

Supporting Information
for
Conformational impact of structural modifications in
2-fluorocyclohexanone

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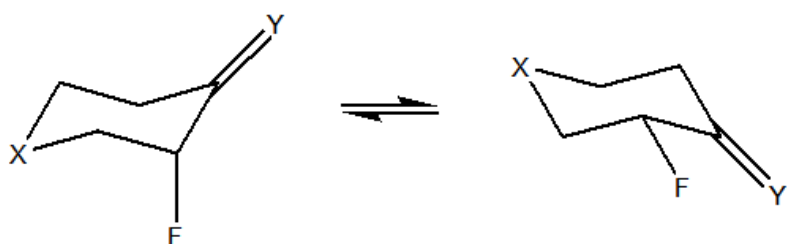
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Computational data

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Table S1. Compounds studied in this work



	Y = O	Y = S	Y = NH _Z	Y = NH _E	Y = CH ₂
X = O	1a and 1e	2a and 2e	3a and 3e	4a and 4e	5a and 5e
X = S	6a and 6e	7a and 7e	8a and 8e	9a and 9e	10a and 10e
X = NH _{ax}	11a and 11e	12a and 12e	13a and 13e	14a and 14e	15a and 15e
X = NH _{eq}	16a and 16e	17a and 17e	18a and 18e	19a and 19e	20a and 20e
X = CH ₂	21a and 21e	22a and 22e	23a and 23e	24a and 24e	25a and 25e

Gas phase

1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.240001	1.266690	0.037134
2	6	0	-0.149394	1.307063	0.700678
3	6	0	-1.058184	0.393506	-0.078436
4	6	0	-0.479860	-1.011476	-0.248379
5	6	0	0.933745	-0.901294	-0.809359
6	1	0	-0.056880	0.934594	1.724958
7	1	0	-0.558595	2.317992	0.710946
8	1	0	1.183814	1.708513	-0.969466
9	1	0	1.958363	1.839814	0.622720
10	1	0	-1.125502	-1.612045	-0.892146
11	1	0	1.410189	-1.882285	-0.805225
12	1	0	0.864162	-0.545187	-1.850005
13	8	0	1.741974	-0.048715	-0.037417
14	9	0	-0.429169	-1.613880	1.006827
15	8	0	-2.083332	0.728288	-0.614215

1e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.263937	-1.425759	-0.260106
2	6	0	0.800410	-0.540611	0.409087
3	6	0	0.519312	0.921449	0.089539
4	6	0	-0.919438	1.307511	0.359718
5	6	0	-1.862402	0.283038	-0.285696
6	1	0	0.752896	-0.677374	1.496010
7	1	0	-0.141973	-1.362229	-1.351254
8	1	0	-0.130740	-2.463225	0.045439
9	1	0	-1.094438	2.313690	-0.024327
10	1	0	-2.895414	0.468204	0.007807
11	1	0	-1.797273	0.352895	-1.381210
12	8	0	-1.553829	-1.029986	0.133309
13	8	0	1.346276	1.662711	-0.368511
14	1	0	-1.088411	1.307279	1.442021
15	9	0	2.045790	-0.919423	-0.025347

2a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.147256	1.545925	0.006139
2	6	0	-0.028634	1.121587	0.910467
3	6	0	-0.773317	0.036820	0.198382
4	6	0	0.129718	-1.119197	-0.169012
5	6	0	1.306552	-0.576176	-0.982133
6	1	0	0.384735	0.728328	1.844579
7	1	0	0.754030	2.002678	-0.914508
8	1	0	1.772981	2.276256	0.518781
9	1	0	-0.410203	-1.888663	-0.722716
10	1	0	2.031467	-1.373360	-1.150426
11	1	0	0.921701	-0.229185	-1.953742
12	8	0	1.979406	0.453531	-0.305064
13	1	0	-0.678835	1.969624	1.125155
14	16	0	-2.306036	0.131219	-0.318713
15	9	0	0.621777	-1.696355	1.001082

2e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.264852	1.112087	-0.388282
2	6	0	-0.017304	0.990047	0.458488
3	6	0	-0.604711	-0.382449	0.266286
4	6	0	0.417770	-1.448925	0.551115
5	6	0	1.676362	-1.185561	-0.290379
6	1	0	0.237022	1.122418	1.517055
7	1	0	0.985530	1.061037	-1.450583
8	1	0	1.740637	2.072899	-0.193772
9	1	0	0.003506	-2.434309	0.337019
10	1	0	2.467077	-1.886685	-0.023873
11	1	0	1.442213	-1.310096	-1.357368
12	8	0	2.185180	0.107799	-0.050746
13	16	0	-2.101493	-0.662909	-0.281142
14	1	0	0.699983	-1.407720	1.609734
15	9	0	-0.872815	2.001712	0.098075

3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.297276	1.240241	0.013165
2	6	0	-0.079816	1.321989	0.683416
3	6	0	-1.031697	0.423680	-0.052146
4	6	0	-0.494644	-0.983714	-0.236583
5	6	0	0.920326	-0.926503	-0.802467
6	1	0	0.014826	0.978832	1.718232
7	1	0	1.244752	1.669251	-0.999364
8	1	0	2.040576	1.796387	0.584234
9	1	0	-1.143568	-1.575658	-0.890317
10	1	0	1.363721	-1.923029	-0.789374
11	1	0	0.853270	-0.581092	-1.847447
12	8	0	1.762994	-0.092489	-0.051579
13	1	0	-0.462282	2.343497	0.677921
14	9	0	-0.466364	-1.615049	1.006424
15	7	0	-2.122682	0.856933	-0.530569
16	1	0	-2.627865	0.114482	-1.017405

3e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.314664	-1.414570	-0.273414
2	6	0	0.753590	-0.565884	0.428119
3	6	0	0.524089	0.896589	0.115128
4	6	0	-0.892580	1.323983	0.387227
5	6	0	-1.858198	0.349090	-0.293732
6	1	0	0.701411	-0.726967	1.509981
7	1	0	-0.167109	-1.336176	-1.360736
8	1	0	-0.220155	-2.460190	0.019710
9	1	0	-1.034377	2.342101	0.021385
10	1	0	-2.890488	0.557015	-0.012558
11	1	0	-1.770150	0.440088	-1.386177
12	8	0	-1.600168	-0.986643	0.098855
13	7	0	1.378425	1.682873	-0.386945
14	1	0	-1.081424	1.308655	1.466315
15	9	0	2.008224	-0.971661	0.000480
16	1	0	2.267224	1.198208	-0.524435

4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.145203	1.365349	0.032066
2	6	0	-0.236424	1.279912	0.699507
3	6	0	-1.073495	0.288839	-0.063379
4	6	0	-0.382975	-1.043023	-0.250255
5	6	0	1.016301	-0.823161	-0.811412
6	1	0	-0.107223	0.926445	1.726857
7	1	0	1.044316	1.802486	-0.973686
8	1	0	1.816042	1.995865	0.615748
9	1	0	-0.977175	-1.687151	-0.900951
10	1	0	1.571623	-1.761594	-0.801338
11	1	0	0.916112	-0.479367	-1.853339
12	8	0	1.758734	0.098800	-0.049435
13	7	0	-2.199896	0.471144	-0.614669
14	1	0	-0.714638	2.262788	0.722471
15	9	0	-0.277376	-1.664094	0.996621
16	1	0	-2.534930	1.421474	-0.446367

4e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.308699	-1.415608	-0.285549
2	6	0	0.771659	-0.575911	0.411828
3	6	0	0.546206	0.887700	0.109764
4	6	0	-0.876709	1.306775	0.403721
5	6	0	-1.852562	0.342596	-0.280909
6	1	0	0.703000	-0.731303	1.495289
7	1	0	-0.169742	-1.332171	-1.373387
8	1	0	-0.211278	-2.462294	0.001697
9	1	0	-1.047818	2.332258	0.065157
10	1	0	-2.881113	0.554707	0.011825
11	1	0	-1.773352	0.446636	-1.373258
12	8	0	-1.595456	-0.992664	0.096571
13	7	0	1.473946	1.594906	-0.379207
14	1	0	-1.051220	1.269992	1.484585
15	9	0	2.005607	-1.013629	-0.004655
16	1	0	1.147710	2.548484	-0.541257

5a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.198756	1.350346	0.002080
2	6	0	-0.168087	1.300263	0.691647
3	6	0	-1.047825	0.315741	-0.026400
4	6	0	-0.392691	-1.021385	-0.235719
5	6	0	1.007547	-0.844596	-0.810681
6	1	0	-0.022568	0.974448	1.726565
7	1	0	1.090107	1.773863	-1.008963
8	1	0	1.897637	1.971081	0.563796
9	1	0	-0.989117	-1.662350	-0.891429
10	1	0	1.538419	-1.797351	-0.793528
11	1	0	0.904011	-0.512778	-1.856702
12	8	0	1.784441	0.066983	-0.073967
13	1	0	-0.622658	2.293982	0.705580
14	9	0	-0.290753	-1.678336	0.997972
15	1	0	-2.703087	1.567069	-0.401721
16	6	0	-2.251523	0.587162	-0.518487
17	1	0	-2.828567	-0.163989	-1.048244

5e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.398653	-1.398464	-0.300207
2	6	0	0.705523	-0.623377	0.427556
3	6	0	-0.824443	1.342171	0.422874
4	6	0	-1.842258	0.449821	-0.291709
5	1	0	0.624406	-0.805418	1.505437
6	1	0	-0.233219	-1.306846	-1.383902
7	1	0	-0.367944	-2.453010	-0.024887
8	1	0	-0.935486	2.379522	0.097329
9	1	0	-2.863486	0.708398	-0.009344
10	1	0	-1.739072	0.567417	-1.380764
11	8	0	-1.667566	-0.908656	0.062495
12	1	0	2.522969	1.156320	-0.575213
13	6	0	1.548993	1.582004	-0.367115
14	1	0	1.396888	2.634058	-0.583476
15	1	0	-1.026521	1.303170	1.499626
16	9	0	1.934387	-1.121748	0.016968
17	6	0	0.569591	0.844741	0.142355

6a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.893932	-1.508511	0.024636
2	6	0	0.475866	-1.341283	0.704682
3	6	0	1.310346	-0.365531	-0.088519
4	6	0	0.758657	1.060105	-0.168785
5	6	0	-0.596546	1.073375	-0.866245
6	1	0	0.331603	-0.959868	1.718885
7	1	0	1.002194	-2.296774	0.742649
8	1	0	-0.770778	-1.909752	-0.985282
9	1	0	-1.509709	-2.210311	0.588590
10	1	0	1.476072	1.684197	-0.706579
11	1	0	-0.991241	2.090606	-0.880519
12	1	0	-0.458113	0.747039	-1.901651
13	16	0	-1.844475	0.040800	-0.039778
14	9	0	0.636633	1.565641	1.120399
15	8	0	2.296942	-0.674705	-0.707230

6e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.257811	-1.337692	-0.375856
2	6	0	0.891611	-0.684108	0.390043
3	6	0	0.988620	0.811827	0.086378
4	6	0	-0.255287	1.620052	0.409489
5	6	0	-1.491415	1.090314	-0.325470
6	1	0	0.737985	-0.813747	1.467598
7	1	0	-0.096010	-1.228253	-1.451511
8	1	0	-0.290653	-2.402230	-0.141003
9	1	0	-0.433240	1.574208	1.489186
10	1	0	-0.055676	2.657387	0.132637
11	1	0	-2.374732	1.667629	-0.048945
12	1	0	-1.362116	1.177871	-1.407626
13	16	0	-1.864107	-0.638613	0.095566
14	9	0	2.068090	-1.311247	0.047737
15	8	0	1.979130	1.297977	-0.388316

7a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.913932	-1.602443	0.111186
2	6	0	0.268016	-1.107144	0.967448
3	6	0	1.026033	-0.058805	0.207309
4	6	0	0.243949	1.210751	-0.063845
5	6	0	-0.952492	0.918610	-0.969446
6	1	0	-0.119917	-0.677663	1.895819
7	1	0	0.929437	-1.941754	1.203258
8	1	0	-0.541114	-2.047529	-0.815468
9	1	0	-1.470180	-2.367943	0.654034
10	1	0	0.890976	1.957747	-0.527190
11	1	0	-1.515545	1.839786	-1.127082
12	1	0	-0.577935	0.573165	-1.937234
13	16	0	-2.111715	-0.289597	-0.265133
14	9	0	-0.201259	1.739092	1.144228
15	16	0	2.498350	-0.282494	-0.432373

7e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.892784	1.252047	-0.447399
2	6	0	-0.313033	1.006979	0.464091
3	6	0	-0.864678	-0.387434	0.266936
4	6	0	0.112875	-1.476380	0.636168
5	6	0	1.371482	-1.421896	-0.241310
6	1	0	-0.011950	1.122297	1.511915
7	1	0	0.587356	1.141197	-1.490987
8	1	0	1.251211	2.270871	-0.296263
9	1	0	0.408345	-1.355114	1.684569
10	1	0	-0.376822	-2.444622	0.522928
11	1	0	2.067243	-2.209235	0.051955
12	1	0	1.108379	-1.576500	-1.291022
13	16	0	2.274755	0.143670	-0.063933
14	9	0	-1.253571	1.977383	0.195428
15	16	0	-2.334018	-0.680247	-0.343746

8a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.939665	1.502881	-0.002970
2	6	0	-0.426673	1.360503	0.678126
3	6	0	-1.297592	0.384230	-0.064389
4	6	0	-0.758070	-1.033555	-0.166255
5	6	0	0.600956	-1.079131	-0.854242
6	1	0	-0.282398	1.009895	1.704236
7	1	0	-0.938886	2.324171	0.701398
8	1	0	0.820288	1.885289	-1.020816
9	1	0	1.567785	2.205019	0.547078
10	1	0	-1.466303	-1.661642	-0.718221
11	1	0	0.974864	-2.104312	-0.854850
12	1	0	0.471843	-0.761670	-1.893879
13	16	0	1.867871	-0.061310	-0.042465
14	9	0	-0.657156	-1.569359	1.114272
15	7	0	-2.374755	0.771526	-0.610220
16	1	0	-2.845170	-0.001808	-1.084035

8e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.271693	-1.336394	-0.372029
2	6	0	0.861559	-0.680437	0.407941
3	6	0	0.972416	0.804202	0.105434
4	6	0	-0.257629	1.614596	0.429728
5	6	0	-1.490058	1.107111	-0.323326
6	1	0	0.711832	-0.826893	1.482443
7	1	0	-0.092983	-1.226046	-1.444899
8	1	0	-0.316694	-2.399944	-0.134623
9	1	0	-0.452442	1.564125	1.506539
10	1	0	-0.050751	2.653569	0.164932
11	1	0	-2.374327	1.683808	-0.047826
12	1	0	-1.347473	1.205191	-1.402850
13	16	0	-1.881945	-0.625796	0.072963
14	9	0	2.053403	-1.315235	0.067841
15	7	0	1.991460	1.354277	-0.403812
16	1	0	2.725549	0.661641	-0.561499

9a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.868406	-1.532409	0.016397
2	6	0	0.493037	-1.320027	0.692989
3	6	0	1.313622	-0.312135	-0.072804
4	6	0	0.714202	1.075273	-0.180584
5	6	0	-0.646252	1.055680	-0.864721
6	1	0	0.335368	-0.956606	1.712361
7	1	0	1.032980	-2.270560	0.745130
8	1	0	-0.733857	-1.922242	-0.996978
9	1	0	-1.462441	-2.255654	0.577109
10	1	0	1.406428	1.713310	-0.733946
11	1	0	-1.068353	2.061762	-0.870187
12	1	0	-0.506638	0.737234	-1.902173
13	16	0	-1.864762	-0.012718	-0.039870
14	9	0	0.585273	1.606793	1.102213
15	7	0	2.404243	-0.523880	-0.683770
16	1	0	2.698327	-1.496028	-0.574589

9e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.289763	-1.329795	-0.387661
2	6	0	0.865171	-0.710037	0.397185
3	6	0	1.004065	0.771447	0.102369
4	6	0	-0.216573	1.594371	0.462722
5	6	0	-1.462040	1.132461	-0.300371
6	1	0	0.690525	-0.844158	1.471217
7	1	0	-0.107017	-1.216207	-1.459414
8	1	0	-0.355639	-2.394039	-0.158583
9	1	0	-0.406358	1.509724	1.537925
10	1	0	-0.015595	2.647193	0.240382
11	1	0	-2.331104	1.725207	-0.010655
12	1	0	-1.317324	1.251258	-1.377770
13	16	0	-1.888745	-0.597139	0.061904
14	9	0	2.018727	-1.391535	0.074973
15	7	0	2.068478	1.204963	-0.426064
16	1	0	2.009378	2.213644	-0.571337

10a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.910104	1.532448	-0.010495
2	6	0	-0.445394	1.341090	0.676788
3	6	0	-1.295690	0.327966	-0.042699
4	6	0	-0.709879	-1.054081	-0.173596
5	6	0	0.653107	-1.062039	-0.854447
6	1	0	-0.277257	1.007881	1.705613
7	1	0	-0.971074	2.299537	0.716293
8	1	0	0.772861	1.905319	-1.029940
9	1	0	1.518856	2.255972	0.534488
10	1	0	-1.391073	-1.698875	-0.737727
11	1	0	1.061109	-2.074076	-0.844580
12	1	0	0.519072	-0.755661	-1.896342
13	16	0	1.889095	0.000121	-0.050620
14	9	0	-0.589340	-1.621096	1.099439
15	6	0	-2.477037	0.611810	-0.581617
16	1	0	-3.062570	-0.143619	-1.095903
17	1	0	-2.902640	1.608282	-0.520538

10e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.328665	-1.329573	-0.384280
2	6	0	0.821519	-0.721708	0.410978
3	6	0	0.995263	0.748227	0.128705
4	6	0	-0.205661	1.595937	0.469228
5	6	0	-1.453060	1.163467	-0.305642
6	1	0	0.647355	-0.875396	1.481915
7	1	0	-0.131384	-1.221030	-1.453893
8	1	0	-0.421646	-2.391045	-0.150602
9	1	0	-0.416673	1.523729	1.542299
10	1	0	0.015631	2.643891	0.246972
11	1	0	-2.316222	1.767324	-0.019801
12	1	0	-1.295707	1.283084	-1.381164
13	16	0	-1.917743	-0.560694	0.042740
14	9	0	1.979614	-1.427139	0.087166
15	6	0	2.108870	1.240387	-0.401262
16	1	0	2.206140	2.302325	-0.600558
17	1	0	2.950277	0.602033	-0.639848

11a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.101648	1.402436	0.022088
2	6	0	-0.284932	1.289231	0.711322
3	6	0	-1.105394	0.287834	-0.056167
4	6	0	-0.414157	-1.062052	-0.220196
5	6	0	0.948489	-0.837019	-0.883645
6	1	0	-0.145085	0.929094	1.735431
7	1	0	-0.804189	2.248429	0.733390
8	1	0	0.971063	1.874592	-0.958202
9	1	0	1.750856	2.055412	0.608025
10	1	0	-1.050805	-1.752470	-0.775434
11	1	0	1.477103	-1.790454	-0.950838
12	1	0	0.776417	-0.482145	-1.906978
13	7	0	1.769714	0.127262	-0.176262
14	1	0	2.070606	-0.259626	0.709911
15	9	0	-0.190602	-1.604576	1.052535
16	8	0	-2.149059	0.530617	-0.609337

11e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.229578	-1.440294	-0.294178
2	6	0	0.810278	-0.542499	0.406426
3	6	0	0.520336	0.919236	0.092870
4	6	0	-0.909137	1.314981	0.394215
5	6	0	-1.879495	0.328152	-0.293075
6	1	0	0.745867	-0.684273	1.493482
7	1	0	-0.066395	-1.364393	-1.374778
8	1	0	-0.057561	-2.480256	-0.011193
9	1	0	-1.067153	1.271796	1.478617
10	1	0	-1.066130	2.342838	0.062323
11	1	0	-2.908766	0.552101	-0.006617
12	1	0	-1.813896	0.462793	-1.378238
13	1	0	-1.838367	-1.291421	0.961464
14	9	0	2.076159	-0.897234	0.006026
15	7	0	-1.597249	-1.065786	0.004155
16	8	0	1.336661	1.656121	-0.393242

12a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.101102	1.583822	-0.016005
2	6	0	-0.057015	1.124837	0.918907
3	6	0	-0.782526	0.016227	0.227357
4	6	0	0.125180	-1.133695	-0.129981
5	6	0	1.241736	-0.598752	-1.043918
6	1	0	0.377727	0.750879	1.851881
7	1	0	-0.732004	1.951539	1.141287
8	1	0	0.663267	2.054120	-0.903352
9	1	0	1.700234	2.340575	0.493772
10	1	0	-0.424337	-1.958327	-0.584165
11	1	0	1.933342	-1.413104	-1.270237
12	1	0	0.786186	-0.272840	-1.985548
13	7	0	1.966946	0.504351	-0.448409
14	1	0	2.532790	0.170305	0.321862
15	9	0	0.734939	-1.621069	1.035988
16	16	0	-2.311946	0.092586	-0.311793

12e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.220886	1.154219	-0.427360
2	6	0	-0.038708	1.000462	0.459452
3	6	0	-0.599635	-0.384349	0.283062
4	6	0	0.427015	-1.435930	0.599395
5	6	0	1.674722	-1.212337	-0.290735
6	1	0	0.236373	1.138865	1.513457
7	1	0	0.893371	1.110481	-1.471689
8	1	0	1.653896	2.141371	-0.256937
9	1	0	0.730657	-1.344583	1.650144
10	1	0	0.003737	-2.429132	0.446506
11	1	0	2.451537	-1.932074	-0.025946
12	1	0	1.399958	-1.398657	-1.334441
13	1	0	2.682457	0.271363	0.693876
14	9	0	-0.933604	1.992043	0.133495
15	7	0	2.214741	0.130043	-0.192818
16	16	0	-2.078651	-0.695545	-0.300598

13a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.202916	1.349832	-0.004099
2	6	0	-0.179331	1.320416	0.683534
3	6	0	-1.072463	0.351721	-0.036880
4	6	0	-0.455643	-1.021491	-0.217023
5	6	0	0.923468	-0.891420	-0.867136
6	1	0	-0.054366	0.988063	1.719969
7	1	0	-0.646910	2.306213	0.687145
8	1	0	1.098241	1.806198	-0.995268
9	1	0	1.891420	1.976557	0.566198
10	1	0	-1.112774	-1.682532	-0.790551
11	1	0	1.393220	-1.876722	-0.912499
12	1	0	0.779562	-0.545824	-1.898320
13	7	0	1.801467	0.033774	-0.177073
14	1	0	2.070320	-0.353301	0.719635
15	9	0	-0.286161	-1.603699	1.048144
16	7	0	-2.188418	0.712845	-0.520683
17	1	0	-2.648296	-0.066042	-0.995685

13e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.285784	-1.432190	-0.300882
2	6	0	0.761767	-0.570317	0.422414
3	6	0	0.528075	0.893759	0.117450
4	6	0	-0.880124	1.334038	0.411579
5	6	0	-1.873313	0.397146	-0.303759
6	1	0	0.698490	-0.732308	1.505431
7	1	0	-0.102070	-1.351127	-1.377966
8	1	0	-0.155868	-2.479806	-0.022592
9	1	0	-1.060059	1.283877	1.492884
10	1	0	-0.999683	2.370918	0.092509
11	1	0	-2.900212	0.648877	-0.030989
12	1	0	-1.783068	0.543863	-1.385750
13	1	0	-1.908373	-1.239979	0.928361
14	9	0	2.035366	-0.956081	0.024394
15	7	0	-1.646326	-1.013704	-0.023581
16	7	0	1.378820	1.676640	-0.397986
17	1	0	2.261353	1.185245	-0.551278

14a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.036970	1.466382	0.015598
2	6	0	-0.339989	1.270357	0.693963
3	6	0	-1.106854	0.207774	-0.047451
4	6	0	-0.334759	-1.078086	-0.228696
5	6	0	1.017405	-0.783198	-0.878283
6	1	0	-0.184725	0.939661	1.726437
7	1	0	-0.902298	2.208395	0.715921
8	1	0	0.885373	1.925458	-0.968470
9	1	0	1.645918	2.157799	0.601822
10	1	0	-0.926682	-1.797696	-0.795770
11	1	0	1.601203	-1.704796	-0.933212
12	1	0	0.833721	-0.446122	-1.905554
13	7	0	1.781075	0.232090	-0.174342
14	1	0	2.094588	-0.132436	0.717059
15	9	0	-0.088332	-1.629566	1.040614
16	7	0	-2.245439	0.307584	-0.597963
17	1	0	-2.638200	1.238746	-0.448411

14e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.273817	-1.430525	-0.321301
2	6	0	0.781509	-0.578185	0.406471
3	6	0	0.547162	0.885934	0.112074
4	6	0	-0.867515	1.312794	0.432809
5	6	0	-1.870266	0.385647	-0.285154
6	1	0	0.694364	-0.737360	1.490102
7	1	0	-0.097072	-1.334870	-1.398269
8	1	0	-0.135819	-2.480841	-0.058015
9	1	0	-1.030264	1.239847	1.515195
10	1	0	-1.019579	2.356732	0.143142
11	1	0	-2.892919	0.634373	0.006394
12	1	0	-1.794258	0.549622	-1.365930
13	1	0	-1.890029	-1.267160	0.921353
14	9	0	2.037428	-0.991664	0.026653
15	7	0	-1.636421	-1.025673	-0.029163
16	7	0	1.464074	1.592168	-0.400505
17	1	0	1.132708	2.545172	-0.555567

15a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.120755	1.434899	-0.015603
2	6	0	-0.247642	1.301373	0.681497
3	6	0	-1.077072	0.259039	-0.016294
4	6	0	-0.364725	-1.048440	-0.220070
5	6	0	1.000353	-0.825674	-0.870839
6	1	0	-0.085092	0.994239	1.721167
7	1	0	-0.768820	2.262417	0.696293
8	1	0	0.974952	1.877953	-1.008145
9	1	0	1.767770	2.111667	0.547439
10	1	0	-0.970698	-1.751417	-0.797901
11	1	0	1.541636	-1.774067	-0.909211
12	1	0	0.831251	-0.498182	-1.903882
13	7	0	1.814561	0.165916	-0.190269
14	1	0	2.110411	-0.197234	0.708068
15	9	0	-0.141343	-1.644265	1.038558
16	6	0	-2.297492	0.463984	-0.501577
17	1	0	-2.843186	-0.323578	-1.011551
18	1	0	-2.793120	1.424085	-0.400112

15e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.369210	-1.417451	-0.329602
2	6	0	0.714002	-0.627621	0.419683
3	6	0	0.572426	0.842375	0.143075
4	6	0	-0.813772	1.349988	0.443267
5	6	0	-1.856746	0.495069	-0.299389
6	1	0	0.619875	-0.809703	1.498721
7	1	0	-0.170427	-1.323109	-1.402960
8	1	0	-0.299805	-2.476239	-0.070969
9	1	0	-1.007567	1.279224	1.521988
10	1	0	-0.903038	2.403044	0.162974
11	1	0	-2.869785	0.795463	-0.021094
12	1	0	-1.752415	0.664049	-1.377175
13	1	0	-1.989292	-1.164567	0.889888
14	9	0	1.963949	-1.105711	0.041521
15	7	0	-1.711590	-0.933590	-0.056730
16	6	0	1.547538	1.579699	-0.375992
17	1	0	1.395273	2.633410	-0.584396
18	1	0	2.517344	1.152608	-0.599808

16a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.275230	-1.267197	0.039915
2	6	0	0.118924	-1.331265	0.688216
3	6	0	1.043914	-0.430196	-0.089520
4	6	0	0.527383	1.003486	-0.239587
5	6	0	-0.887327	0.973385	-0.803544
6	1	0	0.041739	-0.958872	1.713940
7	1	0	0.519298	-2.345380	0.690673
8	1	0	-1.219080	-1.721658	-0.965358
9	1	0	-1.978374	-1.857082	0.630913
10	1	0	1.205040	1.572947	-0.878065
11	1	0	-1.292264	1.987821	-0.802269
12	1	0	-0.803805	0.640751	-1.855284
13	7	0	-1.728357	0.113082	0.007673
14	9	0	0.523600	1.595942	1.020826
15	1	0	-2.695966	0.180182	-0.274091
16	8	0	2.055442	-0.792880	-0.634311

16e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.267536	-1.433704	-0.267863
2	6	0	0.798576	-0.563976	0.403009
3	6	0	0.546422	0.906672	0.083422
4	6	0	-0.877674	1.348394	0.355021
5	6	0	-1.873749	0.369868	-0.278926
6	1	0	0.741194	-0.697779	1.489497
7	1	0	-0.126524	-1.364914	-1.359798
8	1	0	-0.116141	-2.473006	0.028907
9	1	0	-1.035081	1.356573	1.439163
10	1	0	-1.003656	2.361736	-0.028195
11	1	0	-2.890077	0.629687	0.023576
12	1	0	-1.816720	0.465289	-1.376831
13	9	0	2.047698	-0.951018	-0.018710
14	7	0	-1.574285	-0.979936	0.175847
15	1	0	-2.294663	-1.629935	-0.106688
16	8	0	1.397019	1.625942	-0.367518

17a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.148048	-1.570334	0.021868
2	6	0	0.034982	-1.135833	0.908895
3	6	0	0.774900	-0.049594	0.189847
4	6	0	-0.106638	1.133356	-0.157491
5	6	0	-1.298766	0.638267	-0.974609
6	1	0	-0.369297	-0.735922	1.844315
7	1	0	0.696668	-1.974618	1.122494
8	1	0	-0.742899	-2.041542	-0.890883
9	1	0	-1.740659	-2.318371	0.552256
10	1	0	0.457001	1.891017	-0.702955
11	1	0	-1.983314	1.473839	-1.136451
12	1	0	-0.902064	0.322189	-1.956484
13	7	0	-1.985359	-0.418182	-0.257417
14	9	0	-0.560720	1.714799	1.024947
15	1	0	-2.842380	-0.680631	-0.722686
16	16	0	2.302023	-0.158566	-0.341454

17e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.235509	1.153840	-0.389227
2	6	0	-0.036325	0.997490	0.453753
3	6	0	-0.604435	-0.386410	0.256199
4	6	0	0.414108	-1.456969	0.551559
5	6	0	1.685280	-1.214656	-0.274395
6	1	0	0.217201	1.123515	1.513031
7	1	0	0.940484	1.105863	-1.450860
8	1	0	1.662692	2.139336	-0.195862
9	1	0	0.681784	-1.407109	1.613643
10	1	0	-0.012632	-2.437396	0.342335
11	1	0	2.447585	-1.942709	0.009774
12	1	0	1.448368	-1.369517	-1.340639
13	9	0	-0.922612	1.990947	0.110594
14	7	0	2.181307	0.124251	0.000270
15	1	0	3.080967	0.280143	-0.433010
16	16	0	-2.099807	-0.677511	-0.290186

18a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.315780	1.254644	0.016273
2	6	0	-0.067417	1.341513	0.673818
3	6	0	-1.024222	0.446196	-0.061397
4	6	0	-0.528821	-0.981102	-0.226590
5	6	0	0.882645	-0.984361	-0.799845
6	1	0	0.018802	0.997342	1.709123
7	1	0	-0.453062	2.361370	0.663856
8	1	0	1.256697	1.697985	-0.993970
9	1	0	2.035827	1.837566	0.594110
10	1	0	-1.203446	-1.553404	-0.871420
11	1	0	1.266594	-2.007025	-0.791788
12	1	0	0.795151	-0.659609	-1.854217
13	1	0	2.709966	-0.218374	-0.307926
14	7	0	1.749058	-0.133788	-0.007871
15	9	0	-0.532872	-1.600577	1.022317
16	7	0	-2.103291	0.895476	-0.553260
17	1	0	-2.618838	0.156192	-1.034259

18e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.310157	-1.422772	-0.281298
2	6	0	0.753947	-0.582919	0.423331
3	6	0	0.546202	0.885044	0.107930
4	6	0	-0.855722	1.359142	0.387066
5	6	0	-1.868665	0.426360	-0.284712
6	1	0	0.690529	-0.740934	1.504657
7	1	0	-0.143562	-1.338053	-1.368743
8	1	0	-0.190806	-2.469878	0.003428
9	1	0	-1.033126	1.345729	1.468145
10	1	0	-0.955184	2.383813	0.027110
11	1	0	-2.883269	0.704263	0.007921
12	1	0	-1.788476	0.544558	-1.378932
13	1	0	-2.343901	-1.567944	-0.176667
14	9	0	2.014532	-0.993258	0.010883
15	7	0	-1.615191	-0.944327	0.142001
16	7	0	1.419190	1.650791	-0.394517
17	1	0	2.295391	1.143391	-0.531164

19a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.170799	1.373292	0.036495
2	6	0	-0.215254	1.299015	0.694471
3	6	0	-1.066610	0.319454	-0.070486
4	6	0	-0.426851	-1.042158	-0.240945
5	6	0	0.977283	-0.891220	-0.810267
6	1	0	-0.093565	0.939536	1.720567
7	1	0	-0.689852	2.283345	0.717776
8	1	0	1.062897	1.825021	-0.966544
9	1	0	1.823413	2.021247	0.625432
10	1	0	-1.052768	-1.663778	-0.882986
11	1	0	1.469006	-1.866379	-0.807164
12	1	0	0.860116	-0.569320	-1.861653
13	1	0	2.713638	0.065564	-0.306783
14	7	0	1.749017	0.041195	-0.007857
15	9	0	-0.358566	-1.657224	1.011174
16	7	0	-2.180252	0.534756	-0.636982
17	1	0	-2.483352	1.497834	-0.480949

19e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.307579	-1.423870	-0.292175
2	6	0	0.771943	-0.595315	0.407673
3	6	0	0.569522	0.873790	0.103782
4	6	0	-0.837821	1.341059	0.407601
5	6	0	-1.860752	0.425126	-0.273320
6	1	0	0.693144	-0.747459	1.490534
7	1	0	-0.147063	-1.336264	-1.380031
8	1	0	-0.187974	-2.471923	-0.011959
9	1	0	-1.002929	1.300225	1.489739
10	1	0	-0.963888	2.376229	0.080010
11	1	0	-2.871814	0.708297	0.027200
12	1	0	-1.783546	0.557082	-1.366622
13	1	0	-2.343587	-1.565156	-0.186825
14	9	0	2.010590	-1.038417	0.005190
15	7	0	-1.612123	-0.947971	0.138110
16	7	0	1.511537	1.559431	-0.389504
17	1	0	1.204567	2.519762	-0.550365

20a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.217177	1.364535	0.006967
2	6	0	-0.157053	1.318498	0.683794
3	6	0	-1.043511	0.338552	-0.034791
4	6	0	-0.428187	-1.022320	-0.226457
5	6	0	0.974326	-0.904460	-0.809339
6	1	0	-0.019286	0.990039	1.718856
7	1	0	-0.613792	2.310940	0.694923
8	1	0	1.101958	1.802826	-1.001382
9	1	0	1.891470	2.007915	0.576918
10	1	0	-1.051517	-1.646569	-0.872637
11	1	0	1.447622	-1.888973	-0.799898
12	1	0	0.852050	-0.591942	-1.863382
13	1	0	2.732325	0.027252	-0.350619
14	7	0	1.774583	0.021582	-0.029438
15	9	0	-0.357983	-1.671084	1.013198
16	6	0	-2.237080	0.632474	-0.539142
17	1	0	-2.828045	-0.110202	-1.065731
18	1	0	-2.667045	1.623714	-0.435952

20e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.394638	-1.407833	-0.304884
2	6	0	0.706530	-0.638527	0.423366
3	6	0	0.590207	0.832766	0.134936
4	6	0	-0.787147	1.373082	0.424455
5	6	0	-1.848632	0.525329	-0.282786
6	1	0	0.616738	-0.816218	1.500784
7	1	0	-0.209374	-1.313741	-1.388445
8	1	0	-0.336740	-2.464261	-0.034787
9	1	0	-0.979769	1.332150	1.502774
10	1	0	-0.856343	2.416475	0.108328
11	1	0	-2.848523	0.853893	0.010246
12	1	0	-1.748419	0.668501	-1.372795
13	1	0	-2.435856	-1.440038	-0.244643
14	9	0	1.940326	-1.141614	0.025999
15	7	0	-1.680683	-0.868389	0.108068
16	6	0	1.583641	1.549611	-0.377007
17	1	0	1.451293	2.604338	-0.594220
18	1	0	2.549085	1.105586	-0.586183

21a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.159089	1.399298	0.033402
2	6	0	-0.232334	1.319496	0.693011
3	6	0	-1.087235	0.349906	-0.083923
4	6	0	-0.481958	-1.048789	-0.219034
5	6	0	0.891348	-0.952939	-0.866806
6	1	0	-0.125081	0.945788	1.716972
7	1	0	-0.728808	2.289887	0.720319
8	1	0	1.056961	1.857800	-0.957259
9	1	0	1.801058	2.058723	0.622498
10	1	0	-1.168555	-1.695312	-0.767142
11	1	0	1.331003	-1.952531	-0.918228
12	1	0	0.748533	-0.607653	-1.897950
13	1	0	2.760822	0.098025	-0.617720
14	9	0	-0.339320	-1.580788	1.070548
15	6	0	1.799650	0.016189	-0.103819
16	1	0	2.003754	-0.393633	0.890331
17	8	0	-2.114646	0.640879	-0.642967

21e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.216019	-1.455517	-0.299239
2	6	0	0.810153	-0.563296	0.394038
3	6	0	0.546519	0.905940	0.074935
4	6	0	-0.867137	1.349506	0.395423
5	6	0	-1.894895	0.429450	-0.282441
6	1	0	0.737170	-0.687864	1.483243
7	1	0	-0.065229	-1.371433	-1.381128
8	1	0	-0.024548	-2.494947	-0.022686
9	1	0	-1.001633	1.300267	1.483614
10	1	0	-0.978187	2.390008	0.088104
11	1	0	-2.904224	0.726838	0.012935
12	1	0	-1.830392	0.561685	-1.368366
13	1	0	-2.355613	-1.678990	-0.454455
14	9	0	2.084357	-0.924410	0.019808
15	1	0	-1.806239	-1.191654	1.140798
16	6	0	-1.641396	-1.037171	0.067218
17	8	0	1.380792	1.624038	-0.407491

22a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.118116	1.612251	0.012306
2	6	0	-0.056697	1.146345	0.899118
3	6	0	-0.787090	0.044978	0.191004
4	6	0	0.092687	-1.144708	-0.134728
5	6	0	1.252695	-0.696119	-1.017026
6	1	0	0.343698	0.751067	1.839972
7	1	0	-0.737451	1.966626	1.124684
8	1	0	0.709817	2.075278	-0.893375
9	1	0	1.680668	2.385140	0.542013
10	1	0	-0.489584	-1.946542	-0.588516
11	1	0	1.897002	-1.557466	-1.211449
12	1	0	0.834277	-0.375620	-1.977821
13	1	0	2.814270	0.792406	-1.050024
14	9	0	0.616567	-1.646372	1.067378
15	6	0	2.034193	0.448139	-0.366003
16	1	0	2.537843	0.073011	0.530134
17	16	0	-2.316442	0.136758	-0.339379

22e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.187567	1.207948	-0.421478
2	6	0	-0.056470	1.006585	0.445076
3	6	0	-0.602712	-0.388105	0.256888
4	6	0	0.419908	-1.442424	0.594465
5	6	0	1.681708	-1.260320	-0.267238
6	1	0	0.204964	1.125579	1.505771
7	1	0	0.877517	1.148412	-1.470293
8	1	0	1.571038	2.215888	-0.247303
9	1	0	0.694619	-1.334657	1.652664
10	1	0	-0.017892	-2.430960	0.459541
11	1	0	2.425792	-2.007810	0.019023
12	1	0	1.423968	-1.447976	-1.315373
13	1	0	3.101766	0.288061	-0.790565
14	9	0	-0.981733	1.982743	0.148118
15	1	0	2.626707	0.288403	0.900287
16	6	0	2.249639	0.150026	-0.120431
17	16	0	-2.084420	-0.708243	-0.310657

23a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.228636	1.368710	0.006535
2	6	0	-0.156510	1.338026	0.673059
3	6	0	-1.062086	0.387121	-0.059062
4	6	0	-0.500972	-1.016304	-0.211641
5	6	0	0.875991	-0.980995	-0.857428
6	1	0	-0.049482	0.990919	1.707150
7	1	0	-0.621548	2.324209	0.688742
8	1	0	1.133848	1.814493	-0.990897
9	1	0	1.897053	2.015004	0.581327
10	1	0	-1.194418	-1.651391	-0.771307
11	1	0	1.277366	-1.997433	-0.893295
12	1	0	0.745667	-0.644828	-1.893274
13	1	0	2.784019	0.001002	-0.631518
14	9	0	-0.384507	-1.581044	1.068003
15	6	0	1.822459	-0.035825	-0.112850
16	1	0	2.015113	-0.438857	0.886621
17	7	0	-2.161719	0.777566	-0.556724
18	1	0	-2.640128	0.008924	-1.030177

23e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.267170	-1.447843	-0.305695
2	6	0	0.763610	-0.586159	0.411500
3	6	0	0.550867	0.882441	0.099189
4	6	0	-0.840955	1.364362	0.414247
5	6	0	-1.887982	0.490594	-0.291822
6	1	0	0.691637	-0.732598	1.496452
7	1	0	-0.096168	-1.355626	-1.383841
8	1	0	-0.112304	-2.494999	-0.034593
9	1	0	-0.999011	1.306276	1.499242
10	1	0	-0.918823	2.411696	0.120600
11	1	0	-2.893072	0.812704	-0.007125
12	1	0	-1.800321	0.636469	-1.374446
13	1	0	-2.409622	-1.603735	-0.502210
14	9	0	2.046032	-0.976279	0.039409
15	1	0	-1.874283	-1.152658	1.108573
16	6	0	-1.686682	-0.988950	0.039914
17	7	0	1.417043	1.647842	-0.415647
18	1	0	2.288254	1.137405	-0.571795

24a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.073382	1.477836	0.027250
2	6	0	-0.304708	1.291676	0.686335
3	6	0	-1.097426	0.256097	-0.069806
4	6	0	-0.392892	-1.074485	-0.225641
5	6	0	0.973638	-0.887599	-0.867390
6	1	0	-0.166722	0.939799	1.714721
7	1	0	-0.856204	2.234917	0.725468
8	1	0	0.936873	1.925530	-0.964507
9	1	0	1.668116	2.181761	0.615325
10	1	0	-1.028806	-1.762671	-0.783258
11	1	0	1.481714	-1.854490	-0.911360
12	1	0	0.809814	-0.558179	-1.900361
13	1	0	2.765002	0.295437	-0.623486
14	9	0	-0.210788	-1.620436	1.057648
15	1	0	-2.575835	1.352341	-0.492387
16	6	0	1.812123	0.144837	-0.109331
17	1	0	2.046294	-0.245999	0.886096
18	7	0	-2.223979	0.403614	-0.633368

24e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.256873	-1.446308	-0.326404
2	6	0	0.783821	-0.595413	0.396246
3	6	0	0.569858	0.873116	0.095142
4	6	0	-0.827899	1.341489	0.440035
5	6	0	-1.883212	0.482744	-0.272838
6	1	0	0.688376	-0.739467	1.481559
7	1	0	-0.088818	-1.341632	-1.403908
8	1	0	-0.096013	-2.495840	-0.068871
9	1	0	-0.970414	1.254761	1.524829
10	1	0	-0.936163	2.398146	0.181644
11	1	0	-2.884718	0.801179	0.028546
12	1	0	-1.806014	0.646903	-1.353649
13	1	0	-2.401233	-1.606210	-0.517668
14	9	0	2.048456	-1.012270	0.042575
15	1	0	1.182837	2.520659	-0.574579
16	1	0	-1.859496	-1.182317	1.098425
17	6	0	-1.676000	-1.001077	0.031969
18	7	0	1.496770	1.560992	-0.423486

25a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.143241	1.456584	-0.004704
2	6	0	-0.227724	1.317191	0.674024
3	6	0	-1.071208	0.292718	-0.036177
4	6	0	-0.409782	-1.047648	-0.215738
5	6	0	0.961070	-0.914071	-0.863450
6	1	0	-0.078241	0.991973	1.710446
7	1	0	-0.747643	2.277800	0.705249
8	1	0	1.005856	1.889723	-1.003093
9	1	0	1.768349	2.151785	0.562809
10	1	0	-1.051687	-1.728161	-0.780767
11	1	0	1.437338	-1.897846	-0.895068
12	1	0	0.804721	-0.592598	-1.900045
13	1	0	2.793818	0.208095	-0.648649
14	9	0	-0.236997	-1.633406	1.056177
15	6	0	-2.280012	0.531892	-0.534102
16	1	0	-2.845319	-0.241066	-1.045257
17	1	0	-2.747538	1.507144	-0.443198
18	6	0	1.839081	0.099752	-0.126741
19	1	0	2.065328	-0.284710	0.873317

25e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.352464	-1.435077	-0.332258
2	6	0	0.716550	-0.641845	0.409415
3	6	0	0.593903	0.830702	0.125387
4	6	0	-0.774312	1.377059	0.446475
5	6	0	-1.866669	0.586619	-0.287582
6	1	0	0.616751	-0.808640	1.490488
7	1	0	-0.164121	-1.331716	-1.406504
8	1	0	-0.256585	-2.493747	-0.077721
9	1	0	-0.949465	1.296827	1.528097
10	1	0	-0.821318	2.438595	0.192670
11	1	0	-2.854536	0.956185	0.002120
12	1	0	-1.762704	0.753338	-1.365849
13	1	0	-2.500165	-1.471028	-0.553845
14	9	0	1.974075	-1.124362	0.054676
15	6	0	1.581174	1.550354	-0.394584
16	1	0	1.447173	2.606996	-0.601398
17	1	0	2.542688	1.106434	-0.621252
18	1	0	-1.956767	-1.086164	1.071282
19	6	0	-1.749452	-0.909116	0.008118

Implicit DMSO

1a Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.273204	1.252383	0.029502
2	6	0	-0.132772	1.337748	0.649843
3	6	0	-1.051123	0.408302	-0.092514
4	6	0	-0.482678	-1.001425	-0.263207
5	6	0	0.940841	-0.921592	-0.794757
6	1	0	-0.074776	1.011569	1.693000
7	1	0	-0.520153	2.356241	0.614024
8	1	0	1.261450	1.667442	-0.987367
9	1	0	1.981202	1.824420	0.627282
10	1	0	-1.123352	-1.601391	-0.910283
11	1	0	1.394789	-1.912706	-0.783425
12	1	0	0.902471	-0.563602	-1.833996
13	8	0	1.745664	-0.081092	0.001045
14	9	0	-0.466022	-1.598332	1.005432
15	8	0	-2.109697	0.724907	-0.581210

1e Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.281125	-1.430960	-0.252582
2	6	0	0.788318	-0.546984	0.409468
3	6	0	0.523027	0.914446	0.090677
4	6	0	-0.906024	1.320064	0.343593
5	6	0	-1.861724	0.300072	-0.291187
6	1	0	0.756271	-0.681637	1.495421
7	1	0	-0.166216	-1.378769	-1.343875
8	1	0	-0.153647	-2.464618	0.066447
9	1	0	-1.075506	2.321713	-0.053153
10	1	0	-2.888848	0.505249	0.006319
11	1	0	-1.798794	0.353630	-1.385935
12	8	0	-1.565677	-1.015674	0.143761
13	8	0	1.375689	1.645841	-0.352068
14	1	0	-1.074246	1.336100	1.425541
15	9	0	2.038451	-0.930315	-0.038236

2a Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.174916	1.539079	-0.002416
2	6	0	-0.026754	1.145042	0.880812
3	6	0	-0.771953	0.052980	0.184090
4	6	0	0.120766	-1.113928	-0.176310
5	6	0	1.315815	-0.594433	-0.973705
6	1	0	0.359179	0.769722	1.834080
7	1	0	0.814883	1.985226	-0.939310
8	1	0	1.795840	2.266674	0.518185
9	1	0	-0.416263	-1.884325	-0.729033
10	1	0	2.024777	-1.406174	-1.137468
11	1	0	0.952184	-0.236342	-1.947215
12	8	0	1.996602	0.423174	-0.278233
13	1	0	-0.665512	2.007783	1.066391
14	16	0	-2.314637	0.135529	-0.313933
15	9	0	0.591061	-1.692096	1.012036

2e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.268123	1.117643	-0.384645
2	6	0	-0.015777	0.984830	0.459472
3	6	0	-0.599203	-0.385288	0.264158
4	6	0	0.419074	-1.451572	0.542194
5	6	0	1.681457	-1.183685	-0.293808
6	1	0	0.227502	1.120819	1.518348
7	1	0	0.997857	1.067105	-1.448338
8	1	0	1.736215	2.079688	-0.180262
9	1	0	0.013095	-2.437985	0.320454
10	1	0	2.466151	-1.887936	-0.021851
11	1	0	1.455987	-1.300648	-1.361813
12	8	0	2.188186	0.112873	-0.043301
13	16	0	-2.105148	-0.662215	-0.277454
14	1	0	0.694849	-1.414512	1.602026
15	9	0	-0.881869	1.997151	0.092543

3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.310416	1.234599	0.006478
2	6	0	-0.073202	1.337130	0.659962
3	6	0	-1.029922	0.430112	-0.058338
4	6	0	-0.496671	-0.978734	-0.244691
5	6	0	0.918469	-0.936097	-0.802105
6	1	0	0.009361	1.020589	1.704490
7	1	0	1.277058	1.646129	-1.012051
8	1	0	2.047974	1.793256	0.581498
9	1	0	-1.146851	-1.576502	-0.887277
10	1	0	1.350684	-1.937015	-0.793000
11	1	0	0.863805	-0.584469	-1.842982
12	8	0	1.762735	-0.108530	-0.034642
13	1	0	-0.439574	2.364107	0.633010
14	9	0	-0.470968	-1.599288	1.016303
15	7	0	-2.137338	0.845705	-0.518211
16	1	0	-2.638792	0.093735	-0.993643

3e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.320510	-1.416804	-0.270015
2	6	0	0.748221	-0.565665	0.428294
3	6	0	0.525327	0.895688	0.112929
4	6	0	-0.888447	1.328487	0.380775
5	6	0	-1.859511	0.356395	-0.296850
6	1	0	0.702791	-0.721812	1.509883
7	1	0	-0.179165	-1.344459	-1.357485
8	1	0	-0.224849	-2.459376	0.031675
9	1	0	-1.037752	2.344644	0.012987
10	1	0	-2.888012	0.575634	-0.013023
11	1	0	-1.772934	0.437970	-1.388806
12	8	0	-1.606385	-0.981890	0.103787
13	7	0	1.395329	1.674554	-0.380996
14	1	0	-1.073672	1.316303	1.459982
15	9	0	2.005286	-0.975902	-0.004437
16	1	0	2.279320	1.178852	-0.509392

4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.163852	1.361673	0.026692
2	6	0	-0.232030	1.305233	0.662118
3	6	0	-1.070037	0.297236	-0.075389
4	6	0	-0.381654	-1.036604	-0.265260
5	6	0	1.028158	-0.835311	-0.798726
6	1	0	-0.130098	0.990444	1.705281
7	1	0	1.097400	1.774846	-0.989435
8	1	0	1.825236	1.995462	0.616279
9	1	0	-0.964956	-1.683985	-0.920789
10	1	0	1.568919	-1.781893	-0.784259
11	1	0	0.954362	-0.487029	-1.839418
12	8	0	1.763331	0.078505	-0.014181
13	7	0	-2.217394	0.468278	-0.589694
14	1	0	-0.700996	2.291164	0.642432
15	9	0	-0.304056	-1.664190	0.992498
16	1	0	-2.547983	1.419362	-0.417868

4e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.312611	-1.420528	-0.282636
2	6	0	0.764841	-0.576715	0.413541
3	6	0	0.545358	0.885429	0.109807
4	6	0	-0.873415	1.310900	0.395892
5	6	0	-1.852603	0.347748	-0.283277
6	1	0	0.708865	-0.732875	1.495643
7	1	0	-0.179697	-1.340180	-1.370768
8	1	0	-0.212043	-2.465129	0.010343
9	1	0	-1.041424	2.332835	0.049142
10	1	0	-2.877464	0.567531	0.013220
11	1	0	-1.776122	0.440975	-1.374979
12	8	0	-1.597817	-0.992774	0.102310
13	7	0	1.478436	1.595993	-0.371342
14	1	0	-1.044949	1.282903	1.476960
15	9	0	2.008773	-1.016076	-0.011787
16	1	0	1.147932	2.547862	-0.532533

5a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.206622	1.350674	-0.001634
2	6	0	-0.166135	1.316143	0.672915
3	6	0	-1.046970	0.319633	-0.030245
4	6	0	-0.393917	-1.016381	-0.246464
5	6	0	1.009162	-0.850684	-0.809484
6	1	0	-0.032017	1.020931	1.718969
7	1	0	1.115209	1.756689	-1.019433
8	1	0	1.901639	1.974633	0.560358
9	1	0	-0.988855	-1.661463	-0.896094
10	1	0	1.532626	-1.807381	-0.798449
11	1	0	0.917407	-0.510258	-1.851496
12	8	0	1.785664	0.055373	-0.055517
13	1	0	-0.615987	2.311272	0.658713
14	9	0	-0.294742	-1.679506	1.001213
15	1	0	-2.713431	1.560414	-0.388065
16	6	0	-2.260604	0.581088	-0.505677
17	1	0	-2.838176	-0.175102	-1.027744

5e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.397572	-1.401380	-0.299657
2	6	0	0.702485	-0.621907	0.429123
3	6	0	-0.824742	1.341926	0.421922
4	6	0	-1.843520	0.452829	-0.292470
5	1	0	0.627948	-0.804448	1.506180
6	1	0	-0.236393	-1.309534	-1.383336
7	1	0	-0.363003	-2.455075	-0.022088
8	1	0	-0.937548	2.377971	0.095260
9	1	0	-2.862673	0.714658	-0.008127
10	1	0	-1.741906	0.565211	-1.380866
11	8	0	-1.669252	-0.911789	0.063236
12	1	0	2.527032	1.167412	-0.571991
13	6	0	1.549316	1.586154	-0.365134
14	1	0	1.392890	2.637708	-0.580873
15	1	0	-1.024303	1.303396	1.498805
16	9	0	1.937558	-1.124356	0.014638
17	6	0	0.569691	0.845080	0.141117

6a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.908510	-1.511066	0.004458
2	6	0	0.473175	-1.363298	0.663007
3	6	0	1.311114	-0.366307	-0.094020
4	6	0	0.749688	1.055723	-0.183911
5	6	0	-0.610696	1.076908	-0.864470
6	1	0	0.347757	-1.016921	1.692628
7	1	0	0.991772	-2.323212	0.669972
8	1	0	-0.808874	-1.890425	-1.015234
9	1	0	-1.514191	-2.219579	0.569340
10	1	0	1.458916	1.686907	-0.721817
11	1	0	-0.997620	2.096456	-0.879374
12	1	0	-0.487468	0.745168	-1.898977
13	16	0	-1.847727	0.046539	-0.018841
14	9	0	0.642193	1.558291	1.116906
15	8	0	2.338123	-0.649925	-0.664702

6e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.267663	-1.343895	-0.372579
2	6	0	0.881356	-0.684911	0.386287
3	6	0	0.986777	0.808199	0.086414
4	6	0	-0.249750	1.624845	0.387260
5	6	0	-1.493281	1.092952	-0.333858
6	1	0	0.743938	-0.815343	1.464285
7	1	0	-0.115779	-1.239086	-1.449464
8	1	0	-0.303219	-2.405186	-0.126159
9	1	0	-0.420580	1.599380	1.468552
10	1	0	-0.052075	2.657328	0.093295
11	1	0	-2.368524	1.677170	-0.049757
12	1	0	-1.374894	1.168563	-1.417081
13	16	0	-1.866198	-0.631684	0.105293
14	9	0	2.067236	-1.312790	0.033673
15	8	0	2.000068	1.287010	-0.361568

7a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.933747	-1.603996	0.090022
2	6	0	0.267051	-1.133772	0.933063
3	6	0	1.024228	-0.072205	0.193171
4	6	0	0.246449	1.201845	-0.072774
5	6	0	-0.961743	0.928665	-0.964466
6	1	0	-0.099691	-0.725614	1.879603
7	1	0	0.920430	-1.980973	1.142246
8	1	0	-0.585680	-2.033229	-0.852480
9	1	0	-1.484615	-2.372666	0.632240
10	1	0	0.888451	1.952728	-0.533960
11	1	0	-1.512337	1.857248	-1.118546
12	1	0	-0.603365	0.576604	-1.934954
13	16	0	-2.122150	-0.270899	-0.245958
14	9	0	-0.181882	1.726264	1.152744
15	16	0	2.513419	-0.274956	-0.420476

7e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.900688	1.256651	-0.442595
2	6	0	-0.308298	1.001572	0.460652
3	6	0	-0.860562	-0.389521	0.260741
4	6	0	0.112651	-1.482035	0.617542
5	6	0	1.377298	-1.421241	-0.251449
6	1	0	-0.023505	1.119330	1.511070
7	1	0	0.607511	1.147834	-1.489401
8	1	0	1.257010	2.273794	-0.279338
9	1	0	0.397339	-1.371259	1.669577
10	1	0	-0.371320	-2.450922	0.491627
11	1	0	2.067077	-2.211581	0.044443
12	1	0	1.124552	-1.564629	-1.304374
13	16	0	2.277180	0.143789	-0.053260
14	9	0	-1.257415	1.975241	0.183535
15	16	0	-2.344217	-0.675807	-0.332038

8a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.947353	1.504338	-0.013205
2	6	0	-0.424806	1.372917	0.657961
3	6	0	-1.297806	0.385890	-0.067930
4	6	0	-0.755368	-1.030847	-0.173068
5	6	0	0.602453	-1.083384	-0.856614
6	1	0	-0.289442	1.044762	1.692796
7	1	0	-0.927292	2.341856	0.665656
8	1	0	0.840257	1.872579	-1.036650
9	1	0	1.571414	2.209134	0.536629
10	1	0	-1.461322	-1.667299	-0.712933
11	1	0	0.971501	-2.109628	-0.862900
12	1	0	0.477641	-0.759338	-1.893350
13	16	0	1.865993	-0.066800	-0.034773
14	9	0	-0.651758	-1.555402	1.123632
15	7	0	-2.392453	0.753111	-0.595661
16	1	0	-2.856608	-0.029909	-1.058803

8e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.270725	-1.340200	-0.370553
2	6	0	0.858971	-0.676491	0.407264
3	6	0	0.969183	0.806649	0.103113
4	6	0	-0.261076	1.615112	0.424257
5	6	0	-1.495479	1.106235	-0.325071
6	1	0	0.716675	-0.819434	1.482129
7	1	0	-0.097624	-1.231977	-1.443968
8	1	0	-0.314132	-2.401449	-0.125018
9	1	0	-0.450396	1.566430	1.501615
10	1	0	-0.065930	2.655912	0.158288
11	1	0	-2.376709	1.683035	-0.043184
12	1	0	-1.358855	1.200761	-1.404934
13	16	0	-1.880411	-0.627582	0.074755
14	9	0	2.057365	-1.310351	0.065442
15	7	0	1.997795	1.351465	-0.399004
16	1	0	2.727461	0.653100	-0.551018

9a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.878862	-1.536025	0.000996
2	6	0	0.492705	-1.339954	0.658444
3	6	0	1.313299	-0.312934	-0.079877
4	6	0	0.706601	1.071589	-0.197092
5	6	0	-0.659740	1.058256	-0.863231
6	1	0	0.352865	-1.010159	1.692060
7	1	0	1.028845	-2.292330	0.676094
8	1	0	-0.765347	-1.905049	-1.021351
9	1	0	-1.464454	-2.265529	0.560907
10	1	0	1.388355	1.716615	-0.753690
11	1	0	-1.075749	2.066286	-0.872837
12	1	0	-0.534386	0.731168	-1.898912
13	16	0	-1.866805	-0.008135	-0.018606
14	9	0	0.593892	1.609791	1.095757
15	7	0	2.431743	-0.509228	-0.647241
16	1	0	2.727493	-1.479945	-0.531140

9e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.293797	-1.336015	-0.385286
2	6	0	0.857382	-0.709296	0.396373
3	6	0	1.002064	0.769825	0.100726
4	6	0	-0.214410	1.596926	0.452467
5	6	0	-1.463452	1.134520	-0.303420
6	1	0	0.696284	-0.845646	1.470391
7	1	0	-0.118453	-1.224440	-1.458130
8	1	0	-0.360930	-2.398027	-0.148169
9	1	0	-0.397238	1.520815	1.529068
10	1	0	-0.013965	2.646280	0.220229
11	1	0	-2.327850	1.728973	-0.006541
12	1	0	-1.326730	1.248148	-1.381341
13	16	0	-1.888619	-0.595193	0.065936
14	9	0	2.022676	-1.394435	0.067655
15	7	0	2.074943	1.206600	-0.413938
16	1	0	2.011383	2.214961	-0.556973

10a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.916726	1.535926	-0.017555
2	6	0	-0.443677	1.354719	0.660423
3	6	0	-1.295065	0.329930	-0.043927
4	6	0	-0.708514	-1.049750	-0.184409
5	6	0	0.655168	-1.064860	-0.857478
6	1	0	-0.283678	1.048935	1.699421
7	1	0	-0.965913	2.314853	0.676071
8	1	0	0.790506	1.893373	-1.042934
9	1	0	1.523792	2.262216	0.524314
10	1	0	-1.387719	-1.698254	-0.742750
11	1	0	1.059457	-2.077890	-0.857407
12	1	0	0.526547	-0.747736	-1.895708
13	16	0	1.887370	-0.004739	-0.040746
14	9	0	-0.588147	-1.623875	1.101728
15	6	0	-2.487694	0.603194	-0.565414
16	1	0	-3.072716	-0.158011	-1.071763
17	1	0	-2.916531	1.598258	-0.502703

10e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.325146	-1.334745	-0.383873
2	6	0	0.819174	-0.718777	0.412253
3	6	0	0.992947	0.749923	0.127425
4	6	0	-0.209385	1.595017	0.471002
5	6	0	-1.457149	1.164296	-0.303101
6	1	0	0.650899	-0.874023	1.482859
7	1	0	-0.131628	-1.225282	-1.453762
8	1	0	-0.418222	-2.394952	-0.145975
9	1	0	-0.416496	1.521767	1.544472
10	1	0	0.007632	2.642912	0.248090
11	1	0	-2.319954	1.764769	-0.011746
12	1	0	-1.303586	1.284562	-1.378366
13	16	0	-1.915143	-0.564205	0.040553
14	9	0	1.986262	-1.426569	0.088179
15	6	0	2.104784	1.247616	-0.403556
16	1	0	2.195075	2.310229	-0.602381
17	1	0	2.950846	0.616443	-0.646549

11a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.145028	1.377166	0.018542
2	6	0	-0.250613	1.302584	0.695305
3	6	0	-1.091467	0.319649	-0.064394
4	6	0	-0.436144	-1.046989	-0.233583
5	6	0	0.944933	-0.867102	-0.869043
6	1	0	-0.123754	0.945007	1.721899
7	1	0	-0.739586	2.277242	0.713320
8	1	0	1.036218	1.842657	-0.966799
9	1	0	1.796678	2.019179	0.612308
10	1	0	-1.077873	-1.718088	-0.804999
11	1	0	1.441465	-1.838329	-0.916036
12	1	0	0.799526	-0.521224	-1.898708
13	7	0	1.782896	0.081228	-0.155697
14	1	0	2.050046	-0.302735	0.743454
15	9	0	-0.264114	-1.603064	1.046980
16	8	0	-2.144548	0.580428	-0.602293

11e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.244869	-1.444433	-0.288074
2	6	0	0.797670	-0.546946	0.409237
3	6	0	0.521451	0.912418	0.096747
4	6	0	-0.897876	1.323082	0.384131
5	6	0	-1.875952	0.340705	-0.302407
6	1	0	0.747034	-0.691200	1.493824
7	1	0	-0.081713	-1.378737	-1.369182
8	1	0	-0.078731	-2.479902	0.011889
9	1	0	-1.060041	1.281881	1.466906
10	1	0	-1.051796	2.349430	0.047319
11	1	0	-2.898949	0.582856	-0.012131
12	1	0	-1.806922	0.467931	-1.387711
13	1	0	-1.832201	-1.251243	0.980208
14	9	0	2.071457	-0.903758	-0.005733
15	7	0	-1.609014	-1.054729	0.011137
16	8	0	1.360095	1.640869	-0.381910

12a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.106660	1.584579	-0.016327
2	6	0	-0.054283	1.124374	0.917861
3	6	0	-0.778044	0.020914	0.224758
4	6	0	0.122736	-1.131794	-0.138395
5	6	0	1.249916	-0.600107	-1.041088
6	1	0	0.385112	0.749328	1.847622
7	1	0	-0.721730	1.955154	1.144939
8	1	0	0.671014	2.052894	-0.905055
9	1	0	1.698218	2.339699	0.502523
10	1	0	-0.422425	-1.951978	-0.603866
11	1	0	1.936037	-1.420140	-1.260762
12	1	0	0.800210	-0.275455	-1.985255
13	7	0	1.974544	0.502055	-0.439967
14	1	0	2.529197	0.168600	0.339638
15	9	0	0.714825	-1.633707	1.035582
16	16	0	-2.313298	0.098943	-0.312569

12e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.222374	1.157858	-0.426248
2	6	0	-0.036477	0.995129	0.464056
3	6	0	-0.592412	-0.386046	0.287276
4	6	0	0.430023	-1.434226	0.599795
5	6	0	1.676048	-1.208201	-0.297791
6	1	0	0.232398	1.142172	1.515487
7	1	0	0.894057	1.118652	-1.470519
8	1	0	1.650192	2.144016	-0.242068
9	1	0	0.740203	-1.337172	1.646522
10	1	0	0.015273	-2.430649	0.448445
11	1	0	2.447107	-1.930100	-0.026914
12	1	0	1.398244	-1.394293	-1.340263
13	1	0	2.667667	0.270182	0.703787
14	9	0	-0.944216	1.986983	0.128898
15	7	0	2.216519	0.134194	-0.193201
16	16	0	-2.078760	-0.697006	-0.300293

13a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.234765	1.327779	-0.008684
2	6	0	-0.149208	1.327078	0.676960
3	6	0	-1.061766	0.376603	-0.040962
4	6	0	-0.474666	-1.009192	-0.225526
5	6	0	0.912705	-0.915569	-0.859625
6	1	0	-0.027548	0.993992	1.713299
7	1	0	-0.588047	2.326141	0.683801
8	1	0	1.140435	1.779456	-1.002639
9	1	0	1.928037	1.945182	0.564925
10	1	0	-1.138598	-1.655986	-0.803565
11	1	0	1.356966	-1.912642	-0.893038
12	1	0	0.781584	-0.578047	-1.894247
13	7	0	1.808438	-0.003083	-0.168276
14	1	0	2.052601	-0.386424	0.737946
15	9	0	-0.338097	-1.594060	1.050780
16	7	0	-2.178381	0.748818	-0.520296
17	1	0	-2.643942	-0.025471	-0.996486

13e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.291369	-1.432873	-0.298953
2	6	0	0.755061	-0.569243	0.423970
3	6	0	0.527894	0.892930	0.117084
4	6	0	-0.877344	1.335695	0.407707
5	6	0	-1.872725	0.401209	-0.309672
6	1	0	0.696684	-0.729717	1.505263
7	1	0	-0.107862	-1.356648	-1.376362
8	1	0	-0.160889	-2.476639	-0.009188
9	1	0	-1.057321	1.279886	1.487384
10	1	0	-1.005534	2.372289	0.090961
11	1	0	-2.895108	0.662992	-0.032647
12	1	0	-1.780815	0.544731	-1.391798
13	1	0	-1.893900	-1.213550	0.943627
14	9	0	2.033666	-0.958234	0.019808
15	7	0	-1.652636	-1.010806	-0.020141
16	7	0	1.392924	1.669016	-0.393705
17	1	0	2.270634	1.166983	-0.539408

14a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.071434	1.451207	0.013946
2	6	0	-0.315120	1.285257	0.676885
3	6	0	-1.097098	0.233206	-0.059082
4	6	0	-0.349778	-1.066828	-0.246445
5	6	0	1.024714	-0.807301	-0.859366
6	1	0	-0.173764	0.961386	1.713458
7	1	0	-0.858237	2.233302	0.686624
8	1	0	0.940924	1.899336	-0.977263
9	1	0	1.679431	2.137938	0.605008
10	1	0	-0.938338	-1.770375	-0.836067
11	1	0	1.583557	-1.744801	-0.894319
12	1	0	0.870431	-0.476089	-1.892843
13	7	0	1.797713	0.197943	-0.146851
14	1	0	2.072740	-0.162219	0.760021
15	9	0	-0.158821	-1.644156	1.028813
16	7	0	-2.245791	0.352696	-0.588948
17	1	0	-2.615723	1.291207	-0.428970

14e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.278723	-1.435350	-0.316514
2	6	0	0.773725	-0.578697	0.409138
3	6	0	0.545604	0.883473	0.114120
4	6	0	-0.864987	1.314200	0.426982
5	6	0	-1.867118	0.388337	-0.292825
6	1	0	0.701053	-0.741204	1.490294
7	1	0	-0.103181	-1.345657	-1.394401
8	1	0	-0.140131	-2.481902	-0.040551
9	1	0	-1.029830	1.239841	1.507762
10	1	0	-1.014502	2.356364	0.134027
11	1	0	-2.886119	0.646164	-0.000076
12	1	0	-1.787132	0.546949	-1.373667
13	1	0	-1.873898	-1.241395	0.939228
14	9	0	2.041168	-0.993578	0.016244
15	7	0	-1.640841	-1.025636	-0.023803
16	7	0	1.466951	1.594959	-0.391988
17	1	0	1.129453	2.546002	-0.543684

15a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.144634	1.423515	-0.017269
2	6	0	-0.225191	1.309802	0.676523
3	6	0	-1.069969	0.278050	-0.019885
4	6	0	-0.378674	-1.038319	-0.233744
5	6	0	0.999034	-0.843706	-0.860756
6	1	0	-0.064404	1.007897	1.718052
7	1	0	-0.731520	2.278154	0.686924
8	1	0	1.007296	1.858810	-1.013985
9	1	0	1.795053	2.096031	0.545901
10	1	0	-0.987408	-1.727065	-0.822952
11	1	0	1.522268	-1.802257	-0.887697
12	1	0	0.845925	-0.521806	-1.897373
13	7	0	1.825300	0.140851	-0.176754
14	1	0	2.092338	-0.218608	0.733188
15	9	0	-0.189604	-1.656345	1.033323
16	6	0	-2.291674	0.498189	-0.498166
17	1	0	-2.845687	-0.280130	-1.013650
18	1	0	-2.773486	1.464945	-0.391261

15e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.369119	-1.419264	-0.328987
2	6	0	0.709689	-0.626078	0.422070
3	6	0	0.572053	0.842619	0.143516
4	6	0	-0.815015	1.347267	0.444019
5	6	0	-1.855776	0.495594	-0.303877
6	1	0	0.621885	-0.811319	1.498904
7	1	0	-0.169869	-1.325859	-1.402682
8	1	0	-0.297805	-2.475886	-0.063304
9	1	0	-1.010305	1.268213	1.520836
10	1	0	-0.906383	2.400363	0.166784
11	1	0	-2.866425	0.799816	-0.023781
12	1	0	-1.748324	0.664533	-1.381314
13	1	0	-1.970896	-1.148208	0.901721
14	9	0	1.967696	-1.107756	0.037519
15	7	0	-1.714376	-0.936408	-0.056461
16	6	0	1.546523	1.584721	-0.373615
17	1	0	1.389134	2.638122	-0.580268
18	1	0	2.520227	1.165731	-0.598098

16a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.300531	-1.253861	0.034896
2	6	0	0.108377	-1.356182	0.644001
3	6	0	1.039051	-0.439593	-0.101139
4	6	0	0.524639	0.994359	-0.256734
5	6	0	-0.899099	0.983888	-0.787574
6	1	0	0.063727	-1.027062	1.687256
7	1	0	0.491601	-2.376001	0.606011
8	1	0	-1.280996	-1.678986	-0.982123
9	1	0	-1.993412	-1.850179	0.629891
10	1	0	1.193913	1.565129	-0.900925
11	1	0	-1.288119	2.003934	-0.788672
12	1	0	-0.845220	0.643539	-1.836643
13	7	0	-1.736639	0.135949	0.046002
14	9	0	0.557264	1.585103	1.016087
15	1	0	-2.701496	0.205914	-0.249581
16	8	0	2.083309	-0.784442	-0.604089

16e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.288676	-1.435382	-0.260495
2	6	0	0.784644	-0.571248	0.403880
3	6	0	0.551612	0.898934	0.085859
4	6	0	-0.861230	1.361750	0.340845
5	6	0	-1.868963	0.386946	-0.283024
6	1	0	0.744429	-0.702785	1.489926
7	1	0	-0.157337	-1.372765	-1.353054
8	1	0	-0.146680	-2.473727	0.041905
9	1	0	-1.016632	1.387209	1.425040
10	1	0	-0.979486	2.371368	-0.053724
11	1	0	-2.879859	0.666645	0.016258
12	1	0	-1.810508	0.464954	-1.380606
13	9	0	2.039703	-0.964897	-0.030098
14	7	0	-1.588644	-0.963738	0.187761
15	1	0	-2.311896	-1.602855	-0.115254
16	8	0	1.427105	1.605774	-0.354541

17a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.178912	-1.557672	0.017315
2	6	0	0.031350	-1.155779	0.883102
3	6	0	0.773523	-0.066059	0.176133
4	6	0	-0.096994	1.125978	-0.170086
5	6	0	-1.310286	0.651164	-0.962184
6	1	0	-0.342790	-0.770139	1.837372
7	1	0	0.680478	-2.009856	1.070943
8	1	0	-0.806627	-2.013918	-0.914655
9	1	0	-1.764912	-2.308453	0.549175
10	1	0	0.463855	1.880078	-0.720955
11	1	0	-1.976783	1.499518	-1.128800
12	1	0	-0.936806	0.314621	-1.944303
13	7	0	-2.009620	-0.387942	-0.225031
14	9	0	-0.519612	1.718638	1.030535
15	1	0	-2.858363	-0.647451	-0.710369
16	16	0	2.310856	-0.167646	-0.337731

17e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.239355	1.155253	-0.385420
2	6	0	-0.033392	0.992197	0.454681
3	6	0	-0.599513	-0.388703	0.255781
4	6	0	0.414214	-1.459923	0.543553
5	6	0	1.689446	-1.209940	-0.276487
6	1	0	0.207415	1.122572	1.514925
7	1	0	0.953771	1.102206	-1.448625
8	1	0	1.661515	2.141886	-0.190308
9	1	0	0.673645	-1.415807	1.607713
10	1	0	-0.006014	-2.441093	0.327095
11	1	0	2.446846	-1.942129	0.005999
12	1	0	1.459538	-1.353901	-1.344324
13	9	0	-0.930992	1.987237	0.105819
14	7	0	2.186285	0.128011	0.009749
15	1	0	3.077201	0.283866	-0.443640
16	16	0	-2.103728	-0.675758	-0.287632

18a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.327996	1.244615	0.013806
2	6	0	-0.061525	1.353137	0.655270
3	6	0	-1.022766	0.452506	-0.066902
4	6	0	-0.530084	-0.974933	-0.237074
5	6	0	0.883337	-0.989085	-0.795814
6	1	0	0.009573	1.033433	1.700057
7	1	0	-0.431170	2.378736	0.627215
8	1	0	1.284852	1.668436	-1.003739
9	1	0	2.044359	1.833319	0.589061
10	1	0	-1.204294	-1.551398	-0.874181
11	1	0	1.257440	-2.014811	-0.799683
12	1	0	0.810031	-0.652688	-1.844989
13	1	0	2.707276	-0.226818	-0.320134
14	7	0	1.754601	-0.149700	0.011368
15	9	0	-0.544817	-1.587845	1.029309
16	7	0	-2.115999	0.887470	-0.544864
17	1	0	-2.626665	0.140566	-1.018637

18e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.322883	-1.421835	-0.276313
2	6	0	0.746309	-0.584837	0.423596
3	6	0	0.550551	0.882880	0.106794
4	6	0	-0.847105	1.366094	0.381387
5	6	0	-1.865930	0.435895	-0.286961
6	1	0	0.692238	-0.736565	1.505426
7	1	0	-0.165645	-1.339889	-1.364406
8	1	0	-0.207476	-2.468061	0.010513
9	1	0	-1.020358	1.357978	1.462978
10	1	0	-0.950204	2.390129	0.020485
11	1	0	-2.877620	0.726943	-0.000296
12	1	0	-1.782255	0.541178	-1.381055
13	1	0	-2.351533	-1.550082	-0.195210
14	9	0	2.009395	-1.002798	0.006102
15	7	0	-1.625932	-0.935703	0.149878
16	7	0	1.440494	1.638011	-0.390594
17	1	0	2.310719	1.118203	-0.519362

19a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.195785	1.360344	0.034342
2	6	0	-0.206721	1.324452	0.656943
3	6	0	-1.062520	0.331207	-0.082892
4	6	0	-0.427338	-1.032888	-0.258448
5	6	0	0.987939	-0.901327	-0.794744
6	1	0	-0.119417	1.005620	1.700466
7	1	0	-0.668012	2.313931	0.635354
8	1	0	1.124195	1.785567	-0.980848
9	1	0	1.841060	2.013135	0.624344
10	1	0	-1.043079	-1.654926	-0.908548
11	1	0	1.464223	-1.883665	-0.798728
12	1	0	0.898137	-0.566075	-1.842857
13	1	0	2.720006	0.037470	-0.285122
14	7	0	1.759238	0.015868	0.030718
15	9	0	-0.396621	-1.658236	1.004167
16	7	0	-2.198451	0.538422	-0.611131
17	1	0	-2.495911	1.502316	-0.449878

19e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.318603	-1.424712	-0.289445
2	6	0	0.761739	-0.598615	0.409116
3	6	0	0.572555	0.869949	0.104145
4	6	0	-0.828755	1.349035	0.399501
5	6	0	-1.857527	0.433003	-0.272724
6	1	0	0.696168	-0.750551	1.491297
7	1	0	-0.167557	-1.335200	-1.378066
8	1	0	-0.201691	-2.473304	-0.011612
9	1	0	-0.988740	1.322014	1.482685
10	1	0	-0.948157	2.380637	0.061822
11	1	0	-2.864781	0.727032	0.026639
12	1	0	-1.782063	0.552259	-1.365972
13	1	0	-2.347858	-1.551351	-0.204959
14	9	0	2.010452	-1.048330	-0.000123
15	7	0	-1.619902	-0.943152	0.146777
16	7	0	1.522565	1.554201	-0.383899
17	1	0	1.215523	2.514140	-0.544424

20a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.230200	1.356048	0.007843
2	6	0	-0.151867	1.332681	0.667943
3	6	0	-1.042743	0.345468	-0.038056
4	6	0	-0.431364	-1.014492	-0.239704
5	6	0	0.975661	-0.908313	-0.804760
6	1	0	-0.030846	1.034316	1.714943
7	1	0	-0.600021	2.328428	0.651641
8	1	0	1.132848	1.775610	-1.008351
9	1	0	1.903008	2.003687	0.573566
10	1	0	-1.053512	-1.639660	-0.882975
11	1	0	1.440163	-1.896674	-0.810641
12	1	0	0.867427	-0.580206	-1.853430
13	1	0	2.730410	0.017422	-0.360819
14	7	0	1.782174	0.005125	-0.008177
15	9	0	-0.374338	-1.674712	1.014016
16	6	0	-2.244241	0.634753	-0.529257
17	1	0	-2.836403	-0.109735	-1.052131
18	1	0	-2.673126	1.626481	-0.424760

20e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.401859	-1.406787	-0.302556
2	6	0	0.700343	-0.639567	0.424723
3	6	0	0.594609	0.831373	0.134545
4	6	0	-0.781323	1.376712	0.422876
5	6	0	-1.846088	0.531275	-0.281504
6	1	0	0.619318	-0.816963	1.502120
7	1	0	-0.224300	-1.309684	-1.386709
8	1	0	-0.346322	-2.464033	-0.036419
9	1	0	-0.970231	1.341424	1.502171
10	1	0	-0.847678	2.418857	0.103793
11	1	0	-2.844002	0.867496	0.006827
12	1	0	-1.744699	0.665326	-1.371434
13	1	0	-2.436144	-1.428174	-0.272612
14	9	0	1.939601	-1.151446	0.023801
15	7	0	-1.688400	-0.865849	0.112664
16	6	0	1.590945	1.547281	-0.376497
17	1	0	1.458652	2.602045	-0.593904
18	1	0	2.558035	1.105949	-0.586217

21a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.197880	1.375324	0.029934
2	6	0	-0.203559	1.333256	0.672992
3	6	0	-1.073966	0.375277	-0.092219
4	6	0	-0.497186	-1.034242	-0.234499
5	6	0	0.889925	-0.975689	-0.850972
6	1	0	-0.113350	0.967721	1.701828
7	1	0	-0.675831	2.315808	0.691304
8	1	0	1.120234	1.824466	-0.966501
9	1	0	1.841391	2.027028	0.624626
10	1	0	-1.186102	-1.665287	-0.796408
11	1	0	1.302074	-1.987132	-0.889570
12	1	0	0.773774	-0.636025	-1.886808
13	1	0	2.776333	0.032594	-0.585362
14	9	0	-0.404417	-1.575592	1.064102
15	6	0	1.808413	-0.022172	-0.081983
16	1	0	1.992171	-0.423788	0.919589
17	8	0	-2.114997	0.676802	-0.631142

21e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.228698	-1.457942	-0.295987
2	6	0	0.797476	-0.567688	0.396441
3	6	0	0.546396	0.899222	0.077778
4	6	0	-0.856920	1.357657	0.387135
5	6	0	-1.892027	0.439969	-0.286383
6	1	0	0.735404	-0.693480	1.483794
7	1	0	-0.081292	-1.380361	-1.378809
8	1	0	-0.045467	-2.495418	-0.008355
9	1	0	-0.990773	1.311542	1.474924
10	1	0	-0.963944	2.397357	0.075360
11	1	0	-2.894934	0.749026	0.016148
12	1	0	-1.831590	0.567313	-1.372829
13	1	0	-2.366520	-1.663809	-0.450742
14	9	0	2.082858	-0.928501	0.013301
15	1	0	-1.813782	-1.175035	1.144661
16	6	0	-1.649848	-1.025758	0.071232
17	8	0	1.401113	1.608327	-0.400645

22a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.131276	1.608889	0.012556
2	6	0	-0.052799	1.150394	0.893190
3	6	0	-0.782863	0.053209	0.184835
4	6	0	0.088105	-1.141283	-0.147061
5	6	0	1.263806	-0.700543	-1.009029
6	1	0	0.343072	0.754359	1.835613
7	1	0	-0.726644	1.976115	1.118521
8	1	0	0.733510	2.070264	-0.898036
9	1	0	1.688726	2.379912	0.548836
10	1	0	-0.492134	-1.937113	-0.612277
11	1	0	1.900607	-1.568376	-1.197171
12	1	0	0.859646	-0.378698	-1.975108
13	1	0	2.829869	0.778322	-1.032535
14	9	0	0.585122	-1.660856	1.067455
15	6	0	2.044810	0.439963	-0.352260
16	1	0	2.541700	0.068654	0.549323
17	16	0	-2.318654	0.146281	-0.339853

22e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.189677	1.211091	-0.418793
2	6	0	-0.052739	1.001265	0.446374
3	6	0	-0.596036	-0.390312	0.256984
4	6	0	0.421687	-1.444630	0.588213
5	6	0	1.686339	-1.255313	-0.271049
6	1	0	0.199491	1.125654	1.506207
7	1	0	0.886541	1.152912	-1.469724
8	1	0	1.570613	2.217610	-0.234438
9	1	0	0.693529	-1.336707	1.646153
10	1	0	-0.010774	-2.434706	0.449247
11	1	0	2.426399	-2.003185	0.021195
12	1	0	1.434574	-1.441113	-1.320672
13	1	0	3.102288	0.296249	-0.785837
14	9	0	-0.992845	1.978614	0.143695
15	1	0	2.624224	0.290467	0.905912
16	6	0	2.251821	0.153945	-0.115549
17	16	0	-2.087236	-0.708187	-0.308024

23a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.256599	1.347945	0.003361
2	6	0	-0.131249	1.344161	0.666649
3	6	0	-1.051944	0.407977	-0.063544
4	6	0	-0.516137	-1.004591	-0.222094
5	6	0	0.867709	-0.999098	-0.848298
6	1	0	-0.029614	0.997309	1.701411
7	1	0	-0.573016	2.341382	0.685258
8	1	0	1.173305	1.787820	-0.997335
9	1	0	1.930407	1.987036	0.578996
10	1	0	-1.215085	-1.627577	-0.784707
11	1	0	1.247155	-2.023786	-0.877209
12	1	0	0.751360	-0.668786	-1.887089
13	1	0	2.788674	-0.048476	-0.621380
14	9	0	-0.431222	-1.570863	1.070449
15	6	0	1.826432	-0.066691	-0.104130
16	1	0	2.012360	-0.463633	0.899269
17	7	0	-2.153934	0.805480	-0.556050
18	1	0	-2.635468	0.039909	-1.030565

23e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.272489	-1.447298	-0.305106
2	6	0	0.756528	-0.585673	0.412588
3	6	0	0.550210	0.881297	0.098332
4	6	0	-0.838327	1.367285	0.411038
5	6	0	-1.888002	0.493780	-0.293705
6	1	0	0.688366	-0.729645	1.496261
7	1	0	-0.104291	-1.358595	-1.384017
8	1	0	-0.120533	-2.492438	-0.026652
9	1	0	-0.993193	1.305681	1.495350
10	1	0	-0.922223	2.415131	0.119472
11	1	0	-2.889110	0.821361	-0.003720
12	1	0	-1.803915	0.636987	-1.376929
13	1	0	-2.412726	-1.597862	-0.501578
14	9	0	2.047111	-0.977048	0.038315
15	1	0	-1.876185	-1.146117	1.110206
16	6	0	-1.690369	-0.984605	0.041887
17	7	0	1.429883	1.638970	-0.414116
18	1	0	2.295321	1.117434	-0.564613

24a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.107991	1.460604	0.025643
2	6	0	-0.281442	1.307178	0.668392
3	6	0	-1.087706	0.279131	-0.079622
4	6	0	-0.405638	-1.063119	-0.244218
5	6	0	0.978494	-0.906904	-0.849706
6	1	0	-0.160077	0.965079	1.702440
7	1	0	-0.816241	2.259446	0.692202
8	1	0	0.994058	1.898469	-0.972740
9	1	0	1.703722	2.160245	0.616638
10	1	0	-1.039183	-1.737248	-0.821092
11	1	0	1.464474	-1.885339	-0.882704
12	1	0	0.843066	-0.579312	-1.887073
13	1	0	2.786305	0.238802	-0.583546
14	9	0	-0.276016	-1.632535	1.045504
15	1	0	-2.556660	1.397947	-0.470653
16	6	0	1.823098	0.113369	-0.083204
17	1	0	2.033999	-0.270136	0.920553
18	7	0	-2.225444	0.443328	-0.621038

24e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.260839	-1.448870	-0.325482
2	6	0	0.774773	-0.596557	0.398067
3	6	0	0.568203	0.870473	0.096102
4	6	0	-0.824705	1.344858	0.435276
5	6	0	-1.881553	0.483986	-0.274218
6	1	0	0.690161	-0.743185	1.481257
7	1	0	-0.098126	-1.345895	-1.404167
8	1	0	-0.102977	-2.497080	-0.062092
9	1	0	-0.964535	1.260202	1.519742
10	1	0	-0.928987	2.399744	0.171666
11	1	0	-2.878982	0.806845	0.033126
12	1	0	-1.809037	0.646139	-1.355421
13	1	0	-2.402115	-1.604008	-0.515474
14	9	0	2.054706	-1.014021	0.038207
15	1	0	1.180439	2.519705	-0.568105
16	1	0	-1.858969	-1.178388	1.101367
17	6	0	-1.678420	-0.998852	0.035093

18	7	0	1.499431	1.561697	-0.419256
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25a Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.167902	1.442923	-0.004851
2	6	0	-0.206892	1.325634	0.669906
3	6	0	-1.064372	0.310409	-0.038530
4	6	0	-0.422978	-1.037219	-0.230391
5	6	0	0.958812	-0.928214	-0.853365
6	1	0	-0.061434	1.006404	1.709128
7	1	0	-0.713953	2.292968	0.695606
8	1	0	1.040494	1.870201	-1.006845
9	1	0	1.798573	2.133519	0.561482
10	1	0	-1.068483	-1.704455	-0.804650
11	1	0	1.418702	-1.919804	-0.879938
12	1	0	0.818698	-0.609681	-1.892824
13	1	0	2.803647	0.167895	-0.632961
14	9	0	-0.283155	-1.644732	1.051125
15	6	0	-2.273987	0.563969	-0.530756
16	1	0	-2.846817	-0.199956	-1.047432
17	1	0	-2.729031	1.544915	-0.434804
18	6	0	1.845581	0.076375	-0.114767
19	1	0	2.063608	-0.302694	0.889644

25e Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.353407	-1.435531	-0.333459
2	6	0	0.710762	-0.641246	0.410991
3	6	0	0.593837	0.830493	0.125456
4	6	0	-0.774391	1.376982	0.447435
5	6	0	-1.866397	0.586482	-0.287675
6	1	0	0.615558	-0.810679	1.490235
7	1	0	-0.168197	-1.331693	-1.408532
8	1	0	-0.259938	-2.493520	-0.076031
9	1	0	-0.948045	1.292432	1.528283
10	1	0	-0.820714	2.438500	0.194317
11	1	0	-2.852434	0.956822	0.005374
12	1	0	-1.764820	0.754096	-1.366152
13	1	0	-2.498567	-1.470630	-0.557153
14	9	0	1.979839	-1.126546	0.054588
15	6	0	1.581032	1.552843	-0.394927
16	1	0	1.443689	2.609421	-0.600511
17	1	0	2.545365	1.115070	-0.623975
18	1	0	-1.956506	-1.087277	1.070093
19	6	0	-1.750427	-0.908963	0.007639

Vibrational frequencies (gas phase)

1a	1	2	3
	A	A	A
Frequencies --	90.2151	158.2994	229.1940
Red. masses --	6.1826	3.5053	4.6487
Frc consts --	0.0296	0.0518	0.1439
IR Inten --	9.7251	0.5613	5.2886
	4	5	6
	A	A	A
Frequencies --	293.0812	396.0234	440.0788
Red. masses --	3.9482	2.1110	5.0952
Frc consts --	0.1998	0.1951	0.5814
IR Inten --	2.7653	7.8303	1.7235
	7	8	9
	A	A	A
Frequencies --	483.2138	506.0571	653.1741
Red. masses --	5.5501	2.3320	3.9689
Frc consts --	0.7635	0.3519	0.9976
IR Inten --	17.4440	4.1102	15.6659
	10	11	12
	A	A	A
Frequencies --	754.5997	795.8006	873.9698
Red. masses --	4.0653	2.4029	2.9389
Frc consts --	1.3639	0.8966	1.3226
IR Inten --	7.0868	16.1460	14.0293
	13	14	15
	A	A	A
Frequencies --	889.1817	943.5656	1023.4835
Red. masses --	2.3678	2.1215	3.1108
Frc consts --	1.1030	1.1128	1.9199
IR Inten --	16.2294	19.5896	2.0128
	16	17	18
	A	A	A
Frequencies --	1037.8478	1063.9652	1117.6337
Red. masses --	2.2359	2.1085	2.8512
Frc consts --	1.4189	1.4063	2.0984
IR Inten --	45.1435	26.1092	34.2440
	19	20	21
	A	A	A
Frequencies --	1155.5522	1213.4435	1264.4257
Red. masses --	3.7820	1.4356	1.9772
Frc consts --	2.9754	1.2454	1.8625
IR Inten --	33.3133	16.8224	96.2697
	22	23	24
	A	A	A
Frequencies --	1266.9803	1315.2988	1338.7756
Red. masses --	1.4113	1.5277	1.6007
Frc consts --	1.3348	1.5572	1.6903
IR Inten --	7.1947	9.9805	11.3537
	25	26	27
	A	A	A
Frequencies --	1352.8219	1373.5642	1396.9705
Red. masses --	1.2826	1.2265	1.3855
Frc consts --	1.3830	1.3634	1.5930
IR Inten --	5.9858	17.6849	9.6173
	28	29	30
	A	A	A
Frequencies --	1423.1928	1458.8702	1477.3201
Red. masses --	1.3607	1.1154	1.0879
Frc consts --	1.6238	1.3987	1.3990
IR Inten --	13.3370	15.3137	7.2247

	31	32	33
	A	A	A
Frequencies --	1518.1904	1852.6223	2994.7830
Red. masses --	1.0933	11.3679	1.0708
Frc consts --	1.4847	22.9881	5.6582
IR Inten --	4.9707	227.7048	34.8917
	34	35	36
	A	A	A
Frequencies --	2999.4689	3082.1603	3118.1068
Red. masses --	1.0718	1.0606	1.0883
Frc consts --	5.6812	5.9363	6.2340
IR Inten --	58.1900	3.3016	17.0046
	37	38	39
	A	A	A
Frequencies --	3138.7360	3141.0375	3154.9042
Red. masses --	1.0927	1.0942	1.1047
Frc consts --	6.3423	6.3604	6.4785
IR Inten --	24.8336	11.3269	6.9152
1e	1	2	3
	A	A	A
Frequencies --	94.1883	153.0165	272.0407
Red. masses --	5.5425	2.4696	8.0933
Frc consts --	0.0290	0.0341	0.3529
IR Inten --	3.6178	6.3794	0.9925
	4	5	6
	A	A	A
Frequencies --	343.3677	354.6370	410.2270
Red. masses --	3.2946	3.6245	4.4191
Frc consts --	0.2289	0.2686	0.4382
IR Inten --	1.8425	20.2729	1.3111
	7	8	9
	A	A	A
Frequencies --	445.9960	520.7776	609.2475
Red. masses --	2.9505	3.2550	4.5710
Frc consts --	0.3458	0.5201	0.9996
IR Inten --	0.8196	6.0400	14.5056
	10	11	12
	A	A	A
Frequencies --	714.8336	764.8831	876.6929
Red. masses --	2.8265	2.5191	2.5534
Frc consts --	0.8510	0.8683	1.1563
IR Inten --	10.7592	3.3217	17.3645
	13	14	15
	A	A	A
Frequencies --	918.3870	997.4290	1011.3321
Red. masses --	2.6141	1.3716	2.9816
Frc consts --	1.2990	0.8039	1.7967
IR Inten --	16.3680	1.0440	37.9083
	16	17	18
	A	A	A
Frequencies --	1075.8909	1120.4653	1124.8296
Red. masses --	3.3646	3.4560	2.7504
Frc consts --	2.2947	2.5564	2.0503
IR Inten --	7.0021	31.8906	26.2756
	19	20	21
	A	A	A
Frequencies --	1159.8206	1192.9982	1250.5382
Red. masses --	4.3502	1.6962	1.8504
Frc consts --	3.4478	1.4223	1.7049
IR Inten --	105.6293	17.4950	86.3881
	22	23	24
	A	A	A
Frequencies --	1262.7889	1313.8745	1329.9708
Red. masses --	1.3390	1.4279	1.2706
Frc consts --	1.2581	1.4523	1.3241

IR Inten	--	4.1598	6.8478	9.8727
		25	26	27
		A	A	A
Frequencies	--	1355.1818	1362.0086	1410.5360
Red. masses	--	1.2913	1.3040	1.4127
Frc consts	--	1.3972	1.4252	1.6561
IR Inten	--	2.1204	5.5025	11.9437
		28	29	30
		A	A	A
Frequencies	--	1431.6409	1458.8130	1501.7671
Red. masses	--	1.4827	1.1021	1.0757
Frc consts	--	1.7904	1.3818	1.4294
IR Inten	--	3.3600	13.5711	2.0597
		31	32	33
		A	A	A
Frequencies	--	1515.0188	1863.0100	3010.3475
Red. masses	--	1.0984	12.0419	1.0714
Frc consts	--	1.4854	24.6250	5.7203
IR Inten	--	7.2941	235.2296	37.9012
		34	35	36
		A	A	A
Frequencies	--	3014.0865	3063.5376	3070.2136
Red. masses	--	1.0702	1.0762	1.0694
Frc consts	--	5.7282	5.9512	5.9392
IR Inten	--	40.7318	6.4662	20.7866
		37	38	39
		A	A	A
Frequencies	--	3139.0421	3143.4418	3147.4956
Red. masses	--	1.0940	1.1024	1.0962
Frc consts	--	6.3514	6.4177	6.3986
IR Inten	--	25.2180	6.6208	15.8230
2a		1	2	3
		A	A	A
Frequencies	--	85.1817	159.0900	242.9620
Red. masses	--	6.5074	3.9866	4.1267
Frc consts	--	0.0278	0.0594	0.1435
IR Inten	--	3.4478	0.1076	6.9522
		4	5	6
		A	A	A
Frequencies	--	269.3738	353.3672	406.6726
Red. masses	--	5.3602	3.6517	2.3444
Frc consts	--	0.2292	0.2687	0.2284
IR Inten	--	2.5230	2.4451	7.1606
		7	8	9
		A	A	A
Frequencies	--	419.7065	505.8886	634.1389
Red. masses	--	4.8885	2.7032	5.2046
Frc consts	--	0.5074	0.4076	1.2331
IR Inten	--	1.5017	1.1919	5.0280
		10	11	12
		A	A	A
Frequencies	--	711.1176	783.7898	870.0274
Red. masses	--	4.3526	2.2485	3.1448
Frc consts	--	1.2968	0.8139	1.4025
IR Inten	--	22.7696	19.5961	10.4982
		13	14	15
		A	A	A
Frequencies	--	881.7734	937.0309	1014.3188
Red. masses	--	2.5273	2.1656	3.0808
Frc consts	--	1.1578	1.1203	1.8675

IR Inten	--	13.9051	22.9091	11.1093
		16	17	18
		A	A	A
Frequencies	--	1036.7002	1053.6673	1095.9753
Red. masses	--	2.5525	1.7948	2.8046
Frc consts	--	1.6163	1.1740	1.9848
IR Inten	--	60.3124	6.2775	71.0141
		19	20	21
		A	A	A
Frequencies	--	1156.6136	1186.5410	1241.9156
Red. masses	--	3.4481	1.8549	2.7868
Frc consts	--	2.7178	1.5387	2.5324
IR Inten	--	47.0805	22.2945	24.1006
		22	23	24
		A	A	A
Frequencies	--	1265.2864	1270.2297	1323.7035
Red. masses	--	1.5220	1.4393	1.4682
Frc consts	--	1.4356	1.3683	1.5158
IR Inten	--	17.4647	50.1552	34.7541
		25	26	27
		A	A	A
Frequencies	--	1340.6189	1342.2495	1388.1082
Red. masses	--	1.2703	1.2997	1.4790
Frc consts	--	1.3451	1.3796	1.6791
IR Inten	--	16.9430	24.9764	25.8284
		28	29	30
		A	A	A
Frequencies	--	1391.2030	1432.8628	1477.6152
Red. masses	--	1.4619	1.4914	1.1546
Frc consts	--	1.6671	1.8041	1.4852
IR Inten	--	33.5625	1.8888	10.4742
		31	32	33
		A	A	A
Frequencies	--	1481.9536	1512.9413	3002.2585
Red. masses	--	1.0854	1.0967	1.0700
Frc consts	--	1.4045	1.4790	5.6824
IR Inten	--	6.6118	6.9267	26.8751
		34	35	36
		A	A	A
Frequencies	--	3004.2452	3070.8657	3125.4928
Red. masses	--	1.0709	1.0620	1.0888
Frc consts	--	5.6946	5.9007	6.2668
IR Inten	--	55.2867	3.3533	9.0498
		37	38	39
		A	A	A
Frequencies	--	3135.8034	3142.8231	3149.8861
Red. masses	--	1.0938	1.0945	1.1032
Frc consts	--	6.3372	6.3693	6.4488
IR Inten	--	18.2210	20.7415	4.5966
2e		1	2	3
		A	A	A
Frequencies	--	81.4562	161.6959	231.8291
Red. masses	--	5.6144	2.6560	14.3712
Frc consts	--	0.0219	0.0409	0.4551
IR Inten	--	0.9157	3.6077	0.6251
		4	5	6
		A	A	A
Frequencies	--	318.8163	359.8378	387.9086
Red. masses	--	3.6461	4.2610	2.7766
Frc consts	--	0.2184	0.3251	0.2462

IR Inten	--	6.0851	11.4739	3.2429
		7	8	9
		A	A	A
Frequencies	--	447.7094	487.9864	579.6609
Red. masses	--	3.2301	4.3631	4.4945
Frc consts	--	0.3815	0.6121	0.8898
IR Inten	--	0.6646	2.4563	4.1887
		10	11	12
		A	A	A
Frequencies	--	660.7033	742.0612	849.6491
Red. masses	--	3.1308	3.0683	2.1288
Frc consts	--	0.8052	0.9955	0.9054
IR Inten	--	24.9134	2.8600	8.7469
		13	14	15
		A	A	A
Frequencies	--	912.4926	1004.8285	1014.2413
Red. masses	--	2.5849	2.9469	1.4581
Frc consts	--	1.2681	1.7531	0.8837
IR Inten	--	4.1865	50.4676	2.7224
		16	17	18
		A	A	A
Frequencies	--	1052.5530	1096.0734	1120.1109
Red. masses	--	2.9687	2.3888	3.8054
Frc consts	--	1.9378	1.6909	2.8130
IR Inten	--	4.8118	11.6526	27.7486
		19	20	21
		A	A	A
Frequencies	--	1157.2890	1190.5901	1212.9339
Red. masses	--	4.6255	1.7663	1.8974
Frc consts	--	3.6500	1.4751	1.6447
IR Inten	--	119.2508	8.3503	17.6627
		22	23	24
		A	A	A
Frequencies	--	1249.1993	1297.1755	1321.8083
Red. masses	--	1.7677	1.4818	1.2894
Frc consts	--	1.6253	1.4690	1.3274
IR Inten	--	51.3914	2.3220	2.6166
		25	26	27
		A	A	A
Frequencies	--	1340.3996	1354.8454	1367.9799
Red. masses	--	1.3636	1.3918	1.7213
Frc consts	--	1.4435	1.5052	1.8979
IR Inten	--	47.0604	22.3242	65.6792
		28	29	30
		A	A	A
Frequencies	--	1405.1931	1429.3791	1472.9646
Red. masses	--	1.4230	1.4521	1.1176
Frc consts	--	1.6555	1.7480	1.4287
IR Inten	--	4.1666	8.3827	12.4383
		31	32	33
		A	A	A
Frequencies	--	1504.8727	1519.5804	3015.4895
Red. masses	--	1.0758	1.0995	1.0699
Frc consts	--	1.4355	1.4958	5.7318
IR Inten	--	1.4626	9.2009	20.1786
		34	35	36
		A	A	A
Frequencies	--	3016.8531	3051.5115	3064.0367
Red. masses	--	1.0701	1.0673	1.0810
Frc consts	--	5.7384	5.8555	5.9796
IR Inten	--	49.5582	3.5633	25.7750

	37	38	39
	A	A	A
Frequencies --	3141.9844	3144.8122	3145.3704
Red. masses --	1.0947	1.0990	1.0971
Frc consts --	6.3670	6.4038	6.3949
IR Inten --	26.4145	6.1111	13.2714
3a	1	2	3
	A	A	A
Frequencies --	96.0723	162.1047	234.2382
Red. masses --	4.6464	3.5014	4.6083
Frc consts --	0.0253	0.0542	0.1490
IR Inten --	4.3552	0.1430	3.8990
	4	5	6
	A	A	A
Frequencies --	296.8566	397.4849	435.2084
Red. masses --	3.5237	2.0541	3.7027
Frc consts --	0.1830	0.1912	0.4132
IR Inten --	4.6961	9.6806	9.4382
	7	8	9
	A	A	A
Frequencies --	472.8064	503.6122	654.3191
Red. masses --	5.5882	2.1616	4.2204
Frc consts --	0.7360	0.3230	1.0646
IR Inten --	9.3184	4.9816	5.5600
	10	11	12
	A	A	A
Frequencies --	744.6796	798.7577	877.0321
Red. masses --	3.2767	2.5477	2.7158
Frc consts --	1.0706	0.9577	1.2308
IR Inten --	32.2087	9.2357	11.5872
	13	14	15
	A	A	A
Frequencies --	883.7838	939.6472	953.8197
Red. masses --	2.1420	1.9105	1.5695
Frc consts --	0.9858	0.9939	0.8413
IR Inten --	7.1905	92.6773	12.8062
	16	17	18
	A	A	A
Frequencies --	1023.4960	1047.5542	1081.6811
Red. masses --	3.0259	2.2268	1.9449
Frc consts --	1.8676	1.4397	1.3407
IR Inten --	1.4134	46.3468	16.4478
	19	20	21
	A	A	A
Frequencies --	1115.3937	1144.4900	1186.4400
Red. masses --	2.4248	1.7604	3.2351
Frc consts --	1.7774	1.3586	2.6831
IR Inten --	26.7862	52.8334	80.6159
	22	23	24
	A	A	A
Frequencies --	1229.2991	1272.2467	1321.1200
Red. masses --	1.2285	1.3629	1.4726
Frc consts --	1.0938	1.2998	1.5143
IR Inten --	4.2730	49.4622	14.3071
	25	26	27
	A	A	A
Frequencies --	1337.5613	1348.1776	1368.6074
Red. masses --	1.3970	1.3681	1.2534
Frc consts --	1.4726	1.4651	1.3832
IR Inten --	12.4124	2.4568	14.1183
	28	29	30
	A	A	A
Frequencies --	1379.8519	1417.7895	1425.7697
Red. masses --	1.2853	1.6465	1.5171
Frc consts --	1.4419	1.9500	1.8170
IR Inten --	8.5917	24.7868	5.2108

	31	32	33
	A	A	A
Frequencies --	1463.3872	1475.5056	1514.4159
Red. masses --	1.1427	1.0907	1.0953
Frc consts --	1.4417	1.3991	1.4801
IR Inten --	15.4724	7.8643	5.2149
	34	35	36
	A	A	A
Frequencies --	1766.8300	2986.9284	2997.6581
Red. masses --	9.2553	1.0709	1.0717
Frc consts --	17.0228	5.6291	5.6738
IR Inten --	77.0467	37.9166	57.5891
	37	38	39
	A	A	A
Frequencies --	3077.3597	3077.5789	3135.3312
Red. masses --	1.0636	1.0858	1.0924
Frc consts --	5.9345	6.0590	6.3272
IR Inten --	3.2519	36.8276	24.8356
	40	41	42
	A	A	A
Frequencies --	3138.3259	3148.5777	3479.8139
Red. masses --	1.0940	1.1031	1.0745
Frc consts --	6.3482	6.4431	7.6661
IR Inten --	18.7402	7.2695	1.5070
3e	1	2	3
	A	A	A
Frequencies --	111.2512	162.3384	290.9333
Red. masses --	4.4253	2.4835	4.9406
Frc consts --	0.0323	0.0386	0.2464
IR Inten --	0.8022	3.7622	4.1100
	4	5	6
	A	A	A
Frequencies --	346.2823	358.0566	408.0011
Red. masses --	3.3374	3.6330	4.0859
Frc consts --	0.2358	0.2744	0.4007
IR Inten --	5.0409	22.4262	0.5179
	7	8	9
	A	A	A
Frequencies --	449.2057	511.5816	600.8234
Red. masses --	2.8622	3.1644	4.2207
Frc consts --	0.3403	0.4880	0.8977
IR Inten --	0.6060	8.2754	13.9903
	10	11	12
	A	A	A
Frequencies --	704.4835	779.9219	878.8134
Red. masses --	2.5656	2.6139	2.3008
Frc consts --	0.7502	0.9368	1.0470
IR Inten --	13.7191	2.5585	10.7170
	13	14	15
	A	A	A
Frequencies --	907.1956	934.8745	1010.4959
Red. masses --	2.4156	1.2248	2.9127
Frc consts --	1.1713	0.6307	1.7523
IR Inten --	33.0019	41.7178	28.0331
	16	17	18
	A	A	A
Frequencies --	1050.2359	1075.4929	1106.2286
Red. masses --	1.7026	2.2811	2.8797
Frc consts --	1.1065	1.5546	2.0763
IR Inten --	10.0269	44.9244	62.0011
	19	20	21
	A	A	A
Frequencies --	1123.0775	1142.8069	1183.1417
Red. masses --	2.7131	2.7055	3.3177

Frc consts	--	2.0162	2.0818	2.7363
IR Inten	--	4.3655	44.5831	53.8128

		22	23	24
		A	A	A
Frequencies	--	1229.2260	1263.5092	1320.3472
Red. masses	--	1.2021	1.3562	1.3602
Frc consts	--	1.0701	1.2757	1.3971
IR Inten	--	11.3004	36.1156	5.6279

		25	26	27
		A	A	A
Frequencies	--	1327.7333	1335.8567	1367.2404
Red. masses	--	1.3102	1.2065	1.2999
Frc consts	--	1.3608	1.2686	1.4317
IR Inten	--	34.4820	7.4907	2.2529

		28	29	30
		A	A	A
Frequencies	--	1379.0324	1420.9929	1437.2644
Red. masses	--	1.3524	1.4195	1.7021
Frc consts	--	1.5153	1.6887	2.0717
IR Inten	--	4.6817	31.8863	5.0712

		31	32	33
		A	A	A
Frequencies	--	1464.8744	1502.1101	1514.8425
Red. masses	--	1.1346	1.0802	1.0993
Frc consts	--	1.4344	1.4361	1.4863
IR Inten	--	14.7587	2.1409	7.7836

		34	35	36
		A	A	A
Frequencies	--	1772.0739	3007.5790	3010.6178
Red. masses	--	9.9429	1.0710	1.0698
Frc consts	--	18.3962	5.7077	5.7130
IR Inten	--	91.1539	33.5191	47.6643

		37	38	39
		A	A	A
Frequencies	--	3063.5713	3081.2957	3135.7376
Red. masses	--	1.0646	1.0837	1.0942
Frc consts	--	5.8871	6.0622	6.3392
IR Inten	--	8.2569	23.0740	29.1097

		40	41	42
		A	A	A
Frequencies	--	3141.8099	3142.5963	3494.2290
Red. masses	--	1.1006	1.0965	1.0735
Frc consts	--	6.4009	6.3805	7.7227
IR Inten	--	5.6331	21.2168	5.1470

4a

		1	2	3
		A	A	A
Frequencies	--	104.9947	167.9402	234.4443
Red. masses	--	4.7432	3.7659	4.0465
Frc consts	--	0.0308	0.0626	0.1310
IR Inten	--	4.9104	0.8386	6.8122

		4	5	6
		A	A	A
Frequencies	--	298.8838	400.1190	437.3846
Red. masses	--	3.4939	2.0839	4.4104
Frc consts	--	0.1839	0.1966	0.4971
IR Inten	--	1.9791	6.5421	4.5345

		7	8	9
		A	A	A
Frequencies	--	473.1344	506.6870	658.6518
Red. masses	--	4.2648	2.2697	4.1303
Frc consts	--	0.5625	0.3433	1.0557

IR Inten	--	17.2291	1.4407	5.7864
		10	11	12
		A	A	A
Frequencies	--	752.5469	795.8973	875.6270
Red. masses	--	3.8933	2.4634	3.0004
Frc consts	--	1.2991	0.9194	1.3554
IR Inten	--	15.5920	14.1610	11.7044
		13	14	15
		A	A	A
Frequencies	--	885.6564	935.9856	952.7139
Red. masses	--	2.0109	1.7348	1.6087
Frc consts	--	0.9293	0.8955	0.8603
IR Inten	--	32.8281	7.3913	45.1164
		16	17	18
		A	A	A
Frequencies	--	1023.3868	1044.9560	1084.4843
Red. masses	--	3.1625	2.2017	1.9597
Frc consts	--	1.9514	1.4165	1.3580
IR Inten	--	1.8783	27.8017	80.3168
		19	20	21
		A	A	A
Frequencies	--	1112.7668	1145.5979	1183.9292
Red. masses	--	2.4014	1.7063	3.3428
Frc consts	--	1.7519	1.3194	2.7607
IR Inten	--	27.4773	19.4785	83.8751
		22	23	24
		A	A	A
Frequencies	--	1231.8836	1274.2559	1325.0031
Red. masses	--	1.2269	1.3600	1.4534
Frc consts	--	1.0970	1.3010	1.5033
IR Inten	--	2.4901	47.5169	10.9471
		25	26	27
		A	A	A
Frequencies	--	1332.9623	1360.6809	1375.8834
Red. masses	--	1.3894	1.3327	1.2455
Frc consts	--	1.4545	1.4537	1.3892
IR Inten	--	0.1009	2.7078	17.4678
		28	29	30
		A	A	A
Frequencies	--	1378.6885	1426.2719	1428.1978
Red. masses	--	1.3485	1.5675	1.6691
Frc consts	--	1.5102	1.8787	2.0059
IR Inten	--	18.3189	5.6936	51.5133
		31	32	33
		A	A	A
Frequencies	--	1465.0105	1480.5253	1517.3327
Red. masses	--	1.1102	1.0897	1.0958
Frc consts	--	1.4038	1.4074	1.4865
IR Inten	--	13.4626	7.6393	5.0096
		34	35	36
		A	A	A
Frequencies	--	1770.5709	2992.0122	2998.4561
Red. masses	--	9.2331	1.0716	1.0705
Frc consts	--	17.0539	5.6522	5.6707
IR Inten	--	79.2452	48.6078	48.5974
		37	38	39
		A	A	A
Frequencies	--	3069.9226	3120.7733	3126.8172
Red. masses	--	1.0593	1.0883	1.1024
Frc consts	--	5.8820	6.2451	6.3505
IR Inten	--	10.9633	16.3251	18.3448

	40	41	42
	A	A	A
Frequencies --	3133.0197	3139.1061	3484.6586
Red. masses --	1.0966	1.0939	1.0744
Frc consts --	6.3417	6.3508	7.6870
IR Inten --	22.3238	14.6065	1.7274

4e

	1	2	3
	A	A	A
Frequencies --	99.8283	162.7613	283.9303
Red. masses --	4.6959	2.4917	6.0313
Frc consts --	0.0276	0.0389	0.2865
IR Inten --	1.8007	6.0430	0.5030

	4	5	6
	A	A	A
Frequencies --	344.9853	355.5900	409.1262
Red. masses --	3.1287	3.4428	3.8941
Frc consts --	0.2194	0.2565	0.3840
IR Inten --	5.4212	9.5471	4.4659

	7	8	9
	A	A	A
Frequencies --	446.6304	512.5693	597.4297
Red. masses --	2.8478	3.1785	3.9914
Frc consts --	0.3347	0.4920	0.8394
IR Inten --	1.5905	5.5779	17.0482

	10	11	12
	A	A	A
Frequencies --	701.7745	785.5815	876.3017
Red. masses --	2.5833	2.5603	2.6163
Frc consts --	0.7496	0.9309	1.1837
IR Inten --	16.5589	0.5145	16.5574

	13	14	15
	A	A	A
Frequencies --	899.0744	922.9000	1010.1820
Red. masses --	1.5510	1.6572	2.9293
Frc consts --	0.7387	0.8317	1.7612
IR Inten --	20.5502	19.0545	51.1932

	16	17	18
	A	A	A
Frequencies --	1047.6774	1074.9943	1115.4710
Red. masses --	1.6754	2.1208	2.4222
Frc consts --	1.0835	1.4440	1.7757
IR Inten --	13.8074	5.4865	16.4683

	19	20	21
	A	A	A
Frequencies --	1120.8303	1147.6140	1179.6027
Red. masses --	2.7063	3.2033	3.4679
Frc consts --	2.0031	2.4857	2.8431
IR Inten --	15.4935	126.1447	77.9647

	22	23	24
	A	A	A
Frequencies --	1222.1510	1263.6077	1319.4427
Red. masses --	1.1744	1.4100	1.4003
Frc consts --	1.0335	1.3264	1.4363
IR Inten --	1.8374	45.5245	14.6248

	25	26	27
	A	A	A
Frequencies --	1332.5429	1338.1599	1364.3245
Red. masses --	1.3372	1.2394	1.2722
Frc consts --	1.3990	1.3076	1.3952
IR Inten --	2.0945	28.3938	4.0961

	28	29	30
	A	A	A
Frequencies --	1380.0184	1421.3437	1444.4990
Red. masses --	1.3398	1.3977	1.7784

Frc consts	--	1.5033	1.6637	2.1863
IR Inten	--	3.9296	5.4580	11.6305

		31	32	33
		A	A	A
Frequencies	--	1465.3468	1501.7427	1514.7697
Red. masses	--	1.1089	1.0800	1.1003
Frc consts	--	1.4029	1.4350	1.4875
IR Inten	--	15.3814	1.5506	8.0424

		34	35	36
		A	A	A
Frequencies	--	1773.4416	3002.8787	3012.8374
Red. masses	--	9.4693	1.0711	1.0700
Frc consts	--	17.5470	5.6903	5.7223
IR Inten	--	87.4057	43.8404	36.0801

		37	38	39
		A	A	A
Frequencies	--	3057.3493	3062.7041	3118.3222
Red. masses	--	1.0694	1.0745	1.1030
Frc consts	--	5.8894	5.9385	6.3195
IR Inten	--	3.1852	33.5287	20.8167

		40	41	42
		A	A	A
Frequencies	--	3132.7958	3146.4730	3493.5041
Red. masses	--	1.0953	1.0962	1.0747
Frc consts	--	6.3337	6.3945	7.7279
IR Inten	--	26.0481	19.0793	1.8461

5a

		1	2	3
		A	A	A
Frequencies	--	109.0214	168.6143	234.6645
Red. masses	--	3.7429	3.6214	3.8662
Frc consts	--	0.0262	0.0607	0.1254
IR Inten	--	0.8168	0.3277	6.0803

		4	5	6
		A	A	A
Frequencies	--	297.7924	384.2299	414.8383
Red. masses	--	3.1182	2.2622	2.1588
Frc consts	--	0.1629	0.1968	0.2189
IR Inten	--	2.2949	4.5110	4.4487

		7	8	9
		A	A	A
Frequencies	--	461.5955	497.9635	647.0683
Red. masses	--	5.0652	2.2896	4.1129
Frc consts	--	0.6359	0.3345	1.0146
IR Inten	--	5.2773	0.5848	2.7297

		10	11	12
		A	A	A
Frequencies	--	728.5857	762.8337	803.9768
Red. masses	--	1.8220	1.5759	2.4026
Frc consts	--	0.5698	0.5403	0.9150
IR Inten	--	25.3551	14.0612	5.8936

		13	14	15
		A	A	A
Frequencies	--	876.6488	894.0978	932.7303
Red. masses	--	2.7765	2.6029	1.9499
Frc consts	--	1.2572	1.2260	0.9995
IR Inten	--	9.4146	27.4185	22.5944

		16	17	18
		A	A	A
Frequencies	--	966.8468	1011.4759	1022.0257
Red. masses	--	1.3543	1.6215	2.9869
Frc consts	--	0.7459	0.9774	1.8382
IR Inten	--	41.4388	10.5959	1.2832

	19	20	21
	A	A	A
Frequencies --	1050.8963	1083.3141	1113.5639
Red. masses --	2.3895	1.8944	2.2658
Frc consts --	1.5548	1.3099	1.6554
IR Inten --	65.8782	16.2681	25.7992
	22	23	24
	A	A	A
Frequencies --	1183.2299	1237.3854	1277.3354
Red. masses --	4.5779	1.2223	1.3937
Frc consts --	3.7762	1.1026	1.3397
IR Inten --	85.6182	3.0237	40.7029
	25	26	27
	A	A	A
Frequencies --	1313.2463	1328.4850	1350.3641
Red. masses --	1.6222	1.3829	1.5145
Frc consts --	1.6484	1.4380	1.6271
IR Inten --	1.4591	3.5888	4.9869
	28	29	30
	A	A	A
Frequencies --	1368.8423	1370.5887	1401.7002
Red. masses --	1.3041	1.4176	1.4248
Frc consts --	1.4397	1.5690	1.6493
IR Inten --	18.9537	3.8699	2.5132
	31	32	33
	A	A	A
Frequencies --	1427.1165	1459.9967	1477.8969
Red. masses --	1.3757	1.1377	1.1224
Frc consts --	1.6508	1.4288	1.4445
IR Inten --	10.1623	7.5959	6.0154
	34	35	36
	A	A	A
Frequencies --	1479.7124	1512.1504	1753.0715
Red. masses --	1.1205	1.0977	6.0668
Frc consts --	1.4455	1.4788	10.9852
IR Inten --	15.8575	5.5490	12.5635
	37	38	39
	A	A	A
Frequencies --	2988.9457	2991.4745	3066.8325
Red. masses --	1.0714	1.0709	1.0605
Frc consts --	5.6392	5.6461	5.8769
IR Inten --	29.4154	73.1924	14.4663
	40	41	42
	A	A	A
Frequencies --	3087.4056	3122.9285	3130.2421
Red. masses --	1.0873	1.1024	1.0947
Frc consts --	6.1065	6.3347	6.3196
IR Inten --	33.1253	22.9536	32.4132
	43	44	45
	A	A	A
Frequencies --	3135.0211	3147.8794	3235.9538
Red. masses --	1.0936	1.0619	1.1163
Frc consts --	6.3326	6.1994	6.8872
IR Inten --	18.0461	6.8358	10.9902
5e	1	2	3
	A	A	A
Frequencies --	114.4247	173.1093	282.2243
Red. masses --	3.6503	2.4947	3.9039
Frc consts --	0.0282	0.0440	0.1832
IR Inten --	0.1336	2.5177	3.3613
	4	5	6
	A	A	A
Frequencies --	338.1884	357.4635	397.0520

Red. masses	--	2.9374	3.5717	2.8746
Frc consts	--	0.1979	0.2689	0.2670
IR Inten	--	7.4341	11.1300	1.7954

		7	8	9
		A	A	A
Frequencies	--	448.3527	484.9805	575.6142
Red. masses	--	2.7536	3.4771	3.7935
Frc consts	--	0.3261	0.4819	0.7405
IR Inten	--	0.3925	2.2308	6.3441

		10	11	12
		A	A	A
Frequencies	--	681.9401	753.4291	801.8901
Red. masses	--	2.3317	1.1514	2.2725
Frc consts	--	0.6389	0.3851	0.8609
IR Inten	--	23.5889	0.0457	0.2879

		13	14	15
		A	A	A
Frequencies	--	871.7458	896.9981	961.0027
Red. masses	--	2.1615	2.2932	1.3400
Frc consts	--	0.9678	1.0871	0.7291
IR Inten	--	6.0925	8.3826	47.9231

		16	17	18
		A	A	A
Frequencies	--	990.1043	1020.7472	1051.9359
Red. masses	--	2.1295	2.0789	1.5930
Frc consts	--	1.2300	1.2762	1.0386
IR Inten	--	25.2621	22.0481	1.5642

		19	20	21
		A	A	A
Frequencies	--	1098.2265	1100.4775	1126.8432
Red. masses	--	4.1030	2.7186	2.5183
Frc consts	--	2.9157	1.9398	1.8840
IR Inten	--	37.8250	49.3891	18.6462

		22	23	24
		A	A	A
Frequencies	--	1169.8673	1220.3109	1260.9762
Red. masses	--	4.7066	1.2771	1.4683
Frc consts	--	3.7952	1.1205	1.3756
IR Inten	--	80.6696	1.5658	36.7129

		25	26	27
		A	A	A
Frequencies	--	1286.5619	1323.0693	1333.7810
Red. masses	--	1.5394	1.3506	1.2135
Frc consts	--	1.5013	1.3930	1.2719
IR Inten	--	2.5380	4.2769	3.9846

		28	29	30
		A	A	A
Frequencies	--	1365.1205	1378.7629	1408.3859
Red. masses	--	1.3120	1.4168	1.4788
Frc consts	--	1.4406	1.5868	1.7283
IR Inten	--	1.4377	5.9795	3.8097

		31	32	33
		A	A	A
Frequencies	--	1425.4204	1451.1513	1474.3882
Red. masses	--	1.4200	1.1683	1.1321
Frc consts	--	1.6999	1.4495	1.4499
IR Inten	--	7.1697	6.0164	15.2849

		34	35	36
		A	A	A
Frequencies	--	1500.9341	1514.1838	1753.2013
Red. masses	--	1.0797	1.1001	6.3394
Frc consts	--	1.4331	1.4861	11.4805
IR Inten	--	1.0663	8.4688	17.8089

	37	38	39
	A	A	A
Frequencies --	3000.5847	3010.4253	3051.0465
Red. masses --	1.0707	1.0689	1.0642
Frc consts --	5.6795	5.7076	5.8370
IR Inten --	43.9765	41.0884	13.2785
	40	41	42
	A	A	A
Frequencies --	3063.9922	3117.4320	3127.3811
Red. masses --	1.0832	1.0996	1.0953
Frc consts --	5.9917	6.2964	6.3119
IR Inten --	35.9957	24.0042	32.9979
	43	44	45
	A	A	A
Frequencies --	3134.0965	3162.4675	3257.7386
Red. masses --	1.0972	1.0615	1.1162
Frc consts --	6.3498	6.2550	6.9792
IR Inten --	25.0810	6.4718	3.9955
6a	1	2	3
	A	A	A
Frequencies --	83.8067	143.0961	200.9247
Red. masses --	7.2784	4.8657	4.3367
Frc consts --	0.0301	0.0587	0.1032
IR Inten --	10.0548	0.2892	1.5538
	4	5	6
	A	A	A
Frequencies --	251.1251	319.5787	389.5705
Red. masses --	3.0359	2.6139	6.0928
Frc consts --	0.1128	0.1573	0.5448
IR Inten --	5.7049	1.8044	3.6548
	7	8	9
	A	A	A
Frequencies --	419.4072	500.0119	616.1115
Red. masses --	4.3741	3.0137	4.1365
Frc consts --	0.4533	0.4439	0.9251
IR Inten --	3.2871	13.5846	11.0245
	10	11	12
	A	A	A
Frequencies --	670.6127	722.8259	735.6200
Red. masses --	4.6062	4.8290	4.0872
Frc consts --	1.2205	1.4865	1.3031
IR Inten --	6.4431	1.1585	1.6968
	13	14	15
	A	A	A
Frequencies --	776.8414	836.3573	956.7885
Red. masses --	2.3032	1.8151	2.6509
Frc consts --	0.8189	0.7481	1.4298
IR Inten --	4.6751	4.5149	1.4180
	16	17	18
	A	A	A
Frequencies --	980.7752	1006.0292	1009.2999
Red. masses --	2.1956	2.2263	2.0374
Frc consts --	1.2444	1.3276	1.2228
IR Inten --	11.8096	6.8717	8.9577
	19	20	21
	A	A	A
Frequencies --	1081.1430	1151.9242	1165.4700
Red. masses --	3.0900	1.7210	1.1301
Frc consts --	2.1280	1.3455	0.9044
IR Inten --	73.7822	20.9267	2.0620
	22	23	24
	A	A	A
Frequencies --	1238.8514	1277.7554	1291.5596
Red. masses --	1.1785	1.5310	1.4802
Frc consts --	1.0656	1.4727	1.4548

IR Inten	--	1.9033	5.0913	3.7404
		25	26	27
		A	A	A
Frequencies	--	1327.1056	1351.6322	1362.2846
Red. masses	--	1.3411	1.4057	1.6069
Frc consts	--	1.3917	1.5131	1.7570
IR Inten	--	11.9380	11.6995	23.9002
		28	29	30
		A	A	A
Frequencies	--	1364.3135	1453.8903	1469.2615
Red. masses	--	1.3863	1.0894	1.1045
Frc consts	--	1.5203	1.3568	1.4048
IR Inten	--	7.1562	9.1931	16.4710
		31	32	33
		A	A	A
Frequencies	--	1482.2006	1847.2739	3068.4562
Red. masses	--	1.0862	11.3160	1.0643
Frc consts	--	1.4059	22.7513	5.9042
IR Inten	--	6.6642	219.9228	16.2650
		34	35	36
		A	A	A
Frequencies	--	3072.8669	3081.6141	3114.4730
Red. masses	--	1.0635	1.0584	1.0873
Frc consts	--	5.9166	5.9220	6.2137
IR Inten	--	12.8389	5.6798	17.8030
		37	38	39
		A	A	A
Frequencies	--	3139.6284	3143.0010	3147.3311
Red. masses	--	1.1011	1.1017	1.1070
Frc consts	--	6.3947	6.4124	6.4607
IR Inten	--	5.0947	3.5611	5.5039
6e		1	2	3
		A	A	A
Frequencies	--	84.2371	155.2594	253.4167
Red. masses	--	6.9518	2.9427	2.6223
Frc consts	--	0.0291	0.0418	0.0992
IR Inten	--	5.4358	5.4964	1.7428
		4	5	6
		A	A	A
Frequencies	--	285.6834	340.7629	346.4741
Red. masses	--	6.8765	4.5314	4.8440
Frc consts	--	0.3307	0.3100	0.3426
IR Inten	--	0.7054	3.5718	4.5856
		7	8	9
		A	A	A
Frequencies	--	367.5972	467.4034	590.5588
Red. masses	--	6.2049	2.6778	4.9592
Frc consts	--	0.4940	0.3447	1.0190
IR Inten	--	3.1809	0.6979	15.8255
		10	11	12
		A	A	A
Frequencies	--	690.2523	700.9470	760.7463
Red. masses	--	3.7343	3.4985	2.4582
Frc consts	--	1.0483	1.0128	0.8382
IR Inten	--	2.9084	3.5569	0.5388
		13	14	15
		A	A	A
Frequencies	--	788.7417	850.5687	922.8525
Red. masses	--	4.3110	1.9903	1.5779

Frc consts	--	1.5801	0.8484	0.7917
IR Inten	--	6.0880	20.7589	7.0779

		16	17	18
		A	A	A
Frequencies	--	997.5859	1042.7263	1069.0322
Red. masses	--	2.3189	2.2991	3.0877
Frc consts	--	1.3596	1.4728	2.0791
IR Inten	--	11.1621	6.9900	13.0377

		19	20	21
		A	A	A
Frequencies	--	1100.0502	1136.2563	1146.3129
Red. masses	--	2.2125	1.4955	2.0172
Frc consts	--	1.5775	1.1376	1.5617
IR Inten	--	77.4791	47.8140	4.3073

		22	23	24
		A	A	A
Frequencies	--	1218.0184	1262.6481	1284.8627
Red. masses	--	1.2930	1.3377	1.2997
Frc consts	--	1.1302	1.2566	1.2641
IR Inten	--	2.5190	3.3931	3.4648

		25	26	27
		A	A	A
Frequencies	--	1328.1195	1351.7481	1359.6067
Red. masses	--	1.2322	1.4407	1.4192
Frc consts	--	1.2806	1.5510	1.5456
IR Inten	--	11.3299	9.5943	2.2909

		28	29	30
		A	A	A
Frequencies	--	1398.2369	1465.4239	1481.1666
Red. masses	--	1.5445	1.0906	1.0931
Frc consts	--	1.7791	1.3798	1.4129
IR Inten	--	2.1274	13.3639	5.0304

		31	32	33
		A	A	A
Frequencies	--	1489.6624	1858.9758	3062.4899
Red. masses	--	1.0897	11.9656	1.0701
Frc consts	--	1.4247	24.3630	5.9130
IR Inten	--	8.8034	228.0358	2.1207

		34	35	36
		A	A	A
Frequencies	--	3066.8882	3071.0412	3079.1867
Red. masses	--	1.0723	1.0631	1.0632
Frc consts	--	5.9423	5.9076	5.9394
IR Inten	--	4.3218	19.8860	17.4308

		37	38	39
		A	A	A
Frequencies	--	3129.1073	3136.1378	3147.4427
Red. masses	--	1.1014	1.1054	1.1045
Frc consts	--	6.3539	6.4055	6.4463
IR Inten	--	8.7263	6.1247	2.8282

7a

		1	2	3
		A	A	A
Frequencies	--	72.2179	145.8271	200.3857
Red. masses	--	8.1451	5.1793	4.1296
Frc consts	--	0.0250	0.0649	0.0977
IR Inten	--	3.6724	0.2514	1.4879

		4	5	6
		A	A	A
Frequencies	--	248.0833	320.8275	349.0473
Red. masses	--	4.2476	2.7243	7.3232
Frc consts	--	0.1540	0.1652	0.5257

IR Inten	--	6.0415	2.6661	0.3076
		7	8	9
		A	A	A
Frequencies	--	387.3601	439.8468	593.4913
Red. masses	--	4.2191	2.6107	5.4990
Frc consts	--	0.3730	0.2976	1.1412
IR Inten	--	2.9198	0.6468	5.4565
		10	11	12
		A	A	A
Frequencies	--	670.3074	684.8700	712.6719
Red. masses	--	4.3734	5.0202	4.0045
Frc consts	--	1.1577	1.3874	1.1983
IR Inten	--	9.5604	5.1735	1.2848
		13	14	15
		A	A	A
Frequencies	--	767.9373	845.1339	941.8186
Red. masses	--	2.4395	1.8024	2.7717
Frc consts	--	0.8476	0.7585	1.4485
IR Inten	--	3.1348	5.3448	0.9725
		16	17	18
		A	A	A
Frequencies	--	964.3310	989.1551	1012.6535
Red. masses	--	2.2022	2.1791	2.0882
Frc consts	--	1.2066	1.2562	1.2617
IR Inten	--	5.8750	11.6611	14.0562
		19	20	21
		A	A	A
Frequencies	--	1063.4405	1136.1614	1150.9846
Red. masses	--	3.7097	1.5249	1.4028
Frc consts	--	2.4718	1.1598	1.0949
IR Inten	--	108.9551	2.1263	12.1574
		22	23	24
		A	A	A
Frequencies	--	1222.2126	1254.8301	1267.9594
Red. masses	--	1.4346	1.6057	1.5353
Frc consts	--	1.2626	1.4897	1.4543
IR Inten	--	17.7708	52.3446	7.7978
		25	26	27
		A	A	A
Frequencies	--	1300.6157	1319.3374	1341.4760
Red. masses	--	1.5142	1.2648	1.5898
Frc consts	--	1.5091	1.2972	1.6856
IR Inten	--	35.6119	10.8779	6.7160
		28	29	30
		A	A	A
Frequencies	--	1355.6574	1408.9233	1458.2927
Red. masses	--	1.2164	1.8019	1.0858
Frc consts	--	1.3171	2.1074	1.3605
IR Inten	--	6.1338	22.6522	8.9852
		31	32	33
		A	A	A
Frequencies	--	1477.8999	1486.7620	3067.8250
Red. masses	--	1.0794	1.1325	1.0640
Frc consts	--	1.3890	1.4749	5.9001
IR Inten	--	12.5947	9.2573	12.8884
		34	35	36
		A	A	A
Frequencies	--	3073.4149	3074.5340	3118.1027
Red. masses	--	1.0624	1.0598	1.0876
Frc consts	--	5.9126	5.9022	6.2304
IR Inten	--	14.0387	3.5738	10.0012

	37	38	39
	A	A	A
Frequencies --	3137.9603	3142.5128	3145.3839
Red. masses --	1.1012	1.1060	1.1023
Frc consts --	6.3888	6.4353	6.4254
IR Inten --	5.9326	4.5249	2.3355

7e

	1	2	3
	A	A	A
Frequencies --	70.7073	157.3519	239.5141
Red. masses --	7.5651	3.1118	8.1170
Frc consts --	0.0223	0.0454	0.2744
IR Inten --	1.3865	3.5297	0.7651

	4	5	6
	A	A	A
Frequencies --	244.2897	325.4755	344.6357
Red. masses --	3.4392	4.4899	4.0965
Frc consts --	0.1209	0.2802	0.2867
IR Inten --	3.5812	0.1834	5.1757

	7	8	9
	A	A	A
Frequencies --	371.6184	438.2728	555.6053
Red. masses --	5.9816	2.7058	4.9989
Frc consts --	0.4867	0.3062	0.9092
IR Inten --	1.6885	0.4675	6.3804

	10	11	12
	A	A	A
Frequencies --	628.8173	692.3597	731.2761
Red. masses --	4.2683	3.8903	2.8235
Frc consts --	0.9944	1.0987	0.8896
IR Inten --	8.3176	3.4692	1.3777

	13	14	15
	A	A	A
Frequencies --	790.1652	832.4577	940.0558
Red. masses --	4.4349	1.7291	1.6122
Frc consts --	1.6314	0.7060	0.8394
IR Inten --	7.6695	7.7686	6.3535

	16	17	18
	A	A	A
Frequencies --	983.7792	1006.2131	1049.5967
Red. masses --	2.5680	2.2245	2.8256
Frc consts --	1.4643	1.3270	1.8340
IR Inten --	4.1758	23.9671	3.4955

	19	20	21
	A	A	A
Frequencies --	1095.7118	1131.7002	1139.7453
Red. masses --	2.9102	1.3890	1.9323
Frc consts --	2.0586	1.0481	1.4789
IR Inten --	62.3087	39.4004	0.9023

	22	23	24
	A	A	A
Frequencies --	1189.1921	1236.7708	1270.9788
Red. masses --	1.4723	1.5424	1.2575
Frc consts --	1.2268	1.3901	1.1968
IR Inten --	3.8470	21.7276	2.3602

	25	26	27
	A	A	A
Frequencies --	1306.5719	1325.7574	1333.7910
Red. masses --	1.5000	1.5526	1.2815
Frc consts --	1.5087	1.6079	1.3432
IR Inten --	48.3626	10.2682	0.8811

	28	29	30
	A	A	A
Frequencies --	1380.1477	1387.6820	1476.8623
Red. masses --	1.5745	1.7153	1.0846
Frc consts --	1.7671	1.9461	1.3938

IR Inten	--	16.6466	31.5995	2.0614
		31	32	33
		A	A	A
Frequencies	--	1483.4826	1487.6246	3056.8412
Red. masses	--	1.0960	1.0992	1.0664
Frc consts	--	1.4212	1.4333	5.8712
IR Inten	--	20.9376	5.2781	2.5418
		34	35	36
		A	A	A
Frequencies	--	3066.0722	3077.7545	3084.9388
Red. masses	--	1.0797	1.0621	1.0613
Frc consts	--	5.9805	5.9277	5.9506
IR Inten	--	10.0798	15.4312	13.5305
		37	38	39
		A	A	A
Frequencies	--	3131.0061	3145.2679	3153.6422
Red. masses	--	1.1004	1.1044	1.1052
Frc consts	--	6.3556	6.4369	6.4762
IR Inten	--	6.5316	5.5012	2.4411
8a		1	2	3
		A	A	A
Frequencies	--	86.5724	143.5165	205.4713
Red. masses	--	5.0121	4.8979	4.2619
Frc consts	--	0.0221	0.0594	0.1060
IR Inten	--	4.5569	0.1265	1.3736
		4	5	6
		A	A	A
Frequencies	--	256.8985	323.1002	387.9268
Red. masses	--	2.8117	2.6492	5.2273
Frc consts	--	0.1093	0.1629	0.4635
IR Inten	--	5.0645	1.8333	2.2150
		7	8	9
		A	A	A
Frequencies	--	414.8112	487.9826	624.8180
Red. masses	--	3.7271	2.5160	4.2374
Frc consts	--	0.3779	0.3530	0.9747
IR Inten	--	10.5451	13.2935	5.0351
		10	11	12
		A	A	A
Frequencies	--	670.9240	713.3390	724.0267
Red. masses	--	4.7057	3.3804	5.1397
Frc consts	--	1.2480	1.0135	1.5874
IR Inten	--	6.1505	7.1849	3.3784
		13	14	15
		A	A	A
Frequencies	--	782.0098	836.9374	934.0137
Red. masses	--	2.3509	1.7916	1.4601
Frc consts	--	0.8470	0.7394	0.7505
IR Inten	--	3.7718	0.9880	68.2678
		16	17	18
		A	A	A
Frequencies	--	957.1838	981.3958	1023.0024
Red. masses	--	2.6463	2.0410	1.8912
Frc consts	--	1.4285	1.1582	1.1661
IR Inten	--	10.4814	9.2519	4.0422
		19	20	21
		A	A	A
Frequencies	--	1025.7925	1076.2626	1131.1746
Red. masses	--	1.7737	2.8569	1.7961
Frc consts	--	1.0996	1.9498	1.3541
IR Inten	--	12.5608	73.6721	41.3513

	22	23	24
	A	A	A
Frequencies --	1184.6344	1212.7614	1247.5048
Red. masses --	1.1236	1.1882	1.1873
Frc consts --	0.9290	1.0296	1.0886
IR Inten --	5.7487	24.4288	2.9778
	25	26	27
	A	A	A
Frequencies --	1294.7990	1326.7163	1346.4630
Red. masses --	1.5043	1.3083	1.3307
Frc consts --	1.4859	1.3568	1.4215
IR Inten --	8.2928	10.6263	26.2698
	28	29	30
	A	A	A
Frequencies --	1353.6849	1371.6789	1414.6140
Red. masses --	1.2948	1.3922	2.0309
Frc consts --	1.3979	1.5434	2.3945
IR Inten --	6.6094	12.2086	18.1265
	31	32	33
	A	A	A
Frequencies --	1452.9983	1469.5737	1478.2347
Red. masses --	1.0963	1.1142	1.0992
Frc consts --	1.3637	1.4178	1.4152
IR Inten --	8.9641	17.4277	6.7258
	34	35	36
	A	A	A
Frequencies --	1760.8180	3060.8570	3069.1350
Red. masses --	9.1638	1.0754	1.0667
Frc consts --	16.7399	5.9361	5.9202
IR Inten --	72.4364	6.3080	16.7380
	37	38	39
	A	A	A
Frequencies --	3074.0502	3077.8489	3137.9335
Red. masses --	1.0725	1.0597	1.1008
Frc consts --	5.9711	5.9147	6.3864
IR Inten --	44.9992	6.1727	7.1721
	40	41	42
	A	A	A
Frequencies --	3140.8551	3142.6717	3475.7921
Red. masses --	1.1016	1.1050	1.0745
Frc consts --	6.4027	6.4301	7.6481
IR Inten --	5.9668	4.7986	1.4661
8e	1	2	3
	A	A	A
Frequencies --	101.4355	162.4574	256.2731
Red. masses --	5.0399	2.9914	2.5458
Frc consts --	0.0306	0.0465	0.0985
IR Inten --	1.6711	3.8908	3.0378
	4	5	6
	A	A	A
Frequencies --	300.5078	346.4593	349.5318
Red. masses --	4.6675	4.6138	4.7814
Frc consts --	0.2483	0.3263	0.3442
IR Inten --	3.4040	4.4463	7.7486
	7	8	9
	A	A	A
Frequencies --	369.7103	463.5511	579.5649
Red. masses --	5.9136	2.4833	4.3056
Frc consts --	0.4762	0.3144	0.8521
IR Inten --	0.6341	2.7955	18.5691

	10	11	12
	A	A	A
Frequencies --	682.7011	690.0668	771.5966
Red. masses --	3.4060	3.5616	2.6415
Frc consts --	0.9353	0.9993	0.9266
IR Inten --	8.3310	2.4041	2.5384
	13	14	15
	A	A	A
Frequencies --	788.7274	849.0172	910.6160
Red. masses --	3.9815	1.8078	1.4386
Frc consts --	1.4593	0.7678	0.7029
IR Inten --	5.4765	23.4817	34.5774
	16	17	18
	A	A	A
Frequencies --	979.4528	1013.2434	1039.5176
Red. masses --	1.9158	1.4577	2.0409
Frc consts --	1.0828	0.8818	1.2994
IR Inten --	14.9969	30.7562	7.2201
	19	20	21
	A	A	A
Frequencies --	1056.3931	1086.2399	1123.0909
Red. masses --	3.2723	2.6298	2.1040
Frc consts --	2.1516	1.8282	1.5636
IR Inten --	49.6956	47.2758	13.5130
	22	23	24
	A	A	A
Frequencies --	1168.6582	1214.2614	1237.2809
Red. masses --	1.2442	1.2221	1.2721
Frc consts --	1.0012	1.0616	1.1474
IR Inten --	9.7621	2.7866	18.3638
	25	26	27
	A	A	A
Frequencies --	1277.3657	1328.1481	1331.3222
Red. masses --	1.2508	1.2322	1.3193
Frc consts --	1.2025	1.2806	1.3778
IR Inten --	1.4662	1.6798	39.9518
	28	29	30
	A	A	A
Frequencies --	1368.8551	1371.3240	1423.6263
Red. masses --	1.2850	1.3943	1.9508
Frc consts --	1.4187	1.5448	2.3294
IR Inten --	4.8500	5.3316	24.0684
	31	32	33
	A	A	A
Frequencies --	1471.3438	1480.9061	1487.5106
Red. masses --	1.0959	1.1131	1.0933
Frc consts --	1.3979	1.4383	1.4253
IR Inten --	11.3317	7.5327	9.5130
	34	35	36
	A	A	A
Frequencies --	1767.9645	3060.7065	3070.5055
Red. masses --	9.9038	1.0632	1.0619
Frc consts --	18.2389	5.8684	5.8989
IR Inten --	85.4710	7.9606	13.7437
	37	38	39
	A	A	A
Frequencies --	3075.6877	3084.4088	3125.8378
Red. masses --	1.0670	1.0778	1.1007
Frc consts --	5.9470	6.0414	6.3364
IR Inten --	6.7502	19.8817	8.7203
	40	41	42

	A	A	A
Frequencies --	3135.3999	3148.0355	3493.1624
Red. masses --	1.1055	1.1048	1.0734
Frc consts --	6.4031	6.4507	7.7168
IR Inten --	7.6529	4.1553	7.0834

9a

	1	2	3
	A	A	A
Frequencies --	93.3564	146.4966	206.5622
Red. masses --	5.1341	5.0284	4.0463
Frc consts --	0.0264	0.0636	0.1017
IR Inten --	5.1398	0.6194	1.8041

	4	5	6
	A	A	A
Frequencies --	258.5727	324.6502	391.0285
Red. masses --	2.7488	2.6441	5.2052
Frc consts --	0.1083	0.1642	0.4689
IR Inten --	5.7699	2.2404	2.9512

	7	8	9
	A	A	A
Frequencies --	416.4293	490.4948	629.7740
Red. masses --	4.3083	2.3596	4.1879
Frc consts --	0.4402	0.3345	0.9786
IR Inten --	3.3695	12.1097	4.7718

	10	11	12
	A	A	A
Frequencies --	671.7302	718.0716	727.0941
Red. masses --	4.6056	4.0300	4.7665
Frc consts --	1.2244	1.2243	1.4847
IR Inten --	7.5069	4.5002	3.3674

	13	14	15
	A	A	A
Frequencies --	777.8342	838.4363	925.1058
Red. masses --	2.3878	1.7553	1.3589
Frc consts --	0.8512	0.7270	0.6852
IR Inten --	2.6433	10.3360	20.7546

	16	17	18
	A	A	A
Frequencies --	955.0686	976.9658	1022.1750
Red. masses --	2.7507	1.9944	2.0983
Frc consts --	1.4783	1.1216	1.2917
IR Inten --	0.1812	26.9721	15.5383

	19	20	21
	A	A	A
Frequencies --	1027.6970	1074.9338	1130.5753
Red. masses --	1.7344	2.7984	1.7642
Frc consts --	1.0793	1.9051	1.3286
IR Inten --	17.5447	79.4288	31.1783

	22	23	24
	A	A	A
Frequencies --	1182.2007	1206.7887	1243.4090
Red. masses --	1.1315	1.1855	1.1741
Frc consts --	0.9318	1.0172	1.0695
IR Inten --	5.5700	18.9602	2.4338

	25	26	27
	A	A	A
Frequencies --	1299.4665	1327.4592	1340.1995
Red. masses --	1.5160	1.3312	1.3096
Frc consts --	1.5083	1.3820	1.3859
IR Inten --	10.3770	10.9799	1.0283

	28	29	30
	A	A	A
Frequencies --	1360.5791	1367.5042	1418.8187
Red. masses --	1.3124	1.3049	2.3389
Frc consts --	1.4314	1.4377	2.7741
IR Inten --	9.2401	15.8150	60.0263

	31	32	33
	A	A	A
Frequencies --	1454.0450	1473.7595	1479.1981
Red. masses --	1.1032	1.0905	1.0986
Frc consts --	1.3743	1.3955	1.4163
IR Inten --	10.5760	16.8447	6.3108
	34	35	36
	A	A	A
Frequencies --	1764.1371	3061.8964	3064.9962
Red. masses --	9.1476	1.0605	1.0649
Frc consts --	16.7734	5.8581	5.8940
IR Inten --	75.0056	16.6562	23.2694
	37	38	39
	A	A	A
Frequencies --	3074.0698	3115.4567	3119.5261
Red. masses --	1.0633	1.0877	1.1021
Frc consts --	5.9201	6.2203	6.3193
IR Inten --	11.7185	15.5314	9.3818
	40	41	42
	A	A	A
Frequencies --	3138.3864	3145.3206	3486.3499
Red. masses --	1.1023	1.1018	1.0745
Frc consts --	6.3969	6.4221	7.6945
IR Inten --	7.6558	3.5174	1.2771
9e	1	2	3
	A	A	A
Frequencies --	93.5682	162.9627	254.9896
Red. masses --	5.4759	3.0263	2.5510
Frc consts --	0.0282	0.0474	0.0977
IR Inten --	2.4883	5.8346	2.2157
	4	5	6
	A	A	A
Frequencies --	298.4039	344.8053	348.2700
Red. masses --	5.5779	3.5040	5.5835
Frc consts --	0.2926	0.2455	0.3990
IR Inten --	0.1897	2.1917	1.2086
	7	8	9
	A	A	A
Frequencies --	369.2596	471.6816	577.3881
Red. masses --	6.1980	2.4744	3.9966
Frc consts --	0.4979	0.3244	0.7850
IR Inten --	4.1948	2.6880	19.3021
	10	11	12
	A	A	A
Frequencies --	686.2648	692.2537	778.1838
Red. masses --	3.2306	3.7919	2.8275
Frc consts --	0.8964	1.0706	1.0088
IR Inten --	5.9617	0.5431	3.6892
	13	14	15
	A	A	A
Frequencies --	789.2063	850.4512	894.4982
Red. masses --	3.5014	1.8434	1.4003
Frc consts --	1.2849	0.7856	0.6601
IR Inten --	5.2902	10.0843	25.5937
	16	17	18
	A	A	A
Frequencies --	972.3429	1005.4802	1037.6727
Red. masses --	1.6583	1.7188	2.1621
Frc consts --	0.9237	1.0238	1.3717
IR Inten --	24.9756	21.0804	15.4868

	19	20	21
	A	A	A
Frequencies --	1064.2328	1100.5371	1119.8522
Red. masses --	2.5845	2.6948	2.6523
Frc consts --	1.7247	1.9231	1.9597
IR Inten --	8.3269	51.1079	76.8904
	22	23	24
	A	A	A
Frequencies --	1166.3182	1204.5026	1228.5496
Red. masses --	1.2229	1.1595	1.2586
Frc consts --	0.9801	0.9912	1.1192
IR Inten --	17.7623	18.6886	1.3788
	25	26	27
	A	A	A
Frequencies --	1281.5139	1328.7918	1341.6628
Red. masses --	1.2602	1.3113	1.2739
Frc consts --	1.2193	1.3642	1.3511
IR Inten --	2.7289	7.9665	29.1897
	28	29	30
	A	A	A
Frequencies --	1366.0830	1368.6132	1433.0389
Red. masses --	1.3643	1.3639	1.8193
Frc consts --	1.5000	1.5052	2.2012
IR Inten --	11.9926	1.5052	13.5819
	31	32	33
	A	A	A
Frequencies --	1480.1251	1481.7701	1487.7978
Red. masses --	1.1036	1.1047	1.0934
Frc consts --	1.4244	1.4291	1.4260
IR Inten --	5.7067	16.7918	6.9288
	34	35	36
	A	A	A
Frequencies --	1768.9823	3051.7070	3062.6695
Red. masses --	9.4053	1.0605	1.0823
Frc consts --	17.3409	5.8192	5.9811
IR Inten --	80.5693	15.3960	10.1203
	37	38	39
	A	A	A
Frequencies --	3066.8446	3080.9270	3104.3149
Red. masses --	1.0634	1.0622	1.1028
Frc consts --	5.8930	5.9403	6.2614
IR Inten --	15.3424	16.3789	19.0345
	40	41	42
	A	A	A
Frequencies --	3132.6692	3150.4981	3492.4473
Red. masses --	1.1046	1.1046	1.0747
Frc consts --	6.3868	6.4595	7.7233
IR Inten --	7.9219	3.7443	1.4817
10a	1	2	3
	A	A	A
Frequencies --	97.2725	145.6532	207.1900
Red. masses --	3.8294	4.9983	3.7497
Frc consts --	0.0213	0.0625	0.0948
IR Inten --	0.8086	0.3874	3.4645
	4	5	6
	A	A	A
Frequencies --	261.0765	325.5594	385.0631
Red. masses --	2.5707	2.6872	3.5707
Frc consts --	0.1032	0.1678	0.3119
IR Inten --	2.9279	2.6117	1.6893

	7	8	9
	A	A	A
Frequencies --	389.6017	465.8533	626.2455
Red. masses --	3.3100	2.2766	4.1752
Frc consts --	0.2960	0.2911	0.9648
IR Inten --	1.1655	3.0511	1.5277
	10	11	12
	A	A	A
Frequencies --	669.9270	690.7391	723.1214
Red. masses --	4.5188	2.8559	4.7100
Frc consts --	1.1949	0.8028	1.4511
IR Inten --	9.6899	10.3235	3.4693
	13	14	15
	A	A	A
Frequencies --	747.7475	788.9085	847.0296
Red. masses --	1.2631	2.0655	1.8939
Frc consts --	0.4161	0.7574	0.8006
IR Inten --	1.8995	0.9798	7.6642
	16	17	18
	A	A	A
Frequencies --	936.4222	957.2388	963.0057
Red. masses --	2.0621	2.0068	1.4172
Frc consts --	1.0654	1.0834	0.7743
IR Inten --	1.2811	11.7422	42.2799
	19	20	21
	A	A	A
Frequencies --	1002.3842	1028.2128	1039.1630
Red. masses --	1.7968	2.2355	1.9513
Frc consts --	1.0637	1.3925	1.2415
IR Inten --	14.0081	22.2164	27.9969
	22	23	24
	A	A	A
Frequencies --	1068.8620	1185.4999	1198.2138
Red. masses --	2.5915	1.1467	1.3101
Frc consts --	1.7444	0.9495	1.1082
IR Inten --	50.8622	8.6612	4.6097
	25	26	27
	A	A	A
Frequencies --	1247.9673	1298.4826	1324.1560
Red. masses --	1.1752	1.5105	1.4276
Frc consts --	1.0784	1.5006	1.4748
IR Inten --	3.9590	10.7916	11.2653
	28	29	30
	A	A	A
Frequencies --	1334.2957	1355.5036	1363.5177
Red. masses --	1.4465	1.2883	1.2523
Frc consts --	1.5173	1.3947	1.3717
IR Inten --	2.9076	13.0537	9.1247
	31	32	33
	A	A	A
Frequencies --	1379.6000	1452.8600	1462.1024
Red. masses --	2.1195	1.0949	1.1463
Frc consts --	2.3768	1.3617	1.4437
IR Inten --	5.3807	8.2912	12.0172
	34	35	36
	A	A	A
Frequencies --	1473.1543	1483.7537	1747.1392
Red. masses --	1.0937	1.1285	5.9012
Frc consts --	1.3984	1.4638	10.6132
IR Inten --	10.0935	13.9783	11.2664
	37	38	39
	A	A	A

Frequencies --	3061.8545	3063.9299	3067.9146
Red. masses --	1.0599	1.0646	1.0689
Frc consts --	5.8543	5.8885	5.9276
IR Inten --	21.7112	20.1131	1.6940
	40	41	42
	A	A	A
Frequencies --	3081.0465	3112.5628	3136.1418
Red. masses --	1.0800	1.1032	1.1027
Frc consts --	6.0403	6.2968	6.3900
IR Inten --	44.5926	16.5719	11.1285
	43	44	45
	A	A	A
Frequencies --	3142.2068	3151.1834	3238.1856
Red. masses --	1.1017	1.0620	1.1163
Frc consts --	6.4090	6.2130	6.8964
IR Inten --	5.2659	7.0990	10.2566
10e	1	2	3
	A	A	A
Frequencies --	103.5849	169.5804	255.7268
Red. masses --	3.9299	3.0261	2.4713
Frc consts --	0.0248	0.0513	0.0952
IR Inten --	0.0475	3.2060	5.4312
	4	5	6
	A	A	A
Frequencies --	301.5113	340.4264	349.4285
Red. masses --	3.7392	4.4167	3.8981
Frc consts --	0.2003	0.3016	0.2804
IR Inten --	1.4277	0.7943	3.1281
	7	8	9
	A	A	A
Frequencies --	371.6677	448.2121	545.4585
Red. masses --	5.6909	2.1932	3.6757
Frc consts --	0.4632	0.2596	0.6443
IR Inten --	1.4502	1.1945	7.6236
	10	11	12
	A	A	A
Frequencies --	655.8671	687.1146	752.5516
Red. masses --	2.8684	3.9116	1.1799
Frc consts --	0.7270	1.0881	0.3937
IR Inten --	12.7969	2.4581	0.5830
	13	14	15
	A	A	A
Frequencies --	785.9402	792.5091	844.5703
Red. masses --	3.5256	2.2195	1.8607
Frc consts --	1.2831	0.8213	0.7820
IR Inten --	7.9800	0.9134	8.7465
	16	17	18
	A	A	A
Frequencies --	949.2102	965.2485	968.2675
Red. masses --	1.7172	1.3620	1.6245
Frc consts --	0.9116	0.7477	0.8973
IR Inten --	12.5454	46.8550	4.8220
	19	20	21
	A	A	A
Frequencies --	1021.8262	1042.0752	1068.2976
Red. masses --	2.0171	2.0735	5.1316
Frc consts --	1.2409	1.3266	3.4506
IR Inten --	9.6605	5.0228	86.7305
	22	23	24
	A	A	A
Frequencies --	1090.4602	1168.4838	1193.9531
Red. masses --	2.4030	1.1753	1.4028
Frc consts --	1.6835	0.9455	1.1782
IR Inten --	12.1780	7.1760	0.8871

	25	26	27
	A	A	A
Frequencies --	1223.6744	1277.8506	1297.9106
Red. masses --	1.2733	1.2690	1.5277
Frc consts --	1.1233	1.2208	1.5162
IR Inten --	6.4983	1.3866	1.3063
	28	29	30
	A	A	A
Frequencies --	1330.2372	1366.9577	1373.7271
Red. masses --	1.2491	1.3880	1.3256
Frc consts --	1.3023	1.5281	1.4739
IR Inten --	12.4679	0.6092	2.3360
	31	32	33
	A	A	A
Frequencies --	1405.1499	1448.8455	1477.3674
Red. masses --	1.6679	1.1692	1.0979
Frc consts --	1.9403	1.4460	1.4119
IR Inten --	7.0190	9.8595	1.0346
	34	35	36
	A	A	A
Frequencies --	1482.9132	1487.6822	1747.7455
Red. masses --	1.0973	1.1034	6.2127
Frc consts --	1.4217	1.4389	11.1812
IR Inten --	20.7886	6.5089	14.7796
	37	38	39
	A	A	A
Frequencies --	3048.2933	3065.7829	3066.2989
Red. masses --	1.0610	1.0766	1.0683
Frc consts --	5.8089	5.9618	5.9180
IR Inten --	19.1687	3.9380	23.0714
	40	41	42
	A	A	A
Frequencies --	3080.3534	3100.2928	3130.1787
Red. masses --	1.0622	1.1014	1.1053
Frc consts --	5.9380	6.2374	6.3809
IR Inten --	19.7453	24.7154	10.8834
	43	44	45
	A	A	A
Frequencies --	3149.1202	3163.9358	3259.0272
Red. masses --	1.1051	1.0618	1.1158
Frc consts --	6.4573	6.2627	6.9827
IR Inten --	6.1235	6.7353	3.1400
11a	1	2	3
	A	A	A
Frequencies --	101.1767	160.5896	240.0003
Red. masses --	6.1572	3.4545	4.2361
Frc consts --	0.0371	0.0525	0.1438
IR Inten --	7.3175	1.4224	7.2050
	4	5	6
	A	A	A
Frequencies --	294.4307	390.8713	448.9402
Red. masses --	3.0058	1.9420	5.2179
Frc consts --	0.1535	0.1748	0.6196
IR Inten --	5.1155	3.1594	0.9337
	7	8	9
	A	A	A
Frequencies --	488.7561	509.1130	645.3116
Red. masses --	4.7533	2.2922	3.7919
Frc consts --	0.6690	0.3501	0.9304
IR Inten --	15.9616	4.1295	12.5120

	10	11	12
	A	A	A
Frequencies --	734.6312	768.7435	818.1871
Red. masses --	2.1600	2.2971	2.1907
Frc consts --	0.6868	0.7998	0.8640
IR Inten --	24.5046	29.2213	108.8579
	13	14	15
	A	A	A
Frequencies --	861.7334	902.2703	927.2529
Red. masses --	2.3524	2.0509	2.1586
Frc consts --	1.0292	0.9837	1.0935
IR Inten --	13.3246	10.9055	33.0734
	16	17	18
	A	A	A
Frequencies --	1020.0233	1024.6054	1041.9556
Red. masses --	2.0287	2.8893	2.6940
Frc consts --	1.2436	1.7871	1.7232
IR Inten --	9.3755	11.2426	54.6096
	19	20	21
	A	A	A
Frequencies --	1113.2498	1165.8709	1200.0849
Red. masses --	2.2526	2.7364	1.1898
Frc consts --	1.6448	2.1914	1.0096
IR Inten --	22.3706	8.3915	1.3081
	22	23	24
	A	A	A
Frequencies --	1233.5288	1269.9180	1308.6309
Red. masses --	2.1632	1.5032	1.7141
Frc consts --	1.9393	1.4283	1.7295
IR Inten --	42.0672	2.5779	4.1932
	25	26	27
	A	A	A
Frequencies --	1322.2082	1350.5672	1371.9926
Red. masses --	1.3662	1.3213	1.2106
Frc consts --	1.4072	1.4200	1.3427
IR Inten --	13.1265	7.6626	10.3054
	28	29	30
	A	A	A
Frequencies --	1389.4574	1407.9238	1469.5967
Red. masses --	1.5493	1.3863	1.1080
Frc consts --	1.7623	1.6191	1.4099
IR Inten --	10.7065	11.8966	11.9274
	31	32	33
	A	A	A
Frequencies --	1473.8738	1509.7093	1523.1910
Red. masses --	1.0915	1.1010	1.2062
Frc consts --	1.3970	1.4784	1.6488
IR Inten --	11.9471	7.5468	13.3274
	34	35	36
	A	A	A
Frequencies --	1842.7147	3048.3992	3051.8801
Red. masses --	11.2807	1.0674	1.0654
Frc consts --	22.5686	5.8440	5.8467
IR Inten --	241.3275	30.5554	22.3863
	37	38	39
	A	A	A
Frequencies --	3074.3739	3119.7018	3120.9733
Red. masses --	1.0612	1.0993	1.1003
Frc consts --	5.9098	6.3037	6.3146
IR Inten --	5.9076	24.6483	15.0716
	40	41	42
	A	A	A

Frequencies	--	3130.4184	3147.0611	3587.0583
Red. masses	--	1.0887	1.1041	1.0744
Frc consts	--	6.2858	6.4425	8.1454
IR Inten	--	20.4604	12.1021	5.0638

11e

		1	2	3
		A	A	A
Frequencies	--	96.1583	153.2983	276.1603
Red. masses	--	5.4481	2.4283	8.1820
Frc consts	--	0.0297	0.0336	0.3676
IR Inten	--	2.6288	3.2386	0.8472

		4	5	6
		A	A	A
Frequencies	--	330.4282	351.0983	405.2329
Red. masses	--	2.0008	3.5104	5.2860
Frc consts	--	0.1287	0.2550	0.5114
IR Inten	--	10.6106	6.0233	2.6973

		7	8	9
		A	A	A
Frequencies	--	436.7069	525.3327	609.6375
Red. masses	--	2.9897	2.8646	4.2324
Frc consts	--	0.3359	0.4658	0.9268
IR Inten	--	0.6637	5.7098	14.3086

		10	11	12
		A	A	A
Frequencies	--	697.8262	747.3084	772.9128
Red. masses	--	1.8940	1.9030	2.3597
Frc consts	--	0.5434	0.6262	0.8305
IR Inten	--	18.3979	76.8353	81.1575

		13	14	15
		A	A	A
Frequencies	--	878.5272	912.1389	962.7654
Red. masses	--	2.3104	2.3703	1.4830
Frc consts	--	1.0506	1.1619	0.8099
IR Inten	--	22.4525	11.9792	1.2500

		16	17	18
		A	A	A
Frequencies	--	1008.8371	1056.5914	1106.1331
Red. masses	--	2.6632	3.1957	2.5104
Frc consts	--	1.5970	2.1020	1.8097
IR Inten	--	18.1497	3.4362	67.1653

		19	20	21
		A	A	A
Frequencies	--	1130.1363	1158.8543	1177.9298
Red. masses	--	2.6825	2.0342	1.9498
Frc consts	--	2.0186	1.6096	1.5940
IR Inten	--	41.4706	23.8521	6.7875

		22	23	24
		A	A	A
Frequencies	--	1222.9656	1261.7665	1313.8978
Red. masses	--	2.4647	1.3543	1.4973
Frc consts	--	2.1719	1.2703	1.5229
IR Inten	--	34.7423	1.5555	3.3852

		25	26	27
		A	A	A
Frequencies	--	1333.4191	1347.8107	1371.9175
Red. masses	--	1.2431	1.3386	1.1834
Frc consts	--	1.3022	1.4327	1.3123
IR Inten	--	12.5306	2.0073	2.4494

		28	29	30
		A	A	A
Frequencies	--	1395.2219	1419.7182	1463.1314
Red. masses	--	1.4137	1.5853	1.1042
Frc consts	--	1.6214	1.8826	1.3928
IR Inten	--	13.2714	1.2593	15.3465

	31	32	33
	A	A	A
Frequencies --	1493.9267	1504.8305	1512.5884
Red. masses --	1.0833	1.1019	1.2270
Frc consts --	1.4244	1.4701	1.6540
IR Inten --	6.6783	6.9568	11.4320
	34	35	36
	A	A	A
Frequencies --	1856.8614	3040.6316	3051.5699
Red. masses --	11.9196	1.0809	1.0685
Frc consts --	24.2143	5.8882	5.8625
IR Inten --	245.8805	8.0585	6.8760
	37	38	39
	A	A	A
Frequencies --	3057.9669	3062.5102	3120.0895
Red. masses --	1.0632	1.0653	1.1008
Frc consts --	5.8580	5.8867	6.3137
IR Inten --	29.2929	39.5136	24.2353
	40	41	42
	A	A	A
Frequencies --	3130.4550	3136.4316	3580.1637
Red. masses --	1.1027	1.1001	1.0747
Frc consts --	6.3667	6.3762	8.1160
IR Inten --	17.5453	14.3036	1.6657
12a	1	2	3
	A	A	A
Frequencies --	89.9109	157.0795	250.9153
Red. masses --	6.1371	3.5560	4.0955
Frc consts --	0.0292	0.0517	0.1519
IR Inten --	2.1174	1.5328	7.2529
	4	5	6
	A	A	A
Frequencies --	268.2100	355.3750	404.6665
Red. masses --	4.0590	2.9776	2.2982
Frc consts --	0.1720	0.2216	0.2217
IR Inten --	4.0087	1.1303	2.7928
	7	8	9
	A	A	A
Frequencies --	425.4811	506.7107	625.5329
Red. masses --	5.0097	2.5069	5.0632
Frc consts --	0.5344	0.3792	1.1673
IR Inten --	2.5325	1.2232	3.6571
	10	11	12
	A	A	A
Frequencies --	700.5194	749.2140	802.9811
Red. masses --	2.7916	1.8626	2.0534
Frc consts --	0.8071	0.6160	0.7801
IR Inten --	7.6393	66.5568	138.1185
	13	14	15
	A	A	A
Frequencies --	858.3642	886.5778	912.3708
Red. masses --	2.4569	2.3578	2.2178
Frc consts --	1.0665	1.0919	1.0877
IR Inten --	8.6828	8.7061	42.9313
	16	17	18
	A	A	A
Frequencies --	1005.8264	1018.6720	1032.6549
Red. masses --	2.2903	2.6773	2.6312
Frc consts --	1.3652	1.6369	1.6531
IR Inten --	14.4283	22.1546	71.9227

	19	20	21
	A	A	A
Frequencies --	1079.1175	1156.9108	1181.6640
Red. masses --	1.9318	2.5784	1.4863
Frc consts --	1.3254	2.0333	1.2227
IR Inten --	48.0066	19.6747	0.3645
	22	23	24
	A	A	A
Frequencies --	1222.4358	1247.8118	1266.8314
Red. masses --	2.1050	2.0550	1.4599
Frc consts --	1.8533	1.8852	1.3804
IR Inten --	11.7405	27.2696	17.3363
	25	26	27
	A	A	A
Frequencies --	1313.0430	1318.5309	1353.1730
Red. masses --	1.4043	1.5469	1.2888
Frc consts --	1.4265	1.5845	1.3904
IR Inten --	12.3993	83.6645	2.8092
	28	29	30
	A	A	A
Frequencies --	1371.6989	1378.2917	1421.5192
Red. masses --	1.3937	1.3341	1.6862
Frc consts --	1.5450	1.4933	2.0075
IR Inten --	7.0740	30.9851	8.3870
	31	32	33
	A	A	A
Frequencies --	1477.4782	1486.4219	1500.8451
Red. masses --	1.0886	1.1477	1.1043
Frc consts --	1.4001	1.4941	1.4656
IR Inten --	7.5087	13.0150	9.1337
	34	35	36
	A	A	A
Frequencies --	1520.5191	3055.6230	3059.5056
Red. masses --	1.2070	1.0664	1.0642
Frc consts --	1.6441	5.8663	5.8691
IR Inten --	10.9099	26.7491	18.4359
	37	38	39
	A	A	A
Frequencies --	3065.6394	3125.6351	3126.4466
Red. masses --	1.0622	1.1018	1.1009
Frc consts --	5.8815	6.3419	6.3401
IR Inten --	10.3936	11.8725	26.0502
	40	41	42
	A	A	A
Frequencies --	3134.2742	3145.4735	3587.1353
Red. masses --	1.0892	1.1023	1.0745
Frc consts --	6.3045	6.4259	8.1465
IR Inten --	13.6630	7.5802	7.0811
12e	1	2	3
	A	A	A
Frequencies --	82.9310	162.0845	234.0202
Red. masses --	5.3720	2.6000	14.7716
Frc consts --	0.0218	0.0402	0.4766
IR Inten --	0.8452	1.5390	0.8482
	4	5	6
	A	A	A
Frequencies --	315.8577	356.6600	378.0080
Red. masses --	2.3486	3.4902	3.2070
Frc consts --	0.1380	0.2616	0.2700
IR Inten --	7.0449	3.9221	3.1376
	7	8	9
	A	A	A

Frequencies --	437.2959	496.4262	579.8455
Red. masses --	3.3315	3.7744	4.1920
Frc consts --	0.3753	0.5480	0.8304
IR Inten --	0.8442	5.7002	7.3566
	10	11	12
	A	A	A
Frequencies --	657.3817	723.5487	765.6042
Red. masses --	2.3115	2.2886	1.9695
Frc consts --	0.5885	0.7059	0.6802
IR Inten --	3.1970	57.7449	146.2833
	13	14	15
	A	A	A
Frequencies --	848.7270	902.7876	980.8773
Red. masses --	1.8421	2.4780	1.5471
Frc consts --	0.7818	1.1899	0.8770
IR Inten --	11.0477	4.9959	1.1053
	16	17	18
	A	A	A
Frequencies --	998.6195	1028.2587	1089.2228
Red. masses --	2.7837	3.1928	1.9758
Frc consts --	1.6356	1.9890	1.3811
IR Inten --	36.9188	4.6526	16.1018
	19	20	21
	A	A	A
Frequencies --	1112.3706	1151.2553	1170.3478
Red. masses --	3.2407	1.8823	1.9079
Frc consts --	2.3626	1.4699	1.5397
IR Inten --	64.6322	32.7039	16.1583
	22	23	24
	A	A	A
Frequencies --	1209.6892	1232.7866	1293.9365
Red. masses --	2.4331	2.0036	1.4487
Frc consts --	2.0978	1.7941	1.4291
IR Inten --	7.1407	22.0854	1.0835
	25	26	27
	A	A	A
Frequencies --	1318.4107	1333.3274	1348.7071
Red. masses --	1.2816	1.6112	1.5722
Frc consts --	1.3125	1.6876	1.6850
IR Inten --	8.0068	66.8634	57.2981
	28	29	30
	A	A	A
Frequencies --	1360.2035	1397.0953	1413.2685
Red. masses --	1.1850	1.5265	1.5841
Frc consts --	1.2917	1.7555	1.8642
IR Inten --	8.2630	10.3075	8.6173
	31	32	33
	A	A	A
Frequencies --	1484.4503	1494.8531	1506.2273
Red. masses --	1.1203	1.0847	1.1124
Frc consts --	1.4546	1.4280	1.4869
IR Inten --	15.5302	4.8673	9.7181
	34	35	36
	A	A	A
Frequencies --	1516.0952	3037.2031	3045.5619
Red. masses --	1.2085	1.0731	1.0757
Frc consts --	1.6366	5.8324	5.8787
IR Inten --	8.2199	0.4629	24.6021
	37	38	39
	A	A	A
Frequencies --	3059.3675	3061.6074	3126.5485
Red. masses --	1.0642	1.0648	1.1006
Frc consts --	5.8689	5.8807	6.3388
IR Inten --	28.0889	34.0231	24.9606

	40	41	42
	A	A	A
Frequencies --	3129.3038	3133.7732	3581.3270
Red. masses --	1.1037	1.0991	1.0748
Frc consts --	6.3678	6.3594	8.1223
IR Inten --	17.1989	9.3230	2.6124

13a

	1	2	3
	A	A	A
Frequencies --	104.1287	157.9502	240.1499
Red. masses --	4.4807	3.3303	4.3580
Frc consts --	0.0286	0.0490	0.1481
IR Inten --	3.0829	1.8769	6.0572

	4	5	6
	A	A	A
Frequencies --	294.1353	391.7566	440.4326
Red. masses --	2.6830	1.9230	3.6523
Frc consts --	0.1368	0.1739	0.4174
IR Inten --	8.5428	1.9825	10.2410

	7	8	9
	A	A	A
Frequencies --	478.7821	503.5330	647.7356
Red. masses --	4.8511	2.0886	4.2282
Frc consts --	0.6552	0.3120	1.0452
IR Inten --	11.0597	3.8275	4.0342

	10	11	12
	A	A	A
Frequencies --	716.3711	778.0676	809.7841
Red. masses --	1.9909	2.3062	2.0891
Frc consts --	0.6020	0.8226	0.8071
IR Inten --	24.5443	52.3300	101.5154

	13	14	15
	A	A	A
Frequencies --	861.9435	897.7486	934.0462
Red. masses --	2.3288	1.8728	2.0227
Frc consts --	1.0194	0.8893	1.0397
IR Inten --	9.2708	18.5083	39.4008

	16	17	18
	A	A	A
Frequencies --	951.7917	1020.5097	1032.8805
Red. masses --	1.5272	2.9396	1.8901
Frc consts --	0.8151	1.8037	1.1881
IR Inten --	59.1134	1.2207	9.0350

	19	20	21
	A	A	A
Frequencies --	1052.2781	1115.2660	1147.6869
Red. masses --	2.5104	2.0475	1.5931
Frc consts --	1.6378	1.5005	1.2363
IR Inten --	45.3409	13.1350	66.3311

	22	23	24
	A	A	A
Frequencies --	1189.7352	1215.9892	1255.6910
Red. masses --	3.1238	1.1476	1.3414
Frc consts --	2.6051	0.9997	1.2462
IR Inten --	21.5482	3.7347	12.3208

	25	26	27
	A	A	A
Frequencies --	1320.0998	1327.4222	1350.4786
Red. masses --	1.6974	1.4058	1.2345
Frc consts --	1.7428	1.4594	1.3265
IR Inten --	2.2828	11.6533	13.1485

	28	29	30
	A	A	A

Frequencies --	1360.6386	1381.2588	1410.6206
Red. masses --	1.3010	1.2118	1.4007
Frc consts --	1.4191	1.3622	1.6422
IR Inten --	3.5498	5.9099	22.2133
	31	32	33
	A	A	A
Frequencies --	1420.2726	1468.7671	1471.3789
Red. masses --	2.0158	1.1100	1.1112
Frc consts --	2.3957	1.4109	1.4174
IR Inten --	8.1903	4.4598	19.3386
	34	35	36
	A	A	A
Frequencies --	1505.8069	1520.3245	1761.3196
Red. masses --	1.1014	1.2094	9.1855
Frc consts --	1.4714	1.6470	16.7892
IR Inten --	7.1920	13.0588	84.2325
	37	38	39
	A	A	A
Frequencies --	3044.9164	3047.6188	3065.3392
Red. masses --	1.0678	1.0659	1.0634
Frc consts --	5.8330	5.8332	5.8872
IR Inten --	29.8108	19.8426	11.3119
	40	41	42
	A	A	A
Frequencies --	3082.2434	3117.6101	3118.7627
Red. masses --	1.0875	1.0988	1.0999
Frc consts --	6.0871	6.2925	6.3036
IR Inten --	42.4574	33.0881	16.5540
	43	44	45
	A	A	A
Frequencies --	3140.5696	3476.0380	3581.6567
Red. masses --	1.1010	1.0744	1.0743
Frc consts --	6.3982	7.6485	8.1201
IR Inten --	12.2537	2.0660	3.9301
13e	1	2	3
	A	A	A
Frequencies --	111.8163	159.4204	283.4200
Red. masses --	4.2671	2.4339	5.1113
Frc consts --	0.0314	0.0364	0.2419
IR Inten --	0.5166	1.4936	5.0185
	4	5	6
	A	A	A
Frequencies --	329.9288	353.9885	400.5435
Red. masses --	2.0258	3.4506	4.5976
Frc consts --	0.1299	0.2548	0.4346
IR Inten --	14.4163	8.0946	0.4124
	7	8	9
	A	A	A
Frequencies --	439.6790	513.8494	598.3456
Red. masses --	2.8946	2.8580	3.8977
Frc consts --	0.3297	0.4446	0.8222
IR Inten --	2.8930	3.2262	21.5871
	10	11	12
	A	A	A
Frequencies --	685.4339	756.8494	778.8753
Red. masses --	1.8723	1.7578	2.5455
Frc consts --	0.5183	0.5933	0.9098
IR Inten --	13.4391	129.6530	30.8911
	13	14	15
	A	A	A
Frequencies --	876.8031	900.3686	925.7533
Red. masses --	1.9316	2.1692	1.3500
Frc consts --	0.8749	1.0361	0.6817
IR Inten --	23.7020	23.4617	25.5383

	16	17	18
	A	A	A
Frequencies --	1006.9312	1026.2600	1055.8715
Red. masses --	2.6438	1.4944	2.4847
Frc consts --	1.5794	0.9273	1.6321
IR Inten --	14.2166	11.6592	34.0661
	19	20	21
	A	A	A
Frequencies --	1088.5564	1116.9787	1141.9650
Red. masses --	2.9159	2.4006	2.3098
Frc consts --	2.0357	1.7647	1.7747
IR Inten --	69.9101	19.3086	16.0563
	22	23	24
	A	A	A
Frequencies --	1192.2490	1196.5234	1250.9294
Red. masses --	1.5235	2.1566	1.3301
Frc consts --	1.2759	1.8191	1.2263
IR Inten --	8.8930	12.7610	12.0058
	25	26	27
	A	A	A
Frequencies --	1320.2227	1323.2338	1336.5049
Red. masses --	1.3229	1.3451	1.3049
Frc consts --	1.3586	1.3877	1.3733
IR Inten --	17.1784	12.5542	3.7474
	28	29	30
	A	A	A
Frequencies --	1365.2422	1375.3139	1401.1056
Red. masses --	1.3129	1.2050	1.4200
Frc consts --	1.4418	1.3429	1.6425
IR Inten --	2.2554	1.3620	27.4893
	31	32	33
	A	A	A
Frequencies --	1429.7746	1469.0999	1492.8824
Red. masses --	1.8521	1.1279	1.0858
Frc consts --	2.2308	1.4343	1.4258
IR Inten --	12.2328	14.8130	6.1584
	34	35	36
	A	A	A
Frequencies --	1503.2113	1510.7099	1767.4290
Red. masses --	1.1101	1.2140	9.8666
Frc consts --	1.4780	1.6324	18.1595
IR Inten --	8.0040	10.4201	96.7598
	37	38	39
	A	A	A
Frequencies --	3042.7141	3053.1745	3054.6654
Red. masses --	1.0688	1.0747	1.0661
Frc consts --	5.8302	5.9026	5.8609
IR Inten --	7.1456	5.0906	32.6566
	40	41	42
	A	A	A
Frequencies --	3062.8737	3116.0581	3129.3413
Red. masses --	1.0703	1.1013	1.1026
Frc consts --	5.9158	6.3003	6.3617
IR Inten --	49.2197	28.9923	22.2853
	43	44	45
	A	A	A
Frequencies --	3134.3454	3487.4583	3575.6982
Red. masses --	1.0978	1.0736	1.0746
Frc consts --	6.3543	7.6934	8.0950
IR Inten --	13.5870	5.2009	1.1476

14a	1	2	3
	A	A	A
Frequencies --	110.7162	163.8920	243.5637
Red. masses --	4.6246	3.4610	3.7905
Frc consts --	0.0334	0.0548	0.1325
IR Inten --	3.6442	2.3558	7.7007
	4	5	6
	A	A	A
Frequencies --	295.3179	393.0401	442.2362
Red. masses --	2.7870	1.9342	4.4152
Frc consts --	0.1432	0.1760	0.5088
IR Inten --	3.8137	4.0093	4.9427
	7	8	9
	A	A	A
Frequencies --	477.9011	507.7455	650.4429
Red. masses --	4.0176	2.1302	4.0595
Frc consts --	0.5406	0.3236	1.0119
IR Inten --	9.5900	4.9979	6.9613
	10	11	12
	A	A	A
Frequencies --	723.5296	775.7931	814.3616
Red. masses --	2.1217	2.3988	2.0822
Frc consts --	0.6544	0.8506	0.8136
IR Inten --	21.8681	24.5295	114.7400
	13	14	15
	A	A	A
Frequencies --	863.2103	891.1930	931.5357
Red. masses --	2.3246	1.7596	2.0057
Frc consts --	1.0206	0.8234	1.0254
IR Inten --	24.0388	17.1089	36.3824
	16	17	18
	A	A	A
Frequencies --	949.2212	1021.3286	1032.4168
Red. masses --	1.5143	2.9422	1.9518
Frc consts --	0.8039	1.8082	1.2258
IR Inten --	15.7481	1.8614	6.7816
	19	20	21
	A	A	A
Frequencies --	1051.4564	1110.3250	1146.1685
Red. masses --	2.2940	2.1450	1.4600
Frc consts --	1.4942	1.5581	1.1300
IR Inten --	100.0751	29.1538	9.0010
	22	23	24
	A	A	A
Frequencies --	1186.6580	1209.4657	1249.7727
Red. masses --	2.8879	1.1666	1.4312
Frc consts --	2.3960	1.0054	1.3171
IR Inten --	31.3317	2.5626	18.1755
	25	26	27
	A	A	A
Frequencies --	1315.9370	1326.5705	1340.3773
Red. masses --	1.5988	1.4289	1.3071
Frc consts --	1.6312	1.4815	1.3836
IR Inten --	2.5175	1.9331	6.2594
	28	29	30
	A	A	A
Frequencies --	1361.2347	1374.4547	1406.0511
Red. masses --	1.2962	1.1943	1.3778
Frc consts --	1.4151	1.3293	1.6049
IR Inten --	13.6179	7.0007	10.6298
	31	32	33
	A	A	A

Frequencies --	1425.2205	1472.9138	1474.6954
Red. masses --	2.2494	1.0881	1.1049
Frc consts --	2.6921	1.3909	1.4157
IR Inten --	50.3689	1.3679	21.8627
	34	35	36
	A	A	A
Frequencies --	1504.7289	1521.4528	1762.5006
Red. masses --	1.0989	1.2105	9.2147
Frc consts --	1.4660	1.6509	16.8651
IR Inten --	6.5341	13.1038	86.9330
	37	38	39
	A	A	A
Frequencies --	3041.5782	3051.2524	3058.2039
Red. masses --	1.0677	1.0652	1.0595
Frc consts --	5.8198	5.8432	5.8383
IR Inten --	33.0827	24.0629	14.0239
	40	41	42
	A	A	A
Frequencies --	3110.3125	3117.5048	3118.5235
Red. masses --	1.0999	1.1028	1.1019
Frc consts --	6.2694	6.3148	6.3139
IR Inten --	30.4939	10.7068	29.8033
	43	44	45
	A	A	A
Frequencies --	3132.1497	3480.2211	3583.5148
Red. masses --	1.0885	1.0743	1.0744
Frc consts --	6.2916	7.6666	8.1286
IR Inten --	18.1863	1.9634	4.3036
14e	1	2	3
	A	A	A
Frequencies --	102.5665	162.7053	288.7590
Red. masses --	4.5669	2.4508	6.1101
Frc consts --	0.0283	0.0382	0.3002
IR Inten --	1.1790	3.6903	0.3478
	4	5	6
	A	A	A
Frequencies --	330.8755	352.3707	404.7063
Red. masses --	1.9913	3.3188	4.5014
Frc consts --	0.1284	0.2428	0.4344
IR Inten --	7.3688	1.0606	7.8011
	7	8	9
	A	A	A
Frequencies --	439.0916	518.3351	597.1728
Red. masses --	2.9217	2.8064	3.6526
Frc consts --	0.3319	0.4442	0.7675
IR Inten --	1.3245	12.8172	11.1350
	10	11	12
	A	A	A
Frequencies --	684.9638	760.9771	784.8116
Red. masses --	1.9218	1.7041	2.5416
Frc consts --	0.5312	0.5814	0.9224
IR Inten --	9.6964	155.3698	14.2576
	13	14	15
	A	A	A
Frequencies --	876.6862	892.4248	915.2568
Red. masses --	2.0797	1.5993	1.7131
Frc consts --	0.9418	0.7504	0.8455
IR Inten --	15.5711	21.2419	15.9137
	16	17	18
	A	A	A
Frequencies --	1006.8304	1021.9550	1058.5967
Red. masses --	2.5123	1.5684	2.5318
Frc consts --	1.5005	0.9651	1.6716
IR Inten --	21.1545	22.4276	1.5970

	19	20	21
	A	A	A
Frequencies --	1097.5769	1127.3628	1142.6396
Red. masses --	2.1508	2.7785	2.5958
Frc consts --	1.5266	2.0806	1.9968
IR Inten --	19.4432	48.8270	78.9843
	22	23	24
	A	A	A
Frequencies --	1183.7992	1198.1270	1247.3608
Red. masses --	1.5482	1.8946	1.3814
Frc consts --	1.2783	1.6024	1.2663
IR Inten --	17.6453	15.3618	19.0450
	25	26	27
	A	A	A
Frequencies --	1318.9831	1332.4605	1341.9127
Red. masses --	1.3946	1.3953	1.2248
Frc consts --	1.4295	1.4596	1.2995
IR Inten --	6.2308	8.1216	17.9999
	28	29	30
	A	A	A
Frequencies --	1365.2298	1374.4911	1399.7193
Red. masses --	1.3442	1.2117	1.3981
Frc consts --	1.4761	1.3487	1.6139
IR Inten --	8.3201	1.2689	5.6133
	31	32	33
	A	A	A
Frequencies --	1440.9357	1474.2678	1493.1090
Red. masses --	1.8612	1.1051	1.0894
Frc consts --	2.2768	1.4151	1.4310
IR Inten --	12.1857	17.0076	5.2889
	34	35	36
	A	A	A
Frequencies --	1503.5000	1511.4689	1768.5521
Red. masses --	1.0999	1.2263	9.4043
Frc consts --	1.4649	1.6506	17.3305
IR Inten --	7.0159	9.9403	92.6969
	37	38	39
	A	A	A
Frequencies --	3031.5942	3042.8463	3052.3106
Red. masses --	1.0810	1.0658	1.0640
Frc consts --	5.8535	5.8142	5.8404
IR Inten --	13.1814	19.1360	30.8774
	40	41	42
	A	A	A
Frequencies --	3061.4344	3104.7527	3116.4311
Red. masses --	1.0649	1.0997	1.1033
Frc consts --	5.8806	6.2456	6.3131
IR Inten --	33.2446	31.2355	27.7343
	43	44	45
	A	A	A
Frequencies --	3130.8966	3491.8296	3574.9779
Red. masses --	1.1025	1.0746	1.0746
Frc consts --	6.3673	7.7194	8.0917
IR Inten --	21.6670	2.1363	1.1728
15a	1	2	3
	A	A	A
Frequencies --	115.1155	163.5407	241.9274
Red. masses --	3.6576	3.3105	3.6355
Frc consts --	0.0286	0.0522	0.1254
IR Inten --	1.0086	3.0153	6.5719

	4	5	6
	A	A	A
Frequencies --	293.4859	383.9027	412.1519
Red. masses --	2.5470	2.0255	2.2638
Frc consts --	0.1293	0.1759	0.2266
IR Inten --	5.0764	1.8050	1.6549
	7	8	9
	A	A	A
Frequencies --	467.1428	497.9879	640.2622
Red. masses --	4.5725	2.1223	4.0787
Frc consts --	0.5879	0.3101	0.9851
IR Inten --	3.1176	2.8136	1.4725
	10	11	12
	A	A	A
Frequencies --	706.4452	749.9431	789.7344
Red. masses --	1.9095	1.2303	2.1585
Frc consts --	0.5615	0.4077	0.7932
IR Inten --	24.1866	10.2243	28.1735
	13	14	15
	A	A	A
Frequencies --	811.0937	863.9641	908.6924
Red. masses --	2.0101	2.4951	2.0683
Frc consts --	0.7791	1.0973	1.0062
IR Inten --	124.9482	15.1826	0.5656
	16	17	18
	A	A	A
Frequencies --	926.6319	963.0163	1008.1455
Red. masses --	1.8550	1.3600	1.8134
Frc consts --	0.9385	0.7431	1.0859
IR Inten --	31.4421	37.2037	13.1167
	19	20	21
	A	A	A
Frequencies --	1017.5270	1037.6195	1045.4591
Red. masses --	2.6340	2.1358	2.1635
Frc consts --	1.6068	1.3549	1.3932
IR Inten --	8.6577	61.0174	14.7185
	22	23	24
	A	A	A
Frequencies --	1121.5263	1187.6772	1216.3447
Red. masses --	1.8199	3.5651	1.1170
Frc consts --	1.3487	2.9629	0.9737
IR Inten --	12.8328	27.4141	6.5595
	25	26	27
	A	A	A
Frequencies --	1253.6885	1313.4240	1324.9028
Red. masses --	1.4836	1.5888	1.5888
Frc consts --	1.3739	1.6148	1.6432
IR Inten --	9.7095	2.8858	0.1719
	28	29	30
	A	A	A
Frequencies --	1336.0132	1353.8653	1375.6138
Red. masses --	1.3426	1.3836	1.2311
Frc consts --	1.4119	1.4942	1.3725
IR Inten --	3.1613	11.9020	2.5150
	31	32	33
	A	A	A
Frequencies --	1392.1384	1407.5615	1462.8290
Red. masses --	1.7080	1.3943	1.1532
Frc consts --	1.9503	1.6275	1.4539
IR Inten --	2.0469	10.6469	8.4459
	34	35	36
	A	A	A

Frequencies	--	1471.1829	1483.7810	1501.5104
Red. masses	--	1.0888	1.1388	1.0996
Frc consts	--	1.3885	1.4772	1.4607
IR Inten	--	5.8257	16.4734	6.4233

		37	38	39
		A	A	A
Frequencies	--	1518.3770	1747.5293	3037.7926
Red. masses	--	1.2101	5.9775	1.0677
Frc consts	--	1.6437	10.7552	5.8050
IR Inten	--	12.4088	15.6085	34.0980

		40	41	42
		A	A	A
Frequencies	--	3047.6157	3051.0700	3094.8694
Red. masses	--	1.0654	1.0617	1.0877
Frc consts	--	5.8303	5.8234	6.1382
IR Inten	--	21.4050	21.0880	41.3355

		43	44	45
		A	A	A
Frequencies	--	3106.9332	3112.0063	3116.1802
Red. masses	--	1.0969	1.1039	1.1002
Frc consts	--	6.2382	6.2990	6.2948
IR Inten	--	37.5997	26.9726	25.2487

		46	47	48
		A	A	A
Frequencies	--	3145.6342	3233.3573	3578.7116
Red. masses	--	1.0615	1.1164	1.0742
Frc consts	--	6.1886	6.8764	8.1058
IR Inten	--	7.5390	11.9739	3.1375

15e

		1	2	3
		A	A	A
Frequencies	--	115.5288	171.5085	284.3570
Red. masses	--	3.5234	2.4312	3.8951
Frc consts	--	0.0277	0.0421	0.1856
IR Inten	--	1.1009	1.4236	2.9167

		4	5	6
		A	A	A
Frequencies	--	326.6084	352.2894	390.2105
Red. masses	--	2.0312	3.1585	3.2096
Frc consts	--	0.1277	0.2310	0.2879
IR Inten	--	10.0573	1.8898	3.9725

		7	8	9
		A	A	A
Frequencies	--	440.5715	489.4622	574.8299
Red. masses	--	2.8085	3.1213	3.4508
Frc consts	--	0.3212	0.4406	0.6718
IR Inten	--	2.1700	2.8511	9.0231

		10	11	12
		A	A	A
Frequencies	--	664.6529	751.5482	763.9128
Red. masses	--	1.8413	1.1441	1.6106
Frc consts	--	0.4792	0.3807	0.5538
IR Inten	--	12.2754	4.1579	163.2536

		13	14	15
		A	A	A
Frequencies	--	795.0839	866.4412	900.9088
Red. masses	--	2.3174	1.9926	2.0882
Frc consts	--	0.8631	0.8814	0.9986
IR Inten	--	2.1339	6.7347	2.9835

		16	17	18
		A	A	A
Frequencies	--	957.0264	989.6026	1009.8322
Red. masses	--	1.3438	1.9950	1.6149
Frc consts	--	0.7251	1.1511	0.9703
IR Inten	--	46.5221	11.7802	3.6959

	19	20	21
	A	A	A
Frequencies --	1014.8496	1081.3864	1093.4128
Red. masses --	2.1051	2.4495	5.0101
Frc consts --	1.2774	1.6877	3.5291
IR Inten --	12.1148	0.5780	98.5620
	22	23	24
	A	A	A
Frequencies --	1128.2528	1176.5693	1197.1629
Red. masses --	2.0145	2.1803	1.5366
Frc consts --	1.5109	1.7783	1.2976
IR Inten --	2.4434	16.2270	7.8335
	25	26	27
	A	A	A
Frequencies --	1238.8725	1284.0626	1324.8998
Red. masses --	1.6222	1.5054	1.2921
Frc consts --	1.4669	1.4625	1.3363
IR Inten --	7.8224	3.6014	1.0485
	28	29	30
	A	A	A
Frequencies --	1336.7796	1365.2098	1371.7059
Red. masses --	1.3336	1.4008	1.2636
Frc consts --	1.4041	1.5382	1.4008
IR Inten --	1.5186	1.6361	2.7615
	31	32	33
	A	A	A
Frequencies --	1391.4390	1412.4064	1450.4561
Red. masses --	1.4042	1.5676	1.1786
Frc consts --	1.6018	1.8425	1.4609
IR Inten --	4.5671	9.0755	7.0344
	34	35	36
	A	A	A
Frequencies --	1480.8835	1491.1135	1500.7003
Red. masses --	1.1206	1.0856	1.1047
Frc consts --	1.4479	1.4221	1.4658
IR Inten --	16.0484	4.0106	7.9226
	37	38	39
	A	A	A
Frequencies --	1509.7133	1749.7086	3027.4068
Red. masses --	1.2129	6.2834	1.0694
Frc consts --	1.6287	11.3339	5.7747
IR Inten --	8.1761	20.2432	10.6497
	40	41	42
	A	A	A
Frequencies --	3035.5922	3049.3762	3058.3133
Red. masses --	1.0809	1.0639	1.0636
Frc consts --	5.8684	5.8285	5.8613
IR Inten --	38.9117	33.7136	37.3027
	43	44	45
	A	A	A
Frequencies --	3104.3237	3112.1329	3122.9499
Red. masses --	1.0957	1.1032	1.1038
Frc consts --	6.2213	6.2956	6.3426
IR Inten --	34.6420	33.2444	28.4770
	46	47	48
	A	A	A
Frequencies --	3162.4630	3258.5388	3570.9375
Red. masses --	1.0616	1.1158	1.0745
Frc consts --	6.2556	6.9802	8.0725
IR Inten --	7.1459	4.2078	0.6376

16a	1	2	3
	A	A	A
Frequencies --	86.0322	167.8847	224.4395
Red. masses --	5.6158	3.3954	4.3616
Frc consts --	0.0245	0.0564	0.1294
IR Inten --	7.1728	0.0271	3.2755
	4	5	6
	A	A	A
Frequencies --	296.5316	383.1506	431.5751
Red. masses --	3.3160	1.9329	5.3563
Frc consts --	0.1718	0.1672	0.5878
IR Inten --	1.6562	4.1830	7.1492
	7	8	9
	A	A	A
Frequencies --	467.0641	501.3099	621.5657
Red. masses --	2.9185	2.5280	2.5822
Frc consts --	0.3751	0.3743	0.5878
IR Inten --	28.6333	9.9220	47.4737
	10	11	12
	A	A	A
Frequencies --	680.6377	766.6159	814.6839
Red. masses --	2.4909	3.4732	1.9376
Frc consts --	0.6799	1.2026	0.7577
IR Inten --	50.8729	21.0573	13.4884
	13	14	15
	A	A	A
Frequencies --	891.7450	900.3059	955.1618
Red. masses --	2.4432	2.3967	2.1343
Frc consts --	1.1447	1.1446	1.1473
IR Inten --	11.0385	16.0843	29.1377
	16	17	18
	A	A	A
Frequencies --	1018.5561	1055.3135	1066.6637
Red. masses --	2.9589	2.2613	1.7180
Frc consts --	1.8086	1.4838	1.1516
IR Inten --	1.9547	35.7639	2.0297
	19	20	21
	A	A	A
Frequencies --	1112.5589	1173.8730	1200.2035
Red. masses --	2.8499	2.2222	1.6944
Frc consts --	2.0784	1.8042	1.4381
IR Inten --	29.1646	3.6315	7.7612
	22	23	24
	A	A	A
Frequencies --	1215.4847	1268.9336	1305.1986
Red. masses --	1.2286	1.5842	1.3164
Frc consts --	1.0694	1.5030	1.3212
IR Inten --	15.9378	18.1831	3.3829
	25	26	27
	A	A	A
Frequencies --	1329.5489	1350.7215	1372.6730
Red. masses --	1.5663	1.3501	1.5881
Frc consts --	1.6313	1.4513	1.7631
IR Inten --	9.7391	6.1854	15.4360
	28	29	30
	A	A	A
Frequencies --	1382.0727	1428.2446	1458.6296
Red. masses --	1.3852	1.4954	1.1126
Frc consts --	1.5589	1.7973	1.3946
IR Inten --	32.3023	7.1959	16.3282

	31	32	33
	A	A	A
Frequencies --	1481.9163	1496.6108	1521.9606
Red. masses --	1.0871	1.3450	1.1081
Frc consts --	1.4066	1.7750	1.5123
IR Inten --	5.4749	12.4797	3.4216
	34	35	36
	A	A	A
Frequencies --	1849.1168	2940.6593	2947.6456
Red. masses --	11.3514	1.0719	1.0732
Frc consts --	22.8680	5.4612	5.4940
IR Inten --	224.6700	72.4706	72.0422
	37	38	39
	A	A	A
Frequencies --	3080.5968	3112.7692	3113.8828
Red. masses --	1.0612	1.0894	1.0901
Frc consts --	5.9335	6.2194	6.2277
IR Inten --	5.1098	27.6116	15.1577
	40	41	42
	A	A	A
Frequencies --	3123.9465	3155.6293	3615.2036
Red. masses --	1.0882	1.1041	1.0756
Frc consts --	6.2573	6.4779	8.2824
IR Inten --	21.3489	9.2571	5.2881
16e	1	2	3
	A	A	A
Frequencies --	90.2261	163.4368	275.8385
Red. masses --	5.1263	2.4764	7.4553
Frc consts --	0.0246	0.0390	0.3342
IR Inten --	1.9866	3.8319	2.1530
	4	5	6
	A	A	A
Frequencies --	342.1605	358.4817	400.0986
Red. masses --	2.7183	2.9663	4.1376
Frc consts --	0.1875	0.2246	0.3902
IR Inten --	0.7375	11.0417	5.2405
	7	8	9
	A	A	A
Frequencies --	436.6952	513.8487	604.4732
Red. masses --	3.2786	2.4403	3.9550
Frc consts --	0.3684	0.3796	0.8514
IR Inten --	2.0230	14.0498	25.3402
	10	11	12
	A	A	A
Frequencies --	663.3861	757.3671	791.9584
Red. masses --	2.5408	2.3083	1.6537
Frc consts --	0.6588	0.7801	0.6111
IR Inten --	52.9898	8.4607	37.8689
	13	14	15
	A	A	A
Frequencies --	898.6318	914.3751	993.0370
Red. masses --	2.6016	2.5682	1.4455
Frc consts --	1.2378	1.2651	0.8398
IR Inten --	42.7417	7.5675	5.1857
	16	17	18
	A	A	A
Frequencies --	1014.2005	1096.6759	1118.9054
Red. masses --	2.4762	2.1350	2.9675
Frc consts --	1.5007	1.5129	2.1889
IR Inten --	7.7959	0.9274	21.6962
	19	20	21
	A	A	A
Frequencies --	1124.9484	1165.6506	1188.4433
Red. masses --	3.0769	2.8974	1.6949
Frc consts --	2.2942	2.3195	1.4104

IR Inten	--	65.5900	35.0475	2.5403
		22	23	24
		A	A	A
Frequencies	--	1203.6499	1264.5171	1298.2891
Red. masses	--	1.4438	1.3608	1.3766
Frc consts	--	1.2324	1.2820	1.3671
IR Inten	--	24.8991	6.0125	6.3964
		25	26	27
		A	A	A
Frequencies	--	1325.9496	1346.9976	1361.5958
Red. masses	--	1.2522	1.3249	1.3904
Frc consts	--	1.2971	1.4163	1.5187
IR Inten	--	7.2905	4.5238	7.0264
		28	29	30
		A	A	A
Frequencies	--	1398.6684	1434.1231	1458.9927
Red. masses	--	1.7072	1.5548	1.0990
Frc consts	--	1.9677	1.8841	1.3784
IR Inten	--	14.3294	2.2211	14.8886
		31	32	33
		A	A	A
Frequencies	--	1491.3618	1506.5522	1517.4828
Red. masses	--	1.2272	1.1586	1.1035
Frc consts	--	1.6081	1.5493	1.4971
IR Inten	--	12.1037	0.8563	6.6650
		34	35	36
		A	A	A
Frequencies	--	1858.9693	2960.8880	2970.6133
Red. masses	--	12.0496	1.0726	1.0716
Frc consts	--	24.5338	5.5403	5.5716
IR Inten	--	234.8251	74.7112	48.2208
		37	38	39
		A	A	A
Frequencies	--	3064.2875	3070.1740	3111.6604
Red. masses	--	1.0719	1.0745	1.0908
Frc consts	--	5.9300	5.9675	6.2225
IR Inten	--	2.8842	23.4791	27.8036
		40	41	42
		A	A	A
Frequencies	--	3123.3256	3144.8830	3606.6558
Red. masses	--	1.0925	1.1010	1.0755
Frc consts	--	6.2791	6.4158	8.2429
IR Inten	--	19.1993	10.3063	5.5438
17a		1	2	3
		A	A	A
Frequencies	--	82.3767	165.0404	236.2311
Red. masses	--	5.7205	3.7791	3.7428
Frc consts	--	0.0229	0.0606	0.1231
IR Inten	--	2.2924	0.5059	3.0080
		4	5	6
		A	A	A
Frequencies	--	270.1701	352.3308	392.8300
Red. masses	--	4.6396	3.0488	2.3390
Frc consts	--	0.1995	0.2230	0.2127
IR Inten	--	1.4426	2.5933	5.2326
		7	8	9
		A	A	A
Frequencies	--	413.5029	486.1813	596.5183
Red. masses	--	4.8766	2.0323	2.4980
Frc consts	--	0.4913	0.2830	0.5237

IR Inten	--	10.6237	24.6570	65.5939
		10	11	12
		A	A	A
Frequencies	--	650.9503	745.9798	802.4858
Red. masses	--	3.4956	3.1980	1.8075
Frc consts	--	0.8727	1.0485	0.6858
IR Inten	--	23.8533	22.9227	25.9992
		13	14	15
		A	A	A
Frequencies	--	884.9297	893.9685	948.9005
Red. masses	--	2.8989	2.4807	2.1639
Frc consts	--	1.3375	1.1681	1.1480
IR Inten	--	8.2213	17.3291	34.3635
		16	17	18
		A	A	A
Frequencies	--	1007.3557	1047.5545	1067.6355
Red. masses	--	2.7686	1.9134	1.9651
Frc consts	--	1.6553	1.2371	1.3197
IR Inten	--	1.3986	12.9468	11.8603
		19	20	21
		A	A	A
Frequencies	--	1091.2327	1167.5257	1188.0442
Red. masses	--	2.6509	2.0660	1.7325
Frc consts	--	1.8599	1.6593	1.4408
IR Inten	--	61.4668	3.2079	17.0267
		22	23	24
		A	A	A
Frequencies	--	1207.9772	1253.5853	1262.7425
Red. masses	--	1.7907	1.9111	1.4350
Frc consts	--	1.5395	1.7695	1.3481
IR Inten	--	16.8852	38.9914	10.8033
		25	26	27
		A	A	A
Frequencies	--	1304.8629	1335.0394	1347.4665
Red. masses	--	1.3180	1.2485	1.4438
Frc consts	--	1.3221	1.3111	1.5446
IR Inten	--	26.7977	3.6695	18.7115
		28	29	30
		A	A	A
Frequencies	--	1371.8807	1398.7797	1433.7067
Red. masses	--	1.5054	1.8759	1.5510
Frc consts	--	1.6693	2.1625	1.8784
IR Inten	--	16.2561	48.3488	1.6542
		31	32	33
		A	A	A
Frequencies	--	1477.4411	1485.2185	1493.5541
Red. masses	--	1.1444	1.0906	1.3342
Frc consts	--	1.4719	1.4174	1.7535
IR Inten	--	13.1317	6.2919	15.3182
		34	35	36
		A	A	A
Frequencies	--	1515.5144	2950.8648	2954.5783
Red. masses	--	1.1132	1.0715	1.0727
Frc consts	--	1.5064	5.4974	5.5172
IR Inten	--	5.5576	66.4426	59.6196
		37	38	39
		A	A	A
Frequencies	--	3069.5592	3113.3231	3114.1631
Red. masses	--	1.0628	1.0899	1.0911
Frc consts	--	5.8998	6.2242	6.2342
IR Inten	--	3.8510	26.8946	17.3779

	40	41	42
	A	A	A
Frequencies --	3129.9077	3152.3857	3615.2864
Red. masses --	1.0886	1.1021	1.0756
Frc consts --	6.2830	6.4527	8.2826
IR Inten --	14.5392	6.5003	6.5772

17e

	1	2	3
	A	A	A
Frequencies --	77.1469	170.2108	235.7503
Red. masses --	4.9452	2.7000	13.7609
Frc consts --	0.0173	0.0461	0.4506
IR Inten --	0.3633	2.4639	1.0508

	4	5	6
	A	A	A
Frequencies --	316.7612	366.4978	376.0195
Red. masses --	2.9234	3.4132	2.9174
Frc consts --	0.1728	0.2701	0.2430
IR Inten --	2.9289	9.1567	2.1169

	7	8	9
	A	A	A
Frequencies --	438.4577	484.0394	581.1267
Red. masses --	3.4237	3.1845	4.1520
Frc consts --	0.3878	0.4396	0.8261
IR Inten --	1.1278	7.6515	8.9956

	10	11	12
	A	A	A
Frequencies --	607.0457	741.3755	780.8703
Red. masses --	2.3784	3.2230	1.5376
Frc consts --	0.5164	1.0437	0.5524
IR Inten --	62.1060	0.7713	69.4990

	13	14	15
	A	A	A
Frequencies --	862.2925	910.8458	1001.7116
Red. masses --	2.1554	2.6438	1.9476
Frc consts --	0.9442	1.2923	1.1514
IR Inten --	16.9263	3.0765	11.4239

	16	17	18
	A	A	A
Frequencies --	1014.6907	1075.6076	1098.7907
Red. masses --	1.8434	1.9011	2.6520
Frc consts --	1.1182	1.2959	1.8865
IR Inten --	3.0127	16.9277	1.0413

	19	20	21
	A	A	A
Frequencies --	1123.5601	1159.8438	1185.8249
Red. masses --	3.4272	2.8790	1.6663
Frc consts --	2.5491	2.2818	1.3806
IR Inten --	37.1615	52.1185	2.0100

	22	23	24
	A	A	A
Frequencies --	1202.6429	1218.9778	1283.0176
Red. masses --	1.5995	1.7147	1.4076
Frc consts --	1.3631	1.5012	1.3652
IR Inten --	14.1283	25.6448	3.7958

	25	26	27
	A	A	A
Frequencies --	1318.7400	1335.6444	1342.7501
Red. masses --	1.2914	1.3397	1.4164
Frc consts --	1.3232	1.4081	1.5046
IR Inten --	0.7106	21.7167	27.4851

	28	29	30
	A	A	A
Frequencies --	1367.7080	1396.5414	1431.5367
Red. masses --	2.0942	1.6161	1.5259
Frc consts --	2.3081	1.8571	1.8424

IR Inten	--	51.0011	17.2157	4.9214
		31	32	33
		A	A	A
Frequencies	--	1473.7800	1490.2634	1509.7844
Red. masses	--	1.1109	1.2747	1.1200
Frc consts	--	1.4216	1.6679	1.5042
IR Inten	--	14.4214	16.7291	1.2427
		34	35	36
		A	A	A
Frequencies	--	1522.8448	2968.3730	2972.8991
Red. masses	--	1.1034	1.0720	1.0711
Frc consts	--	1.5077	5.5652	5.5776
IR Inten	--	8.4876	67.6726	39.9675
		37	38	39
		A	A	A
Frequencies	--	3052.0411	3065.8618	3114.6570
Red. masses	--	1.0671	1.0816	1.0913
Frc consts	--	5.8564	5.9900	6.2378
IR Inten	--	4.0986	21.4018	29.2002
		40	41	42
		A	A	A
Frequencies	--	3119.9680	3147.8535	3607.7580
Red. masses	--	1.0930	1.0980	1.0754
Frc consts	--	6.2688	6.4103	8.2471
IR Inten	--	19.4489	6.9987	6.3080
18a		1	2	3
		A	A	A
Frequencies	--	95.0521	171.6274	231.6182
Red. masses	--	4.2885	3.3917	4.3211
Frc consts	--	0.0228	0.0589	0.1366
IR Inten	--	3.0313	0.3619	3.1069
		4	5	6
		A	A	A
Frequencies	--	300.5078	387.2857	429.6379
Red. masses	--	3.0286	1.9209	3.9667
Frc consts	--	0.1611	0.1698	0.4314
IR Inten	--	1.0783	5.3710	19.1640
		7	8	9
		A	A	A
Frequencies	--	461.0815	496.3925	631.2419
Red. masses	--	3.3324	2.1126	2.6528
Frc consts	--	0.4174	0.3067	0.6228
IR Inten	--	15.0011	16.4883	46.4403
		10	11	12
		A	A	A
Frequencies	--	666.7291	779.1152	808.2298
Red. masses	--	2.5968	3.2080	1.8070
Frc consts	--	0.6801	1.1473	0.6955
IR Inten	--	28.6933	35.8520	18.9837
		13	14	15
		A	A	A
Frequencies	--	888.3876	903.9383	938.0761
Red. masses	--	2.0103	2.4332	1.7641
Frc consts	--	0.9348	1.1714	0.9147
IR Inten	--	7.0798	8.3435	117.8907
		16	17	18
		A	A	A
Frequencies	--	964.7816	1020.3984	1071.6963
Red. masses	--	1.6847	3.1250	1.9024
Frc consts	--	0.9239	1.9171	1.2874
IR Inten	--	3.0236	2.4741	18.4644

	19	20	21
	A	A	A
Frequencies --	1074.8126	1110.9249	1141.5224
Red. masses --	1.7859	2.4702	1.6707
Frc consts --	1.2156	1.7962	1.2827
IR Inten --	2.2289	26.7049	52.7336
	22	23	24
	A	A	A
Frequencies --	1201.6806	1219.1678	1227.7239
Red. masses --	2.7425	1.1925	1.0970
Frc consts --	2.3334	1.0443	0.9742
IR Inten --	14.6426	9.7662	8.0645
	25	26	27
	A	A	A
Frequencies --	1309.3616	1333.6635	1339.7821
Red. masses --	1.2989	1.5278	1.3231
Frc consts --	1.3120	1.6011	1.3994
IR Inten --	9.2202	18.9685	10.5789
	28	29	30
	A	A	A
Frequencies --	1368.8014	1374.3435	1416.3391
Red. masses --	1.3920	1.2559	2.1189
Frc consts --	1.5366	1.3976	2.5043
IR Inten --	13.1233	15.9024	21.7338
	31	32	33
	A	A	A
Frequencies --	1428.9792	1464.2319	1480.9107
Red. masses --	1.5245	1.1361	1.0872
Frc consts --	1.8342	1.4351	1.4048
IR Inten --	7.0229	16.4901	5.1259
	34	35	36
	A	A	A
Frequencies --	1497.5558	1518.4871	1763.8807
Red. masses --	1.3472	1.1134	9.2590
Frc consts --	1.7801	1.5126	16.9729
IR Inten --	12.4366	3.6294	75.8026
	37	38	39
	A	A	A
Frequencies --	2933.7725	2946.2650	3076.1146
Red. masses --	1.0720	1.0730	1.0627
Frc consts --	5.4362	5.4876	5.9247
IR Inten --	70.5366	77.3283	7.6055
	40	41	42
	A	A	A
Frequencies --	3078.1611	3111.2436	3112.7248
Red. masses --	1.0874	1.0893	1.0900
Frc consts --	6.0705	6.2126	6.2225
IR Inten --	35.4233	39.6083	13.3548
	43	44	45
	A	A	A
Frequencies --	3149.8396	3477.5311	3609.7408
Red. masses --	1.1024	1.0744	1.0755
Frc consts --	6.4439	7.6551	8.2568
IR Inten --	9.4717	1.9074	4.0270
18e	1	2	3
	A	A	A
Frequencies --	109.2360	171.3759	297.5640
Red. masses --	4.1136	2.4925	4.4607
Frc consts --	0.0289	0.0431	0.2327
IR Inten --	0.4881	2.3669	6.0088

	4	5	6
	A	A	A
Frequencies --	345.9156	362.9932	399.8600
Red. masses --	2.7110	3.0931	4.1638
Frc consts --	0.1911	0.2401	0.3922
IR Inten --	0.4385	14.5743	1.3955
	7	8	9
	A	A	A
Frequencies --	438.6448	507.1783	597.2567
Red. masses --	3.1494	2.4071	3.6043
Frc consts --	0.3570	0.3648	0.7575
IR Inten --	0.3387	25.1567	19.1949
	10	11	12
	A	A	A
Frequencies --	658.8293	777.7470	786.9070
Red. masses --	2.4478	2.5024	1.5428
Frc consts --	0.6260	0.8918	0.5629
IR Inten --	38.4974	3.3322	62.3576
	13	14	15
	A	A	A
Frequencies --	896.3407	906.3728	936.6738
Red. masses --	2.4166	2.1075	1.2792
Frc consts --	1.1439	1.0201	0.6612
IR Inten --	51.8107	5.3059	40.3021
	16	17	18
	A	A	A
Frequencies --	1005.0258	1055.1168	1092.3604
Red. masses --	2.4531	1.5424	2.5408
Frc consts --	1.4599	1.0117	1.7863
IR Inten --	5.3239	17.7508	51.9483
	19	20	21
	A	A	A
Frequencies --	1100.9096	1117.3823	1139.4004
Red. masses --	2.1808	2.4376	2.5600
Frc consts --	1.5573	1.7932	1.9581
IR Inten --	19.3475	9.0925	24.0775
	22	23	24
	A	A	A
Frequencies --	1191.6527	1212.1804	1240.5538
Red. masses --	2.9589	1.1117	1.2216
Frc consts --	2.4756	0.9625	1.1077
IR Inten --	11.9892	8.0459	14.4130
	25	26	27
	A	A	A
Frequencies --	1299.6238	1326.2802	1332.7231
Red. masses --	1.3504	1.2852	1.2312
Frc consts --	1.3438	1.3319	1.2884
IR Inten --	3.8829	9.5709	29.0432
	28	29	30
	A	A	A
Frequencies --	1362.1945	1367.5226	1422.9311
Red. masses --	1.3508	1.3506	1.7339
Frc consts --	1.4768	1.4881	2.0685
IR Inten --	6.9072	2.7006	34.5005
	31	32	33
	A	A	A
Frequencies --	1436.4012	1464.7780	1490.2617
Red. masses --	1.7253	1.1214	1.2280
Frc consts --	2.0973	1.4176	1.6068
IR Inten --	2.9920	16.0877	10.7881
	34	35	36

	A	A	A
Frequencies --	1506.7847	1516.8584	1769.8599
Red. masses --	1.1655	1.1034	9.9738
Frc consts --	1.5591	1.4958	18.4073
IR Inten --	0.8837	7.2957	91.1079
	37	38	39
	A	A	A
Frequencies --	2960.0459	2968.1875	3063.5561
Red. masses --	1.0724	1.0713	1.0650
Frc consts --	5.5361	5.5609	5.8892
IR Inten --	71.7907	51.4204	9.5161
	40	41	42
	A	A	A
Frequencies --	3084.0962	3110.1554	3121.1627
Red. masses --	1.0839	1.0909	1.0926
Frc consts --	6.0741	6.2174	6.2712
IR Inten --	19.9031	32.7152	23.3839
	43	44	45
	A	A	A
Frequencies --	3144.3942	3494.0377	3603.5650
Red. masses --	1.0997	1.0734	1.0755
Frc consts --	6.4061	7.7209	8.2286
IR Inten --	10.2201	4.6127	4.4678
19a	1	2	3
	A	A	A
Frequencies --	103.4099	174.7959	231.3072
Red. masses --	4.3917	3.5505	3.8267
Frc consts --	0.0277	0.0639	0.1206
IR Inten --	3.3055	0.0878	2.6257
	4	5	6
	A	A	A
Frequencies --	302.8111	387.7483	433.3181
Red. masses --	3.0624	1.9475	4.8529
Frc consts --	0.1654	0.1725	0.5369
IR Inten --	3.2210	3.9799	3.6818
	7	8	9
	A	A	A
Frequencies --	464.0761	497.5276	635.8278
Red. masses --	3.1047	2.0309	2.5345
Frc consts --	0.3940	0.2962	0.6037
IR Inten --	42.5566	1.5821	38.8144
	10	11	12
	A	A	A
Frequencies --	672.1465	779.7012	809.9965
Red. masses --	2.7591	3.4274	1.8738
Frc consts --	0.7344	1.2276	0.7243
IR Inten --	42.4275	20.5169	24.9852
	13	14	15
	A	A	A
Frequencies --	890.6358	903.3979	933.8443
Red. masses --	1.9406	2.4617	1.6889
Frc consts --	0.9070	1.1837	0.8678
IR Inten --	26.8146	14.0432	12.8326
	16	17	18
	A	A	A
Frequencies --	964.2067	1021.0987	1073.5147
Red. masses --	1.6840	3.1446	1.7536
Frc consts --	0.9224	1.9318	1.1907
IR Inten --	41.0781	1.3306	6.4482
	19	20	21
	A	A	A
Frequencies --	1076.7453	1109.2027	1143.2348
Red. masses --	2.0351	2.4701	1.6496
Frc consts --	1.3901	1.7906	1.2703
IR Inten --	71.6712	23.2233	15.8734

	22	23	24
	A	A	A
Frequencies --	1201.1942	1220.0856	1235.9702
Red. masses --	2.8367	1.1707	1.1052
Frc consts --	2.4115	1.0268	0.9948
IR Inten --	21.7326	3.7327	10.9208
	25	26	27
	A	A	A
Frequencies --	1314.1856	1331.1100	1358.4788
Red. masses --	1.2645	1.4273	1.4800
Frc consts --	1.2867	1.4901	1.6092
IR Inten --	4.3255	10.2040	16.8982
	28	29	30
	A	A	A
Frequencies --	1366.1349	1385.7166	1423.1810
Red. masses --	1.3084	1.2376	2.3892
Frc consts --	1.4388	1.4001	2.8512
IR Inten --	7.2301	20.1611	49.3497
	31	32	33
	A	A	A
Frequencies --	1437.7279	1466.3434	1484.0629
Red. masses --	1.4989	1.1079	1.0886
Frc consts --	1.8254	1.4036	1.4126
IR Inten --	11.1481	14.1807	5.8353
	34	35	36
	A	A	A
Frequencies --	1502.2919	1521.3915	1767.6604
Red. masses --	1.3366	1.1181	9.1975
Frc consts --	1.7774	1.5248	16.9324
IR Inten --	12.7301	3.3573	78.0436
	37	38	39
	A	A	A
Frequencies --	2939.5078	2945.9353	3069.7989
Red. masses --	1.0727	1.0722	1.0595
Frc consts --	5.4613	5.4822	5.8829
IR Inten --	85.6308	62.6362	13.2990
	40	41	42
	A	A	A
Frequencies --	3104.0296	3115.0661	3122.8446
Red. masses --	1.0895	1.0899	1.0887
Frc consts --	6.1849	6.2310	6.2557
IR Inten --	35.1274	13.9732	22.9382
	43	44	45
	A	A	A
Frequencies --	3128.0090	3482.9566	3614.0729
Red. masses --	1.1055	1.0743	1.0755
Frc consts --	6.3730	7.6788	8.2768
IR Inten --	12.7273	1.9569	4.1339
19e	1	2	3
	A	A	A
Frequencies --	97.0669	172.3516	288.4591
Red. masses --	4.3818	2.5062	5.5796
Frc consts --	0.0243	0.0439	0.2735
IR Inten --	0.7992	3.7193	0.2375
	4	5	6
	A	A	A
Frequencies --	343.5006	360.4944	400.8312
Red. masses --	2.5943	2.8939	3.8603
Frc consts --	0.1804	0.2216	0.3654
IR Inten --	3.3279	5.5179	11.5421

	7	8	9
	A	A	A
Frequencies --	436.9536	508.9983	593.0026
Red. masses --	3.1365	2.4210	3.3839
Frc consts --	0.3528	0.3696	0.7011
IR Inten --	2.4690	4.9880	36.5698
	10	11	12
	A	A	A
Frequencies --	658.1601	782.1276	786.4170
Red. masses --	2.4999	1.9987	1.7946
Frc consts --	0.6380	0.7204	0.6539
IR Inten --	36.6492	23.8968	40.0860
	13	14	15
	A	A	A
Frequencies --	893.3469	903.6409	923.4983
Red. masses --	2.5409	1.5398	1.6878
Frc consts --	1.1947	0.7408	0.8481
IR Inten --	18.4992	31.3426	11.1324
	16	17	18
	A	A	A
Frequencies --	1003.6624	1053.1885	1089.8497
Red. masses --	2.3983	1.5539	1.8340
Frc consts --	1.4234	1.0155	1.2834
IR Inten --	25.7225	14.2866	22.7081
	19	20	21
	A	A	A
Frequencies --	1107.6602	1116.2478	1146.0952
Red. masses --	2.1767	2.8335	3.2787
Frc consts --	1.5735	2.0802	2.5374
IR Inten --	11.2190	9.2055	101.8248
	22	23	24
	A	A	A
Frequencies --	1193.1984	1211.5119	1226.7350
Red. masses --	3.0737	1.1239	1.1526
Frc consts --	2.5783	0.9720	1.0220
IR Inten --	17.5633	6.2509	11.8782
	25	26	27
	A	A	A
Frequencies --	1297.8995	1330.5647	1336.9054
Red. masses --	1.3663	1.2406	1.3203
Frc consts --	1.3561	1.2941	1.3903
IR Inten --	6.7353	6.3658	26.2603
	28	29	30
	A	A	A
Frequencies --	1359.9475	1368.2468	1423.1444
Red. masses --	1.3074	1.4221	1.7105
Frc consts --	1.4246	1.5686	2.0412
IR Inten --	10.1623	12.8916	2.5430
	31	32	33
	A	A	A
Frequencies --	1441.4968	1466.1619	1490.1407
Red. masses --	1.7464	1.1083	1.2394
Frc consts --	2.1381	1.4037	1.6215
IR Inten --	9.9346	15.7906	11.9832
	34	35	36
	A	A	A
Frequencies --	1506.0515	1517.1425	1770.7197
Red. masses --	1.1583	1.1046	9.5005
Frc consts --	1.5480	1.4979	17.5508
IR Inten --	0.9174	7.3254	86.8360
	37	38	39

	A	A	A
Frequencies --	2954.9397	2971.5015	3058.5132
Red. masses --	1.0725	1.0713	1.0663
Frc consts --	5.5174	5.5733	5.8769
IR Inten --	73.0232	50.2649	3.9862
	40	41	42
	A	A	A
Frequencies --	3064.5411	3108.2616	3120.2485
Red. masses --	1.0783	1.0903	1.1037
Frc consts --	5.9662	6.2064	6.3312
IR Inten --	31.1415	33.6501	20.5215
	43	44	45
	A	A	A
Frequencies --	3123.8957	3490.3587	3603.1219
Red. masses --	1.0925	1.0746	1.0755
Frc consts --	6.2817	7.7132	8.2264
IR Inten --	22.1865	2.0872	4.4604
20a	1	2	3
	A	A	A
Frequencies --	106.8183	175.5039	230.9133
Red. masses --	3.4805	3.4521	3.6094
Frc consts --	0.0234	0.0626	0.1134
IR Inten --	0.7190	0.9267	2.2733
	4	5	6
	A	A	A
Frequencies --	301.2841	381.5738	404.0571
Red. masses --	2.7998	2.0552	2.3808
Frc consts --	0.1497	0.1763	0.2290
IR Inten --	1.0312	4.2588	2.8228
	7	8	9
	A	A	A
Frequencies --	454.3725	486.1609	640.7943
Red. masses --	3.7803	1.9763	3.1794
Frc consts --	0.4598	0.2752	0.7692
IR Inten --	25.0760	8.3041	22.2904
	10	11	12
	A	A	A
Frequencies --	646.5897	743.6523	794.4739
Red. masses --	2.2476	1.2009	2.6189
Frc consts --	0.5536	0.3913	0.9739
IR Inten --	43.4355	10.8875	31.8985
	13	14	15
	A	A	A
Frequencies --	807.8572	894.3995	907.7320
Red. masses --	1.7688	2.3417	2.5327
Frc consts --	0.6801	1.1037	1.2296
IR Inten --	19.7277	27.3745	6.7199
	16	17	18
	A	A	A
Frequencies --	939.0477	962.7435	1013.2341
Red. masses --	1.9056	1.3614	1.8991
Frc consts --	0.9900	0.7435	1.1487
IR Inten --	36.9328	37.6732	10.3345
	19	20	21
	A	A	A
Frequencies --	1020.9351	1063.8205	1084.3782
Red. masses --	2.5161	2.0784	1.8067
Frc consts --	1.5451	1.3859	1.2517
IR Inten --	5.8372	46.8445	0.7629
	22	23	24
	A	A	A
Frequencies --	1108.2548	1202.9159	1222.6635
Red. masses --	2.2303	2.8357	1.2938
Frc consts --	1.6140	2.4176	1.1396
IR Inten --	19.9358	17.5839	4.7472

	25	26	27
	A	A	A
Frequencies --	1235.8991	1312.9124	1323.4976
Red. masses --	1.1056	1.4060	1.3656
Frc consts --	0.9950	1.4279	1.4093
IR Inten --	6.0580	1.8935	3.6662
	28	29	30
	A	A	A
Frequencies --	1338.9427	1366.7597	1377.1485
Red. masses --	1.6116	1.3253	1.2661
Frc consts --	1.7023	1.4586	1.4147
IR Inten --	24.9835	4.4062	16.7774
	31	32	33
	A	A	A
Frequencies --	1389.8821	1437.0580	1460.1050
Red. masses --	1.8500	1.5241	1.1390
Frc consts --	2.1056	1.8544	1.4307
IR Inten --	7.9430	4.1056	8.2355
	34	35	36
	A	A	A
Frequencies --	1478.5503	1483.4183	1502.1574
Red. masses --	1.1485	1.0918	1.3366
Frc consts --	1.4792	1.4155	1.7769
IR Inten --	13.9982	6.6735	11.9920
	37	38	39
	A	A	A
Frequencies --	1517.0504	1751.2315	2938.0250
Red. masses --	1.1259	6.0142	1.0728
Frc consts --	1.5267	10.8672	5.4558
IR Inten --	3.8402	12.4205	78.7328
	40	41	42
	A	A	A
Frequencies --	2939.0640	3067.1072	3086.9378
Red. masses --	1.0720	1.0608	1.0875
Frc consts --	5.4557	5.8798	6.1057
IR Inten --	77.0577	14.8543	33.6412
	43	44	45
	A	A	A
Frequencies --	3101.9654	3111.7010	3123.8999
Red. masses --	1.0893	1.0895	1.1042
Frc consts --	6.1756	6.2154	6.3486
IR Inten --	42.4611	25.6719	18.9772
	46	47	48
	A	A	A
Frequencies --	3147.8638	3235.1627	3610.1438
Red. masses --	1.0618	1.1161	1.0754
Frc consts --	6.1992	6.8826	8.2581
IR Inten --	8.3533	12.1994	2.7422
20e	1	2	3
	A	A	A
Frequencies --	113.0675	183.0919	289.9914
Red. masses --	3.4310	2.5053	3.7091
Frc consts --	0.0258	0.0495	0.1838
IR Inten --	1.0453	1.4608	4.0375
	4	5	6
	A	A	A
Frequencies --	337.7101	363.9578	390.2033
Red. masses --	2.5478	2.8754	3.0814
Frc consts --	0.1712	0.2244	0.2764

IR Inten	--	3.3185	7.8357	4.3591
		7	8	9
		A	A	A
Frequencies	--	440.8414	481.9789	572.7861
Red. masses	--	3.0147	2.5976	3.0410
Frc consts	--	0.3452	0.3555	0.5878
IR Inten	--	0.2518	10.1187	20.9278
		10	11	12
		A	A	A
Frequencies	--	638.6733	751.2685	779.9709
Red. masses	--	2.2974	1.1802	1.5412
Frc consts	--	0.5521	0.3925	0.5524
IR Inten	--	29.9023	0.7153	74.5920
		13	14	15
		A	A	A
Frequencies	--	805.1218	879.9792	911.7408
Red. masses	--	2.0626	2.0154	2.3654
Frc consts	--	0.7877	0.9195	1.1585
IR Inten	--	2.8017	14.7166	2.6244
		16	17	18
		A	A	A
Frequencies	--	959.8195	982.1115	1029.2201
Red. masses	--	1.3437	2.1109	1.7138
Frc consts	--	0.7294	1.1996	1.0696
IR Inten	--	46.9959	21.9430	5.8559
		19	20	21
		A	A	A
Frequencies	--	1046.2846	1094.1347	1108.4801
Red. masses	--	1.6996	2.9952	2.4545
Frc consts	--	1.0962	2.1126	1.7769
IR Inten	--	4.9420	49.8817	12.6855
		22	23	24
		A	A	A
Frequencies	--	1124.8932	1190.5898	1208.8615
Red. masses	--	2.6205	3.3762	1.3734
Frc consts	--	1.9537	2.8197	1.1825
IR Inten	--	27.7822	17.1259	1.6503
		25	26	27
		A	A	A
Frequencies	--	1213.5416	1287.7449	1303.1842
Red. masses	--	1.0932	1.4834	1.3453
Frc consts	--	0.9485	1.4494	1.3461
IR Inten	--	5.3874	2.4790	4.0551
		28	29	30
		A	A	A
Frequencies	--	1327.5651	1361.3157	1366.2335
Red. masses	--	1.2465	1.3549	1.3687
Frc consts	--	1.2943	1.4794	1.5053
IR Inten	--	6.5820	8.1170	11.1120
		31	32	33
		A	A	A
Frequencies	--	1403.8800	1430.3700	1452.5516
Red. masses	--	1.7811	1.5492	1.1564
Frc consts	--	2.0682	1.8674	1.4376
IR Inten	--	1.4594	2.9223	5.2119
		34	35	36
		A	A	A
Frequencies	--	1475.7242	1487.6088	1504.9656
Red. masses	--	1.1299	1.2402	1.1609
Frc consts	--	1.4498	1.6170	1.5491
IR Inten	--	15.7826	10.5219	1.0868
		37	38	39

	A	A	A
Frequencies --	1515.0745	1751.9618	2954.1869
Red. masses --	1.1038	6.2435	1.0724
Frc consts --	1.4928	11.2909	5.5141
IR Inten --	7.8577	17.9500	71.7318
	40	41	42
	A	A	A
Frequencies --	2969.4304	3051.5387	3068.3578
Red. masses --	1.0706	1.0638	1.0837
Frc consts --	5.5620	5.8364	6.0112
IR Inten --	55.9552	15.7114	29.1316
	43	44	45
	A	A	A
Frequencies --	3105.6868	3113.5425	3116.9219
Red. masses --	1.0906	1.0931	1.1007
Frc consts --	6.1975	6.2434	6.3006
IR Inten --	41.3306	29.4674	23.0573
	46	47	48
	A	A	A
Frequencies --	3162.0300	3257.3726	3602.6783
Red. masses --	1.0616	1.1158	1.0754
Frc consts --	6.2537	6.9753	8.2240
IR Inten --	7.7851	4.5290	3.2553
21a	1	2	3
	A	A	A
Frequencies --	96.7339	154.8942	234.7893
Red. masses --	5.4967	3.2610	4.0258
Frc consts --	0.0303	0.0461	0.1308
IR Inten --	6.3116	0.5396	5.3804
	4	5	6
	A	A	A
Frequencies --	286.7747	369.9112	436.9408
Red. masses --	2.5663	2.0634	4.6860
Frc consts --	0.1243	0.1664	0.5271
IR Inten --	2.2809	1.3659	2.3782
	7	8	9
	A	A	A
Frequencies --	467.3242	499.4383	620.8526
Red. masses --	2.5896	2.9778	3.3574
Frc consts --	0.3332	0.4376	0.7625
IR Inten --	4.4385	12.8106	8.9923
	10	11	12
	A	A	A
Frequencies --	709.4216	763.0406	827.6799
Red. masses --	2.7086	2.9490	1.6331
Frc consts --	0.8032	1.0116	0.6591
IR Inten --	2.2208	4.9153	4.4343
	13	14	15
	A	A	A
Frequencies --	852.7177	903.0581	941.6732
Red. masses --	2.6382	2.0735	1.6112
Frc consts --	1.1302	0.9963	0.8418
IR Inten --	0.8591	3.3207	12.8288
	16	17	18
	A	A	A
Frequencies --	991.8758	1014.4124	1045.7281
Red. masses --	2.4424	2.8818	1.9694
Frc consts --	1.4157	1.7472	1.2689
IR Inten --	39.7459	21.8381	9.6037
	19	20	21
	A	A	A
Frequencies --	1093.3514	1111.4381	1154.5276
Red. masses --	1.6274	2.4073	1.4244
Frc consts --	1.1462	1.7521	1.1187

IR Inten	--	2.9214	25.9266	14.8879
		22	23	24
		A	A	A
Frequencies	--	1176.9417	1250.4722	1283.2474
Red. masses	--	1.4966	1.6319	1.3135
Frc consts	--	1.2214	1.5034	1.2744
IR Inten	--	3.9584	7.2901	5.0145
		25	26	27
		A	A	A
Frequencies	--	1296.4668	1346.0894	1355.7236
Red. masses	--	1.3736	1.3119	1.6603
Frc consts	--	1.3603	1.4005	1.7980
IR Inten	--	4.5628	2.5804	14.0034
		28	29	30
		A	A	A
Frequencies	--	1362.6906	1381.3357	1394.1783
Red. masses	--	1.3427	1.5325	1.5170
Frc consts	--	1.4690	1.7229	1.7373
IR Inten	--	7.4850	2.9069	0.6645
		31	32	33
		A	A	A
Frequencies	--	1399.5503	1472.4418	1475.9414
Red. masses	--	1.4675	1.0954	1.1000
Frc consts	--	1.6936	1.3993	1.4118
IR Inten	--	2.1848	4.6577	19.1511
		34	35	36
		A	A	A
Frequencies	--	1503.8581	1512.9170	1847.6189
Red. masses	--	1.0800	1.0957	11.2985
Frc consts	--	1.4391	1.4777	22.7246
IR Inten	--	7.2674	4.5192	226.1074
		37	38	39
		A	A	A
Frequencies	--	3043.3059	3053.9195	3064.2449
Red. masses	--	1.0670	1.0641	1.0626
Frc consts	--	5.8223	5.8469	5.8785
IR Inten	--	23.5005	13.5826	16.8483
		40	41	42
		A	A	A
Frequencies	--	3069.3062	3103.7337	3108.2806
Red. masses	--	1.0630	1.0968	1.0995
Frc consts	--	5.9002	6.2248	6.2586
IR Inten	--	9.4677	31.4071	23.7668
		43	44	45
		A	A	A
Frequencies	--	3115.6941	3129.4225	3146.8524
Red. masses	--	1.1046	1.0887	1.1016
Frc consts	--	6.3177	6.2816	6.4276
IR Inten	--	29.8743	22.1042	12.0722
21e		1	2	3
		A	A	A
Frequencies	--	93.2051	151.2463	279.5732
Red. masses	--	4.9938	2.4730	7.3259
Frc consts	--	0.0256	0.0333	0.3374
IR Inten	--	1.4524	2.4705	0.9443
		4	5	6
		A	A	A
Frequencies	--	312.7370	350.0942	396.7097
Red. masses	--	1.8936	3.5198	4.4994
Frc consts	--	0.1091	0.2542	0.4172
IR Inten	--	0.3189	5.3131	2.2324

	7	8	9
	A	A	A
Frequencies --	423.3384	508.8918	602.6018
Red. masses --	2.8835	2.2938	4.0539
Frc consts --	0.3045	0.3500	0.8673
IR Inten --	0.7767	2.0861	15.9648
	10	11	12
	A	A	A
Frequencies --	679.9319	750.7814	851.1205
Red. masses --	2.9108	2.1920	1.7460
Frc consts --	0.7929	0.7280	0.7452
IR Inten --	2.7447	2.0866	11.8949
	13	14	15
	A	A	A
Frequencies --	872.0839	900.5492	930.0562
Red. masses --	2.5241	1.8068	1.7068
Frc consts --	1.1310	0.8634	0.8698
IR Inten --	1.2065	22.0001	8.3587
	16	17	18
	A	A	A
Frequencies --	974.7945	1058.2528	1093.9797
Red. masses --	2.4044	1.4630	1.5838
Frc consts --	1.3461	0.9653	1.1168
IR Inten --	3.2827	8.5794	4.8823
	19	20	21
	A	A	A
Frequencies --	1095.6244	1133.4165	1146.4257
Red. masses --	2.4406	3.3529	1.8026
Frc consts --	1.7261	2.5378	1.3959
IR Inten --	23.3070	96.9103	3.2514
	22	23	24
	A	A	A
Frequencies --	1159.8628	1249.2716	1271.7533
Red. masses --	2.3375	1.4904	1.3812
Frc consts --	1.8528	1.3704	1.3162
IR Inten --	3.3806	2.7725	0.5655
	25	26	27
	A	A	A
Frequencies --	1292.1921	1336.9858	1357.8528
Red. masses --	1.2587	1.2493	1.3953
Frc consts --	1.2383	1.3157	1.5157
IR Inten --	0.8489	4.0276	4.9165
	28	29	30
	A	A	A
Frequencies --	1363.9084	1377.4663	1398.9474
Red. masses --	1.4134	1.4985	1.4595
Frc consts --	1.5491	1.6752	1.6829
IR Inten --	1.6098	3.1115	0.5472
	31	32	33
	A	A	A
Frequencies --	1411.2181	1469.5087	1495.4483
Red. masses --	1.6296	1.0946	1.0932
Frc consts --	1.9122	1.3926	1.4405
IR Inten --	6.3283	11.9048	5.7368
	34	35	36
	A	A	A
Frequencies --	1499.6685	1511.0876	1859.7425
Red. masses --	1.0846	1.0979	11.9970
Frc consts --	1.4371	1.4771	24.4472
IR Inten --	9.6696	3.8949	235.4443
	37	38	39
	A	A	A
Frequencies --	3032.4776	3041.7451	3045.2577
Red. masses --	1.0806	1.0704	1.0694
Frc consts --	5.8545	5.8348	5.8430
IR Inten --	6.9285	19.5341	8.0023

	40	41	42
	A	A	A
Frequencies --	3054.2344	3059.7246	3107.8681
Red. masses --	1.0625	1.0621	1.0980
Frc consts --	5.8394	5.8586	6.2487
IR Inten --	31.4919	27.7931	31.5542

	43	44	45
	A	A	A
Frequencies --	3110.9844	3118.1644	3140.7045
Red. masses --	1.0979	1.1039	1.0968
Frc consts --	6.2604	6.3239	6.3741
IR Inten --	33.4864	27.1040	12.7500

22a

	1	2	3
	A	A	A
Frequencies --	87.7194	151.9116	245.6554
Red. masses --	5.2557	3.4312	3.3726
Frc consts --	0.0238	0.0467	0.1199
IR Inten --	1.5091	1.1024	3.9316

	4	5	6
	A	A	A
Frequencies --	262.5357	343.4632	389.6157
Red. masses --	3.6785	2.8707	2.5829
Frc consts --	0.1494	0.1995	0.2310
IR Inten --	2.0716	0.5339	2.6278

	7	8	9
	A	A	A
Frequencies --	417.9795	473.2700	604.5443
Red. masses --	4.4298	2.1009	4.0720
Frc consts --	0.4560	0.2772	0.8768
IR Inten --	1.6668	1.8255	3.3326

	10	11	12
	A	A	A
Frequencies --	664.6653	745.7642	821.5901
Red. masses --	3.1141	2.6136	1.5635
Frc consts --	0.8106	0.8564	0.6218
IR Inten --	2.7275	3.5922	4.3047

	13	14	15
	A	A	A
Frequencies --	848.2188	891.2723	933.8438
Red. masses --	2.8386	2.2705	1.6024
Frc consts --	1.2033	1.0626	0.8233
IR Inten --	1.5599	6.8506	13.5356

	16	17	18
	A	A	A
Frequencies --	978.0672	1003.1850	1045.6500
Red. masses --	2.6410	2.5565	1.9648
Frc consts --	1.4885	1.5158	1.2658
IR Inten --	19.7097	49.2797	1.4702

	19	20	21
	A	A	A
Frequencies --	1074.5744	1092.6893	1143.5241
Red. masses --	1.9566	1.7712	1.5893
Frc consts --	1.3311	1.2460	1.2244
IR Inten --	39.4770	13.1454	9.7075

	22	23	24
	A	A	A
Frequencies --	1171.6762	1230.4473	1245.5298
Red. masses --	1.6056	1.9360	1.7835
Frc consts --	1.2987	1.7269	1.6302
IR Inten --	5.0324	37.6523	13.9684

	25	26	27
	A	A	A
Frequencies --	1280.1951	1310.7673	1340.8870
Red. masses --	1.3992	1.3474	1.3980
Frc consts --	1.3511	1.3640	1.4810
IR Inten --	12.3421	29.6251	7.5493
	28	29	30
	A	A	A
Frequencies --	1345.5232	1369.1376	1379.1352
Red. masses --	1.4020	1.4140	1.4656
Frc consts --	1.4955	1.5617	1.6424
IR Inten --	3.3604	2.6572	10.0744
	31	32	33
	A	A	A
Frequencies --	1398.0080	1419.7426	1475.1376
Red. masses --	1.5174	1.8015	1.0899
Frc consts --	1.7473	2.1395	1.3973
IR Inten --	3.3049	18.2324	7.2616
	34	35	36
	A	A	A
Frequencies --	1488.5218	1496.5714	1507.5523
Red. masses --	1.1238	1.0785	1.1023
Frc consts --	1.4670	1.4233	1.4760
IR Inten --	11.7946	7.1674	5.9843
	37	38	39
	A	A	A
Frequencies --	3049.6620	3056.4825	3057.8176
Red. masses --	1.0666	1.0632	1.0629
Frc consts --	5.8444	5.8518	5.8558
IR Inten --	15.2673	13.7981	13.1794
	40	41	42
	A	A	A
Frequencies --	3067.2399	3105.7001	3110.4778
Red. masses --	1.0626	1.0988	1.1014
Frc consts --	5.8899	6.2445	6.2784
IR Inten --	21.2615	30.2813	21.1125
	43	44	45
	A	A	A
Frequencies --	3119.0319	3134.2604	3145.8296
Red. masses --	1.1047	1.0890	1.0989
Frc consts --	6.3320	6.3028	6.4076
IR Inten --	31.8467	14.6628	7.3276
22e	1	2	3
	A	A	A
Frequencies --	81.0435	155.4921	236.9758
Red. masses --	4.5944	2.6544	14.3566
Frc consts --	0.0178	0.0378	0.4750
IR Inten --	0.0224	1.2643	0.5803
	4	5	6
	A	A	A
Frequencies --	292.8982	354.3188	377.3020
Red. masses --	2.0347	3.1127	3.8824
Frc consts --	0.1028	0.2302	0.3256
IR Inten --	0.2174	2.7112	0.9260
	7	8	9
	A	A	A
Frequencies --	415.8603	484.2445	573.9140
Red. masses --	3.0186	2.8198	3.8498
Frc consts --	0.3076	0.3896	0.7471
IR Inten --	0.5354	2.8167	7.3052

	10	11	12
	A	A	A
Frequencies --	616.0010	732.3572	831.0794
Red. masses --	2.7503	3.0386	1.6327
Frc consts --	0.6149	0.9602	0.6644
IR Inten --	3.5204	1.4767	6.6463
	13	14	15
	A	A	A
Frequencies --	860.2545	886.6189	936.1310
Red. masses --	2.1266	2.1515	1.5480
Frc consts --	0.9273	0.9965	0.7993
IR Inten --	5.8279	9.4055	0.4152
	16	17	18
	A	A	A
Frequencies --	966.3479	1050.0905	1072.6170
Red. masses --	2.4115	1.8752	1.6408
Frc consts --	1.3268	1.2183	1.1122
IR Inten --	4.8499	11.4834	9.1636
	19	20	21
	A	A	A
Frequencies --	1093.8330	1126.7631	1135.8216
Red. masses --	1.6050	3.9270	1.8576
Frc consts --	1.1314	2.9375	1.4120
IR Inten --	1.6133	77.7283	6.7064
	22	23	24
	A	A	A
Frequencies --	1147.8397	1218.2480	1262.7365
Red. masses --	2.1239	1.8830	1.4233
Frc consts --	1.6487	1.6465	1.3372
IR Inten --	1.7983	12.5001	0.6266
	25	26	27
	A	A	A
Frequencies --	1280.3754	1320.8613	1331.0770
Red. masses --	1.3674	1.2954	1.5851
Frc consts --	1.3208	1.3316	1.6547
IR Inten --	11.4959	17.9522	13.7009
	28	29	30
	A	A	A
Frequencies --	1353.5033	1364.6671	1385.2015
Red. masses --	1.3985	1.6191	1.5186
Frc consts --	1.5095	1.7765	1.7168
IR Inten --	1.0674	32.3732	15.7362
	31	32	33
	A	A	A
Frequencies --	1397.1571	1404.8496	1486.0996
Red. masses --	1.4935	1.6672	1.1023
Frc consts --	1.7176	1.9386	1.4343
IR Inten --	14.0323	12.9972	6.5037
	34	35	36
	A	A	A
Frequencies --	1493.9531	1497.4597	1511.4409
Red. masses --	1.0831	1.0953	1.0979
Frc consts --	1.4243	1.4471	1.4777
IR Inten --	12.4310	5.3530	5.9355
	37	38	39
	A	A	A
Frequencies --	3028.7192	3037.9997	3044.2821
Red. masses --	1.0753	1.0750	1.0694
Frc consts --	5.8114	5.8457	5.8395
IR Inten --	0.2130	22.1485	23.0354

	40	41	42
	A	A	A
Frequencies --	3055.9588	3062.2072	3108.9376
Red. masses --	1.0625	1.0621	1.0950
Frc consts --	5.8461	5.8678	6.2356
IR Inten --	27.4048	20.5982	34.6386

	43	44	45
	A	A	A
Frequencies --	3112.5462	3121.9380	3136.3730
Red. masses --	1.1019	1.1040	1.0960
Frc consts --	6.2898	6.3397	6.3519
IR Inten --	31.4039	26.7830	8.3018

23a

	1	2	3
	A	A	A
Frequencies --	102.2293	154.3367	236.3825
Red. masses --	4.1419	3.1316	4.0852
Frc consts --	0.0255	0.0440	0.1345
IR Inten --	2.3313	0.9641	4.7989

	4	5	6
	A	A	A
Frequencies --	288.2266	373.6395	431.4981
Red. masses --	2.4093	2.0360	3.6161
Frc consts --	0.1179	0.1675	0.3967
IR Inten --	1.8070	1.9472	9.6419

	7	8	9
	A	A	A
Frequencies --	462.9537	488.9661	628.0359
Red. masses --	2.8795	2.3755	3.7097
Frc consts --	0.3636	0.3346	0.8621
IR Inten --	3.2910	10.4879	4.6445

	10	11	12
	A	A	A
Frequencies --	685.9433	773.8041	822.8547
Red. masses --	2.5000	3.0265	1.5346
Frc consts --	0.6931	1.0677	0.6122
IR Inten --	2.5566	4.1812	3.3223

	13	14	15
	A	A	A
Frequencies --	858.7042	894.5700	938.3222
Red. masses --	2.5916	1.9370	1.5905
Frc consts --	1.1259	0.9133	0.8251
IR Inten --	5.4401	4.2845	32.2591

	16	17	18
	A	A	A
Frequencies --	944.5129	997.1094	1017.7946
Red. masses --	1.5779	2.1330	2.4922
Frc consts --	0.8294	1.2495	1.5211
IR Inten --	83.5763	4.3855	22.1710

	19	20	21
	A	A	A
Frequencies --	1054.8422	1090.0120	1113.2561
Red. masses --	1.8967	1.4853	2.3002
Frc consts --	1.2435	1.0398	1.6796
IR Inten --	6.2107	10.5662	20.0546

	22	23	24
	A	A	A
Frequencies --	1144.1147	1183.3956	1199.4266
Red. masses --	1.7394	1.3456	1.2457
Frc consts --	1.3415	1.1102	1.0558
IR Inten --	41.4821	6.5316	17.8021

	25	26	27
	A	A	A
Frequencies --	1276.9723	1294.1017	1342.4920
Red. masses --	1.2915	1.2753	1.2820
Frc consts --	1.2408	1.2584	1.3613

IR Inten	--	4.6582	3.1183	10.3151
		28	29	30
		A	A	A
Frequencies	--	1348.0474	1368.0323	1374.8781
Red. masses	--	1.3350	1.5457	1.3551
Frc consts	--	1.4293	1.7044	1.5092
IR Inten	--	8.1999	5.1339	6.6955
		31	32	33
		A	A	A
Frequencies	--	1393.7469	1396.9406	1417.4003
Red. masses	--	1.5325	1.4512	2.0686
Frc consts	--	1.7539	1.6685	2.4486
IR Inten	--	2.4051	0.9640	16.2466
		34	35	36
		A	A	A
Frequencies	--	1472.3625	1475.9900	1501.8568
Red. masses	--	1.0896	1.1229	1.0812
Frc consts	--	1.3917	1.4414	1.4368
IR Inten	--	1.0283	22.4003	7.4678
		37	38	39
		A	A	A
Frequencies	--	1510.9065	1762.6393	3041.0605
Red. masses	--	1.0985	9.2036	1.0671
Frc consts	--	1.4775	16.8475	5.8145
IR Inten	--	4.3111	75.4234	23.8691
		40	41	42
		A	A	A
Frequencies	--	3051.8545	3061.4612	3062.4197
Red. masses	--	1.0648	1.0640	1.0638
Frc consts	--	5.8431	5.8756	5.8780
IR Inten	--	9.9588	14.9608	15.6548
		43	44	45
		A	A	A
Frequencies	--	3082.8387	3101.6825	3107.6965
Red. masses	--	1.0874	1.0969	1.0988
Frc consts	--	6.0889	6.2173	6.2522
IR Inten	--	44.8851	35.9137	30.7842
		46	47	48
		A	A	A
Frequencies	--	3113.9388	3142.3086	3473.6881
Red. masses	--	1.1043	1.0991	1.0743
Frc consts	--	6.3088	6.3940	7.6379
IR Inten	--	32.1969	11.8481	2.3841
23e		1	2	3
		A	A	A
Frequencies	--	111.9789	157.9850	304.8343
Red. masses	--	3.9891	2.4604	2.5979
Frc consts	--	0.0295	0.0362	0.1422
IR Inten	--	0.0292	1.0660	0.6458
		4	5	6
		A	A	A
Frequencies	--	321.5384	358.4563	395.6937
Red. masses	--	2.6252	3.9137	4.5184
Frc consts	--	0.1599	0.2963	0.4168
IR Inten	--	2.7620	8.2990	0.0335
		7	8	9
		A	A	A
Frequencies	--	427.4739	503.6101	594.5605
Red. masses	--	2.8290	2.2841	3.6225
Frc consts	--	0.3046	0.3413	0.7545
IR Inten	--	2.1670	1.5292	21.7299

	10	11	12
	A	A	A
Frequencies --	666.2133	767.5230	849.5265
Red. masses --	2.6363	2.3179	1.6433
Frc consts --	0.6894	0.8045	0.6988
IR Inten --	1.1394	2.7690	15.4671
	13	14	15
	A	A	A
Frequencies --	869.6601	893.4302	910.7659
Red. masses --	2.2694	1.8332	1.5298
Frc consts --	1.0112	0.8622	0.7477
IR Inten --	3.4160	21.7792	28.8342
	16	17	18
	A	A	A
Frequencies --	972.0240	994.0085	1065.2628
Red. masses --	2.4038	1.2597	1.6305
Frc consts --	1.3381	0.7333	1.0902
IR Inten --	2.2113	26.9834	20.0673
	19	20	21
	A	A	A
Frequencies --	1080.5569	1096.7274	1112.5881
Red. masses --	2.3727	2.0318	2.4435
Frc consts --	1.6322	1.4399	1.7821
IR Inten --	30.2245	33.3401	21.5314
	22	23	24
	A	A	A
Frequencies --	1141.3145	1173.5658	1223.8770
Red. masses --	2.1632	1.4900	1.3668
Frc consts --	1.6602	1.2091	1.2062
IR Inten --	8.3687	2.7116	10.3273
	25	26	27
	A	A	A
Frequencies --	1275.7113	1287.8439	1330.9372
Red. masses --	1.3387	1.2558	1.2951
Frc consts --	1.2836	1.2271	1.3516
IR Inten --	0.8976	3.9162	20.4211
	28	29	30
	A	A	A
Frequencies --	1345.9184	1367.7638	1372.1819
Red. masses --	1.1877	1.4086	1.3960
Frc consts --	1.2677	1.5526	1.5486
IR Inten --	4.6865	1.8380	2.0264
	31	32	33
	A	A	A
Frequencies --	1389.8648	1396.8140	1432.7304
Red. masses --	1.4800	1.4611	1.8688
Frc consts --	1.6845	1.6796	2.2601
IR Inten --	12.8274	1.6105	29.4420
	34	35	36
	A	A	A
Frequencies --	1476.0809	1495.5402	1499.8887
Red. masses --	1.1064	1.1047	1.0871
Frc consts --	1.4203	1.4557	1.4409
IR Inten --	11.9715	7.1411	8.9726
	37	38	39
	A	A	A
Frequencies --	1510.4797	1769.9126	3036.7636
Red. masses --	1.0997	9.9732	1.0700
Frc consts --	1.4782	18.4073	5.8140
IR Inten --	4.1809	90.5318	7.7928
	40	41	42

	A	A	A
Frequencies --	3040.4626	3050.3774	3052.6178
Red. masses --	1.0692	1.0792	1.0638
Frc consts --	5.8238	5.9163	5.8408
IR Inten --	17.7743	5.2822	37.4402
	43	44	45
	A	A	A
Frequencies --	3061.3274	3106.4147	3109.0366
Red. masses --	1.0642	1.0966	1.0995
Frc consts --	5.8764	6.2347	6.2619
IR Inten --	33.0093	37.4442	37.7771
	46	47	48
	A	A	A
Frequencies --	3119.4934	3136.8028	3496.3642
Red. masses --	1.1037	1.0956	1.0732
Frc consts --	6.3283	6.3514	7.7296
IR Inten --	31.0128	12.1487	4.5179
24a	1	2	3
	A	A	A
Frequencies --	109.9164	158.6231	239.6836
Red. masses --	4.2735	3.2338	3.5710
Frc consts --	0.0304	0.0479	0.1209
IR Inten --	2.6824	0.8275	4.1796
	4	5	6
	A	A	A
Frequencies --	288.3635	374.8406	435.1566
Red. masses --	2.4232	2.0733	4.3760
Frc consts --	0.1187	0.1716	0.4882
IR Inten --	3.2005	1.1402	5.0542
	7	8	9
	A	A	A
Frequencies --	462.0431	490.4157	633.3462
Red. masses --	2.7287	2.2320	3.5840
Frc consts --	0.3432	0.3163	0.8470
IR Inten --	4.0167	9.6915	4.9011
	10	11	12
	A	A	A
Frequencies --	690.9434	770.7504	825.9322
Red. masses --	2.6727	2.9798	1.6119
Frc consts --	0.7518	1.0430	0.6478
IR Inten --	1.5624	4.2595	4.6076
	13	14	15
	A	A	A
Frequencies --	856.7602	890.9136	937.0183
Red. masses --	2.4636	1.8151	1.5933
Frc consts --	1.0655	0.8488	0.8242
IR Inten --	0.6872	17.7642	27.7366
	16	17	18
	A	A	A
Frequencies --	942.9602	998.5712	1019.1330
Red. masses --	1.6606	2.0827	2.3485
Frc consts --	0.8700	1.2236	1.4372
IR Inten --	6.2664	27.0361	55.0377
	19	20	21
	A	A	A
Frequencies --	1055.7271	1091.3177	1110.3815
Red. masses --	1.9555	1.5579	2.3806
Frc consts --	1.2842	1.0932	1.7294
IR Inten --	15.4762	10.9088	33.8744
	22	23	24
	A	A	A
Frequencies --	1142.4284	1182.0057	1199.1776
Red. masses --	1.5177	1.4186	1.2359
Frc consts --	1.1670	1.1677	1.0471
IR Inten --	11.0975	5.2891	16.3925

	25	26	27
	A	A	A
Frequencies --	1275.1769	1291.5037	1341.6571
Red. masses --	1.3041	1.2698	1.3270
Frc consts --	1.2494	1.2479	1.4073
IR Inten --	0.1744	1.8186	5.2705
	28	29	30
	A	A	A
Frequencies --	1350.0977	1366.8441	1375.7456
Red. masses --	1.2711	1.3978	1.4548
Frc consts --	1.3651	1.5386	1.6223
IR Inten --	5.5528	4.8541	11.6825
	31	32	33
	A	A	A
Frequencies --	1394.6548	1398.9966	1423.4997
Red. masses --	1.5100	1.5043	2.2570
Frc consts --	1.7304	1.7347	2.6946
IR Inten --	0.3808	2.4575	51.6569
	34	35	36
	A	A	A
Frequencies --	1475.1525	1479.4848	1500.5805
Red. masses --	1.0954	1.1000	1.0824
Frc consts --	1.4044	1.4186	1.4360
IR Inten --	5.6069	18.8746	5.4271
	37	38	39
	A	A	A
Frequencies --	1509.6665	1765.3810	3038.8933
Red. masses --	1.0972	9.1955	1.0673
Frc consts --	1.4734	16.8851	5.8073
IR Inten --	4.7913	77.6767	25.2520
	40	41	42
	A	A	A
Frequencies --	3054.7613	3057.8610	3063.5115
Red. masses --	1.0643	1.0604	1.0622
Frc consts --	5.8513	5.8417	5.8733
IR Inten --	15.0053	13.3310	22.0608
	43	44	45
	A	A	A
Frequencies --	3101.2730	3107.8642	3112.2916
Red. masses --	1.0957	1.1003	1.1039
Frc consts --	6.2088	6.2616	6.3001
IR Inten --	40.2332	34.7514	2.2707
	46	47	48
	A	A	A
Frequencies --	3116.0573	3132.8632	3481.4947
Red. masses --	1.1047	1.0888	1.0743
Frc consts --	6.3196	6.2961	7.6720
IR Inten --	43.5598	17.9907	2.0663
24e	1	2	3
	A	A	A
Frequencies --	102.0738	162.1378	293.0035
Red. masses --	4.2699	2.4860	5.3646
Frc consts --	0.0262	0.0385	0.2714
IR Inten --	0.2432	2.5019	0.1391
	4	5	6
	A	A	A
Frequencies --	314.1878	352.9295	397.1884
Red. masses --	1.9214	3.2782	4.3289
Frc consts --	0.1118	0.2406	0.4024
IR Inten --	0.1748	0.5865	4.4733

	7	8	9
	A	A	A
Frequencies --	427.6658	505.5153	589.4419
Red. masses --	2.7477	2.2677	3.3519
Frc consts --	0.2961	0.3414	0.6862
IR Inten --	0.3070	8.1994	15.9129
	10	11	12
	A	A	A
Frequencies --	666.7807	775.2390	850.2402
Red. masses --	2.7042	2.2612	1.7237
Frc consts --	0.7084	0.8007	0.7341
IR Inten --	1.3544	0.1758	6.5786
	13	14	15
	A	A	A
Frequencies --	871.8657	891.3823	896.6487
Red. masses --	1.9587	1.4824	2.0854
Frc consts --	0.8773	0.6940	0.9878
IR Inten --	12.3844	19.2527	15.4247
	16	17	18
	A	A	A
Frequencies --	973.3765	984.1552	1066.8363
Red. masses --	2.3790	1.3227	1.5514
Frc consts --	1.3280	0.7548	1.0403
IR Inten --	9.5682	24.5108	7.3104
	19	20	21
	A	A	A
Frequencies --	1075.6575	1098.9611	1131.1607
Red. masses --	2.0215	1.8560	3.5892
Frc consts --	1.3781	1.3206	2.7058
IR Inten --	20.0352	4.1101	96.1245
	22	23	24
	A	A	A
Frequencies --	1134.3699	1170.9461	1206.3218
Red. masses --	2.1237	1.4963	1.3017
Frc consts --	1.6101	1.2088	1.1161
IR Inten --	14.9923	8.7179	18.0724
	25	26	27
	A	A	A
Frequencies --	1275.3707	1287.7914	1330.8083
Red. masses --	1.3500	1.2583	1.3207
Frc consts --	1.2938	1.2295	1.3781
IR Inten --	0.7721	0.9796	14.4260
	28	29	30
	A	A	A
Frequencies --	1351.4233	1364.8196	1369.6283
Red. masses --	1.2095	1.3837	1.4288
Frc consts --	1.3015	1.5186	1.5792
IR Inten --	14.7744	3.9533	3.4134
	31	32	33
	A	A	A
Frequencies --	1386.2318	1398.3239	1437.2838
Red. masses --	1.5834	1.4552	1.8312
Frc consts --	1.7927	1.6765	2.2288
IR Inten --	9.0816	0.7750	10.1940
	34	35	36
	A	A	A
Frequencies --	1483.1308	1494.1882	1500.9386
Red. masses --	1.0977	1.0991	1.0880
Frc consts --	1.4226	1.4457	1.4441
IR Inten --	13.6806	4.4684	10.5558
	37	38	39

	A	A	A
Frequencies --	1511.2789	1770.5138	3026.6578
Red. masses --	1.1004	9.4826	1.0808
Frc consts --	1.4808	17.5136	5.8333
IR Inten --	3.1172	86.0018	9.4553
	40	41	42
	A	A	A
Frequencies --	3038.5622	3040.7658	3052.1237
Red. masses --	1.0678	1.0696	1.0621
Frc consts --	5.8087	5.8269	5.8296
IR Inten --	20.4422	22.1571	28.2967
	43	44	45
	A	A	A
Frequencies --	3060.3880	3104.9475	3106.9177
Red. masses --	1.0624	1.0971	1.0972
Frc consts --	5.8626	6.2318	6.2404
IR Inten --	24.1670	35.6548	38.6215
	46	47	48
	A	A	A
Frequencies --	3110.9806	3119.9819	3489.5566
Red. masses --	1.1009	1.1035	1.0745
Frc consts --	6.2775	6.3289	7.7091
IR Inten --	25.6621	32.5364	2.2741
25a	1	2	3
	A	A	A
Frequencies --	114.0818	161.2919	239.1231
Red. masses --	3.4428	3.0615	3.4207
Frc consts --	0.0264	0.0469	0.1152
IR Inten --	0.6467	1.8057	3.4074
	4	5	6
	A	A	A
Frequencies --	289.5739	373.8027	404.0799
Red. masses --	2.3298	2.0081	2.5044
Frc consts --	0.1151	0.1653	0.2409
IR Inten --	1.2353	1.7555	0.8809
	7	8	9
	A	A	A
Frequencies --	456.6925	474.7704	630.7319
Red. masses --	3.3429	2.0430	4.0891
Frc consts --	0.4108	0.2713	0.9585
IR Inten --	2.0668	3.0091	2.0731
	10	11	12
	A	A	A
Frequencies --	665.0632	743.7750	784.4801
Red. masses --	2.2857	1.2327	2.3212
Frc consts --	0.5957	0.4018	0.8416
IR Inten --	6.8090	1.2405	2.2673
	13	14	15
	A	A	A
Frequencies --	827.1020	867.1159	895.6638
Red. masses --	1.6784	2.4645	2.1773
Frc consts --	0.6765	1.0918	1.0291
IR Inten --	4.8890	2.9239	12.8923
	16	17	18
	A	A	A
Frequencies --	925.0929	962.4695	981.5992
Red. masses --	1.4897	1.3928	2.4502
Frc consts --	0.7511	0.7602	1.3910
IR Inten --	20.9892	27.6528	50.7964
	19	20	21
	A	A	A
Frequencies --	1006.0698	1014.4067	1060.0956
Red. masses --	1.5486	2.7430	1.8653
Frc consts --	0.9235	1.6630	1.2351
IR Inten --	14.5558	28.2220	4.6479

	22	23	24
	A	A	A
Frequencies --	1102.5290	1117.8357	1184.1525
Red. masses --	1.7111	1.8303	1.2635
Frc consts --	1.2254	1.3475	1.0439
IR Inten --	11.0452	8.8665	11.5846
	25	26	27
	A	A	A
Frequencies --	1190.9744	1277.1755	1295.0062
Red. masses --	1.4995	1.3541	1.2435
Frc consts --	1.2531	1.3014	1.2287
IR Inten --	4.1667	0.1323	1.5958
	28	29	30
	A	A	A
Frequencies --	1323.7411	1346.3096	1363.2667
Red. masses --	1.5650	1.2502	1.3470
Frc consts --	1.6158	1.3351	1.4749
IR Inten --	2.9227	7.0448	5.3636
	31	32	33
	A	A	A
Frequencies --	1375.1300	1382.4243	1396.6860
Red. masses --	1.6105	1.6157	1.5364
Frc consts --	1.7943	1.8192	1.7659
IR Inten --	4.1457	4.5701	1.5617
	34	35	36
	A	A	A
Frequencies --	1398.9316	1465.1725	1474.0142
Red. masses --	1.6183	1.1621	1.0965
Frc consts --	1.8660	1.4698	1.4037
IR Inten --	0.5707	6.6788	8.5476
	37	38	39
	A	A	A
Frequencies --	1487.0279	1499.0609	1509.4389
Red. masses --	1.1228	1.0832	1.0958
Frc consts --	1.4629	1.4342	1.4710
IR Inten --	16.1860	6.6687	4.0773
	40	41	42
	A	A	A
Frequencies --	1748.6808	3035.5996	3051.0937
Red. masses --	5.9596	1.0670	1.0630
Frc consts --	10.7372	5.7932	5.8304
IR Inten --	11.9865	26.3319	16.7427
	43	44	45
	A	A	A
Frequencies --	3052.5558	3059.6897	3094.6732
Red. masses --	1.0639	1.0624	1.0887
Frc consts --	5.8407	5.8602	6.1432
IR Inten --	14.2919	22.3382	63.6511
	46	47	48
	A	A	A
Frequencies --	3096.9608	3104.4292	3110.5234
Red. masses --	1.0957	1.0997	1.1012
Frc consts --	6.1915	6.2445	6.2772
IR Inten --	20.6773	47.1315	2.5457
	49	50	51
	A	A	A
Frequencies --	3112.7719	3145.6809	3232.2725
Red. masses --	1.1035	1.0616	1.1162
Frc consts --	6.2999	6.1892	6.8710
IR Inten --	51.9840	8.7889	12.8270
25e	1	2	3
	A	A	A
Frequencies --	114.8073	171.0738	294.4932
Red. masses --	3.3337	2.4394	3.4184

Frc consts	--	0.0259	0.0421	0.1747
IR Inten	--	1.1628	0.4184	2.0913

		4	5	6
		A	A	A
Frequencies	--	312.9655	355.2174	390.6705
Red. masses	--	1.9932	3.1155	3.6243
Frc consts	--	0.1150	0.2316	0.3259
IR Inten	--	0.9210	1.6835	1.2224

		7	8	9
		A	A	A
Frequencies	--	426.0272	482.5561	566.3530
Red. masses	--	2.5722	2.4846	2.9425
Frc consts	--	0.2751	0.3409	0.5561
IR Inten	--	0.4742	2.3544	9.8770

		10	11	12
		A	A	A
Frequencies	--	641.4912	749.9727	789.3686
Red. masses	--	2.3796	1.1675	2.0173
Frc consts	--	0.5769	0.3869	0.7406
IR Inten	--	6.0737	0.2346	1.0649

		13	14	15
		A	A	A
Frequencies	--	844.9504	878.5069	879.8423
Red. masses	--	1.6832	2.1063	1.9481
Frc consts	--	0.7080	0.9578	0.8885
IR Inten	--	8.0904	3.4869	9.0312

		16	17	18
		A	A	A
Frequencies	--	954.2103	958.7318	966.3581
Red. masses	--	1.7790	1.3690	1.8413
Frc consts	--	0.9544	0.7414	1.0131
IR Inten	--	5.2317	43.0575	9.4344

		19	20	21
		A	A	A
Frequencies	--	1008.0048	1070.0492	1094.9440
Red. masses	--	1.6148	1.7652	3.6347
Frc consts	--	0.9667	1.1908	2.5675
IR Inten	--	5.8077	12.9809	76.3105

		22	23	24
		A	A	A
Frequencies	--	1098.7330	1124.4088	1171.9819
Red. masses	--	2.0042	1.7278	1.5341
Frc consts	--	1.4255	1.2870	1.2415
IR Inten	--	3.1328	4.0481	2.4991

		25	26	27
		A	A	A
Frequencies	--	1186.2302	1276.9733	1279.8233
Red. masses	--	1.5568	1.4074	1.3839
Frc consts	--	1.2907	1.3522	1.3355
IR Inten	--	1.0424	0.3211	2.5950

		28	29	30
		A	A	A
Frequencies	--	1294.8532	1343.9998	1365.1830
Red. masses	--	1.3547	1.2104	1.3891
Frc consts	--	1.3383	1.2882	1.5253
IR Inten	--	0.1347	0.1923	1.1265

		31	32	33
		A	A	A
Frequencies	--	1371.6328	1385.0016	1396.1376
Red. masses	--	1.4603	1.5439	1.4535
Frc consts	--	1.6187	1.7449	1.6693
IR Inten	--	1.2176	2.6647	0.1168

34

35

36

	A	A	A
Frequencies --	1410.3041	1455.9635	1488.0481
Red. masses --	1.6681	1.1673	1.1080
Frc consts --	1.9548	1.4579	1.4455
IR Inten --	14.0130	5.8322	10.2704
	37	38	39
	A	A	A
Frequencies --	1492.7502	1499.3677	1509.9190
Red. masses --	1.0997	1.0863	1.0995
Frc consts --	1.4437	1.4389	1.4769
IR Inten --	6.4779	10.3503	3.3999
	40	41	42
	A	A	A
Frequencies --	1751.9798	3024.5846	3033.0365
Red. masses --	6.2121	1.0702	1.0798
Frc consts --	11.2343	5.7685	5.8524
IR Inten --	17.1252	9.7443	21.6268
	43	44	45
	A	A	A
Frequencies --	3036.8166	3048.6274	3058.8846
Red. masses --	1.0702	1.0621	1.0619
Frc consts --	5.8149	5.8157	5.8542
IR Inten --	37.8454	29.6426	24.1336
	46	47	48
	A	A	A
Frequencies --	3100.0809	3102.3070	3107.3487
Red. masses --	1.0954	1.0989	1.0984
Frc consts --	6.2023	6.2314	6.2488
IR Inten --	45.1766	48.1851	21.7139
	49	50	51
	A	A	A
Frequencies --	3116.5491	3162.2109	3258.5360
Red. masses --	1.1042	1.0618	1.1155
Frc consts --	6.3190	6.2554	6.9783
IR Inten --	40.3702	8.3538	4.5577

Vibrational frequencies (implicit DMSO)

1a			
	1	2	3
	A	A	A
Frequencies --	79.4945	158.0562	227.3005
Red. masses --	6.0240	3.3364	4.8661
Frc consts --	0.0224	0.0491	0.1481
IR Inten --	16.8227	1.3962	7.4769
	4	5	6
	A	A	A
Frequencies --	291.9247	400.5551	435.7659
Red. masses --	4.0419	2.1720	4.8323
Frc consts --	0.2029	0.2053	0.5406
IR Inten --	4.7004	13.4629	3.4851
	7	8	9
	A	A	A
Frequencies --	477.5911	507.6887	651.1146
Red. masses --	5.7165	2.2605	3.9490
Frc consts --	0.7682	0.3433	0.9864
IR Inten --	29.2819	7.8584	26.2191
	10	11	12
	A	A	A
Frequencies --	747.0564	790.6997	868.8744
Red. masses --	4.0451	2.4781	2.8697
Frc consts --	1.3301	0.9128	1.2764
IR Inten --	14.9574	30.1885	23.0007
	13	14	15
	A	A	A
Frequencies --	888.0910	943.7780	1012.3503
Red. masses --	2.5009	2.1586	3.3404
Frc consts --	1.1622	1.1328	2.0170
IR Inten --	41.6439	28.6458	2.9358
	16	17	18
	A	A	A
Frequencies --	1027.1320	1053.6446	1105.5931
Red. masses --	2.4238	2.0278	2.4963
Frc consts --	1.5066	1.3264	1.7978
IR Inten --	112.9408	26.2755	29.6881
	19	20	21
	A	A	A
Frequencies --	1149.2298	1207.8180	1257.1782
Red. masses --	4.4413	1.4234	1.7581
Frc consts --	3.4560	1.2234	1.6372
IR Inten --	74.9094	22.2429	140.8987
	22	23	24
	A	A	A
Frequencies --	1268.6505	1315.8987	1339.3320
Red. masses --	1.4698	1.4806	1.6554
Frc consts --	1.3938	1.5105	1.7496
IR Inten --	4.1214	20.8499	17.3923
	25	26	27
	A	A	A
Frequencies --	1351.1199	1368.6698	1397.2699
Red. masses --	1.2866	1.2134	1.3925
Frc consts --	1.3838	1.3392	1.6018
IR Inten --	7.6562	23.2642	12.4812
	28	29	30
	A	A	A
Frequencies --	1422.2167	1445.9309	1473.5060
Red. masses --	1.3548	1.1149	1.0856
Frc consts --	1.6145	1.3733	1.3888

IR Inten	--	24.3831	23.1945	12.1167
		31	32	33
		A	A	A
Frequencies	--	1511.8945	1825.5921	3017.6694
Red. masses	--	1.0919	11.3060	1.0699
Frc consts	--	1.4706	22.2007	5.7401
IR Inten	--	8.0888	420.1456	50.8208
		34	35	36
		A	A	A
Frequencies	--	3025.3454	3076.7079	3132.2814
Red. masses	--	1.0706	1.0626	1.0886
Frc consts	--	5.7732	5.9266	6.2927
IR Inten	--	70.4699	5.6768	22.6191
		37	38	39
		A	A	A
Frequencies	--	3144.5651	3149.5949	3154.5480
Red. masses	--	1.0947	1.0955	1.1027
Frc consts	--	6.3780	6.4031	6.4651
IR Inten	--	27.4441	22.8260	10.6193
1e		1	2	3
		A	A	A
Frequencies	--	96.0657	153.0802	278.5646
Red. masses	--	5.5544	2.5132	8.1429
Frc consts	--	0.0302	0.0347	0.3723
IR Inten	--	6.5510	12.0572	2.0516
		4	5	6
		A	A	A
Frequencies	--	343.4734	353.0514	409.2507
Red. masses	--	3.2453	3.6455	4.5702
Frc consts	--	0.2256	0.2677	0.4510
IR Inten	--	6.8448	31.0038	2.1453
		7	8	9
		A	A	A
Frequencies	--	447.9679	520.9053	607.4852
Red. masses	--	3.0650	3.1684	4.5958
Frc consts	--	0.3624	0.5065	0.9993
IR Inten	--	1.5758	10.5264	26.9936
		10	11	12
		A	A	A
Frequencies	--	717.2358	766.5935	877.1134
Red. masses	--	2.8945	2.5167	2.5177
Frc consts	--	0.8773	0.8714	1.1412
IR Inten	--	21.6542	7.1658	27.3569
		13	14	15
		A	A	A
Frequencies	--	914.8942	996.9423	1003.7645
Red. masses	--	2.7425	1.4088	2.7885
Frc consts	--	1.3525	0.8250	1.6553
IR Inten	--	35.6661	7.4953	61.4134
		16	17	18
		A	A	A
Frequencies	--	1073.9311	1104.1337	1123.1127
Red. masses	--	3.6582	3.6955	2.7751
Frc consts	--	2.4858	2.6544	2.0624
IR Inten	--	35.9414	134.2966	0.3164
		19	20	21
		A	A	A
Frequencies	--	1148.2358	1187.7875	1247.3114
Red. masses	--	4.2494	1.7370	1.6651
Frc consts	--	3.3010	1.4439	1.5263
IR Inten	--	94.0156	38.9158	113.9691
		22	23	24
		A	A	A
Frequencies	--	1266.7460	1313.8000	1331.7185

Red. masses	--	1.3405	1.4156	1.2602
Frc consts	--	1.2674	1.4396	1.3168
IR Inten	--	3.2607	12.6376	15.2376

		25	26	27
		A	A	A
Frequencies	--	1355.5282	1363.5649	1409.9666
Red. masses	--	1.2756	1.3203	1.4077
Frc consts	--	1.3809	1.4463	1.6489
IR Inten	--	6.0955	8.0283	20.4205

		28	29	30
		A	A	A
Frequencies	--	1430.3507	1452.8447	1497.7867
Red. masses	--	1.4510	1.1047	1.0761
Frc consts	--	1.7491	1.3738	1.4223
IR Inten	--	8.0244	20.2919	3.3856

		31	32	33
		A	A	A
Frequencies	--	1511.0539	1824.7785	3024.0332
Red. masses	--	1.0960	11.9475	1.0695
Frc consts	--	1.4744	23.4394	5.7622
IR Inten	--	10.4168	450.2216	58.7916

		34	35	36
		A	A	A
Frequencies	--	3029.2083	3072.3680	3089.9463
Red. masses	--	1.0703	1.0633	1.0831
Frc consts	--	5.7865	5.9136	6.0929
IR Inten	--	63.9080	4.9091	21.5320

		37	38	39
		A	A	A
Frequencies	--	3146.3785	3150.1677	3152.8525
Red. masses	--	1.0993	1.0987	1.0975
Frc consts	--	6.4117	6.4237	6.4277
IR Inten	--	23.7838	19.1117	21.6996

2a

		1	2	3
		A	A	A
Frequencies	--	77.0683	157.4106	238.2260
Red. masses	--	6.3929	3.8677	4.1114
Frc consts	--	0.0224	0.0565	0.1375
IR Inten	--	6.6618	0.1397	11.6816

		4	5	6
		A	A	A
Frequencies	--	268.7886	350.6183	406.3305
Red. masses	--	5.6464	3.8148	2.7447
Frc consts	--	0.2403	0.2763	0.2670
IR Inten	--	4.0960	3.8823	14.4729

		7	8	9
		A	A	A
Frequencies	--	417.2906	503.2886	633.2173
Red. masses	--	3.6777	2.6218	5.2349
Frc consts	--	0.3773	0.3913	1.2367
IR Inten	--	2.0469	2.4330	10.6308

		10	11	12
		A	A	A
Frequencies	--	704.4912	778.0639	865.4249
Red. masses	--	4.3268	2.2804	3.0416
Frc consts	--	1.2652	0.8134	1.3422
IR Inten	--	40.3416	34.5498	17.3652

		13	14	15
		A	A	A
Frequencies	--	877.9695	933.0409	1004.4689

Red. masses	--	2.7226	2.2329	3.2475
Frc consts	--	1.2365	1.1453	1.9305
IR Inten	--	47.2310	35.2458	13.2787

		16	17	18
		A	A	A
Frequencies	--	1021.3217	1046.4565	1080.8860
Red. masses	--	2.8390	1.8137	2.3403
Frc consts	--	1.7448	1.1702	1.6109
IR Inten	--	161.5318	13.8234	91.9415

		19	20	21
		A	A	A
Frequencies	--	1147.1870	1178.8926	1236.3048
Red. masses	--	4.2410	1.8256	3.1057
Frc consts	--	3.2885	1.4948	2.7968
IR Inten	--	98.9431	36.2636	63.7813

		22	23	24
		A	A	A
Frequencies	--	1257.6626	1267.2299	1319.2820
Red. masses	--	1.4798	1.3676	1.4920
Frc consts	--	1.3790	1.2940	1.5300
IR Inten	--	44.5807	50.4486	99.0491

		25	26	27
		A	A	A
Frequencies	--	1338.7622	1339.8592	1384.0888
Red. masses	--	1.3895	1.1781	1.5807
Frc consts	--	1.4673	1.2460	1.7841
IR Inten	--	54.9981	6.0047	80.5779

		28	29	30
		A	A	A
Frequencies	--	1389.6948	1430.4507	1464.0051
Red. masses	--	1.3122	1.4322	1.1768
Frc consts	--	1.4931	1.7266	1.4861
IR Inten	--	15.5587	3.1708	15.3890

		31	32	33
		A	A	A
Frequencies	--	1476.6226	1509.1106	3021.7064
Red. masses	--	1.0836	1.0954	1.0698
Frc consts	--	1.3921	1.4698	5.7552
IR Inten	--	10.7375	10.9877	81.3611

		34	35	36
		A	A	A
Frequencies	--	3023.8332	3068.9413	3138.8638
Red. masses	--	1.0694	1.0639	1.0900
Frc consts	--	5.7610	5.9039	6.3274
IR Inten	--	34.7163	6.0275	11.6079

		37	38	39
		A	A	A
Frequencies	--	3143.9051	3152.7961	3155.5606
Red. masses	--	1.0947	1.0955	1.1016
Frc consts	--	6.3752	6.4157	6.4627
IR Inten	--	27.9931	30.1294	6.2503

2e

		1	2	3
		A	A	A
Frequencies	--	81.6613	157.4221	237.2004
Red. masses	--	5.5898	2.6604	13.9630
Frc consts	--	0.0220	0.0388	0.4629
IR Inten	--	2.0097	6.9103	1.3304

		4	5	6
		A	A	A
Frequencies	--	316.6825	357.3404	385.5046

Red. masses	--	3.6689	4.3233	2.7674
Frc consts	--	0.2168	0.3253	0.2423
IR Inten	--	10.4746	21.3036	5.9102

		7	8	9
		A	A	A
Frequencies	--	446.3850	486.4910	576.3928
Red. masses	--	3.2973	4.3492	4.4775
Frc consts	--	0.3871	0.6065	0.8764
IR Inten	--	1.3850	4.5731	7.3746

		10	11	12
		A	A	A
Frequencies	--	657.3603	743.1863	845.6887
Red. masses	--	3.2092	3.1182	2.1341
Frc consts	--	0.8171	1.0147	0.8992
IR Inten	--	49.6104	4.3124	17.7408

		13	14	15
		A	A	A
Frequencies	--	909.9734	994.4687	1011.8297
Red. masses	--	2.6468	3.0367	1.4609
Frc consts	--	1.2913	1.7694	0.8813
IR Inten	--	12.0412	106.1039	3.8508

		16	17	18
		A	A	A
Frequencies	--	1049.4814	1087.3826	1105.5302
Red. masses	--	2.9701	2.6697	3.6700
Frc consts	--	1.9274	1.8598	2.6428
IR Inten	--	8.1727	67.5493	70.8348

		19	20	21
		A	A	A
Frequencies	--	1143.0319	1185.1618	1209.0216
Red. masses	--	4.5282	1.8177	2.0762
Frc consts	--	3.4857	1.5043	1.7881
IR Inten	--	128.8777	22.8133	57.4202

		22	23	24
		A	A	A
Frequencies	--	1246.6490	1293.7883	1322.3411
Red. masses	--	1.6357	1.4908	1.2657
Frc consts	--	1.4978	1.4703	1.3039
IR Inten	--	70.3085	2.0699	5.3562

		25	26	27
		A	A	A
Frequencies	--	1334.0231	1353.6567	1363.0382
Red. masses	--	1.6420	1.4369	1.2867
Frc consts	--	1.7217	1.5513	1.4085
IR Inten	--	191.1923	73.2026	35.5175

		28	29	30
		A	A	A
Frequencies	--	1404.7529	1430.1850	1464.2058
Red. masses	--	1.3793	1.4237	1.1292
Frc consts	--	1.6036	1.7157	1.4264
IR Inten	--	5.1334	11.5003	19.8845

		31	32	33
		A	A	A
Frequencies	--	1500.3780	1514.4317	3023.4198
Red. masses	--	1.0765	1.0974	1.0689
Frc consts	--	1.4278	1.4830	5.7567
IR Inten	--	2.0727	12.5126	53.5424

		34	35	36
		A	A	A
Frequencies	--	3031.5789	3059.0887	3084.8334
Red. masses	--	1.0700	1.0663	1.0829
Frc consts	--	5.7941	5.8791	6.0715

IR Inten	--	63.1543	8.2726	22.4081
		37	38	39
		A	A	A
Frequencies	--	3152.0085	3153.1485	3155.0605
Red. masses	--	1.0964	1.0981	1.0980
Frc consts	--	6.4181	6.4324	6.4398
IR Inten	--	37.1768	0.7833	25.2041

3a

		1	2	3
		A	A	A
Frequencies	--	99.8112	163.2068	235.0889
Red. masses	--	4.6909	3.3997	4.7495
Frc consts	--	0.0275	0.0534	0.1547
IR Inten	--	8.3974	0.3335	6.4185

		4	5	6
		A	A	A
Frequencies	--	296.6955	401.1395	435.8214
Red. masses	--	3.5929	2.1003	3.6516
Frc consts	--	0.1863	0.1991	0.4086
IR Inten	--	8.0381	17.5252	12.7803

		7	8	9
		A	A	A
Frequencies	--	472.5644	506.5008	652.6620
Red. masses	--	5.7043	2.1319	4.2068
Frc consts	--	0.7505	0.3222	1.0558
IR Inten	--	15.3261	10.0375	10.5717

		10	11	12
		A	A	A
Frequencies	--	740.7283	794.8065	870.2047
Red. masses	--	3.2955	2.5932	2.7726
Frc consts	--	1.0653	0.9652	1.2370
IR Inten	--	55.7398	17.3025	22.1792

		13	14	15
		A	A	A
Frequencies	--	884.9251	929.5587	953.7319
Red. masses	--	2.2192	1.9014	1.6627
Frc consts	--	1.0239	0.9680	0.8911
IR Inten	--	15.3316	189.1231	15.3603

		16	17	18
		A	A	A
Frequencies	--	1013.3056	1040.7517	1069.8466
Red. masses	--	3.1743	2.3020	1.9440
Frc consts	--	1.9204	1.4691	1.3109
IR Inten	--	1.7858	82.7634	21.9195

		19	20	21
		A	A	A
Frequencies	--	1105.4503	1145.1895	1173.3113
Red. masses	--	2.1939	1.9414	3.0207
Frc consts	--	1.5796	1.5001	2.4501
IR Inten	--	28.6513	73.2838	142.5948

		22	23	24
		A	A	A
Frequencies	--	1224.8545	1267.4248	1319.9065
Red. masses	--	1.2176	1.2850	1.4347
Frc consts	--	1.0763	1.2161	1.4727
IR Inten	--	7.3456	59.8282	28.0045

		25	26	27
		A	A	A
Frequencies	--	1342.7703	1351.4117	1368.5121
Red. masses	--	1.3005	1.5100	1.2358
Frc consts	--	1.3815	1.6248	1.3637
IR Inten	--	11.6430	5.0235	19.3892

		28	29	30
		A	A	A
Frequencies	--	1380.6786	1420.4460	1426.0076
Red. masses	--	1.2581	1.4439	1.6702
Frc consts	--	1.4131	1.7165	2.0011

IR Inten	--	11.0580	42.1574	4.6937
		31	32	33
		A	A	A
Frequencies	--	1455.4020	1472.5076	1507.6991
Red. masses	--	1.1651	1.0883	1.0947
Frc consts	--	1.4541	1.3903	1.4662
IR Inten	--	24.3388	13.3455	8.0365
		34	35	36
		A	A	A
Frequencies	--	1758.5030	3015.1378	3016.7502
Red. masses	--	9.2322	1.0698	1.0707
Frc consts	--	16.8206	5.7302	5.7412
IR Inten	--	149.6740	64.0131	65.0820
		37	38	39
		A	A	A
Frequencies	--	3074.2510	3108.2259	3141.9282
Red. masses	--	1.0630	1.0881	1.0946
Frc consts	--	5.9191	6.1935	6.3666
IR Inten	--	12.6609	33.8412	42.6912
		40	41	42
		A	A	A
Frequencies	--	3144.3543	3146.4246	3488.3164
Red. masses	--	1.0961	1.1015	1.0746
Frc consts	--	6.3849	6.4249	7.7041
IR Inten	--	15.2713	20.3859	1.6574
3e		1	2	3
		A	A	A
Frequencies	--	109.5353	160.9863	284.7147
Red. masses	--	4.4183	2.5086	5.1862
Frc consts	--	0.0312	0.0383	0.2477
IR Inten	--	1.5034	7.2834	8.9916
		4	5	6
		A	A	A
Frequencies	--	343.9930	356.1399	406.2585
Red. masses	--	3.2547	3.6099	4.0868
Frc consts	--	0.2269	0.2698	0.3974
IR Inten	--	7.2830	40.6053	1.2605
		7	8	9
		A	A	A
Frequencies	--	448.9761	511.2871	597.5293
Red. masses	--	2.8932	3.1026	4.2191
Frc consts	--	0.3436	0.4779	0.8875
IR Inten	--	1.0801	13.6105	22.7144
		10	11	12
		A	A	A
Frequencies	--	705.7978	778.9827	876.4179
Red. masses	--	2.5990	2.5902	2.2643
Frc consts	--	0.7628	0.9261	1.0247
IR Inten	--	23.6167	5.5977	18.6059
		13	14	15
		A	A	A
Frequencies	--	902.0984	922.0369	1001.8429
Red. masses	--	2.2729	1.3011	2.8655
Frc consts	--	1.0898	0.6517	1.6945
IR Inten	--	71.5415	64.8809	50.4336
		16	17	18
		A	A	A
Frequencies	--	1045.5023	1065.0801	1093.2857
Red. masses	--	1.6533	2.7360	2.8550
Frc consts	--	1.0648	1.8287	2.0106
IR Inten	--	15.5645	86.5472	101.5334
		19	20	21
		A	A	A
Frequencies	--	1121.1862	1136.3538	1172.2605
Red. masses	--	2.7275	2.4904	3.5795

Frc consts	--	2.0201	1.8947	2.8982
IR Inten	--	7.0215	47.0075	83.7718
		22	23	24
		A	A	A
Frequencies	--	1228.0429	1262.5189	1320.0974
Red. masses	--	1.1906	1.3043	1.3733
Frc consts	--	1.0579	1.2249	1.4100
IR Inten	--	18.3891	46.3116	9.7949
		25	26	27
		A	A	A
Frequencies	--	1328.2203	1336.4024	1366.1241
Red. masses	--	1.3124	1.1922	1.2913
Frc consts	--	1.3642	1.2545	1.4199
IR Inten	--	51.5863	6.2226	4.9212
		28	29	30
		A	A	A
Frequencies	--	1380.8808	1419.6457	1437.5498
Red. masses	--	1.3409	1.4136	1.6700
Frc consts	--	1.5065	1.6786	2.0334
IR Inten	--	4.5309	50.3582	4.0590
		31	32	33
		A	A	A
Frequencies	--	1458.5289	1497.2984	1510.3250
Red. masses	--	1.1439	1.0809	1.0976
Frc consts	--	1.4338	1.4278	1.4751
IR Inten	--	21.8034	3.4245	10.9777
		34	35	36
		A	A	A
Frequencies	--	1757.8249	3019.8009	3020.3873
Red. masses	--	10.0146	1.0691	1.0703
Frc consts	--	18.2319	5.7443	5.7526
IR Inten	--	190.5423	52.5090	78.0685
		37	38	39
		A	A	A
Frequencies	--	3069.0784	3097.4421	3141.9144
Red. masses	--	1.0639	1.0843	1.0969
Frc consts	--	5.9043	6.1290	6.3799
IR Inten	--	12.6212	24.4317	35.2811
		40	41	42
		A	A	A
Frequencies	--	3144.5029	3148.0286	3490.7463
Red. masses	--	1.1000	1.0973	1.0736
Frc consts	--	6.4083	6.4070	7.7076
IR Inten	--	19.3244	28.4208	9.0377
4a		1	2	3
		A	A	A
Frequencies	--	101.8050	167.3342	232.0004
Red. masses	--	4.7422	3.6192	4.2057
Frc consts	--	0.0290	0.0597	0.1334
IR Inten	--	9.4985	1.8451	10.0434
		4	5	6
		A	A	A
Frequencies	--	300.3188	403.5836	435.1130
Red. masses	--	3.5539	2.1471	4.2143
Frc consts	--	0.1889	0.2060	0.4701
IR Inten	--	3.2769	10.9876	8.0638
		7	8	9
		A	A	A
Frequencies	--	469.4509	507.5457	656.4325
Red. masses	--	4.4655	2.2074	4.1648
Frc consts	--	0.5798	0.3350	1.0574
IR Inten	--	26.6796	2.4608	11.6847
		10	11	12
		A	A	A

Frequencies	--	746.2480	791.1427	870.5095
Red. masses	--	3.9072	2.5039	2.9732
Frc consts	--	1.2820	0.9234	1.3274
IR Inten	--	28.2318	23.8764	19.0793

		13	14	15
		A	A	A
Frequencies	--	884.5445	927.1296	956.0215
Red. masses	--	2.1817	1.7225	1.6677
Frc consts	--	1.0057	0.8724	0.8981
IR Inten	--	77.3333	16.9608	61.2163

		16	17	18
		A	A	A
Frequencies	--	1011.4785	1038.0373	1070.6042
Red. masses	--	3.2169	2.2901	1.9671
Frc consts	--	1.9391	1.4539	1.3284
IR Inten	--	4.8052	97.5194	106.3472

		19	20	21
		A	A	A
Frequencies	--	1106.0048	1147.7440	1172.2330
Red. masses	--	2.1998	1.8465	3.2635
Frc consts	--	1.5854	1.4332	2.6422
IR Inten	--	14.2747	37.0209	138.5160

		22	23	24
		A	A	A
Frequencies	--	1230.2664	1271.4659	1324.7132
Red. masses	--	1.1922	1.2815	1.4329
Frc consts	--	1.0632	1.2206	1.4815
IR Inten	--	1.8927	56.9637	17.1558

		25	26	27
		A	A	A
Frequencies	--	1336.7668	1360.5347	1369.9986
Red. masses	--	1.4057	1.3319	1.2124
Frc consts	--	1.4800	1.4526	1.3407
IR Inten	--	0.6969	3.5729	25.8632

		28	29	30
		A	A	A
Frequencies	--	1380.8307	1425.8338	1430.4721
Red. masses	--	1.3585	1.4163	1.8862
Frc consts	--	1.5262	1.6965	2.2740
IR Inten	--	28.7902	2.9126	85.7123

		31	32	33
		A	A	A
Frequencies	--	1455.1739	1476.2377	1512.5778
Red. masses	--	1.1047	1.0874	1.0946
Frc consts	--	1.3782	1.3962	1.4755
IR Inten	--	20.4463	11.8912	8.9561

		34	35	36
		A	A	A
Frequencies	--	1759.8949	3016.1532	3017.9874
Red. masses	--	9.2676	1.0700	1.0699
Frc consts	--	16.9119	5.7353	5.7416
IR Inten	--	150.9799	92.7695	37.3490

		37	38	39
		A	A	A
Frequencies	--	3073.7094	3131.4806	3134.5867
Red. masses	--	1.0611	1.0892	1.1010
Frc consts	--	5.9064	6.2933	6.3740
IR Inten	--	11.4218	28.7845	22.4253

		40	41	42
		A	A	A
Frequencies	--	3140.1603	3142.4764	3491.0827
Red. masses	--	1.0976	1.0956	1.0745
Frc consts	--	6.3765	6.3745	7.7157

IR Inten	--	33.5082	20.5044	2.1083
4e				
		1	2	3
		A	A	A
Frequencies	--	98.6630	160.4623	291.0184
Red. masses	--	4.6627	2.5180	5.8033
Frc consts	--	0.0267	0.0382	0.2896
IR Inten	--	3.5612	11.2115	0.9366
		4	5	6
		A	A	A
Frequencies	--	345.5015	354.1084	408.5985
Red. masses	--	3.2195	3.5037	3.9340
Frc consts	--	0.2264	0.2589	0.3870
IR Inten	--	7.7935	18.4816	6.2703
		7	8	9
		A	A	A
Frequencies	--	447.4889	513.6473	594.3130
Red. masses	--	2.9166	3.1278	4.0282
Frc consts	--	0.3441	0.4862	0.8383
IR Inten	--	2.8146	9.5795	28.7183
		10	11	12
		A	A	A
Frequencies	--	704.1221	785.0283	875.8357
Red. masses	--	2.6120	2.5492	2.6025
Frc consts	--	0.7630	0.9256	1.1762
IR Inten	--	27.9038	1.7645	28.2390
		13	14	15
		A	A	A
Frequencies	--	893.9234	919.1432	1001.7659
Red. masses	--	1.4836	1.8125	2.8022
Frc consts	--	0.6985	0.9022	1.6568
IR Inten	--	41.8581	34.8385	90.7313
		16	17	18
		A	A	A
Frequencies	--	1045.9081	1073.7472	1097.5521
Red. masses	--	1.6356	2.6209	3.4675
Frc consts	--	1.0542	1.7803	2.4610
IR Inten	--	23.3291	8.6173	156.5402
		19	20	21
		A	A	A
Frequencies	--	1118.5380	1133.7133	1171.5322
Red. masses	--	2.6660	2.2542	3.7070
Frc consts	--	1.9652	1.7071	2.9977
IR Inten	--	13.1365	81.3524	117.2048
		22	23	24
		A	A	A
Frequencies	--	1223.1716	1262.6604	1320.0202
Red. masses	--	1.1559	1.3187	1.3912
Frc consts	--	1.0189	1.2387	1.4283
IR Inten	--	4.0245	57.0062	20.6767
		25	26	27
		A	A	A
Frequencies	--	1336.3742	1341.2995	1364.5964
Red. masses	--	1.2431	1.2818	1.2695
Frc consts	--	1.3080	1.3587	1.3928
IR Inten	--	7.0200	33.3142	7.2800
		28	29	30
		A	A	A
Frequencies	--	1383.6046	1420.4753	1443.6339
Red. masses	--	1.3243	1.3976	1.7491
Frc consts	--	1.4937	1.6615	2.1477
IR Inten	--	6.8634	11.3868	19.8664
		31	32	33
		A	A	A
Frequencies	--	1460.2211	1497.4478	1510.9516
Red. masses	--	1.1183	1.0817	1.0983
Frc consts	--	1.4049	1.4291	1.4774

IR Inten	--	25.2677	2.7195	11.3667
		34	35	36
		A	A	A
Frequencies	--	1759.9695	3017.8159	3021.0551
Red. masses	--	9.5298	1.0693	1.0702
Frc consts	--	17.3917	5.7375	5.7549
IR Inten	--	185.4009	60.9777	70.0532
		37	38	39
		A	A	A
Frequencies	--	3067.5556	3085.2366	3131.1063
Red. masses	--	1.0623	1.0836	1.1025
Frc consts	--	5.8897	6.0772	6.3684
IR Inten	--	8.9248	30.7736	24.4242
		40	41	42
		A	A	A
Frequencies	--	3144.2190	3148.1631	3501.4604
Red. masses	--	1.0965	1.0971	1.0746
Frc consts	--	6.3869	6.4062	7.7622
IR Inten	--	34.6227	28.4378	2.9390
5a				
		1	2	3
		A	A	A
Frequencies	--	107.0120	168.0789	233.6731
Red. masses	--	3.6967	3.6044	3.9326
Frc consts	--	0.0249	0.0600	0.1265
IR Inten	--	1.5446	0.5051	10.5770
		4	5	6
		A	A	A
Frequencies	--	298.6678	383.8461	415.8988
Red. masses	--	3.1409	2.3188	2.1306
Frc consts	--	0.1651	0.2013	0.2171
IR Inten	--	3.9748	7.2049	8.4312
		7	8	9
		A	A	A
Frequencies	--	459.7700	498.5154	643.0518
Red. masses	--	5.2436	2.2547	4.1543
Frc consts	--	0.6531	0.3301	1.0121
IR Inten	--	8.5805	1.5122	4.9291
		10	11	12
		A	A	A
Frequencies	--	724.7031	761.5314	800.3644
Red. masses	--	1.9989	1.4966	2.3610
Frc consts	--	0.6185	0.5114	0.8911
IR Inten	--	51.7862	20.3961	10.1861
		13	14	15
		A	A	A
Frequencies	--	866.3554	884.9859	926.6468
Red. masses	--	2.7922	3.0486	1.9618
Frc consts	--	1.2348	1.4068	0.9925
IR Inten	--	25.0173	84.7469	35.5508
		16	17	18
		A	A	A
Frequencies	--	975.2587	1004.7511	1013.0059
Red. masses	--	1.3530	2.6199	1.7880
Frc consts	--	0.7582	1.5583	1.0810
IR Inten	--	69.5267	18.7772	4.6254
		19	20	21
		A	A	A
Frequencies	--	1034.1583	1075.6197	1102.6694
Red. masses	--	2.4385	1.8401	2.0404
Frc consts	--	1.5366	1.2543	1.4617
IR Inten	--	126.9543	13.5186	17.8635
		22	23	24
		A	A	A
Frequencies	--	1166.2236	1233.5903	1272.0451

Red. masses	--	5.1705	1.2156	1.3271
Frc consts	--	4.1433	1.0899	1.2652
IR Inten	--	148.7730	6.3671	48.1791

		25	26	27
		A	A	A
Frequencies	--	1313.7589	1327.7607	1352.5728
Red. masses	--	1.6379	1.3398	1.5352
Frc consts	--	1.6656	1.3917	1.6548
IR Inten	--	2.1213	9.1154	10.5048

		28	29	30
		A	A	A
Frequencies	--	1364.8050	1369.1793	1400.6401
Red. masses	--	1.2031	1.5575	1.4076
Frc consts	--	1.3203	1.7203	1.6270
IR Inten	--	25.8463	6.2515	2.7711

		31	32	33
		A	A	A
Frequencies	--	1426.3973	1455.5140	1471.8745
Red. masses	--	1.3801	1.1318	1.1475
Frc consts	--	1.6544	1.4127	1.4646
IR Inten	--	17.3029	11.5055	16.2684

		34	35	36
		A	A	A
Frequencies	--	1475.0941	1505.7399	1746.9086
Red. masses	--	1.0992	1.0965	6.0796
Frc consts	--	1.4091	1.4647	10.9311
IR Inten	--	17.7933	8.6856	19.3233

		37	38	39
		A	A	A
Frequencies	--	3009.8359	3014.2177	3063.9246
Red. masses	--	1.0703	1.0695	1.0630
Frc consts	--	5.7128	5.7253	5.8793
IR Inten	--	86.9126	55.7030	27.6723

		40	41	42
		A	A	A
Frequencies	--	3110.7838	3125.9346	3134.9737
Red. masses	--	1.0879	1.1006	1.0957
Frc consts	--	6.2027	6.3364	6.3446
IR Inten	--	38.8195	33.4073	49.7235

		43	44	45
		A	A	A
Frequencies	--	3137.5700	3146.9124	3236.6683
Red. masses	--	1.0956	1.0622	1.1168
Frc consts	--	6.3544	6.1977	6.8930
IR Inten	--	30.8727	9.8604	14.1555

5e

		1	2	3
		A	A	A
Frequencies	--	112.0832	171.6266	286.0770
Red. masses	--	3.6431	2.5145	3.9348
Frc consts	--	0.0270	0.0436	0.1897
IR Inten	--	0.2087	4.6937	6.2019

		4	5	6
		A	A	A
Frequencies	--	338.0123	355.2970	396.3061
Red. masses	--	2.9819	3.5806	2.9162
Frc consts	--	0.2007	0.2663	0.2699
IR Inten	--	14.1189	18.5370	2.8629

		7	8	9
		A	A	A
Frequencies	--	447.7333	484.9141	573.0979

Red. masses	--	2.7773	3.4034	3.7912
Frc consts	--	0.3280	0.4715	0.7336
IR Inten	--	0.6001	3.4823	11.0716

		10	11	12
		A	A	A
Frequencies	--	681.3230	750.2469	800.8316
Red. masses	--	2.3345	1.1517	2.2781
Frc consts	--	0.6385	0.3820	0.8608
IR Inten	--	39.8130	0.2416	0.5023

		13	14	15
		A	A	A
Frequencies	--	869.7201	894.1062	953.4400
Red. masses	--	2.1897	2.3473	1.3481
Frc consts	--	0.9759	1.1056	0.7220
IR Inten	--	12.4736	19.5551	82.3703

		16	17	18
		A	A	A
Frequencies	--	981.0173	1018.0532	1047.7886
Red. masses	--	2.2883	1.9107	1.6630
Frc consts	--	1.2975	1.1667	1.0757
IR Inten	--	61.9782	27.1610	2.5531

		19	20	21
		A	A	A
Frequencies	--	1071.9773	1097.6033	1123.1930
Red. masses	--	4.5758	2.5307	2.4401
Frc consts	--	3.0981	1.7963	1.8137
IR Inten	--	163.0206	7.6866	13.5786

		22	23	24
		A	A	A
Frequencies	--	1158.7977	1218.2073	1258.5775
Red. masses	--	5.3194	1.2955	1.3895
Frc consts	--	4.2085	1.1327	1.2968
IR Inten	--	120.7813	3.5825	43.9613

		25	26	27
		A	A	A
Frequencies	--	1286.1253	1322.6004	1334.9999
Red. masses	--	1.5192	1.3481	1.2018
Frc consts	--	1.4805	1.3894	1.2619
IR Inten	--	4.1732	8.7605	6.2964

		28	29	30
		A	A	A
Frequencies	--	1364.5190	1379.5211	1405.7865
Red. masses	--	1.3066	1.4418	1.4570
Frc consts	--	1.4334	1.6166	1.6965
IR Inten	--	3.5368	8.4359	5.6605

		31	32	33
		A	A	A
Frequencies	--	1424.1131	1447.4724	1468.7630
Red. masses	--	1.4005	1.1568	1.1358
Frc consts	--	1.6735	1.4279	1.4436
IR Inten	--	13.7569	6.4750	22.7389

		34	35	36
		A	A	A
Frequencies	--	1496.1005	1509.3304	1746.5805
Red. masses	--	1.0802	1.0987	6.3666
Frc consts	--	1.4245	1.4746	11.4429
IR Inten	--	1.4928	11.7379	37.5385

		37	38	39
		A	A	A
Frequencies	--	3013.0594	3014.6722	3055.4536
Red. masses	--	1.0699	1.0683	1.0645
Frc consts	--	5.7226	5.7203	5.8555

IR Inten	--	64.6240	78.8439	28.8708
		40	41	42
		A	A	A
Frequencies	--	3077.2834	3125.2066	3133.9569
Red. masses	--	1.0841	1.0993	1.0967
Frc consts	--	6.0485	6.3258	6.3462
IR Inten	--	45.9745	35.6795	41.1437
		43	44	45
		A	A	A
Frequencies	--	3136.0147	3160.3895	3253.7217
Red. masses	--	1.0975	1.0614	1.1165
Frc consts	--	6.3591	6.2464	6.9644
IR Inten	--	44.7123	8.1905	7.6362
6a		1	2	3
		A	A	A
Frequencies	--	72.0032	147.8959	202.9739
Red. masses	--	7.0805	4.7381	4.6261
Frc consts	--	0.0216	0.0611	0.1123
IR Inten	--	17.5717	0.6560	2.4925
		4	5	6
		A	A	A
Frequencies	--	249.2078	323.5439	385.8771
Red. masses	--	3.0080	2.6325	6.1761
Frc consts	--	0.1101	0.1624	0.5418
IR Inten	--	8.7334	3.1766	5.9381
		7	8	9
		A	A	A
Frequencies	--	415.6996	499.0087	615.0839
Red. masses	--	4.3352	2.9506	4.1273
Frc consts	--	0.4414	0.4329	0.9200
IR Inten	--	6.7529	24.4700	18.5256
		10	11	12
		A	A	A
Frequencies	--	668.3859	721.5615	729.7600
Red. masses	--	4.6742	4.9091	4.0751
Frc consts	--	1.2303	1.5059	1.2786
IR Inten	--	13.3734	2.7742	3.3563
		13	14	15
		A	A	A
Frequencies	--	775.5375	835.2100	951.4171
Red. masses	--	2.3295	1.8184	2.6496
Frc consts	--	0.8255	0.7474	1.4131
IR Inten	--	8.8132	9.7725	5.0926
		16	17	18
		A	A	A
Frequencies	--	976.6431	1001.8880	1010.1219
Red. masses	--	2.1806	2.5628	1.9784
Frc consts	--	1.2254	1.5157	1.1893
IR Inten	--	37.9459	24.9952	16.2620
		19	20	21
		A	A	A
Frequencies	--	1061.4708	1153.5456	1163.4875
Red. masses	--	3.0453	1.5673	1.1667
Frc consts	--	2.0216	1.2288	0.9306
IR Inten	--	111.6282	29.8958	1.1388
		22	23	24
		A	A	A
Frequencies	--	1237.4183	1282.3497	1294.6721
Red. masses	--	1.1646	1.5476	1.4653
Frc consts	--	1.0507	1.4995	1.4471
IR Inten	--	1.3688	9.5243	8.8565
		25	26	27
		A	A	A
Frequencies	--	1323.6721	1352.8194	1360.1949

Red. masses	--	1.3285	1.3924	1.4118
Frc consts	--	1.3715	1.5013	1.5389
IR Inten	--	18.3466	35.5941	30.3651

		28	29	30
		A	A	A
Frequencies	--	1362.6722	1449.8213	1456.0626
Red. masses	--	1.5958	1.0883	1.1065
Frc consts	--	1.7458	1.3478	1.3822
IR Inten	--	9.4631	12.5752	29.4656

		31	32	33
		A	A	A
Frequencies	--	1474.7511	1819.9459	3080.8850
Red. masses	--	1.0855	11.2249	1.0640
Frc consts	--	1.3909	21.9054	5.9503
IR Inten	--	11.7522	420.6176	17.2436

		34	35	36
		A	A	A
Frequencies	--	3083.6950	3087.2656	3127.6249
Red. masses	--	1.0598	1.0617	1.0875
Frc consts	--	5.9375	5.9622	6.2679
IR Inten	--	14.8469	16.3846	26.5957

		37	38	39
		A	A	A
Frequencies	--	3147.3983	3153.1010	3154.9382
Red. masses	--	1.1032	1.1040	1.1045
Frc consts	--	6.4388	6.4670	6.4773
IR Inten	--	11.4190	6.0289	4.1985

6e

		1	2	3
		A	A	A
Frequencies	--	84.4209	154.0399	253.2386
Red. masses	--	6.8026	2.9333	2.5959
Frc consts	--	0.0286	0.0410	0.0981
IR Inten	--	9.9764	9.6789	2.7791

		4	5	6
		A	A	A
Frequencies	--	295.0869	341.4988	345.9978
Red. masses	--	6.4477	3.7657	6.7551
Frc consts	--	0.3308	0.2587	0.4765
IR Inten	--	1.1516	12.6681	2.1358

		7	8	9
		A	A	A
Frequencies	--	367.4065	467.6097	587.4874
Red. masses	--	6.4209	2.7011	5.1140
Frc consts	--	0.5107	0.3480	1.0399
IR Inten	--	5.3539	1.4348	30.6477

		10	11	12
		A	A	A
Frequencies	--	686.9113	702.0723	762.8583
Red. masses	--	3.7807	3.5787	2.4945
Frc consts	--	1.0511	1.0393	0.8553
IR Inten	--	6.4858	7.4304	1.4550

		13	14	15
		A	A	A
Frequencies	--	789.1984	849.5363	921.3827
Red. masses	--	4.3048	1.9921	1.5605
Frc consts	--	1.5797	0.8471	0.7805
IR Inten	--	12.9439	40.3951	14.3409

		16	17	18
		A	A	A
Frequencies	--	996.7474	1041.9005	1059.3886

Red. masses	--	2.3637	2.2877	4.2232
Frc consts	--	1.3836	1.4632	2.7926
IR Inten	--	27.6302	12.9867	105.2869

		19	20	21
		A	A	A
Frequencies	--	1085.6651	1132.7350	1151.0608
Red. masses	--	2.4634	1.3266	1.8171
Frc consts	--	1.7107	1.0029	1.4185
IR Inten	--	76.9728	23.0638	17.9351

		22	23	24
		A	A	A
Frequencies	--	1220.2875	1265.8944	1287.2731
Red. masses	--	1.2898	1.3407	1.2969
Frc consts	--	1.1316	1.2659	1.2662
IR Inten	--	4.2830	4.7765	8.0481

		25	26	27
		A	A	A
Frequencies	--	1327.9089	1352.0814	1359.2273
Red. masses	--	1.2225	1.3975	1.4411
Frc consts	--	1.2701	1.5052	1.5687
IR Inten	--	21.9901	14.2571	5.4772

		28	29	30
		A	A	A
Frequencies	--	1395.6778	1454.2615	1476.3675
Red. masses	--	1.5376	1.0942	1.0970
Frc consts	--	1.7647	1.3634	1.4088
IR Inten	--	2.6286	21.2161	7.8704

		31	32	33
		A	A	A
Frequencies	--	1483.7023	1824.3227	3070.0086
Red. masses	--	1.0862	11.9285	1.0623
Frc consts	--	1.4088	23.3904	5.8989
IR Inten	--	14.0651	450.7478	7.1058

		34	35	36
		A	A	A
Frequencies	--	3079.1446	3083.1534	3089.6731
Red. masses	--	1.0635	1.0658	1.0768
Frc consts	--	5.9408	5.9690	6.0564
IR Inten	--	17.1844	12.7780	26.1974

		37	38	39
		A	A	A
Frequencies	--	3135.7522	3147.4708	3154.4583
Red. masses	--	1.1018	1.1056	1.1057
Frc consts	--	6.3830	6.4530	6.4824
IR Inten	--	15.2822	7.4769	3.6755

7a

		1	2	3
		A	A	A
Frequencies	--	67.1821	146.1682	200.7949
Red. masses	--	7.9245	5.0307	4.2255
Frc consts	--	0.0211	0.0633	0.1004
IR Inten	--	7.2911	0.4524	2.5402

		4	5	6
		A	A	A
Frequencies	--	244.1094	317.7835	344.0834
Red. masses	--	4.1919	2.7819	7.1240
Frc consts	--	0.1472	0.1655	0.4969
IR Inten	--	10.6645	4.8781	0.3880

		7	8	9
		A	A	A
Frequencies	--	383.9294	438.1561	592.3502

Red. masses	--	4.2184	2.5857	5.5834
Frc consts	--	0.3664	0.2925	1.1543
IR Inten	--	5.5674	1.3024	11.6627

		10	11	12
		A	A	A
Frequencies	--	667.6530	680.3170	710.6886
Red. masses	--	4.3041	5.1051	3.9564
Frc consts	--	1.1304	1.3921	1.1774
IR Inten	--	20.3030	7.2621	2.2804

		13	14	15
		A	A	A
Frequencies	--	764.7230	841.7730	936.9637
Red. masses	--	2.4952	1.8129	2.8526
Frc consts	--	0.8597	0.7569	1.4755
IR Inten	--	5.3715	13.8548	3.7434

		16	17	18
		A	A	A
Frequencies	--	960.2620	986.6050	1007.1334
Red. masses	--	2.1232	2.2730	2.2442
Frc consts	--	1.1535	1.3036	1.3412
IR Inten	--	19.4749	26.1248	71.7547

		19	20	21
		A	A	A
Frequencies	--	1040.6986	1132.8079	1149.9126
Red. masses	--	3.5567	1.4435	1.4385
Frc consts	--	2.2696	1.0914	1.1207
IR Inten	--	174.3686	9.6967	17.6724

		22	23	24
		A	A	A
Frequencies	--	1217.0353	1248.0017	1266.9240
Red. masses	--	1.4906	1.5936	1.5027
Frc consts	--	1.3008	1.4624	1.4211
IR Inten	--	45.6117	119.7291	8.3118

		25	26	27
		A	A	A
Frequencies	--	1298.7531	1314.9923	1336.8800
Red. masses	--	1.5058	1.2393	1.6376
Frc consts	--	1.4965	1.2626	1.7244
IR Inten	--	56.2792	20.8142	15.2663

		28	29	30
		A	A	A
Frequencies	--	1353.1027	1405.9083	1452.7980
Red. masses	--	1.2041	1.7301	1.0846
Frc consts	--	1.2989	2.0149	1.3487
IR Inten	--	12.4823	40.9194	14.5946

		31	32	33
		A	A	A
Frequencies	--	1468.5054	1474.1216	3071.3902
Red. masses	--	1.0870	1.1327	1.0635
Frc consts	--	1.3812	1.4502	5.9109
IR Inten	--	22.2545	10.9286	8.3868

		34	35	36
		A	A	A
Frequencies	--	3077.9046	3083.5570	3132.6917
Red. masses	--	1.0615	1.0623	1.0879
Frc consts	--	5.9246	5.9511	6.2904
IR Inten	--	21.3962	15.8447	16.1900

		37	38	39
		A	A	A
Frequencies	--	3144.3164	3149.4829	3153.8525
Red. masses	--	1.1014	1.1050	1.1035
Frc consts	--	6.4158	6.4581	6.4668

IR Inten	--	8.9700	7.0316	2.8685
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7e

		1	2	3
		A	A	A
Frequencies	--	69.4268	154.2965	240.5783
Red. masses	--	7.4601	3.0963	3.2035
Frc consts	--	0.0212	0.0434	0.1092
IR Inten	--	3.0363	6.3863	5.3540
		4	5	6
		A	A	A
Frequencies	--	245.6976	322.8389	343.5864
Red. masses	--	9.6311	4.5315	4.1292
Frc consts	--	0.3426	0.2783	0.2872
IR Inten	--	2.6007	0.3923	9.7071
		7	8	9
		A	A	A
Frequencies	--	370.6517	436.1545	551.3342
Red. masses	--	6.1068	2.7217	5.0470
Frc consts	--	0.4943	0.3050	0.9039
IR Inten	--	3.3353	0.8914	12.5072
		10	11	12
		A	A	A
Frequencies	--	624.7191	690.0380	732.9669
Red. masses	--	4.3734	3.9411	2.8346
Frc consts	--	1.0056	1.1056	0.8972
IR Inten	--	17.4909	7.3146	1.5993
		13	14	15
		A	A	A
Frequencies	--	790.0481	830.5534	936.2074
Red. masses	--	4.5845	1.7277	1.6164
Frc consts	--	1.6860	0.7022	0.8347
IR Inten	--	15.2924	17.6660	15.6896
		16	17	18
		A	A	A
Frequencies	--	982.8267	1002.4030	1047.6395
Red. masses	--	2.5629	2.2674	3.0128
Frc consts	--	1.4586	1.3424	1.9483
IR Inten	--	12.0281	55.3031	8.3677
		19	20	21
		A	A	A
Frequencies	--	1071.8835	1128.1114	1142.0242
Red. masses	--	4.0021	1.3238	1.6944
Frc consts	--	2.7091	0.9926	1.3020
IR Inten	--	143.1611	26.0771	2.9278
		22	23	24
		A	A	A
Frequencies	--	1188.0549	1233.4015	1272.3322
Red. masses	--	1.5181	1.5897	1.2457
Frc consts	--	1.2625	1.4248	1.1881
IR Inten	--	14.2379	62.5050	7.5260
		25	26	27
		A	A	A
Frequencies	--	1302.6027	1324.4051	1330.0364
Red. masses	--	1.5943	1.4420	1.2752
Frc consts	--	1.5939	1.4902	1.3291
IR Inten	--	120.4759	10.3046	6.0505
		28	29	30
		A	A	A
Frequencies	--	1377.7954	1380.9390	1471.0502
Red. masses	--	1.4301	1.7172	1.0840

Frc consts	--	1.5995	1.9294	1.3821
IR Inten	--	13.8161	72.1903	4.2613

		31	32	33
		A	A	A
Frequencies	--	1475.1969	1480.2130	3063.9196
Red. masses	--	1.1035	1.0974	1.0640
Frc consts	--	1.4149	1.4166	5.8848
IR Inten	--	29.3127	8.0852	6.0296

		34	35	36
		A	A	A
Frequencies	--	3082.7581	3087.6908	3091.1023
Red. masses	--	1.0727	1.0673	1.0658
Frc consts	--	6.0064	5.9951	6.0001
IR Inten	--	0.8313	28.1855	27.5192

		37	38	39
		A	A	A
Frequencies	--	3137.1255	3156.7102	3160.9736
Red. masses	--	1.1007	1.1052	1.1053
Frc consts	--	6.3826	6.4886	6.5069
IR Inten	--	11.3888	7.7559	2.9719

8a

		1	2	3
		A	A	A
Frequencies	--	82.0928	148.7560	208.2145
Red. masses	--	5.0032	4.7945	4.3575
Frc consts	--	0.0199	0.0625	0.1113
IR Inten	--	8.3910	0.2987	2.2036

		4	5	6
		A	A	A
Frequencies	--	257.7576	325.7414	386.5937
Red. masses	--	2.8583	2.6835	5.2686
Frc consts	--	0.1119	0.1678	0.4639
IR Inten	--	8.7451	3.3879	4.2417

		7	8	9
		A	A	A
Frequencies	--	413.2399	491.0041	622.8270
Red. masses	--	3.6997	2.5128	4.2485
Frc consts	--	0.3722	0.3569	0.9710
IR Inten	--	17.0552	23.4002	9.7586

		10	11	12
		A	A	A
Frequencies	--	667.8810	710.8739	722.5647
Red. masses	--	4.7140	3.3785	5.1881
Frc consts	--	1.2389	1.0059	1.5959
IR Inten	--	12.9791	13.0199	5.6335

		13	14	15
		A	A	A
Frequencies	--	780.1139	835.8122	925.7057
Red. masses	--	2.3690	1.8034	1.4651
Frc consts	--	0.8494	0.7423	0.7397
IR Inten	--	6.6941	3.6856	143.1321

		16	17	18
		A	A	A
Frequencies	--	951.5412	976.7210	1018.7672
Red. masses	--	2.8333	2.0550	2.0268
Frc consts	--	1.5115	1.1550	1.2394
IR Inten	--	16.0546	25.4205	20.6712

		19	20	21
		A	A	A
Frequencies	--	1024.5352	1056.6311	1133.2149
Red. masses	--	1.7904	2.6936	1.7687
Frc consts	--	1.1072	1.7719	1.3382
IR Inten	--	30.6482	89.1912	60.3974

		22	23	24
		A	A	A

Frequencies	--	1181.5908	1213.0800	1244.8811
Red. masses	--	1.1150	1.1549	1.1804
Frc consts	--	0.9172	1.0013	1.0778
IR Inten	--	8.0321	36.3289	2.6477

		25	26	27
		A	A	A
Frequencies	--	1297.6321	1327.0017	1346.3736
Red. masses	--	1.4889	1.3148	1.3248
Frc consts	--	1.4771	1.3641	1.4150
IR Inten	--	14.4712	17.8848	40.3878

		28	29	30
		A	A	A
Frequencies	--	1352.6727	1371.1206	1418.4122
Red. masses	--	1.2589	1.4258	1.9279
Frc consts	--	1.3572	1.5793	2.2853
IR Inten	--	7.1867	23.9493	25.5953

		31	32	33
		A	A	A
Frequencies	--	1448.9615	1460.9862	1471.0107
Red. masses	--	1.0973	1.1248	1.1034
Frc consts	--	1.3574	1.4146	1.4067
IR Inten	--	14.5421	28.3596	10.9605

		34	35	36
		A	A	A
Frequencies	--	1753.1875	3076.2230	3079.6187
Red. masses	--	9.1462	1.0636	1.0612
Frc consts	--	16.5633	5.9302	5.9295
IR Inten	--	145.2013	15.3003	26.6179

		37	38	39
		A	A	A
Frequencies	--	3084.9132	3100.8271	3138.1889
Red. masses	--	1.0631	1.0856	1.1026
Frc consts	--	5.9611	6.1503	6.3979
IR Inten	--	9.3293	46.1117	16.6740

		40	41	42
		A	A	A
Frequencies	--	3151.0573	3152.5880	3486.9986
Red. masses	--	1.1041	1.1035	1.0746
Frc consts	--	6.4590	6.4618	7.6986
IR Inten	--	11.4547	3.7227	1.2373

8e

		1	2	3
		A	A	A
Frequencies	--	99.5583	160.4967	255.1383
Red. masses	--	4.9771	3.0130	2.5404
Frc consts	--	0.0291	0.0457	0.0974
IR Inten	--	3.3143	7.1415	5.1008

		4	5	6
		A	A	A
Frequencies	--	307.7665	344.9462	351.9556
Red. masses	--	4.4705	3.8878	6.4161
Frc consts	--	0.2495	0.2726	0.4683
IR Inten	--	4.0892	15.1109	7.4047

		7	8	9
		A	A	A
Frequencies	--	368.6976	463.7197	577.6804
Red. masses	--	5.9582	2.5347	4.3238
Frc consts	--	0.4772	0.3211	0.8501
IR Inten	--	1.2627	4.5198	32.0774

		10	11	12
		A	A	A

Frequencies	--	682.9275	689.9493	772.0723
Red. masses	--	3.6366	3.3907	2.6836
Frc consts	--	0.9993	0.9510	0.9425
IR Inten	--	17.4811	2.0376	4.3102

		13	14	15
		A	A	A
Frequencies	--	787.4989	847.3159	902.3498
Red. masses	--	3.9745	1.8058	1.3951
Frc consts	--	1.4522	0.7639	0.6693
IR Inten	--	12.0177	42.6645	69.1695

		16	17	18
		A	A	A
Frequencies	--	975.4370	1005.7475	1037.0611
Red. masses	--	1.7779	1.7019	2.0829
Frc consts	--	0.9967	1.0143	1.3199
IR Inten	--	33.8478	54.4869	11.0688

		19	20	21
		A	A	A
Frequencies	--	1043.5032	1079.9376	1124.9582
Red. masses	--	3.7266	2.4036	1.9686
Frc consts	--	2.3908	1.6516	1.4678
IR Inten	--	104.2967	35.7039	16.9217

		22	23	24
		A	A	A
Frequencies	--	1169.1591	1215.6898	1239.3466
Red. masses	--	1.2469	1.2258	1.2636
Frc consts	--	1.0042	1.0674	1.1435
IR Inten	--	15.0406	2.1943	26.5115

		25	26	27
		A	A	A
Frequencies	--	1279.7355	1328.6941	1335.7896
Red. masses	--	1.2467	1.2373	1.2993
Frc consts	--	1.2029	1.2870	1.3659
IR Inten	--	2.6452	24.2124	37.7950

		28	29	30
		A	A	A
Frequencies	--	1366.9323	1369.9667	1428.4241
Red. masses	--	1.3073	1.3398	1.8573
Frc consts	--	1.4391	1.4815	2.2327
IR Inten	--	3.4882	13.8176	35.6481

		31	32	33
		A	A	A
Frequencies	--	1462.8104	1475.9881	1480.5552
Red. masses	--	1.1054	1.1238	1.0916
Frc consts	--	1.3936	1.4425	1.4098
IR Inten	--	18.4552	11.6237	14.5724

		34	35	36
		A	A	A
Frequencies	--	1755.2926	3066.2345	3077.0235
Red. masses	--	10.0189	1.0624	1.0619
Frc consts	--	18.1874	5.8849	5.9240
IR Inten	--	183.9407	14.2064	24.7299

		37	38	39
		A	A	A
Frequencies	--	3082.5968	3096.6972	3128.4784
Red. masses	--	1.0623	1.0829	1.1018
Frc consts	--	5.9475	6.1183	6.3538
IR Inten	--	15.4435	21.7150	19.1774

		40	41	42
		A	A	A
Frequencies	--	3144.6807	3154.5847	3495.3666
Red. masses	--	1.1053	1.1058	1.0731

Frc consts	--	6.4402	6.4835	7.7246
IR Inten	--	11.0556	5.8356	11.3814

9a		1	2	3
		A	A	A
Frequencies	--	81.9750	150.4343	209.3898
Red. masses	--	5.0444	4.8857	4.1477
Frc consts	--	0.0200	0.0651	0.1071
IR Inten	--	9.2707	1.1681	2.9334
		4	5	6
		A	A	A
Frequencies	--	258.6112	327.0195	388.2848
Red. masses	--	2.7861	2.6712	5.2265
Frc consts	--	0.1098	0.1683	0.4643
IR Inten	--	9.6823	3.9289	5.2902
		7	8	9
		A	A	A
Frequencies	--	412.8388	490.3554	627.6291
Red. masses	--	4.2599	2.3471	4.1707
Frc consts	--	0.4278	0.3325	0.9680
IR Inten	--	6.4030	18.2783	9.3328
		10	11	12
		A	A	A
Frequencies	--	668.2751	716.9876	722.6003
Red. masses	--	4.6965	4.0440	4.8787
Frc consts	--	1.2358	1.2249	1.5009
IR Inten	--	14.7767	7.5908	6.5237
		13	14	15
		A	A	A
Frequencies	--	775.0435	835.8119	915.9417
Red. masses	--	2.4069	1.7617	1.3691
Frc consts	--	0.8519	0.7251	0.6767
IR Inten	--	4.4023	20.5211	30.8296
		16	17	18
		A	A	A
Frequencies	--	948.7802	973.0053	1018.3501
Red. masses	--	2.8862	2.0237	2.2073
Frc consts	--	1.5308	1.1289	1.3487
IR Inten	--	5.0063	73.4725	54.3853
		19	20	21
		A	A	A
Frequencies	--	1026.9695	1056.1549	1135.0766
Red. masses	--	1.7397	2.6199	1.7258
Frc consts	--	1.0810	1.7219	1.3100
IR Inten	--	31.5105	111.1044	32.7808
		22	23	24
		A	A	A
Frequencies	--	1181.8042	1208.4776	1241.1071
Red. masses	--	1.1454	1.1530	1.1649
Frc consts	--	0.9426	0.9921	1.0572
IR Inten	--	7.0639	25.1232	1.5887
		25	26	27
		A	A	A
Frequencies	--	1301.8570	1327.5123	1340.1888
Red. masses	--	1.5007	1.3403	1.3246
Frc consts	--	1.4986	1.3917	1.4017
IR Inten	--	18.9934	16.2177	1.0315
		28	29	30
		A	A	A
Frequencies	--	1359.4912	1365.4775	1420.6621

Red. masses	--	1.2011	1.4132	2.2370
Frc consts	--	1.3080	1.5525	2.6600
IR Inten	--	25.2980	17.0821	91.5390

		31	32	33
		A	A	A
Frequencies	--	1449.0929	1464.3454	1471.8518
Red. masses	--	1.1133	1.0924	1.0976
Frc consts	--	1.3773	1.3801	1.4010
IR Inten	--	19.3214	27.8445	10.7397

		34	35	36
		A	A	A
Frequencies	--	1754.8055	3070.6776	3079.6553
Red. masses	--	9.1910	1.0600	1.0634
Frc consts	--	16.6752	5.8886	5.9421
IR Inten	--	146.7220	20.9059	23.9156

		37	38	39
		A	A	A
Frequencies	--	3085.3313	3121.8590	3125.3250
Red. masses	--	1.0624	1.0884	1.1029
Frc consts	--	5.9586	6.2499	6.3473
IR Inten	--	17.6398	27.8406	19.1997

		40	41	42
		A	A	A
Frequencies	--	3150.6259	3153.4443	3491.3040
Red. masses	--	1.1044	1.1032	1.0745
Frc consts	--	6.4589	6.4633	7.7170
IR Inten	--	10.6981	4.3400	2.1251

9e

		1	2	3
		A	A	A
Frequencies	--	99.9991	160.5538	254.4467
Red. masses	--	5.4575	3.0252	2.5401
Frc consts	--	0.0322	0.0459	0.0969
IR Inten	--	5.2833	10.4944	3.4663

		4	5	6
		A	A	A
Frequencies	--	305.6364	343.0717	348.8685
Red. masses	--	5.3541	3.5472	5.8794
Frc consts	--	0.2947	0.2460	0.4216
IR Inten	--	0.1684	5.0757	1.0979

		7	8	9
		A	A	A
Frequencies	--	368.4299	471.2688	575.0380
Red. masses	--	6.3668	2.5116	4.0629
Frc consts	--	0.5092	0.3286	0.7916
IR Inten	--	7.3867	3.6791	33.4703

		10	11	12
		A	A	A
Frequencies	--	686.3932	690.5674	779.4667
Red. masses	--	3.6065	3.4715	2.9018
Frc consts	--	1.0011	0.9754	1.0387
IR Inten	--	10.1221	1.9253	5.1907

		13	14	15
		A	A	A
Frequencies	--	789.7157	850.0531	892.6434
Red. masses	--	3.4436	1.8648	1.3716
Frc consts	--	1.2653	0.7939	0.6439
IR Inten	--	11.4052	22.3541	47.0662

		16	17	18
		A	A	A
Frequencies	--	969.1444	1006.0389	1037.3406
Red. masses	--	1.6452	1.8460	2.1470
Frc consts	--	0.9104	1.1008	1.3612
IR Inten	--	50.8065	39.9591	27.5591

19

20

21

	A	A	A
Frequencies --	1059.5967	1076.9766	1117.9074
Red. masses --	3.7390	2.7847	1.9807
Frc consts --	2.4734	1.9030	1.4584
IR Inten --	67.8463	112.5144	39.1100

	22	23	24
	A	A	A
Frequencies --	1167.7856	1208.7328	1230.6711
Red. masses --	1.2084	1.1631	1.2394
Frc consts --	0.9709	1.0012	1.1060
IR Inten --	19.5566	24.6399	2.0082

	25	26	27
	A	A	A
Frequencies --	1283.7283	1329.1801	1347.6654
Red. masses --	1.2487	1.2798	1.2789
Frc consts --	1.2124	1.3321	1.3685
IR Inten --	3.7038	16.3040	37.2167

	28	29	30
	A	A	A
Frequencies --	1366.3464	1368.7987	1434.0089
Red. masses --	1.2949	1.3894	1.8082
Frc consts --	1.4243	1.5338	2.1908
IR Inten --	17.1538	2.7065	23.3963

	31	32	33
	A	A	A
Frequencies --	1473.5120	1476.2560	1481.3880
Red. masses --	1.0962	1.1284	1.0940
Frc consts --	1.4023	1.4490	1.4145
IR Inten --	31.2298	5.9091	11.2782

	34	35	36
	A	A	A
Frequencies --	1757.1454	3062.2992	3076.8161
Red. masses --	9.4572	1.0604	1.0633
Frc consts --	17.2040	5.8587	5.9307
IR Inten --	176.3734	18.4131	17.3678

	37	38	39
	A	A	A
Frequencies --	3080.2113	3087.4974	3116.1807
Red. masses --	1.0694	1.0752	1.1036
Frc consts --	5.9779	6.0388	6.3139
IR Inten --	11.3325	34.7352	25.8127

	40	41	42
	A	A	A
Frequencies --	3144.7189	3155.2402	3501.2872
Red. masses --	1.1053	1.1051	1.0746
Frc consts --	6.4404	6.4819	7.7616
IR Inten --	10.5943	6.1092	2.5906

10a

	1	2	3
	A	A	A
Frequencies --	95.8492	150.4319	207.7320
Red. masses --	3.8202	4.9454	3.8833
Frc consts --	0.0207	0.0659	0.0987
IR Inten --	1.5895	0.7383	6.4076

	4	5	6
	A	A	A
Frequencies --	260.5130	326.8823	383.6966
Red. masses --	2.5319	2.7298	3.7918
Frc consts --	0.1012	0.1719	0.3289
IR Inten --	4.7947	4.8153	3.5686

7

8

9

	A	A	A
Frequencies --	387.8086	466.3763	621.7961
Red. masses --	3.1535	2.2716	4.2356
Frc consts --	0.2794	0.2911	0.9649
IR Inten --	1.6594	5.9082	3.0987

	10	11	12
	A	A	A
Frequencies --	664.4488	688.1356	718.7438
Red. masses --	4.5628	2.9342	4.7427
Frc consts --	1.1869	0.8186	1.4435
IR Inten --	19.9930	18.0614	8.3735

	13	14	15
	A	A	A
Frequencies --	748.7091	786.3570	840.1792
Red. masses --	1.2801	2.0184	1.9696
Frc consts --	0.4228	0.7354	0.8192
IR Inten --	2.9159	1.7335	25.3079

	16	17	18
	A	A	A
Frequencies --	929.7126	952.6847	971.4176
Red. masses --	2.3221	2.0473	1.3604
Frc consts --	1.1826	1.0948	0.7564
IR Inten --	13.4206	20.6356	79.8020

	19	20	21
	A	A	A
Frequencies --	990.4705	1015.3751	1035.5571
Red. masses --	1.9848	2.2136	2.0617
Frc consts --	1.1472	1.3446	1.3026
IR Inten --	102.0719	60.6939	13.1873

	22	23	24
	A	A	A
Frequencies --	1058.6235	1182.3271	1196.1615
Red. masses --	2.0119	1.1321	1.2729
Frc consts --	1.3285	0.9324	1.0731
IR Inten --	31.6390	11.7781	5.6255

	25	26	27
	A	A	A
Frequencies --	1244.0179	1300.4221	1324.7804
Red. masses --	1.1710	1.4967	1.4514
Frc consts --	1.0677	1.4912	1.5008
IR Inten --	4.4251	19.3541	17.2410

	28	29	30
	A	A	A
Frequencies --	1331.9121	1353.9394	1359.2308
Red. masses --	1.4445	1.2069	1.3122
Frc consts --	1.5098	1.3035	1.4284
IR Inten --	6.4743	26.1727	13.1664

	31	32	33
	A	A	A
Frequencies --	1377.5075	1447.1910	1456.9770
Red. masses --	2.1342	1.0949	1.1351
Frc consts --	2.3861	1.3511	1.4197
IR Inten --	9.5954	14.1226	16.6057

	34	35	36
	A	A	A
Frequencies --	1465.5109	1476.4601	1741.1728
Red. masses --	1.0968	1.1372	5.9106
Frc consts --	1.3879	1.4606	10.5576
IR Inten --	15.3294	21.8364	16.9681

	37	38	39	
	A	A	A	
Frequencies --	3062.0448	3075.0340	3083.1218	

Red. masses	--	1.0614	1.0631	1.0631
Frc consts	--	5.8634	5.9225	5.9538
IR Inten	--	31.6858	29.1833	10.3520

		40	41	42
		A	A	A
Frequencies	--	3101.8820	3115.2891	3145.8674
Red. masses	--	1.0857	1.1021	1.1040
Frc consts	--	6.1550	6.3018	6.4375
IR Inten	--	50.0370	32.5810	17.8384

		43	44	45
		A	A	A
Frequencies	--	3150.2243	3150.8103	3239.2358
Red. masses	--	1.0693	1.0962	1.1167
Frc consts	--	6.2523	6.4117	6.9036
IR Inten	--	14.2503	4.2529	13.6740

10e

		1	2	3
		A	A	A
Frequencies	--	102.5678	167.9450	254.3239
Red. masses	--	3.9183	3.0593	2.4826
Frc consts	--	0.0243	0.0508	0.0946
IR Inten	--	0.0943	5.9569	9.5767

		4	5	6
		A	A	A
Frequencies	--	301.8444	339.7697	348.1284
Red. masses	--	3.7082	4.3349	4.0628
Frc consts	--	0.1991	0.2949	0.2901
IR Inten	--	2.2839	1.5579	5.6210

		7	8	9
		A	A	A
Frequencies	--	370.5412	447.6036	541.6603
Red. masses	--	5.6685	2.1983	3.6688
Frc consts	--	0.4586	0.2595	0.6342
IR Inten	--	2.7148	2.1947	13.8490

		10	11	12
		A	A	A
Frequencies	--	655.8224	683.2703	749.8270
Red. masses	--	2.8767	3.9413	1.1726
Frc consts	--	0.7290	1.0841	0.3884
IR Inten	--	22.5448	5.3075	0.8297

		13	14	15
		A	A	A
Frequencies	--	784.5890	792.0827	842.8425
Red. masses	--	3.9373	2.1487	1.8556
Frc consts	--	1.4280	0.7943	0.7767
IR Inten	--	16.2783	1.5782	18.5341

		16	17	18
		A	A	A
Frequencies	--	945.3434	958.5266	967.2173
Red. masses	--	1.7051	1.3516	1.6988
Frc consts	--	0.8978	0.7316	0.9364
IR Inten	--	32.2754	83.0930	7.6671

		19	20	21
		A	A	A
Frequencies	--	1015.8798	1040.8947	1042.2095
Red. masses	--	2.2281	2.2584	3.4041
Frc consts	--	1.3548	1.4417	2.1785
IR Inten	--	57.7042	23.7715	97.5798

		22	23	24
		A	A	A
Frequencies	--	1088.7387	1169.0434	1194.2190
Red. masses	--	2.4014	1.1564	1.4177
Frc consts	--	1.6771	0.9312	1.1913
IR Inten	--	15.7031	9.3621	1.4207

25

26

27

	A	A	A
Frequencies --	1222.5159	1278.9410	1295.8927
Red. masses --	1.2696	1.2704	1.5258
Frc consts --	1.1180	1.2243	1.5096
IR Inten --	10.0524	2.8458	2.9572

	28	29	30
	A	A	A
Frequencies --	1329.6536	1366.8452	1371.3029
Red. masses --	1.2413	1.3862	1.3170
Frc consts --	1.2930	1.5258	1.4592
IR Inten --	22.4101	1.4221	4.4666

	31	32	33
	A	A	A
Frequencies --	1401.4940	1444.3965	1471.7741
Red. masses --	1.6472	1.1682	1.0985
Frc consts --	1.9062	1.4359	1.4020
IR Inten --	9.6917	11.7790	1.6400

	34	35	36
	A	A	A
Frequencies --	1475.8437	1480.7135	1741.3856
Red. masses --	1.0974	1.1039	6.2682
Frc consts --	1.4084	1.4261	11.1990
IR Inten --	30.1073	9.5401	31.6922

	37	38	39
	A	A	A
Frequencies --	3052.5463	3073.1080	3076.0689
Red. masses --	1.0619	1.0622	1.0780
Frc consts --	5.8300	5.9101	6.0098
IR Inten --	31.5118	21.2083	18.8761

	40	41	42
	A	A	A
Frequencies --	3083.6684	3107.7014	3138.9803
Red. masses --	1.0667	1.1014	1.1057
Frc consts --	5.9761	6.2672	6.4192
IR Inten --	42.4969	38.1096	17.0460

	43	44	45
	A	A	A
Frequencies --	3153.4156	3161.9704	3254.6276
Red. masses --	1.1055	1.0617	1.1163
Frc consts --	6.4772	6.2539	6.9668
IR Inten --	10.7631	8.8531	6.8049

11a

	1	2	3
	A	A	A
Frequencies --	91.3670	157.4635	236.5761
Red. masses --	6.0921	3.4414	4.3785
Frc consts --	0.0300	0.0503	0.1444
IR Inten --	13.0050	2.6359	11.3794

	4	5	6
	A	A	A
Frequencies --	291.6676	389.4762	445.7576
Red. masses --	2.9656	1.9621	5.0535
Frc consts --	0.1486	0.1754	0.5916
IR Inten --	8.5042	5.1074	2.0092

	7	8	9
	A	A	A
Frequencies --	486.9410	508.8812	645.5312
Red. masses --	4.8340	2.2908	3.7680
Frc consts --	0.6753	0.3495	0.9251
IR Inten --	26.7564	7.9959	21.8963

10

11

12

	A	A	A
Frequencies --	735.8126	774.4019	818.2192
Red. masses --	2.4265	2.2035	2.1782
Frc consts --	0.7740	0.7786	0.8592
IR Inten --	23.4167	39.3397	206.9821

	13	14	15
	A	A	A
Frequencies --	858.0504	904.1149	927.2674
Red. masses --	2.3769	2.0082	2.2154
Frc consts --	1.0311	0.9672	1.1223
IR Inten --	27.1845	22.9705	48.8101

	16	17	18
	A	A	A
Frequencies --	1014.2019	1016.3521	1031.7175
Red. masses --	3.1637	2.0802	2.6122
Frc consts --	1.9173	1.2660	1.6382
IR Inten --	71.4622	17.1815	53.1056

	19	20	21
	A	A	A
Frequencies --	1111.5104	1164.4047	1201.1212
Red. masses --	2.0740	2.9775	1.1894
Frc consts --	1.5097	2.3786	1.0110
IR Inten --	28.8723	16.7433	1.4768

	22	23	24
	A	A	A
Frequencies --	1232.4187	1274.3941	1309.0783
Red. masses --	2.0369	1.5100	1.6660
Frc consts --	1.8228	1.4449	1.6821
IR Inten --	61.9138	5.7221	10.4745

	25	26	27
	A	A	A
Frequencies --	1324.7025	1353.7550	1372.3118
Red. masses --	1.4031	1.2722	1.1995
Frc consts --	1.4506	1.3737	1.3309
IR Inten --	25.3912	12.0815	15.2477

	28	29	30
	A	A	A
Frequencies --	1393.3738	1411.9080	1459.1760
Red. masses --	1.5380	1.3852	1.1182
Frc consts --	1.7593	1.6270	1.4028
IR Inten --	13.4582	24.5431	21.2557

	31	32	33
	A	A	A
Frequencies --	1467.0057	1505.9682	1516.7352
Red. masses --	1.0903	1.0972	1.2107
Frc consts --	1.3825	1.4661	1.6410
IR Inten --	17.1744	10.1608	24.5331

	34	35	36
	A	A	A
Frequencies --	1810.5120	3053.9383	3059.2857
Red. masses --	11.0818	1.0672	1.0651
Frc consts --	21.4025	5.8643	5.8735
IR Inten --	460.4108	49.9217	32.6153

	37	38	39
	A	A	A
Frequencies --	3076.9456	3127.6283	3128.0774
Red. masses --	1.0616	1.1008	1.0998
Frc consts --	5.9218	6.3442	6.3405
IR Inten --	8.2745	20.7478	36.0250

	40	41	42
	A	A	A
Frequencies --	3135.0089	3150.1578	3577.9091

Red. masses	--	1.0891	1.1037	1.0746
Frc consts	--	6.3066	6.4531	8.1052
IR Inten	--	28.5825	20.3972	8.6070

11e		1	2	3
		A	A	A
Frequencies	--	96.2131	153.0606	282.2793
Red. masses	--	5.4914	2.4800	7.9461
Frc consts	--	0.0300	0.0342	0.3730
IR Inten	--	4.9405	6.8111	1.5553
		4	5	6
		A	A	A
Frequencies	--	330.4580	351.0852	403.6034
Red. masses	--	2.0725	3.5317	5.3415
Frc consts	--	0.1333	0.2565	0.5127
IR Inten	--	14.9828	12.3705	2.9562
		7	8	9
		A	A	A
Frequencies	--	440.5634	527.0952	608.8856
Red. masses	--	3.0999	2.8347	4.3543
Frc consts	--	0.3545	0.4640	0.9511
IR Inten	--	0.8628	11.1788	27.2886
		10	11	12
		A	A	A
Frequencies	--	710.6410	761.2949	797.1168
Red. masses	--	2.3349	2.1014	1.8573
Frc consts	--	0.6947	0.7176	0.6953
IR Inten	--	1.8057	28.0311	267.7971
		13	14	15
		A	A	A
Frequencies	--	879.7068	912.4964	963.9217
Red. masses	--	2.2914	2.3059	1.4878
Frc consts	--	1.0448	1.1312	0.8145
IR Inten	--	44.3929	25.7244	2.8252
		16	17	18
		A	A	A
Frequencies	--	1005.6143	1055.6619	1088.3914
Red. masses	--	2.6036	3.2355	4.0158
Frc consts	--	1.5513	2.1244	2.8028
IR Inten	--	30.4338	9.6764	179.0933
		19	20	21
		A	A	A
Frequencies	--	1123.4600	1156.2524	1175.0714
Red. masses	--	2.1026	1.9717	1.8905
Frc consts	--	1.5636	1.5531	1.5380
IR Inten	--	14.5654	4.8893	7.4575
		22	23	24
		A	A	A
Frequencies	--	1222.2044	1265.5167	1313.3034
Red. masses	--	2.2686	1.3585	1.5281
Frc consts	--	1.9966	1.2819	1.5529
IR Inten	--	52.7126	3.1192	12.3042
		25	26	27
		A	A	A
Frequencies	--	1334.9687	1349.0567	1370.4143
Red. masses	--	1.2036	1.3127	1.1753
Frc consts	--	1.2638	1.4076	1.3005
IR Inten	--	16.9264	5.0705	5.9157
		28	29	30
		A	A	A

Frequencies --	1395.0300	1419.5409	1458.9507
Red. masses --	1.4092	1.5737	1.1115
Frc consts --	1.6158	1.8684	1.3939
IR Inten --	25.1097	0.9683	24.8710
	31	32	33
	A	A	A
Frequencies --	1489.1057	1499.3576	1512.0546
Red. masses --	1.0790	1.0981	1.2267
Frc consts --	1.4097	1.4544	1.6525
IR Inten --	6.3316	10.2060	23.2094
	34	35	36
	A	A	A
Frequencies --	1813.5947	3058.3533	3060.0742
Red. masses --	11.7402	1.0672	1.0668
Frc consts --	22.7513	5.8813	5.8855
IR Inten --	487.2899	30.3104	38.0620
	37	38	39
	A	A	A
Frequencies --	3064.9446	3080.5291	3131.2636
Red. masses --	1.0631	1.0819	1.0999
Frc consts --	5.8841	6.0490	6.3540
IR Inten --	16.6579	34.9739	32.6813
	40	41	42
	A	A	A
Frequencies --	3137.2026	3141.3944	3570.3352
Red. masses --	1.1020	1.1022	1.0750
Frc consts --	6.3902	6.4083	8.0741
IR Inten --	27.2159	22.4810	6.4005
12a	1	2	3
	A	A	A
Frequencies --	87.9829	153.4391	248.9821
Red. masses --	6.1790	3.5748	4.1319
Frc consts --	0.0282	0.0496	0.1509
IR Inten --	4.7637	2.3821	12.3486
	4	5	6
	A	A	A
Frequencies --	264.6963	352.8336	402.9509
Red. masses --	4.0356	3.0519	2.3089
Frc consts --	0.1666	0.2239	0.2209
IR Inten --	6.0440	1.7440	5.4200
	7	8	9
	A	A	A
Frequencies --	423.6778	506.6199	625.6742
Red. masses --	4.9020	2.5162	5.0851
Frc consts --	0.5184	0.3805	1.1729
IR Inten --	4.7939	2.4658	7.2762
	10	11	12
	A	A	A
Frequencies --	701.1737	755.0026	802.3211
Red. masses --	3.0513	1.8533	2.0469
Frc consts --	0.8839	0.6224	0.7763
IR Inten --	10.0492	94.2604	297.1072
	13	14	15
	A	A	A
Frequencies --	854.5481	884.9707	907.7443
Red. masses --	2.4793	2.3479	2.2821
Frc consts --	1.0667	1.0834	1.1079
IR Inten --	18.1990	23.2120	68.4896
	16	17	18
	A	A	A
Frequencies --	999.2408	1007.3091	1021.5986
Red. masses --	2.1755	4.1905	2.2055
Frc consts --	1.2798	2.5052	1.3562
IR Inten --	44.4054	156.2171	64.2635

	19	20	21
	A	A	A
Frequencies --	1072.6065	1151.7606	1179.3358
Red. masses --	1.7688	2.7280	1.5122
Frc consts --	1.1990	2.1322	1.2392
IR Inten --	78.9666	43.0811	1.0258

	22	23	24
	A	A	A
Frequencies --	1220.4235	1242.3472	1264.9638
Red. masses --	1.9652	2.1642	1.4455
Frc consts --	1.7245	1.9681	1.3627
IR Inten --	20.4864	65.0811	33.7604

	25	26	27
	A	A	A
Frequencies --	1303.6855	1312.9569	1350.9988
Red. masses --	1.5709	1.3802	1.2467
Frc consts --	1.5731	1.4018	1.3407
IR Inten --	192.9818	27.3208	5.7718

	28	29	30
	A	A	A
Frequencies --	1372.7189	1376.7135	1421.5178
Red. masses --	1.3845	1.3276	1.6029
Frc consts --	1.5371	1.4825	1.9083
IR Inten --	13.9386	47.9126	10.4009

	31	32	33
	A	A	A
Frequencies --	1471.0073	1480.1328	1493.8287
Red. masses --	1.0869	1.1610	1.0994
Frc consts --	1.3857	1.4986	1.4454
IR Inten --	8.6448	22.9509	10.7520

	34	35	36
	A	A	A
Frequencies --	1516.6311	3060.4953	3066.1656
Red. masses --	1.2108	1.0665	1.0639
Frc consts --	1.6409	5.8857	5.8932
IR Inten --	20.4264	46.0185	30.8764

	37	38	39
	A	A	A
Frequencies --	3072.0484	3133.1088	3137.2819
Red. masses --	1.0622	1.1021	1.1004
Frc consts --	5.9064	6.3740	6.3814
IR Inten --	13.6469	17.8993	40.6446

	40	41	42
	A	A	A
Frequencies --	3140.9040	3151.2630	3579.7024
Red. masses --	1.0896	1.1028	1.0748
Frc consts --	6.3334	6.4526	8.1149
IR Inten --	17.7675	13.4863	13.1976

12e

	1	2	3
	A	A	A
Frequencies --	81.4479	157.4116	238.1948
Red. masses --	5.3995	2.6076	14.4019
Frc consts --	0.0211	0.0381	0.4814
IR Inten --	1.9092	3.0071	1.8008

	4	5	6
	A	A	A
Frequencies --	316.3326	356.5163	377.9297
Red. masses --	2.4618	3.7947	3.0351
Frc consts --	0.1451	0.2842	0.2554
IR Inten --	11.3907	8.8599	3.1705

	7	8	9
	A	A	A
Frequencies --	437.6584	496.9242	577.3330
Red. masses --	3.3859	3.8668	4.2349
Frc consts --	0.3821	0.5626	0.8317
IR Inten --	1.0143	13.8905	13.5513
	10	11	12
	A	A	A
Frequencies --	659.5289	734.7551	794.4229
Red. masses --	2.6513	2.7545	1.7071
Frc consts --	0.6795	0.8762	0.6348
IR Inten --	18.3402	24.8464	351.0151
	13	14	15
	A	A	A
Frequencies --	847.3889	900.9934	978.8476
Red. masses --	1.7826	2.4484	1.5530
Frc consts --	0.7542	1.1710	0.8767
IR Inten --	33.3904	17.3593	1.5480
	16	17	18
	A	A	A
Frequencies --	990.7416	1021.8209	1083.1862
Red. masses --	2.8383	3.2757	2.0303
Frc consts --	1.6415	2.0152	1.4035
IR Inten --	84.3997	11.9979	44.1911
	19	20	21
	A	A	A
Frequencies --	1089.9377	1144.4425	1165.8709
Red. masses --	3.8735	1.9348	1.6431
Frc consts --	2.7112	1.4931	1.3159
IR Inten --	165.2783	23.8982	12.9740
	22	23	24
	A	A	A
Frequencies --	1208.0933	1230.0973	1288.6339
Red. masses --	2.4238	2.1402	1.4609
Frc consts --	2.0842	1.9080	1.4294
IR Inten --	33.1437	44.8733	2.1330
	25	26	27
	A	A	A
Frequencies --	1312.9577	1321.9360	1344.2895
Red. masses --	1.3231	1.8226	1.2631
Frc consts --	1.3438	1.8766	1.3449
IR Inten --	92.3646	204.0808	28.5741
	28	29	30
	A	A	A
Frequencies --	1357.6514	1395.4850	1413.9587
Red. masses --	1.1616	1.4648	1.5471
Frc consts --	1.2615	1.6807	1.8224
IR Inten --	8.2246	9.9375	10.1260
	31	32	33
	A	A	A
Frequencies --	1480.2942	1490.1142	1501.3957
Red. masses --	1.1287	1.0827	1.1046
Frc consts --	1.4573	1.4164	1.4670
IR Inten --	24.0867	4.9137	12.7411
	34	35	36
	A	A	A
Frequencies --	1519.2781	3055.4219	3057.9135
Red. masses --	1.2141	1.0670	1.0658
Frc consts --	1.6512	5.8688	5.8721
IR Inten --	18.1115	14.1348	25.0412
	37	38	39
	A	A	A

Frequencies --	3063.6455	3079.1710	3138.1514
Red. masses --	1.0651	1.0821	1.1014
Frc consts --	5.8901	6.0446	6.3906
IR Inten --	48.4694	37.1910	30.7773

	40	41	42
	A	A	A
Frequencies --	3139.1226	3142.7371	3575.9565
Red. masses --	1.0997	1.1018	1.0752
Frc consts --	6.3846	6.4119	8.1008
IR Inten --	28.7855	15.6683	9.7597

13a

	1	2	3
	A	A	A
Frequencies --	104.4161	153.7493	238.9112
Red. masses --	4.5144	3.3003	4.5098
Frc consts --	0.0290	0.0460	0.1517
IR Inten --	6.1583	3.1141	10.7260

	4	5	6
	A	A	A
Frequencies --	291.2268	389.9025	440.3723
Red. masses --	2.6750	1.9408	3.7129
Frc consts --	0.1337	0.1738	0.4242
IR Inten --	14.0155	3.3446	14.3090

	7	8	9
	A	A	A
Frequencies --	479.0635	503.9598	647.5880
Red. masses --	4.8005	2.0925	4.1881
Frc consts --	0.6491	0.3131	1.0348
IR Inten --	19.0669	8.2624	8.2881

	10	11	12
	A	A	A
Frequencies --	718.0195	780.8806	812.0856
Red. masses --	2.1551	2.3348	2.0112
Frc consts --	0.6546	0.8388	0.7815
IR Inten --	31.9378	56.7663	193.4045

	13	14	15
	A	A	A
Frequencies --	858.1479	898.3454	929.7332
Red. masses --	2.4156	1.7979	2.0319
Frc consts --	1.0481	0.8549	1.0348
IR Inten --	22.0674	41.8167	97.1135

	16	17	18
	A	A	A
Frequencies --	948.8757	1015.5734	1029.1697
Red. masses --	1.6863	2.9016	1.7732
Frc consts --	0.8945	1.7632	1.1066
IR Inten --	80.0208	3.5523	14.7118

	19	20	21
	A	A	A
Frequencies --	1037.9265	1113.1529	1151.0022
Red. masses --	2.6005	1.9688	1.6456
Frc consts --	1.6506	1.4374	1.2845
IR Inten --	71.6202	13.7972	99.6612

	22	23	24
	A	A	A
Frequencies --	1183.8181	1213.0016	1253.2303
Red. masses --	3.0921	1.1484	1.3181
Frc consts --	2.5531	0.9956	1.2197
IR Inten --	37.7872	6.2684	16.8627

	25	26	27
	A	A	A
Frequencies --	1319.7216	1330.7141	1354.9894
Red. masses --	1.5971	1.4641	1.2062
Frc consts --	1.6389	1.5275	1.3048
IR Inten --	10.0415	14.5611	13.8887

	28	29	30
	A	A	A
Frequencies --	1363.5585	1380.2468	1411.3064
Red. masses --	1.2722	1.2231	1.3869
Frc consts --	1.3937	1.3728	1.6275
IR Inten --	4.3563	11.8981	33.8152

	31	32	33
	A	A	A
Frequencies --	1425.3363	1461.0971	1465.6488
Red. masses --	1.8980	1.1411	1.1082
Frc consts --	2.2718	1.4352	1.4026
IR Inten --	14.7365	13.1384	25.4940

	34	35	36
	A	A	A
Frequencies --	1499.9838	1513.0015	1750.1633
Red. masses --	1.0958	1.2157	9.1318
Frc consts --	1.4526	1.6397	16.4803
IR Inten --	8.4472	24.9517	170.1800

	37	38	39
	A	A	A
Frequencies --	3047.0295	3057.5454	3066.7762
Red. masses --	1.0678	1.0650	1.0630
Frc consts --	5.8413	5.8660	5.8904
IR Inten --	51.5375	33.3784	18.5491

	40	41	42
	A	A	A
Frequencies --	3105.7795	3123.1944	3125.5419
Red. masses --	1.0882	1.0987	1.1008
Frc consts --	6.1845	6.3145	6.3362
IR Inten --	48.0483	44.6283	26.0283

	43	44	45
	A	A	A
Frequencies --	3137.7210	3485.7691	3571.8290
Red. masses --	1.1019	1.0744	1.0745
Frc consts --	6.3918	7.6915	8.0769
IR Inten --	25.7080	1.2467	6.3460

13e

	1	2	3
	A	A	A
Frequencies --	110.3511	158.5560	305.9338
Red. masses --	4.2906	2.4571	4.3251
Frc consts --	0.0308	0.0364	0.2385
IR Inten --	1.1930	3.2203	2.5528

	4	5	6
	A	A	A
Frequencies --	332.5609	354.3144	404.1016
Red. masses --	2.1601	3.7874	4.9503
Frc consts --	0.1408	0.2801	0.4763
IR Inten --	25.5371	16.3137	0.3428

	7	8	9
	A	A	A
Frequencies --	441.5718	519.0023	598.5448
Red. masses --	2.9470	2.7946	3.9703
Frc consts --	0.3386	0.4435	0.8380
IR Inten --	3.8823	5.1431	35.1572

	10	11	12
	A	A	A
Frequencies --	695.4821	774.3160	800.6197
Red. masses --	2.1589	2.2805	1.8189
Frc consts --	0.6152	0.8056	0.6869
IR Inten --	5.5426	22.4063	254.6875

13

14

15

	A	A	A
Frequencies --	877.2362	897.1274	920.4935
Red. masses --	1.8388	1.8486	1.5000
Frc consts --	0.8337	0.8766	0.7488
IR Inten --	48.5336	68.4030	21.0661

	16	17	18
	A	A	A
Frequencies --	1004.2305	1018.3916	1054.8711
Red. masses --	2.5776	1.5270	3.0411
Frc consts --	1.5315	0.9331	1.9938
IR Inten --	27.2929	13.7270	76.9608

	19	20	21
	A	A	A
Frequencies --	1074.3650	1116.6754	1145.0972
Red. masses --	3.2287	2.0783	2.2316
Frc consts --	2.1958	1.5269	1.7241
IR Inten --	97.5389	7.8314	25.7758

	22	23	24
	A	A	A
Frequencies --	1191.7363	1196.2302	1252.9152
Red. masses --	2.9369	1.2910	1.3066
Frc consts --	2.4575	1.0885	1.2085
IR Inten --	24.7867	8.2281	13.2069

	25	26	27
	A	A	A
Frequencies --	1322.3492	1331.5403	1339.7239
Red. masses --	1.4258	1.2996	1.2184
Frc consts --	1.4690	1.3576	1.2884
IR Inten --	1.0533	35.8202	4.3980

	28	29	30
	A	A	A
Frequencies --	1367.7190	1373.6482	1401.7481
Red. masses --	1.2736	1.1933	1.3899
Frc consts --	1.4037	1.3266	1.6090
IR Inten --	4.2607	3.4056	46.0336

	31	32	33
	A	A	A
Frequencies --	1438.5289	1465.6246	1487.4107
Red. masses --	1.7809	1.1472	1.0870
Frc consts --	2.1713	1.4519	1.4169
IR Inten --	22.2356	24.4809	6.3026

	34	35	36
	A	A	A
Frequencies --	1497.0714	1509.7048	1749.7943
Red. masses --	1.0988	1.2224	9.9328
Frc consts --	1.4510	1.6416	17.9182
IR Inten --	10.0398	22.6815	212.3200

	37	38	39
	A	A	A
Frequencies --	3051.8423	3057.8637	3058.5942
Red. masses --	1.0675	1.0659	1.0636
Frc consts --	5.8580	5.8724	5.8624
IR Inten --	33.6614	49.6496	21.0818

	40	41	42
	A	A	A
Frequencies --	3084.2855	3124.3360	3134.4308
Red. masses --	1.0836	1.0996	1.1011
Frc consts --	6.0732	6.3244	6.3736
IR Inten --	35.5112	41.3841	48.3204

	43	44	45	
	A	A	A	
Frequencies --	3134.9897	3494.4898	3566.4295	

Red. masses	--	1.1015	1.0732	1.0748
Frc consts	--	6.3781	7.7211	8.0549
IR Inten	--	15.1940	8.1658	4.5801

14a

		1	2	3
		A	A	A
Frequencies	--	104.7498	162.0635	240.7467
Red. masses	--	4.6431	3.4521	3.8858
Frc consts	--	0.0300	0.0534	0.1327
IR Inten	--	6.9315	4.3349	12.7264
		4	5	6
		A	A	A
Frequencies	--	292.8771	392.9824	439.8581
Red. masses	--	2.7502	1.9513	4.3650
Frc consts	--	0.1390	0.1775	0.4976
IR Inten	--	6.2995	6.9845	7.7942
		7	8	9
		A	A	A
Frequencies	--	475.2036	507.1378	650.7198
Red. masses	--	4.0502	2.1171	4.0736
Frc consts	--	0.5389	0.3208	1.0163
IR Inten	--	15.2689	8.8868	12.7954
		10	11	12
		A	A	A
Frequencies	--	724.6372	778.3909	818.0090
Red. masses	--	2.3389	2.3893	2.0477
Frc consts	--	0.7236	0.8529	0.8073
IR Inten	--	23.3903	21.4021	211.5886
		13	14	15
		A	A	A
Frequencies	--	859.0899	892.0673	930.6291
Red. masses	--	2.3951	1.6571	2.0447
Frc consts	--	1.0415	0.7770	1.0433
IR Inten	--	48.6878	34.2984	30.6467
		16	17	18
		A	A	A
Frequencies	--	942.9107	1015.6221	1032.8802
Red. masses	--	1.6376	2.8523	1.8227
Frc consts	--	0.8578	1.7335	1.1457
IR Inten	--	44.6079	21.1007	30.6784
		19	20	21
		A	A	A
Frequencies	--	1035.4029	1111.5987	1150.0534
Red. masses	--	2.4598	2.0515	1.4917
Frc consts	--	1.5537	1.4936	1.1624
IR Inten	--	146.9464	33.9043	12.1202
		22	23	24
		A	A	A
Frequencies	--	1182.4487	1210.8781	1251.9395
Red. masses	--	3.1757	1.1637	1.3445
Frc consts	--	2.6161	1.0053	1.2416
IR Inten	--	53.1234	3.4386	26.1985
		25	26	27
		A	A	A
Frequencies	--	1317.8064	1329.0361	1346.5977
Red. masses	--	1.6063	1.4372	1.2648
Frc consts	--	1.6435	1.4957	1.3512
IR Inten	--	3.7427	3.5443	9.3709
		28	29	30
		A	A	A

Frequencies --	1366.7817	1374.1519	1409.7668
Red. masses --	1.2905	1.1881	1.3783
Frc consts --	1.4204	1.3218	1.6140
IR Inten --	20.3875	11.7247	16.4337
	31	32	33
	A	A	A
Frequencies --	1429.8361	1464.3637	1467.0384
Red. masses --	2.2035	1.0917	1.0998
Frc consts --	2.6543	1.3793	1.3946
IR Inten --	78.5816	7.4513	28.3971
	34	35	36
	A	A	A
Frequencies --	1499.9793	1511.8559	1751.5664
Red. masses --	1.0948	1.2170	9.1720
Frc consts --	1.4513	1.6390	16.5794
IR Inten --	8.1637	24.7955	171.0476
	37	38	39
	A	A	A
Frequencies --	3048.8486	3056.9153	3064.6197
Red. masses --	1.0675	1.0649	1.0607
Frc consts --	5.8462	5.8633	5.8696
IR Inten --	52.9572	36.6884	16.8842
	40	41	42
	A	A	A
Frequencies --	3121.2085	3123.8853	3126.7252
Red. masses --	1.0990	1.1008	1.1044
Frc consts --	6.3079	6.3294	6.3616
IR Inten --	48.0765	21.5976	34.6504
	43	44	45
	A	A	A
Frequencies --	3132.8065	3488.8443	3573.4694
Red. masses --	1.0888	1.0743	1.0744
Frc consts --	6.2958	7.7041	8.0836
IR Inten --	32.4303	1.9984	6.1435
14e	1	2	3
	A	A	A
Frequencies --	99.5871	158.8273	295.7095
Red. masses --	4.5734	2.4853	5.8429
Frc consts --	0.0267	0.0369	0.3010
IR Inten --	2.3389	7.6079	0.5962
	4	5	6
	A	A	A
Frequencies --	329.7248	352.0252	403.6376
Red. masses --	2.0638	3.3938	4.5865
Frc consts --	0.1322	0.2478	0.4403
IR Inten --	11.0579	2.8605	9.9688
	7	8	9
	A	A	A
Frequencies --	441.8712	521.0796	595.0039
Red. masses --	3.0058	2.7699	3.7407
Frc consts --	0.3458	0.4431	0.7803
IR Inten --	1.4644	22.7331	20.5831
	10	11	12
	A	A	A
Frequencies --	694.4590	781.8678	802.5171
Red. masses --	2.1846	2.1882	1.8409
Frc consts --	0.6208	0.7881	0.6985
IR Inten --	4.1787	29.8353	255.0780
	13	14	15
	A	A	A
Frequencies --	877.6002	889.8392	918.8837
Red. masses --	1.9099	1.6102	1.7545
Frc consts --	0.8667	0.7512	0.8728
IR Inten --	34.3896	39.2317	30.1118

	16	17	18
	A	A	A
Frequencies --	1003.7296	1018.9483	1060.6448
Red. masses --	2.3801	1.6232	2.7082
Frc consts --	1.4128	0.9930	1.7950
IR Inten --	36.4943	35.3256	2.5515

	19	20	21
	A	A	A
Frequencies --	1083.1926	1110.7283	1139.7468
Red. masses --	3.7481	2.2545	1.9807
Frc consts --	2.5910	1.6388	1.5160
IR Inten --	135.4074	76.7008	10.9011

	22	23	24
	A	A	A
Frequencies --	1185.3916	1194.6548	1249.1571
Red. masses --	2.0890	1.4703	1.3153
Frc consts --	1.7295	1.2364	1.2092
IR Inten --	38.2234	12.2528	28.7673

	25	26	27
	A	A	A
Frequencies --	1320.7192	1338.8925	1344.7070
Red. masses --	1.4255	1.3447	1.2001
Frc consts --	1.4650	1.4202	1.2786
IR Inten --	8.3510	4.7033	29.0473

	28	29	30
	A	A	A
Frequencies --	1367.3506	1373.1579	1399.6196
Red. masses --	1.3060	1.2026	1.3964
Frc consts --	1.4387	1.3360	1.6116
IR Inten --	15.4925	3.0000	11.9465

	31	32	33
	A	A	A
Frequencies --	1442.6066	1472.1257	1488.3348
Red. masses --	1.8607	1.1085	1.0854
Frc consts --	2.2815	1.4153	1.4166
IR Inten --	18.7371	29.0718	4.6712

	34	35	36
	A	A	A
Frequencies --	1496.7242	1508.9543	1751.8927
Red. masses --	1.1006	1.2261	9.4036
Frc consts --	1.4527	1.6449	17.0043
IR Inten --	10.3811	20.3321	205.2505

	37	38	39
	A	A	A
Frequencies --	3052.8743	3055.7316	3057.3762
Red. masses --	1.0666	1.0670	1.0623
Frc consts --	5.8572	5.8703	5.8508
IR Inten --	29.5226	28.2099	34.4993

	40	41	42
	A	A	A
Frequencies --	3072.6856	3119.3303	3127.0476
Red. masses --	1.0820	1.1005	1.1025
Frc consts --	6.0190	6.3088	6.3518
IR Inten --	50.3487	39.8314	37.8314

	43	44	45
	A	A	A
Frequencies --	3133.5206	3499.1804	3564.1286
Red. masses --	1.1016	1.0743	1.0749
Frc consts --	6.3728	7.7503	8.0447
IR Inten --	34.5115	2.5259	4.6803

15a

1	2	3
A	A	A

Frequencies --	112.0054	161.3559	239.1748
Red. masses --	3.6618	3.3167	3.6928
Frc consts --	0.0271	0.0509	0.1245
IR Inten --	1.8313	4.9600	12.3013
	4	5	6
	A	A	A
Frequencies --	290.6711	381.1965	410.4414
Red. masses --	2.5080	2.0687	2.2405
Frc consts --	0.1248	0.1771	0.2224
IR Inten --	8.7256	2.9241	2.8658
	7	8	9
	A	A	A
Frequencies --	464.9786	495.3259	638.3620
Red. masses --	4.4905	2.1191	4.1703
Frc consts --	0.5720	0.3063	1.0013
IR Inten --	5.0518	5.6046	2.7485
	10	11	12
	A	A	A
Frequencies --	704.7139	751.5753	790.3145
Red. masses --	2.0096	1.2449	2.2145
Frc consts --	0.5880	0.4143	0.8149
IR Inten --	42.0508	8.7643	16.7487
	13	14	15
	A	A	A
Frequencies --	816.2167	854.7650	907.3406
Red. masses --	1.9470	2.7514	2.0730
Frc consts --	0.7642	1.1844	1.0055
IR Inten --	228.8770	47.6127	5.6438
	16	17	18
	A	A	A
Frequencies --	921.3015	968.1195	996.3964
Red. masses --	1.8810	1.3648	2.5407
Frc consts --	0.9407	0.7537	1.4862
IR Inten --	53.7539	59.9396	83.3151
	19	20	21
	A	A	A
Frequencies --	1011.6038	1024.4982	1044.2395
Red. masses --	1.6945	2.4866	1.9434
Frc consts --	1.0217	1.5377	1.2486
IR Inten --	15.8392	59.7592	9.6345
	22	23	24
	A	A	A
Frequencies --	1118.1729	1180.7915	1215.5940
Red. masses --	1.7580	3.7429	1.1129
Frc consts --	1.2951	3.0747	0.9689
IR Inten --	16.7836	46.2914	11.6622
	25	26	27
	A	A	A
Frequencies --	1253.3914	1313.9399	1326.4980
Red. masses --	1.4558	1.6046	1.5008
Frc consts --	1.3475	1.6322	1.5560
IR Inten --	14.8857	4.0483	0.1532
	28	29	30
	A	A	A
Frequencies --	1340.7613	1355.0843	1373.9768
Red. masses --	1.4218	1.3559	1.2227
Frc consts --	1.5059	1.4669	1.3600
IR Inten --	5.6767	19.3706	4.2386
	31	32	33
	A	A	A
Frequencies --	1393.3046	1410.4900	1456.8269
Red. masses --	1.6585	1.3890	1.1517
Frc consts --	1.8970	1.6282	1.4402
IR Inten --	2.6388	17.9959	13.4350
	34	35	36
	A	A	A
Frequencies --	1464.5815	1475.7682	1495.0454

Red. masses	--	1.0865	1.1460	1.0951
Frc consts	--	1.3731	1.4706	1.4421
IR Inten	--	7.1267	27.3629	7.3103

		37	38	39
		A	A	A
Frequencies	--	1508.8131	1741.4496	3040.7900
Red. masses	--	1.2154	6.0004	1.0675
Frc consts	--	1.6302	10.7214	5.8156
IR Inten	--	23.4493	25.8144	52.3579

		40	41	42
		A	A	A
Frequencies	--	3050.7114	3054.7268	3108.8451
Red. masses	--	1.0630	1.0646	1.0888
Frc consts	--	5.8288	5.8530	6.2001
IR Inten	--	41.4206	37.6097	73.6631

		43	44	45
		A	A	A
Frequencies	--	3112.1368	3115.8487	3120.1572
Red. masses	--	1.0965	1.1030	1.1009
Frc consts	--	6.2571	6.3093	6.3145
IR Inten	--	33.7993	50.8396	35.4788

		46	47	48
		A	A	A
Frequencies	--	3143.4664	3232.5223	3566.5598
Red. masses	--	1.0618	1.1167	1.0743
Frc consts	--	6.1819	6.8752	8.0512
IR Inten	--	12.1406	16.3155	4.2034

15e

		1	2	3
		A	A	A
Frequencies	--	113.2588	170.1147	285.7459
Red. masses	--	3.5228	2.4456	3.9551
Frc consts	--	0.0266	0.0417	0.1903
IR Inten	--	1.8871	2.7207	5.0671

		4	5	6
		A	A	A
Frequencies	--	327.3473	351.8401	390.0516
Red. masses	--	2.0742	3.2441	3.1931
Frc consts	--	0.1310	0.2366	0.2862
IR Inten	--	17.4852	4.0002	5.1334

		7	8	9
		A	A	A
Frequencies	--	439.9635	488.4404	571.9613
Red. masses	--	2.7979	3.1005	3.4553
Frc consts	--	0.3191	0.4358	0.6660
IR Inten	--	3.0933	5.3608	16.1719

		10	11	12
		A	A	A
Frequencies	--	669.5975	748.1263	793.8872
Red. masses	--	1.9973	1.1308	2.0477
Frc consts	--	0.5276	0.3729	0.7604
IR Inten	--	17.3120	0.2944	31.3651

		13	14	15
		A	A	A
Frequencies	--	802.4881	865.8334	903.1034
Red. masses	--	1.8337	1.9895	1.9737
Frc consts	--	0.6958	0.8787	0.9484
IR Inten	--	238.1623	16.2802	9.7889

		16	17	18
		A	A	A
Frequencies	--	945.3924	985.1855	1006.3824
Red. masses	--	1.3552	2.0318	1.6476
Frc consts	--	0.7136	1.1619	0.9832
IR Inten	--	81.9170	31.6571	8.5577

	19	20	21
	A	A	A
Frequencies --	1013.2573	1062.1477	1080.7119
Red. masses --	2.0494	4.6062	2.4384
Frc consts --	1.2397	3.0617	1.6780
IR Inten --	14.3580	158.6221	0.2857
	22	23	24
	A	A	A
Frequencies --	1129.3112	1173.4105	1195.1910
Red. masses --	1.9616	2.8894	1.3581
Frc consts --	1.4740	2.3440	1.1431
IR Inten --	4.3687	28.3412	7.0891
	25	26	27
	A	A	A
Frequencies --	1237.9257	1284.0512	1326.0607
Red. masses --	1.5937	1.5008	1.3453
Frc consts --	1.4390	1.4579	1.3937
IR Inten --	10.7212	5.9350	1.4002
	28	29	30
	A	A	A
Frequencies --	1338.2260	1365.2026	1370.5930
Red. masses --	1.2652	1.3904	1.2477
Frc consts --	1.3350	1.5268	1.3809
IR Inten --	3.0396	2.1330	4.5623
	31	32	33
	A	A	A
Frequencies --	1390.5572	1410.9339	1445.3138
Red. masses --	1.4191	1.5216	1.1803
Frc consts --	1.6167	1.7847	1.4526
IR Inten --	9.1575	12.6494	7.9779
	34	35	36
	A	A	A
Frequencies --	1476.3565	1485.5794	1494.5111
Red. masses --	1.1186	1.0820	1.1002
Frc consts --	1.4365	1.4070	1.4478
IR Inten --	24.0876	3.3842	10.0142
	37	38	39
	A	A	A
Frequencies --	1507.5953	1741.1713	3038.9001
Red. masses --	1.2167	6.3284	1.0667
Frc consts --	1.6293	11.3038	5.8039
IR Inten --	18.0225	46.5763	31.1256
	40	41	42
	A	A	A
Frequencies --	3049.3005	3051.0834	3062.6762
Red. masses --	1.0642	1.0670	1.0812
Frc consts --	5.8299	5.8521	5.9750
IR Inten --	58.9041	30.8606	72.1217
	43	44	45
	A	A	A
Frequencies --	3111.4970	3118.2094	3123.3646
Red. masses --	1.0974	1.1021	1.1027
Frc consts --	6.2597	6.3137	6.3383
IR Inten --	52.6646	51.1667	47.1651
	46	47	48
	A	A	A
Frequencies --	3159.3693	3252.9538	3560.9027
Red. masses --	1.0614	1.1161	1.0747
Frc consts --	6.2424	6.9583	8.0287
IR Inten --	9.7218	8.8926	2.4278

16a

	1	2	3
	A	A	A
Frequencies --	76.8374	170.3370	223.3085
Red. masses --	5.4649	3.2296	4.5915
Frc consts --	0.0190	0.0552	0.1349
IR Inten --	12.4323	0.0886	5.2913
	4	5	6
	A	A	A
Frequencies --	298.5010	389.1577	428.4253
Red. masses --	3.4523	1.9141	5.2739
Frc consts --	0.1812	0.1708	0.5703
IR Inten --	2.8045	8.0368	10.3162
	7	8	9
	A	A	A
Frequencies --	467.3947	503.2114	629.0584
Red. masses --	3.4467	2.3871	2.9949
Frc consts --	0.4436	0.3561	0.6983
IR Inten --	42.4661	16.2330	56.0395
	10	11	12
	A	A	A
Frequencies --	688.1657	766.6775	820.6711
Red. masses --	2.4075	3.3153	1.8642
Frc consts --	0.6717	1.1481	0.7397
IR Inten --	91.0127	43.8696	30.2911
	13	14	15
	A	A	A
Frequencies --	888.3069	901.2581	954.7008
Red. masses --	2.4635	2.3011	2.1970
Frc consts --	1.1453	1.1012	1.1798
IR Inten --	54.8837	21.2136	57.9191
	16	17	18
	A	A	A
Frequencies --	1013.8687	1034.8438	1068.2531
Red. masses --	3.4138	2.2228	1.6651
Frc consts --	2.0675	1.4025	1.1195
IR Inten --	2.1672	68.7948	2.2501
	19	20	21
	A	A	A
Frequencies --	1100.6371	1175.8117	1190.5954
Red. masses --	2.5151	2.4321	1.5833
Frc consts --	1.7951	1.9811	1.3224
IR Inten --	23.4044	6.1716	10.7774
	22	23	24
	A	A	A
Frequencies --	1210.3624	1270.5991	1302.7837
Red. masses --	1.2285	1.6044	1.3098
Frc consts --	1.0603	1.5261	1.3098
IR Inten --	25.4190	29.9798	7.4090
	25	26	27
	A	A	A
Frequencies --	1327.3721	1348.5143	1369.3168
Red. masses --	1.4583	1.4422	1.5017
Frc consts --	1.5138	1.5453	1.6590
IR Inten --	18.0244	10.1655	16.7913
	28	29	30
	A	A	A
Frequencies --	1377.4914	1427.1303	1446.6174
Red. masses --	1.4582	1.5076	1.1121
Frc consts --	1.6302	1.8090	1.3712
IR Inten --	53.1708	11.8833	23.4990
	31	32	33
	A	A	A

Frequencies --	1476.7544	1493.3903	1516.6477
Red. masses --	1.0860	1.3348	1.1062
Frc consts --	1.3954	1.7540	1.4992
IR Inten --	10.4799	20.3220	5.4095
	34	35	36
	A	A	A
Frequencies --	1819.9592	2960.8019	2972.0357
Red. masses --	11.2718	1.0718	1.0728
Frc consts --	21.9972	5.5357	5.5831
IR Inten --	418.4170	109.5545	99.1024
	37	38	39
	A	A	A
Frequencies --	3071.3003	3120.0874	3122.3750
Red. masses --	1.0632	1.0904	1.0915
Frc consts --	5.9090	6.2544	6.2694
IR Inten --	9.1931	27.1208	33.8507
	40	41	42
	A	A	A
Frequencies --	3135.1784	3151.8288	3600.8573
Red. masses --	1.0885	1.1014	1.0755
Frc consts --	6.3038	6.4463	8.2159
IR Inten --	29.3657	17.3345	13.4079
16e	1	2	3
	A	A	A
Frequencies --	90.2036	163.5648	282.9371
Red. masses --	5.1424	2.4987	7.0443
Frc consts --	0.0247	0.0394	0.3323
IR Inten --	3.7413	7.5036	4.8008
	4	5	6
	A	A	A
Frequencies --	344.0789	357.6006	401.2311
Red. masses --	2.7849	2.9897	4.2037
Frc consts --	0.1943	0.2253	0.3987
IR Inten --	1.7783	19.9618	7.3950
	7	8	9
	A	A	A
Frequencies --	438.7553	514.8450	601.7492
Red. masses --	3.3308	2.4404	4.0349
Frc consts --	0.3778	0.3811	0.8608
IR Inten --	3.4890	22.5940	44.5876
	10	11	12
	A	A	A
Frequencies --	668.0186	759.4189	804.4417
Red. masses --	2.6274	2.3543	1.6138
Frc consts --	0.6908	0.8000	0.6153
IR Inten --	90.5454	11.7112	68.3788
	13	14	15
	A	A	A
Frequencies --	898.1513	912.5821	990.4794
Red. masses --	2.7025	2.4733	1.4554
Frc consts --	1.2844	1.2136	0.8412
IR Inten --	91.8888	5.1410	11.0653
	16	17	18
	A	A	A
Frequencies --	1013.3758	1095.9847	1097.1535
Red. masses --	2.4259	2.1984	3.7582
Frc consts --	1.4678	1.5558	2.6654
IR Inten --	14.6460	19.6457	123.0380
	19	20	21
	A	A	A
Frequencies --	1122.8661	1159.1207	1183.7749
Red. masses --	2.5926	2.5412	1.8921
Frc consts --	1.9259	2.0116	1.5622
IR Inten --	19.4822	21.1408	6.2241

	22		23		24
	A		A		A
Frequencies --	1200.3642		1265.7038		1295.5088
Red. masses --	1.3334		1.3770		1.3799
Frc consts --	1.1320		1.2997		1.3645
IR Inten --	30.8376		11.5949		11.7146

	25		26		27
	A		A		A
Frequencies --	1323.3069		1342.3985		1359.1679
Red. masses --	1.2315		1.3112		1.4034
Frc consts --	1.2706		1.3921		1.5274
IR Inten --	9.4024		7.7527		11.1232

	28		29		30
	A		A		A
Frequencies --	1394.2072		1429.6516		1451.6447
Red. masses --	1.7416		1.5371		1.1006
Frc consts --	1.9946		1.8510		1.3665
IR Inten --	24.3306		6.9952		20.4850

	31		32		33
	A		A		A
Frequencies --	1488.4705		1503.1364		1512.4039
Red. masses --	1.2187		1.1644		1.0998
Frc consts --	1.5908		1.5501		1.4821
IR Inten --	21.2761		1.2389		9.1981

	34		35		36
	A		A		A
Frequencies --	1819.5297		2974.8504		2977.9718
Red. masses --	11.9733		1.0712		1.0727
Frc consts --	23.3550		5.5855		5.6051
IR Inten --	452.1956		168.8958		38.2289

	37		38		39
	A		A		A
Frequencies --	3067.3619		3087.4870		3124.7998
Red. masses --	1.0640		1.0831		1.0915
Frc consts --	5.8983		6.0834		6.2792
IR Inten --	8.2688		24.1019		35.8851

	40		41		42
	A		A		A
Frequencies --	3130.7333		3145.4644		3599.0264
Red. masses --	1.0929		1.1007		1.0755
Frc consts --	6.3111		6.4164		8.2081
IR Inten --	26.7025		17.4985		14.9887

17a

	1		2		3
	A		A		A
Frequencies --	75.2394		168.0481		233.8647
Red. masses --	5.6334		3.6161		3.8040
Frc consts --	0.0188		0.0602		0.1226
IR Inten --	4.7393		0.5918		5.1823

	4		5		6
	A		A		A
Frequencies --	271.3886		351.5573		395.1949
Red. masses --	5.0030		3.1951		2.1854
Frc consts --	0.2171		0.2327		0.2011
IR Inten --	2.4994		5.2923		8.3899

	7		8		9
	A		A		A
Frequencies --	410.9961		488.0010		607.5585
Red. masses --	5.2961		2.1357		3.0491
Frc consts --	0.5271		0.2997		0.6631
IR Inten --	12.6165		34.3966		89.0160

	10	11	12
	A	A	A
Frequencies --	656.9512	750.0439	808.7467
Red. masses --	3.1784	2.9337	1.7460
Frc consts --	0.8082	0.9724	0.6728
IR Inten --	54.4969	42.1806	59.8140

	13	14	15
	A	A	A
Frequencies --	880.6099	890.9969	946.2046
Red. masses --	2.7661	2.5387	2.2683
Frc consts --	1.2638	1.1875	1.1965
IR Inten --	52.4099	31.5952	73.8803

	16	17	18
	A	A	A
Frequencies --	1000.7279	1032.4086	1063.3076
Red. masses --	3.1287	1.9821	2.0661
Frc consts --	1.8461	1.2448	1.3763
IR Inten --	1.8127	46.9530	40.4844

	19	20	21
	A	A	A
Frequencies --	1077.6979	1165.0574	1179.1451
Red. masses --	2.0023	2.0288	1.8788
Frc consts --	1.3702	1.6225	1.5391
IR Inten --	55.2734	7.4589	36.5623

	22	23	24
	A	A	A
Frequencies --	1201.5824	1243.7561	1260.6715
Red. masses --	1.7296	1.9810	1.4383
Frc consts --	1.4713	1.8056	1.3468
IR Inten --	33.1330	100.5830	9.6246

	25	26	27
	A	A	A
Frequencies --	1300.3583	1327.0086	1342.6027
Red. masses --	1.3442	1.2371	1.4273
Frc consts --	1.3391	1.2836	1.5159
IR Inten --	58.2012	6.4613	29.7017

	28	29	30
	A	A	A
Frequencies --	1367.7157	1393.2839	1431.5844
Red. masses --	1.4943	1.8020	1.5139
Frc consts --	1.6470	2.0610	1.8280
IR Inten --	23.6929	88.1165	2.8706

	31	32	33
	A	A	A
Frequencies --	1463.7892	1480.0236	1491.2055
Red. masses --	1.1635	1.0834	1.3250
Frc consts --	1.4689	1.3983	1.7360
IR Inten --	17.0119	10.6094	27.3211

	34	35	36
	A	A	A
Frequencies --	1509.6874	2969.1682	2973.2002
Red. masses --	1.1133	1.0713	1.0724
Frc consts --	1.4950	5.5643	5.5855
IR Inten --	7.3699	148.8308	48.0028

	37	38	39
	A	A	A
Frequencies --	3064.4568	3121.1085	3124.2119
Red. masses --	1.0646	1.0910	1.0918
Frc consts --	5.8905	6.2614	6.2788
IR Inten --	8.1161	25.3686	38.0189

40	41	42
A	A	A

Frequencies	--	3142.5974	3155.0557	3601.0029
Red. masses	--	1.0889	1.0999	1.0753
Frc consts	--	6.3358	6.4510	8.2156
IR Inten	--	22.6269	11.3070	16.3572

17e

		1	2	3
		A	A	A
Frequencies	--	78.5891	169.1511	241.0245
Red. masses	--	4.9094	2.7073	13.3638
Frc consts	--	0.0179	0.0456	0.4574
IR Inten	--	0.7963	4.9081	2.4459

		4	5	6
		A	A	A
Frequencies	--	315.9817	363.4978	376.8533
Red. masses	--	3.0067	3.4789	2.8264
Frc consts	--	0.1769	0.2708	0.2365
IR Inten	--	5.5043	17.9600	2.6516

		7	8	9
		A	A	A
Frequencies	--	438.0018	482.0726	577.3692
Red. masses	--	3.3863	3.2243	4.0371
Frc consts	--	0.3828	0.4415	0.7929
IR Inten	--	2.6121	11.7421	18.7665

		10	11	12
		A	A	A
Frequencies	--	604.9038	741.9473	789.7241
Red. masses	--	2.5222	3.2336	1.5446
Frc consts	--	0.5437	1.0488	0.5676
IR Inten	--	115.0552	0.7070	117.3936

		13	14	15
		A	A	A
Frequencies	--	858.7996	908.8358	998.5530
Red. masses	--	2.1990	2.6208	1.8151
Frc consts	--	0.9556	1.2754	1.0663
IR Inten	--	41.1919	5.3274	21.9123

		16	17	18
		A	A	A
Frequencies	--	1012.1836	1068.5425	1095.0340
Red. masses	--	1.9971	2.0256	2.7310
Frc consts	--	1.2055	1.3627	1.9294
IR Inten	--	8.8851	56.0291	12.4579

		19	20	21
		A	A	A
Frequencies	--	1106.6425	1149.3040	1182.2280
Red. masses	--	3.3239	2.5132	1.7968
Frc consts	--	2.3983	1.9559	1.4796
IR Inten	--	77.4931	39.1814	5.5317

		22	23	24
		A	A	A
Frequencies	--	1200.1204	1213.1709	1279.7905
Red. masses	--	1.5647	1.7796	1.4390
Frc consts	--	1.3278	1.5432	1.3887
IR Inten	--	23.2988	70.1934	6.5941

		25	26	27
		A	A	A
Frequencies	--	1317.2837	1327.1706	1336.9859
Red. masses	--	1.2887	1.4819	1.3197
Frc consts	--	1.3176	1.5379	1.3898
IR Inten	--	1.5511	89.8422	37.6396

28

29

30

	A	A	A
Frequencies --	1359.9798	1390.3095	1430.8320
Red. masses --	1.8688	1.5146	1.5114
Frc consts --	2.0364	1.7250	1.8230
IR Inten --	104.0990	22.9347	6.7014
	31	32	33
	A	A	A
Frequencies --	1464.1085	1487.0208	1505.8058
Red. masses --	1.1202	1.2701	1.1207
Frc consts --	1.4148	1.6547	1.4972
IR Inten --	19.5981	31.4133	1.5078
	34	35	36
	A	A	A
Frequencies --	1517.3558	2977.5229	2982.1503
Red. masses --	1.1007	1.0705	1.0723
Frc consts --	1.4931	5.5918	5.6188
IR Inten --	10.8948	123.0110	69.9992
	37	38	39
	A	A	A
Frequencies --	3055.4328	3082.7464	3127.4077
Red. masses --	1.0667	1.0827	1.0920
Frc consts --	5.8675	6.0624	6.2928
IR Inten --	8.6506	23.6836	37.6837
	40	41	42
	A	A	A
Frequencies --	3128.6731	3152.9645	3599.2289
Red. masses --	1.0930	1.0978	1.0754
Frc consts --	6.3037	6.4298	8.2081
IR Inten --	28.9083	12.8817	17.2093
18a	1	2	3
	A	A	A
Frequencies --	98.5574	176.3633	232.6496
Red. masses --	4.2638	3.3324	4.3739
Frc consts --	0.0244	0.0611	0.1395
IR Inten --	5.9343	0.3523	5.6333
	4	5	6
	A	A	A
Frequencies --	303.5284	392.6514	430.6830
Red. masses --	3.1600	1.9078	3.9428
Frc consts --	0.1715	0.1733	0.4309
IR Inten --	1.7636	11.4103	25.0983
	7	8	9
	A	A	A
Frequencies --	465.3115	501.3814	637.6232
Red. masses --	3.7637	2.1107	3.3336
Frc consts --	0.4801	0.3126	0.7985
IR Inten --	21.6508	26.7530	44.2562
	10	11	12
	A	A	A
Frequencies --	677.9673	780.4526	816.9266
Red. masses --	2.3488	3.2370	1.7022
Frc consts --	0.6361	1.1617	0.6693
IR Inten --	64.6384	53.3993	54.1450
	13	14	15
	A	A	A
Frequencies --	885.5679	904.4906	925.2274
Red. masses --	2.1820	2.2301	1.8247
Frc consts --	1.0082	1.0749	0.9203
IR Inten --	21.1430	57.6321	194.8969
	16	17	18
	A	A	A
Frequencies --	966.4156	1015.7664	1054.7709
Red. masses --	1.6945	3.3859	2.0038
Frc consts --	0.9324	2.0583	1.3135
IR Inten --	4.6837	5.6181	32.4885

	19	20	21
	A	A	A
Frequencies --	1075.1120	1100.6745	1144.0807
Red. masses --	1.6872	2.1970	1.6801
Frc consts --	1.1490	1.5682	1.2957
IR Inten --	2.4980	25.4395	73.6119

	22	23	24
	A	A	A
Frequencies --	1191.5380	1214.4293	1224.1648
Red. masses --	2.6499	1.2106	1.0928
Frc consts --	2.2166	1.0520	0.9649
IR Inten --	20.7688	19.8531	11.9498

	25	26	27
	A	A	A
Frequencies --	1304.8704	1333.0554	1340.2981
Red. masses --	1.3047	1.4545	1.3377
Frc consts --	1.3089	1.5228	1.4159
IR Inten --	16.5401	31.0417	9.6287

	28	29	30
	A	A	A
Frequencies --	1370.0186	1372.3802	1420.1812
Red. masses --	1.4410	1.2283	2.0126
Frc consts --	1.5935	1.3631	2.3916
IR Inten --	20.7550	22.2602	26.5583

	31	32	33
	A	A	A
Frequencies --	1427.5394	1456.3071	1477.2475
Red. masses --	1.5220	1.1519	1.0857
Frc consts --	1.8274	1.4394	1.3959
IR Inten --	14.2420	24.3543	10.0256

	34	35	36
	A	A	A
Frequencies --	1495.1338	1512.3547	1754.0766
Red. masses --	1.3324	1.1149	9.2383
Frc consts --	1.7549	1.5024	16.7471
IR Inten --	20.6589	4.8476	149.8616

	37	38	39
	A	A	A
Frequencies --	2960.8979	2964.2164	3069.0019
Red. masses --	1.0713	1.0731	1.0637
Frc consts --	5.5336	5.5556	5.9031
IR Inten --	159.9199	58.4093	17.1959

	40	41	42
	A	A	A
Frequencies --	3108.1234	3117.9472	3119.6064
Red. masses --	1.0882	1.0903	1.0911
Frc consts --	6.1939	6.2449	6.2562
IR Inten --	38.5415	60.9070	17.1925

	43	44	45
	A	A	A
Frequencies --	3143.3996	3485.7530	3596.1655
Red. masses --	1.1009	1.0745	1.0754
Frc consts --	6.4090	7.6920	8.1940
IR Inten --	21.7348	1.0410	10.3131

18e

	1	2	3
	A	A	A
Frequencies --	106.1149	170.8066	289.3884
Red. masses --	4.1074	2.5023	4.8794
Frc consts --	0.0273	0.0430	0.2408
IR Inten --	1.0248	4.7275	13.0926

	4	5	6
	A	A	A
Frequencies --	345.1997	361.6299	399.2877
Red. masses --	2.7528	3.0081	3.9805
Frc consts --	0.1933	0.2318	0.3739
IR Inten --	0.2363	26.8086	1.8762

	7	8	9
	A	A	A
Frequencies --	439.1426	505.8509	593.2765
Red. masses --	3.0667	2.4360	3.6310
Frc consts --	0.3484	0.3673	0.7530
IR Inten --	0.6741	39.7133	32.5542

	10	11	12
	A	A	A
Frequencies --	663.9893	776.4378	799.0367
Red. masses --	2.5044	2.4766	1.5348
Frc consts --	0.6505	0.8797	0.5773
IR Inten --	61.9836	7.1691	109.5661

	13	14	15
	A	A	A
Frequencies --	891.1364	904.1611	926.1839
Red. masses --	2.5391	1.7474	1.4062
Frc consts --	1.1880	0.8417	0.7107
IR Inten --	105.0988	15.3001	56.4240

	16	17	18
	A	A	A
Frequencies --	1002.1877	1047.1241	1079.1086
Red. masses --	2.4056	1.6514	3.1552
Frc consts --	1.4235	1.0669	2.1647
IR Inten --	10.9704	31.5000	105.7863

	19	20	21
	A	A	A
Frequencies --	1093.9694	1113.3750	1130.8376
Red. masses --	1.8371	2.2914	2.4473
Frc consts --	1.2954	1.6736	1.8439
IR Inten --	10.3720	16.1220	20.4044

	22	23	24
	A	A	A
Frequencies --	1186.7205	1208.8801	1234.7534
Red. masses --	3.0192	1.1158	1.2164
Frc consts --	2.5052	0.9607	1.0926
IR Inten --	16.7912	12.9500	24.5346

	25	26	27
	A	A	A
Frequencies --	1296.9597	1323.1887	1327.3517
Red. masses --	1.3658	1.3143	1.2040
Frc consts --	1.3536	1.3558	1.2498
IR Inten --	5.6245	19.7092	36.1985

	28	29	30
	A	A	A
Frequencies --	1356.3177	1363.6114	1418.7484
Red. masses --	1.3146	1.3821	1.8181
Frc consts --	1.4248	1.5141	2.1562
IR Inten --	8.3790	6.5772	46.5153

	31	32	33
	A	A	A
Frequencies --	1431.9769	1456.9132	1488.2101
Red. masses --	1.6699	1.1254	1.2153
Frc consts --	2.0174	1.4074	1.5858
IR Inten --	0.7484	21.4891	19.0896

34

35

36

	A	A	A
Frequencies --	1503.2162	1512.0554	1752.8920
Red. masses --	1.1761	1.1008	10.0780
Frc consts --	1.5657	1.4828	18.2447
IR Inten --	1.5054	9.8283	193.7460
	37	38	39
	A	A	A
Frequencies --	2969.1009	2975.3417	3065.5982
Red. masses --	1.0720	1.0715	1.0646
Frc consts --	5.5680	5.5885	5.8947
IR Inten --	142.3483	72.6163	16.7645
	40	41	42
	A	A	A
Frequencies --	3095.2558	3120.4120	3128.3643
Red. masses --	1.0841	1.0912	1.0930
Frc consts --	6.1196	6.2603	6.3021
IR Inten --	26.7593	43.7679	34.6105
	43	44	45
	A	A	A
Frequencies --	3142.0753	3489.7448	3600.6973
Red. masses --	1.1001	1.0733	1.0754
Frc consts --	6.3993	7.7012	8.2150
IR Inten --	22.0670	8.5588	11.9594
19a	1	2	3
	A	A	A
Frequencies --	95.9087	176.3350	229.7553
Red. masses --	4.3121	3.4350	3.9290
Frc consts --	0.0234	0.0629	0.1222
IR Inten --	6.3540	0.1746	4.2252
	4	5	6
	A	A	A
Frequencies --	304.3152	396.9740	430.5785
Red. masses --	3.1925	1.9189	4.7064
Frc consts --	0.1742	0.1782	0.5141
IR Inten --	5.3571	6.8540	6.9662
	7	8	9
	A	A	A
Frequencies --	463.5558	499.8030	642.0673
Red. masses --	3.5173	2.0436	3.2518
Frc consts --	0.4453	0.3008	0.7898
IR Inten --	58.6913	2.6960	31.8184
	10	11	12
	A	A	A
Frequencies --	681.4167	777.6253	817.9302
Red. masses --	2.4754	3.1809	1.8354
Frc consts --	0.6772	1.1333	0.7234
IR Inten --	86.8235	32.4521	57.6128
	13	14	15
	A	A	A
Frequencies --	887.0657	904.5395	923.4142
Red. masses --	2.1505	2.1784	1.7121
Frc consts --	0.9970	1.0501	0.8602
IR Inten --	93.1472	21.5831	14.2074
	16	17	18
	A	A	A
Frequencies --	965.8731	1014.8957	1055.1643
Red. masses --	1.6985	3.4615	2.0355
Frc consts --	0.9336	2.1006	1.3353
IR Inten --	70.5563	2.2051	143.8736
	19	20	21
	A	A	A
Frequencies --	1075.3008	1101.2357	1147.3333
Red. masses --	1.6891	2.2214	1.6614
Frc consts --	1.1507	1.5873	1.2886
IR Inten --	1.8744	8.2834	23.2982

	22	23	24
	A	A	A
Frequencies --	1192.0122	1217.3399	1232.3950
Red. masses --	2.7518	1.1838	1.1019
Frc consts --	2.3037	1.0336	0.9860
IR Inten --	30.7409	7.8880	14.2410

	25	26	27
	A	A	A
Frequencies --	1310.9243	1329.9354	1357.7225
Red. masses --	1.2699	1.4230	1.3351
Frc consts --	1.2858	1.4829	1.4501
IR Inten --	7.7715	21.0768	20.4753

	28	29	30
	A	A	A
Frequencies --	1362.2169	1379.3215	1424.3438
Red. masses --	1.4306	1.2275	2.3970
Frc consts --	1.5641	1.3759	2.8652
IR Inten --	4.8035	30.3094	82.3813

	31	32	33
	A	A	A
Frequencies --	1436.2550	1455.3627	1479.3825
Red. masses --	1.5083	1.1025	1.0858
Frc consts --	1.8332	1.3758	1.4001
IR Inten --	15.8055	20.5093	9.9435

	34	35	36
	A	A	A
Frequencies --	1499.2567	1515.4865	1756.3504
Red. masses --	1.3290	1.1171	9.2583
Frc consts --	1.7601	1.5116	16.8269
IR Inten --	20.1041	5.7157	151.2755

	37	38	39
	A	A	A
Frequencies --	2962.6715	2966.7669	3069.7915
Red. masses --	1.0713	1.0729	1.0613
Frc consts --	5.5404	5.5638	5.8925
IR Inten --	173.9712	45.2391	16.3049

	40	41	42
	A	A	A
Frequencies --	3114.2488	3119.9403	3129.4644
Red. masses --	1.0909	1.0905	1.0922
Frc consts --	6.2334	6.2540	6.3021
IR Inten --	48.7040	24.4340	37.2451

	43	44	45
	A	A	A
Frequencies --	3131.9046	3488.3956	3599.6138
Red. masses --	1.1000	1.0744	1.0754
Frc consts --	6.3574	7.7029	8.2101
IR Inten --	19.5578	1.5644	10.5523

19e

	1	2	3
	A	A	A
Frequencies --	96.3852	171.1527	296.3543
Red. masses --	4.3375	2.5135	5.3722
Frc consts --	0.0237	0.0434	0.2780
IR Inten --	1.9117	7.2058	0.8374

	4	5	6
	A	A	A
Frequencies --	346.2757	359.8987	401.7152
Red. masses --	2.7775	2.8579	3.9031
Frc consts --	0.1962	0.2181	0.3711
IR Inten --	4.8326	12.5869	15.2707

	7 A	8 A	9 A
Frequencies --	438.2161	509.9484	590.0768
Red. masses --	3.1053	2.4576	3.5132
Frc consts --	0.3513	0.3765	0.7207
IR Inten --	4.3225	8.0917	57.3120

	10 A	11 A	12 A
Frequencies --	664.3587	782.3249	799.6645
Red. masses --	2.5494	2.3463	1.5713
Frc consts --	0.6630	0.8461	0.5920
IR Inten --	61.3249	8.8078	103.4305

	13 A	14 A	15 A
Frequencies --	890.9432	901.0712	922.9936
Red. masses --	2.1427	1.6086	1.8272
Frc consts --	1.0021	0.7695	0.9171
IR Inten --	35.0445	76.8579	10.3115

	16 A	17 A	18 A
Frequencies --	1001.9957	1048.4477	1090.7862
Red. masses --	2.3106	1.6564	3.3599
Frc consts --	1.3668	1.0728	2.3554
IR Inten --	44.5581	29.4039	105.3078

	19 A	20 A	21 A
Frequencies --	1093.6625	1112.8941	1129.8906
Red. masses --	1.8956	2.3034	2.4038
Frc consts --	1.3358	1.6809	1.8081
IR Inten --	25.3880	15.8193	69.1894

	22 A	23 A	24 A
Frequencies --	1188.1778	1209.3568	1227.6283
Red. masses --	3.0700	1.1185	1.1422
Frc consts --	2.5536	0.9639	1.0142
IR Inten --	23.8190	7.1211	14.2093

	25 A	26 A	27 A
Frequencies --	1296.5669	1327.8142	1340.9777
Red. masses --	1.3711	1.2152	1.3136
Frc consts --	1.3581	1.2623	1.3917
IR Inten --	11.1393	14.8388	27.9009

	28 A	29 A	30 A
Frequencies --	1357.0720	1365.8938	1422.6477
Red. masses --	1.2802	1.4158	1.7102
Frc consts --	1.3891	1.5562	2.0393
IR Inten --	17.4872	15.7494	5.2701

	31 A	32 A	33 A
Frequencies --	1437.6379	1459.3667	1488.9111
Red. masses --	1.7566	1.1130	1.2195
Frc consts --	2.1391	1.3966	1.5929
IR Inten --	22.1801	22.9509	20.3461

	34 A	35 A	36 A
Frequencies --	1503.3755	1512.5509	1755.7493
Red. masses --	1.1750	1.1022	9.5582
Frc consts --	1.5647	1.4857	17.3600
IR Inten --	1.8854	9.7483	186.9804

37

38

39

	A	A	A
Frequencies --	2969.4805	2972.9608	3064.3447
Red. masses --	1.0716	1.0719	1.0628
Frc consts --	5.5672	5.5818	5.8797
IR Inten --	162.0711	53.8806	13.7406

	40	41	42
	A	A	A
Frequencies --	3082.8832	3120.2141	3127.1153
Red. masses --	1.0836	1.0911	1.0929
Frc consts --	6.0679	6.2585	6.2966
IR Inten --	33.2838	44.5607	39.0423

	43	44	45
	A	A	A
Frequencies --	3129.4905	3498.2651	3597.9303
Red. masses --	1.1025	1.0745	1.0754
Frc consts --	6.3615	7.7475	8.2022
IR Inten --	22.0830	2.1388	11.6267

20a

	1	2	3
	A	A	A
Frequencies --	108.1769	180.4559	232.8482
Red. masses --	3.4378	3.4239	3.6207
Frc consts --	0.0237	0.0657	0.1157
IR Inten --	1.4152	1.3939	4.0610

	4	5	6
	A	A	A
Frequencies --	304.6629	384.8590	407.0704
Red. masses --	2.9199	2.1725	2.2050
Frc consts --	0.1597	0.1896	0.2153
IR Inten --	1.6370	7.1088	5.2499

	7	8	9
	A	A	A
Frequencies --	456.7423	490.1165	637.8266
Red. masses --	4.1950	2.0225	4.1437
Frc consts --	0.5156	0.2862	0.9932
IR Inten --	32.0787	15.3325	7.7638

	10	11	12
	A	A	A
Frequencies --	663.9272	744.7859	796.5375
Red. masses --	2.0861	1.2239	2.5431
Frc consts --	0.5418	0.4000	0.9507
IR Inten --	80.9647	22.5081	20.4717

	13	14	15
	A	A	A
Frequencies --	817.5590	877.9035	907.8791
Red. masses --	1.6966	2.7927	2.2664
Frc consts --	0.6681	1.2681	1.1006
IR Inten --	79.7964	122.3383	4.8148

	16	17	18
	A	A	A
Frequencies --	933.6161	970.2023	1003.5943
Red. masses --	1.9262	1.3606	2.3370
Frc consts --	0.9892	0.7546	1.3868
IR Inten --	66.8100	61.4158	16.6451

	19	20	21
	A	A	A
Frequencies --	1019.0741	1042.8745	1084.5617
Red. masses --	2.2131	1.8926	1.7503
Frc consts --	1.3541	1.2127	1.2130
IR Inten --	20.8896	64.3217	1.5403

	22	23	24
	A	A	A
Frequencies --	1097.7852	1191.6395	1218.9651
Red. masses --	1.9988	2.7498	1.3147
Frc consts --	1.4192	2.3006	1.1510
IR Inten --	12.1565	26.3817	11.6218

	25	26	27
	A	A	A
Frequencies --	1230.6690	1310.1667	1321.8546
Red. masses --	1.1031	1.3574	1.4293
Frc consts --	0.9844	1.3728	1.4714
IR Inten --	6.8346	5.0903	6.2803

	28	29	30
	A	A	A
Frequencies --	1337.7112	1362.4806	1372.1472
Red. masses --	1.5839	1.2999	1.2666
Frc consts --	1.6699	1.4217	1.4050
IR Inten --	41.4524	4.8895	21.8933

	31	32	33
	A	A	A
Frequencies --	1386.4081	1435.8092	1455.7879
Red. masses --	1.8647	1.5392	1.1355
Frc consts --	2.1117	1.8695	1.4179
IR Inten --	13.3376	6.2945	11.5134

	34	35	36
	A	A	A
Frequencies --	1472.8456	1479.1409	1498.9478
Red. masses --	1.1532	1.0871	1.3190
Frc consts --	1.4739	1.4014	1.7461
IR Inten --	21.5979	10.1807	19.9902

	37	38	39
	A	A	A
Frequencies --	1510.4079	1744.1536	2956.3823
Red. masses --	1.1314	6.0201	1.0719
Frc consts --	1.5208	10.7901	5.5198
IR Inten --	5.1293	19.9038	161.3424

	40	41	42
	A	A	A
Frequencies --	2963.2847	3061.2014	3107.4166
Red. masses --	1.0722	1.0632	1.0885
Frc consts --	5.5470	5.8701	6.1926
IR Inten --	74.5732	31.6745	65.8404

	43	44	45
	A	A	A
Frequencies --	3108.3320	3115.5641	3123.5269
Red. masses --	1.0903	1.0903	1.1011
Frc consts --	6.2066	6.2353	6.3294
IR Inten --	35.1044	48.1097	31.0113

	46	47	48
	A	A	A
Frequencies --	3146.7088	3235.5986	3593.4411
Red. masses --	1.0621	1.1165	1.0753
Frc consts --	6.1965	6.8867	8.1810
IR Inten --	12.6502	16.0845	7.3498

20e

	1	2	3
	A	A	A
Frequencies --	110.4868	183.9585	286.8028
Red. masses --	3.4140	2.5219	3.7903
Frc consts --	0.0246	0.0503	0.1837
IR Inten --	1.6220	2.8809	7.0574

	4	5	6
	A	A	A
Frequencies --	338.9542	363.0867	391.8364
Red. masses --	2.5885	2.8866	3.0426
Frc consts --	0.1752	0.2242	0.2752
IR Inten --	5.7854	15.2046	5.0055

	7	8	9
	A	A	A
Frequencies --	441.3262	481.7671	570.0411
Red. masses --	2.9217	2.6757	3.1357
Frc consts --	0.3353	0.3659	0.6003
IR Inten --	0.5401	14.9469	33.8020
	10	11	12
	A	A	A
Frequencies --	643.6523	747.4837	793.4869
Red. masses --	2.3017	1.1757	1.6601
Frc consts --	0.5618	0.3870	0.6158
IR Inten --	46.3186	1.9665	108.3991
	13	14	15
	A	A	A
Frequencies --	805.7960	876.8060	912.3015
Red. masses --	1.8878	2.0429	2.2964
Frc consts --	0.7222	0.9254	1.1261
IR Inten --	28.1319	33.5079	8.3803
	16	17	18
	A	A	A
Frequencies --	950.7733	976.0127	1025.8350
Red. masses --	1.3515	2.1021	1.7219
Frc consts --	0.7198	1.1798	1.0676
IR Inten --	81.3671	47.0811	14.0243
	19	20	21
	A	A	A
Frequencies --	1040.3212	1073.1870	1104.0110
Red. masses --	1.9218	3.1792	2.0291
Frc consts --	1.2254	2.1573	1.4571
IR Inten --	25.1976	96.9763	9.2264
	22	23	24
	A	A	A
Frequencies --	1120.5356	1185.2506	1205.1228
Red. masses --	2.5057	3.4241	1.3787
Frc consts --	1.8537	2.8341	1.1798
IR Inten --	14.6218	24.4393	4.2033
	25	26	27
	A	A	A
Frequencies --	1211.4239	1285.3684	1301.1501
Red. masses --	1.0935	1.4955	1.3446
Frc consts --	0.9455	1.4558	1.3412
IR Inten --	5.9239	3.4419	8.3437
	28	29	30
	A	A	A
Frequencies --	1324.9444	1357.3929	1362.1809
Red. masses --	1.2403	1.3424	1.3587
Frc consts --	1.2828	1.4573	1.4855
IR Inten --	11.9805	14.7614	12.6908
	31	32	33
	A	A	A
Frequencies --	1398.4899	1427.2604	1444.5897
Red. masses --	1.7888	1.5363	1.1632
Frc consts --	2.0612	1.8439	1.4302
IR Inten --	1.9548	5.0577	6.5307
	34	35	36
	A	A	A
Frequencies --	1468.0075	1486.5977	1501.6916
Red. masses --	1.1265	1.2217	1.1753
Frc consts --	1.4304	1.5908	1.5615
IR Inten --	21.4869	18.3698	2.2271
	37	38	39

	A	A	A
Frequencies --	1510.4325	1743.5528	2963.3107
Red. masses --	1.1021	6.3491	1.0720
Frc consts --	1.4813	11.3718	5.5462
IR Inten --	10.0978	39.0984	141.7087
	40	41	42
	A	A	A
Frequencies --	2971.0485	3050.8789	3076.5242
Red. masses --	1.0707	1.0647	1.0840
Frc consts --	5.5685	5.8391	6.0448
IR Inten --	89.5050	33.9460	47.1533
	43	44	45
	A	A	A
Frequencies --	3113.0692	3115.8407	3120.8664
Red. masses --	1.0911	1.0932	1.0995
Frc consts --	6.2298	6.2534	6.3096
IR Inten --	59.6075	50.9173	31.9175
	46	47	48
	A	A	A
Frequencies --	3159.1809	3252.0596	3594.0723
Red. masses --	1.0615	1.1162	1.0754
Frc consts --	6.2418	6.9553	8.1846
IR Inten --	10.2554	8.8907	8.6728
21a	1	2	3
	A	A	A
Frequencies --	86.8233	149.4038	231.7497
Red. masses --	5.4480	3.1658	4.2457
Frc consts --	0.0242	0.0416	0.1344
IR Inten --	10.7418	0.9557	8.7811
	4	5	6
	A	A	A
Frequencies --	283.9763	371.9860	432.2632
Red. masses --	2.5804	2.0436	4.6455
Frc consts --	0.1226	0.1666	0.5114
IR Inten --	3.3905	2.3458	4.8511
	7	8	9
	A	A	A
Frequencies --	466.5274	499.2205	620.2244
Red. masses --	2.6932	2.8907	3.3256
Frc consts --	0.3454	0.4245	0.7537
IR Inten --	8.1076	21.4316	15.2341
	10	11	12
	A	A	A
Frequencies --	706.8278	763.3791	823.3109
Red. masses --	2.6880	2.9599	1.6576
Frc consts --	0.7912	1.0163	0.6620
IR Inten --	4.6705	9.2528	10.7121
	13	14	15
	A	A	A
Frequencies --	854.1750	901.0867	935.7361
Red. masses --	2.6234	2.0258	1.6687
Frc consts --	1.1278	0.9691	0.8609
IR Inten --	1.4877	9.4194	24.7130
	16	17	18
	A	A	A
Frequencies --	973.9026	1009.4125	1040.9596
Red. masses --	2.7459	2.9513	1.8466
Frc consts --	1.5345	1.7718	1.1789
IR Inten --	108.1907	18.5229	10.5826
	19	20	21
	A	A	A
Frequencies --	1089.5437	1104.5368	1150.9598
Red. masses --	1.5606	2.2671	1.3953
Frc consts --	1.0915	1.6296	1.0890
IR Inten --	4.7017	31.4985	21.9949

	22	23	24
	A	A	A
Frequencies --	1173.0656	1248.0332	1281.2863
Red. masses --	1.5355	1.5865	1.3140
Frc consts --	1.2450	1.4560	1.2709
IR Inten --	5.7635	10.0862	7.3673

	25	26	27
	A	A	A
Frequencies --	1293.9946	1344.3044	1351.5879
Red. masses --	1.3933	1.3725	1.5424
Frc consts --	1.3746	1.4613	1.6602
IR Inten --	11.3578	1.3119	31.2666

	28	29	30
	A	A	A
Frequencies --	1362.3801	1379.8672	1392.2189
Red. masses --	1.3655	1.5526	1.5043
Frc consts --	1.4933	1.7417	1.7179
IR Inten --	8.4457	5.1427	1.5624

	31	32	33
	A	A	A
Frequencies --	1395.8165	1460.7763	1468.1764
Red. masses --	1.4924	1.1076	1.0956
Frc consts --	1.7132	1.3925	1.3914
IR Inten --	4.5255	16.3335	21.8913

	34	35	36
	A	A	A
Frequencies --	1495.8910	1505.0115	1815.6586
Red. masses --	1.0825	1.0956	11.1350
Frc consts --	1.4272	1.4621	21.6277
IR Inten --	10.4449	6.7510	427.1177

	37	38	39
	A	A	A
Frequencies --	3049.9600	3060.1889	3063.8606
Red. masses --	1.0669	1.0647	1.0627
Frc consts --	5.8476	5.8746	5.8776
IR Inten --	36.4121	18.0517	38.7588

	40	41	42
	A	A	A
Frequencies --	3067.6498	3110.3821	3113.5405
Red. masses --	1.0633	1.0975	1.0995
Frc consts --	5.8955	6.2557	6.2797
IR Inten --	14.5974	45.8965	37.0542

	43	44	45
	A	A	A
Frequencies --	3118.8574	3133.9592	3146.2600
Red. masses --	1.1041	1.0887	1.1009
Frc consts --	6.3275	6.3002	6.4206
IR Inten --	50.2780	36.3890	22.6423

21e

	1	2	3
	A	A	A
Frequencies --	93.6415	151.8839	285.2133
Red. masses --	5.0778	2.4923	6.6345
Frc consts --	0.0262	0.0339	0.3180
IR Inten --	2.4491	4.7246	1.8888

	4	5	6
	A	A	A
Frequencies --	312.9156	350.4984	396.1428
Red. masses --	1.9392	3.5559	4.6822
Frc consts --	0.1119	0.2574	0.4329
IR Inten --	0.6799	9.4691	3.8797

	7	8	9
	A	A	A
Frequencies --	426.2739	510.2743	600.5536
Red. masses --	2.9446	2.2568	4.1397
Frc consts --	0.3153	0.3462	0.8797
IR Inten --	1.7769	3.4934	30.8625
	10	11	12
	A	A	A
Frequencies --	683.5881	753.7755	851.4823
Red. masses --	2.9175	2.1718	1.7649
Frc consts --	0.8032	0.7270	0.7539
IR Inten --	6.9120	4.9144	21.9883
	13	14	15
	A	A	A
Frequencies --	872.6901	897.5701	928.5386
Red. masses --	2.5195	1.8167	1.6892
Frc consts --	1.1305	0.8623	0.8581
IR Inten --	2.0288	41.8346	15.9450
	16	17	18
	A	A	A
Frequencies --	972.6046	1058.0023	1086.3724
Red. masses --	2.4113	1.5275	3.8245
Frc consts --	1.3439	1.0074	2.6594
IR Inten --	7.6807	22.1193	121.3794
	19	20	21
	A	A	A
Frequencies --	1092.9023	1108.7045	1146.0129
Red. masses --	1.5975	2.1488	1.7508
Frc consts --	1.1243	1.5562	1.3548
IR Inten --	5.0011	48.1646	9.0831
	22	23	24
	A	A	A
Frequencies --	1159.3087	1249.8628	1270.3171
Red. masses --	2.2904	1.5036	1.3810
Frc consts --	1.8137	1.3839	1.3131
IR Inten --	7.7148	6.0819	1.3519
	25	26	27
	A	A	A
Frequencies --	1289.9369	1335.1973	1354.5601
Red. masses --	1.2629	1.2414	1.3594
Frc consts --	1.2381	1.3040	1.4696
IR Inten --	2.5426	6.9133	8.1687
	28	29	30
	A	A	A
Frequencies --	1362.9839	1375.1369	1398.7331
Red. masses --	1.4130	1.5055	1.4844
Frc consts --	1.5466	1.6774	1.7110
IR Inten --	4.0906	7.9444	2.1807
	31	32	33
	A	A	A
Frequencies --	1406.0719	1463.4075	1488.9209
Red. masses --	1.5771	1.1010	1.0960
Frc consts --	1.8370	1.3892	1.4315
IR Inten --	4.0706	18.7998	8.9664
	34	35	36
	A	A	A
Frequencies --	1492.8572	1503.5093	1816.2623
Red. masses --	1.0865	1.0988	11.8787
Frc consts --	1.4266	1.4634	23.0875
IR Inten --	14.1610	4.7463	461.3508
	37	38	39

	A	A	A
Frequencies --	3049.6327	3051.8628	3056.7492
Red. masses --	1.0699	1.0684	1.0637
Frc consts --	5.8625	5.8628	5.8559
IR Inten --	6.7203	18.6634	23.7321

	40	41	42
	A	A	A
Frequencies --	3057.6194	3067.4955	3115.3586
Red. masses --	1.0635	1.0794	1.0965
Frc consts --	5.8579	5.9839	6.2702
IR Inten --	50.5041	46.3620	43.0808

	43	44	45
	A	A	A
Frequencies --	3117.1017	3122.2943	3139.7403
Red. masses --	1.1002	1.1033	1.0982
Frc consts --	6.2982	6.3371	6.3787
IR Inten --	48.2304	46.6919	24.4233

22a

	1	2	3
	A	A	A
Frequencies --	82.9917	150.6587	242.1800
Red. masses --	5.2999	3.3789	3.4482
Frc consts --	0.0215	0.0452	0.1192
IR Inten --	3.1617	1.4603	7.1767

	4	5	6
	A	A	A
Frequencies --	260.4137	339.9125	385.8860
Red. masses --	3.6571	2.8265	2.5893
Frc consts --	0.1461	0.1924	0.2272
IR Inten --	3.0177	0.9343	4.9609

	7	8	9
	A	A	A
Frequencies --	415.4764	470.6482	602.9471
Red. masses --	4.4504	2.0899	3.9939
Frc consts --	0.4526	0.2727	0.8555
IR Inten --	2.7542	3.4146	7.1574

	10	11	12
	A	A	A
Frequencies --	664.3959	743.7529	817.2812
Red. masses --	3.1637	2.6210	1.5874
Frc consts --	0.8228	0.8542	0.6247
IR Inten --	4.5489	6.2474	11.8203

	13	14	15
	A	A	A
Frequencies --	847.7587	888.1191	927.9734
Red. masses --	2.8617	2.2658	1.6759
Frc consts --	1.2118	1.0530	0.8503
IR Inten --	3.2367	23.2925	27.3829

	16	17	18
	A	A	A
Frequencies --	963.9000	994.7225	1041.6424
Red. masses --	2.6543	2.7185	1.9238
Frc consts --	1.4530	1.5849	1.2298
IR Inten --	85.1330	58.9639	2.4027

	19	20	21
	A	A	A
Frequencies --	1063.5559	1088.3038	1138.9317
Red. masses --	1.9360	1.6371	1.5654
Frc consts --	1.2903	1.1424	1.1964
IR Inten --	85.2132	11.6241	18.7033

	22	23	24
	A	A	A
Frequencies --	1166.9910	1222.8651	1241.3209
Red. masses --	1.6165	2.1094	1.7107
Frc consts --	1.2971	1.8585	1.5531
IR Inten --	8.2303	101.0213	14.5837

	25	26	27
	A	A	A
Frequencies --	1275.6548	1301.2089	1331.7114
Red. masses --	1.4366	1.3282	1.3901
Frc consts --	1.3774	1.3250	1.4525
IR Inten --	33.6992	53.9990	19.9205

	28	29	30
	A	A	A
Frequencies --	1341.9703	1367.9623	1375.1785
Red. masses --	1.3876	1.4147	1.4753
Frc consts --	1.4723	1.5598	1.6438
IR Inten --	6.7325	5.2958	22.5197

	31	32	33
	A	A	A
Frequencies --	1395.0227	1416.3914	1466.2011
Red. masses --	1.5202	1.7212	1.0892
Frc consts --	1.7431	2.0344	1.3796
IR Inten --	4.7386	31.6261	12.3833

	34	35	36
	A	A	A
Frequencies --	1479.5268	1487.9690	1497.9014
Red. masses --	1.1356	1.0819	1.1009
Frc consts --	1.4646	1.4113	1.4553
IR Inten --	17.5408	9.1076	7.8651

	37	38	39
	A	A	A
Frequencies --	3051.8481	3057.7578	3061.7347
Red. masses --	1.0673	1.0632	1.0635
Frc consts --	5.8569	5.8568	5.8740
IR Inten --	14.6055	35.6995	20.1572

	40	41	42
	A	A	A
Frequencies --	3067.7488	3112.1399	3115.4038
Red. masses --	1.0628	1.0981	1.1015
Frc consts --	5.8930	6.2664	6.2987
IR Inten --	38.6709	43.2793	33.1352

	43	44	45
	A	A	A
Frequencies --	3121.4282	3140.0714	3146.8786
Red. masses --	1.1047	1.0891	1.0986
Frc consts --	6.3415	6.3272	6.4096
IR Inten --	58.6752	28.7357	12.4769

22e

	1	2	3
	A	A	A
Frequencies --	79.4454	151.7083	240.8727
Red. masses --	4.5372	2.6474	14.0987
Frc consts --	0.0169	0.0359	0.4820
IR Inten --	0.0983	2.3489	1.3424

	4	5	6
	A	A	A
Frequencies --	288.5819	351.8323	376.1327
Red. masses --	2.0556	3.1232	3.8686
Frc consts --	0.1009	0.2278	0.3225
IR Inten --	0.3955	5.5376	1.7851

	7	8	9
	A	A	A
Frequencies --	413.0449	482.8470	569.5170
Red. masses --	3.0324	2.8708	3.8276
Frc consts --	0.3048	0.3943	0.7315
IR Inten --	1.0345	5.7302	13.9385

	10	11	12
	A	A	A
Frequencies --	614.6591	732.9574	828.5342
Red. masses --	2.8124	3.0579	1.6598
Frc consts --	0.6260	0.9679	0.6713
IR Inten --	9.0489	2.3740	14.6188

	13	14	15
	A	A	A
Frequencies --	859.5106	884.6214	934.0559
Red. masses --	2.0657	2.1812	1.5390
Frc consts --	0.8991	1.0057	0.7911
IR Inten --	11.9973	18.9259	1.3446

	16	17	18
	A	A	A
Frequencies --	963.5457	1044.3984	1068.1597
Red. masses --	2.4606	1.9431	1.8303
Frc consts --	1.3460	1.2488	1.2304
IR Inten --	12.7243	38.2681	30.1433

	19	20	21
	A	A	A
Frequencies --	1090.5756	1096.5177	1133.4900
Red. masses --	1.7554	2.6612	1.8357
Frc consts --	1.2301	1.8852	1.3896
IR Inten --	32.6921	91.8451	5.5578

	22	23	24
	A	A	A
Frequencies --	1144.7937	1212.0599	1258.2806
Red. masses --	2.0915	2.0314	1.4370
Frc consts --	1.6149	1.7583	1.3404
IR Inten --	1.4396	45.4394	2.6003

	25	26	27
	A	A	A
Frequencies --	1274.4245	1313.9055	1323.1992
Red. masses --	1.3991	1.3945	1.4675
Frc consts --	1.3388	1.4184	1.5138
IR Inten --	30.1194	72.6272	11.0220

	28	29	30
	A	A	A
Frequencies --	1348.5798	1356.7785	1382.6229
Red. masses --	1.5116	1.4282	1.4707
Frc consts --	1.6198	1.5490	1.6565
IR Inten --	21.5616	67.2887	22.8604

	31	32	33
	A	A	A
Frequencies --	1391.6327	1404.0648	1478.3039
Red. masses --	1.4544	1.5813	1.1084
Frc consts --	1.6596	1.8367	1.4272
IR Inten --	18.6431	14.6952	9.5781

	34	35	36
	A	A	A
Frequencies --	1485.1122	1491.1880	1503.6657
Red. masses --	1.0868	1.0979	1.0970
Frc consts --	1.4123	1.4384	1.4614
IR Inten --	21.0174	5.3525	7.1713

	37	38	39
	A	A	A
Frequencies --	3042.8749	3054.5638	3058.4053
Red. masses --	1.0684	1.0700	1.0655
Frc consts --	5.8282	5.8822	5.8720
IR Inten --	5.4838	26.1520	26.9117

40	41	42
----	----	----

	A	A	A
Frequencies --	3059.7445	3066.7364	3117.2502
Red. masses --	1.0650	1.0757	1.0962
Frc consts --	5.8744	5.9607	6.2760
IR Inten --	32.3827	53.9667	46.1022
	43	44	45
	A	A	A
Frequencies --	3120.4216	3126.6796	3139.5372
Red. masses --	1.1014	1.1033	1.0972
Frc consts --	6.3189	6.3550	6.3720
IR Inten --	46.3634	48.1642	16.4084
23a	1	2	3
	A	A	A
Frequencies --	101.3503	152.6902	236.3914
Red. masses --	4.2064	3.0933	4.1580
Frc consts --	0.0255	0.0425	0.1369
IR Inten --	4.4886	1.3386	8.5445
	4	5	6
	A	A	A
Frequencies --	286.9464	374.5495	429.8574
Red. masses --	2.4268	2.0379	3.6273
Frc consts --	0.1177	0.1684	0.3949
IR Inten --	2.8141	3.4492	14.2560
	7	8	9
	A	A	A
Frequencies --	462.5456	491.7234	626.7545
Red. masses --	2.8530	2.4033	3.6401
Frc consts --	0.3596	0.3424	0.8425
IR Inten --	5.6420	19.0916	8.9218
	10	11	12
	A	A	A
Frequencies --	685.8283	772.3640	818.9751
Red. masses --	2.5024	3.0258	1.5545
Frc consts --	0.6935	1.0635	0.6143
IR Inten --	3.8297	9.3862	6.3295
	13	14	15
	A	A	A
Frequencies --	858.4601	893.6147	924.8834
Red. masses --	2.5619	1.9190	1.8038
Frc consts --	1.1124	0.9029	0.9091
IR Inten --	11.6955	5.0417	203.8745
	16	17	18
	A	A	A
Frequencies --	936.8132	986.5306	1010.4330
Red. masses --	1.6695	1.8079	2.7493
Frc consts --	0.8633	1.0367	1.6538
IR Inten --	36.1233	10.7255	23.9762
	19	20	21
	A	A	A
Frequencies --	1050.5253	1086.6575	1105.0565
Red. masses --	1.8258	1.4464	2.1673
Frc consts --	1.1872	1.0063	1.5593
IR Inten --	7.5776	11.8851	23.9292
	22	23	24
	A	A	A
Frequencies --	1145.1079	1176.9557	1197.4827
Red. masses --	1.7811	1.3126	1.2680
Frc consts --	1.3760	1.0713	1.0713
IR Inten --	61.0047	12.7585	25.7612
	25	26	27
	A	A	A
Frequencies --	1271.9793	1287.7044	1343.0414
Red. masses --	1.2852	1.2694	1.2789
Frc consts --	1.2251	1.2401	1.3592
IR Inten --	8.8657	2.8760	14.5561

	28	29	30
	A	A	A
Frequencies --	1346.0984	1367.2652	1373.5554
Red. masses --	1.3527	1.5047	1.3661
Frc consts --	1.4442	1.6573	1.5185
IR Inten --	9.0091	6.5564	14.5611

	31	32	33
	A	A	A
Frequencies --	1391.9955	1393.2074	1421.6861
Red. masses --	1.5264	1.4817	1.9483
Frc consts --	1.7426	1.6945	2.3202
IR Inten --	7.0148	0.4486	20.6711

	34	35	36
	A	A	A
Frequencies --	1465.2926	1468.6920	1493.2541
Red. masses --	1.0981	1.1333	1.0841
Frc consts --	1.3892	1.4403	1.4242
IR Inten --	2.4158	34.4301	11.1006

	37	38	39
	A	A	A
Frequencies --	1502.0147	1751.0600	3044.1235
Red. masses --	1.0995	9.1812	1.0672
Frc consts --	1.4615	16.5864	5.8269
IR Inten --	5.8823	153.7269	38.7794

	40	41	42
	A	A	A
Frequencies --	3058.9360	3060.2717	3060.8513
Red. masses --	1.0654	1.0639	1.0628
Frc consts --	5.8737	5.8706	5.8664
IR Inten --	16.6927	33.0741	32.6928

	43	44	45
	A	A	A
Frequencies --	3104.6651	3106.5181	3111.9376
Red. masses --	1.0901	1.0967	1.0975
Frc consts --	6.1907	6.2355	6.2621
IR Inten --	95.5403	15.0387	50.1442

	46	47	48
	A	A	A
Frequencies --	3116.3545	3135.5055	3482.6552
Red. masses --	1.1037	1.0995	1.0744
Frc consts --	6.3151	6.3691	7.6777
IR Inten --	52.2466	27.9561	0.8745

23e

	1	2	3
	A	A	A
Frequencies --	110.7049	158.0871	289.1920
Red. masses --	4.0316	2.4600	4.8132
Frc consts --	0.0291	0.0362	0.2372
IR Inten --	0.0710	1.9318	8.5799

	4	5	6
	A	A	A
Frequencies --	314.0729	355.4461	393.4042
Red. masses --	1.9287	3.4348	4.5619
Frc consts --	0.1121	0.2557	0.4160
IR Inten --	2.1682	15.0840	0.2934

	7	8	9
	A	A	A
Frequencies --	427.1427	501.9294	588.1792
Red. masses --	2.7431	2.2650	3.5721
Frc consts --	0.2949	0.3362	0.7281
IR Inten --	3.5552	3.0692	37.2475

	10	11	12
	A	A	A
Frequencies --	669.4544	768.0273	847.7167
Red. masses --	2.6428	2.3048	1.6377
Frc consts --	0.6979	0.8010	0.6934
IR Inten --	2.1585	5.7717	30.1576

	13	14	15
	A	A	A
Frequencies --	868.2908	888.4306	902.0707
Red. masses --	2.1535	1.8756	1.4930
Frc consts --	0.9566	0.8723	0.7158
IR Inten --	10.6486	47.7259	46.2951

	16	17	18
	A	A	A
Frequencies --	969.5360	982.4248	1057.0021
Red. masses --	2.4198	1.3214	2.2212
Frc consts --	1.3401	0.7514	1.4622
IR Inten --	4.8650	40.2748	92.1209

	19	20	21
	A	A	A
Frequencies --	1070.4529	1084.4323	1101.1680
Red. masses --	2.0550	1.9561	1.9744
Frc consts --	1.3874	1.3553	1.4106
IR Inten --	28.6786	33.7274	7.0674

	22	23	24
	A	A	A
Frequencies --	1135.8570	1171.1016	1214.3786
Red. masses --	2.0430	1.4902	1.3827
Frc consts --	1.5530	1.2042	1.2014
IR Inten --	16.3535	4.3426	19.9472

	25	26	27
	A	A	A
Frequencies --	1273.7646	1283.7449	1321.2924
Red. masses --	1.3384	1.2585	1.3295
Frc consts --	1.2794	1.2220	1.3675
IR Inten --	1.3064	6.7477	32.1903

	28	29	30
	A	A	A
Frequencies --	1344.0526	1365.7960	1367.8008
Red. masses --	1.1737	1.3748	1.4239
Frc consts --	1.2493	1.5109	1.5695
IR Inten --	3.4540	2.8054	2.9958

	31	32	33
	A	A	A
Frequencies --	1383.2199	1396.3430	1424.3061
Red. masses --	1.5066	1.4640	1.8987
Frc consts --	1.6984	1.6818	2.2694
IR Inten --	17.2056	2.5409	23.3681

	34	35	36
	A	A	A
Frequencies --	1471.5846	1488.4589	1493.0033
Red. masses --	1.1078	1.1074	1.0907
Frc consts --	1.4134	1.4456	1.4325
IR Inten --	17.2899	10.3240	13.0951

	37	38	39
	A	A	A
Frequencies --	1503.0833	1752.2032	3046.0432
Red. masses --	1.0996	10.0710	1.0695
Frc consts --	1.4638	18.2175	5.8464
IR Inten --	4.6724	198.0567	13.0381

40	41	42
A	A	A

Frequencies --	3049.8665	3053.5346	3058.2352
Red. masses --	1.0677	1.0629	1.0634
Frc consts --	5.8514	5.8393	5.8600
IR Inten --	22.0049	63.1569	29.5143

	43	44	45
	A	A	A
Frequencies --	3075.8119	3111.9645	3114.9372
Red. masses --	1.0825	1.0976	1.0990
Frc consts --	6.0338	6.2627	6.2825
IR Inten --	36.7900	55.6860	56.6046

	46	47	48
	A	A	A
Frequencies --	3123.0647	3131.9387	3488.9552
Red. masses --	1.1030	1.0977	1.0732
Frc consts --	6.3384	6.3440	7.6971
IR Inten --	53.4488	28.5395	8.2339

24a

	1	2	3
	A	A	A
Frequencies --	101.3645	156.2007	237.1415
Red. masses --	4.2667	3.1553	3.7013
Frc consts --	0.0258	0.0454	0.1226
IR Inten --	4.8802	1.3623	6.9263

	4	5	6
	A	A	A
Frequencies --	288.9864	374.1964	431.5744
Red. masses --	2.4367	2.0431	4.3059
Frc consts --	0.1199	0.1686	0.4725
IR Inten --	4.9718	2.1494	8.6682

	7	8	9
	A	A	A
Frequencies --	460.2427	488.5875	631.4663
Red. masses --	2.8510	2.1865	3.5734
Frc consts --	0.3558	0.3075	0.8395
IR Inten --	7.5548	13.9083	9.0218

	10	11	12
	A	A	A
Frequencies --	690.2650	768.4771	822.0974
Red. masses --	2.6880	2.9573	1.6522
Frc consts --	0.7546	1.0290	0.6579
IR Inten --	3.1114	7.4585	12.3662

	13	14	15
	A	A	A
Frequencies --	857.2282	889.7706	925.2831
Red. masses --	2.4105	1.7524	1.9093
Frc consts --	1.0436	0.8174	0.9631
IR Inten --	1.6887	36.8012	35.7449

	16	17	18
	A	A	A
Frequencies --	933.7002	990.1084	1011.6146
Red. masses --	1.6707	1.7525	2.7378
Frc consts --	0.8582	1.0122	1.6508
IR Inten --	28.3374	106.7407	58.7152

	19	20	21
	A	A	A
Frequencies --	1051.3685	1089.3292	1104.8187
Red. masses --	1.8474	1.5120	2.2564
Frc consts --	1.2032	1.0571	1.6228
IR Inten --	17.2784	13.6586	37.4264

	22	23	24
	A	A	A
Frequencies --	1144.2769	1178.7622	1198.7820
Red. masses --	1.5567	1.4009	1.2514
Frc consts --	1.2009	1.1469	1.0595
IR Inten --	15.8681	6.0319	25.4013

	25	26	27
	A	A	A
Frequencies --	1270.3263	1288.5459	1344.5580
Red. masses --	1.2942	1.2446	1.3220
Frc consts --	1.2305	1.2175	1.4081
IR Inten --	0.1410	2.4957	3.7638

	28	29	30
	A	A	A
Frequencies --	1350.9392	1363.5770	1374.4554
Red. masses --	1.3156	1.3546	1.4638
Frc consts --	1.4146	1.4839	1.6293
IR Inten --	6.3701	9.7106	20.1673

	31	32	33
	A	A	A
Frequencies --	1395.1033	1396.1431	1425.4189
Red. masses --	1.4708	1.5661	2.2064
Frc consts --	1.6866	1.7985	2.6413
IR Inten --	3.2636	1.8978	77.9709

	34	35	36
	A	A	A
Frequencies --	1467.1782	1468.8636	1493.7125
Red. masses --	1.0999	1.1025	1.0854
Frc consts --	1.3950	1.4015	1.4268
IR Inten --	7.8845	31.1428	8.0813

	37	38	39
	A	A	A
Frequencies --	1501.9331	1752.5213	3044.1400
Red. masses --	1.0983	9.1867	1.0675
Frc consts --	1.4597	16.6241	5.8285
IR Inten --	6.8319	154.5221	38.4091

	40	41	42
	A	A	A
Frequencies --	3058.3544	3058.7338	3060.4010
Red. masses --	1.0647	1.0618	1.0621
Frc consts --	5.8674	5.8532	5.8608
IR Inten --	27.3729	16.8821	42.6886

	43	44	45
	A	A	A
Frequencies --	3106.9167	3109.4724	3115.5376
Red. masses --	1.0961	1.1007	1.1027
Frc consts --	6.2338	6.2706	6.3065
IR Inten --	56.1480	55.1206	38.4758

	46	47	48
	A	A	A
Frequencies --	3119.3027	3129.7378	3486.0369
Red. masses --	1.1033	1.0889	1.0743
Frc consts --	6.3251	6.2842	7.6920
IR Inten --	45.9462	34.8613	1.5376

24e

	1	2	3
	A	A	A
Frequencies --	100.3533	161.3729	299.6674
Red. masses --	4.2879	2.4929	4.7060
Frc consts --	0.0254	0.0382	0.2490
IR Inten --	0.5734	4.5474	0.1062

	4	5	6
	A	A	A
Frequencies --	315.5065	352.2852	395.8687
Red. masses --	2.0178	3.3528	4.4471
Frc consts --	0.1183	0.2452	0.4106
IR Inten --	0.2089	1.4710	7.7939

	7	8	9
	A	A	A
Frequencies --	429.3925	507.1764	586.5205
Red. masses --	2.8141	2.2475	3.4180
Frc consts --	0.3057	0.3406	0.6928
IR Inten --	0.6530	12.7069	28.7735

	10	11	12
	A	A	A
Frequencies --	670.7833	775.9939	850.5048
Red. masses --	2.7100	2.2438	1.7343
Frc consts --	0.7184	0.7961	0.7391
IR Inten --	2.7249	1.1480	12.7110

	13	14	15
	A	A	A
Frequencies --	870.2718	890.1072	895.0580
Red. masses --	1.7924	1.5893	2.0576
Frc consts --	0.7998	0.7419	0.9712
IR Inten --	29.8248	30.6342	28.4634

	16	17	18
	A	A	A
Frequencies --	970.3193	980.0178	1062.8605
Red. masses --	2.2104	1.4110	1.8186
Frc consts --	1.2262	0.7984	1.2104
IR Inten --	24.4551	38.9713	34.8941

	19	20	21
	A	A	A
Frequencies --	1077.8371	1088.3317	1102.4056
Red. masses --	2.1570	2.4354	2.1305
Frc consts --	1.4764	1.6996	1.5255
IR Inten --	24.2903	125.7000	32.0246

	22	23	24
	A	A	A
Frequencies --	1134.8370	1169.7037	1207.1571
Red. masses --	1.9295	1.4819	1.2954
Frc consts --	1.4641	1.1946	1.1122
IR Inten --	5.1604	12.4546	21.2954

	25	26	27
	A	A	A
Frequencies --	1273.5370	1285.0970	1334.9203
Red. masses --	1.3443	1.2507	1.2927
Frc consts --	1.2846	1.2170	1.3572
IR Inten --	0.7836	1.1339	12.9174

	28	29	30
	A	A	A
Frequencies --	1353.0462	1362.7945	1368.1347
Red. masses --	1.2048	1.3716	1.4140
Frc consts --	1.2996	1.5008	1.5594
IR Inten --	24.4908	8.6666	3.0356

	31	32	33
	A	A	A
Frequencies --	1382.4567	1397.5723	1436.1398
Red. masses --	1.5464	1.4703	1.8207
Frc consts --	1.7413	1.6920	2.2126
IR Inten --	14.0860	1.3084	16.1827

	34	35	36
	A	A	A
Frequencies --	1479.1338	1487.6303	1494.4426
Red. masses --	1.1011	1.1028	1.0948
Frc consts --	1.4194	1.4380	1.4406
IR Inten --	23.5671	6.9143	15.4881

37	38	39
A	A	A

Frequencies	--	1504.1161	1753.6432	3046.2885
Red. masses	--	1.1016	9.5319	1.0672
Frc consts	--	1.4683	17.2708	5.8351
IR Inten	--	2.7419	190.7894	13.1581

		40	41	42
		A	A	A
Frequencies	--	3049.9050	3054.4122	3055.6871
Red. masses	--	1.0690	1.0645	1.0644
Frc consts	--	5.8587	5.8510	5.8556
IR Inten	--	25.4770	28.3552	36.8274

		43	44	45
		A	A	A
Frequencies	--	3064.1856	3112.3030	3114.5661
Red. masses	--	1.0783	1.0974	1.0984
Frc consts	--	5.9649	6.2630	6.2779
IR Inten	--	63.4004	52.6388	60.7210

		46	47	48
		A	A	A
Frequencies	--	3118.6537	3121.4430	3496.4271
Red. masses	--	1.1008	1.1030	1.0743
Frc consts	--	6.3081	6.3322	7.7381
IR Inten	--	26.9535	61.8374	1.8493

25a

		1	2	3
		A	A	A
Frequencies	--	111.7562	159.8149	235.7105
Red. masses	--	3.4420	3.0324	3.4841
Frc consts	--	0.0253	0.0456	0.1141
IR Inten	--	1.1432	2.8309	6.2133

		4	5	6
		A	A	A
Frequencies	--	288.6735	372.8275	401.5685
Red. masses	--	2.3235	2.0077	2.4986
Frc consts	--	0.1141	0.1644	0.2374
IR Inten	--	1.9559	3.3384	1.3488

		7	8	9
		A	A	A
Frequencies	--	454.9616	472.7757	627.1738
Red. masses	--	3.4016	2.0170	4.1580
Frc consts	--	0.4148	0.2656	0.9636
IR Inten	--	3.6948	5.8941	4.0442

		10	11	12
		A	A	A
Frequencies	--	662.9997	743.4937	782.4418
Red. masses	--	2.2880	1.2573	2.2210
Frc consts	--	0.5926	0.4095	0.8011
IR Inten	--	12.2342	4.0245	4.1547

		13	14	15
		A	A	A
Frequencies	--	821.3493	866.3992	886.7568
Red. masses	--	1.7714	2.5147	2.2646
Frc consts	--	0.7041	1.1122	1.0492
IR Inten	--	16.2669	6.0646	60.4916

		16	17	18
		A	A	A
Frequencies	--	918.0352	955.5894	967.7950
Red. masses	--	1.6097	2.1623	1.3906
Frc consts	--	0.7993	1.1633	0.7674
IR Inten	--	38.7827	56.6822	105.1978

		19	20	21
		A	A	A
Frequencies	--	1000.8618	1009.1885	1056.2365
Red. masses	--	1.6760	2.4633	1.7935
Frc consts	--	0.9892	1.4781	1.1789
IR Inten	--	23.3180	16.9089	4.9976

	22	23	24
	A	A	A
Frequencies --	1095.9723	1111.4064	1177.5467
Red. masses --	1.6768	1.7238	1.2197
Frc consts --	1.1867	1.2545	0.9965
IR Inten --	15.1722	8.8164	16.2292
	25	26	27
	A	A	A
Frequencies --	1188.1527	1271.7383	1290.5853
Red. masses --	1.5572	1.3451	1.2283
Frc consts --	1.2952	1.2818	1.2054
IR Inten --	7.6762	0.2332	1.8686
	28	29	30
	A	A	A
Frequencies --	1322.9748	1347.4438	1359.8126
Red. masses --	1.5835	1.2712	1.3181
Frc consts --	1.6330	1.3598	1.4361
IR Inten --	5.0591	10.4311	7.2006
	31	32	33
	A	A	A
Frequencies --	1372.2000	1380.1766	1392.8627
Red. masses --	1.6303	1.5931	1.6044
Frc consts --	1.8086	1.7880	1.8340
IR Inten --	9.8520	7.7542	1.6274
	34	35	36
	A	A	A
Frequencies --	1397.7001	1458.9447	1466.5458
Red. masses --	1.5845	1.1581	1.0969
Frc consts --	1.8238	1.4523	1.3899
IR Inten --	1.7805	9.0477	14.0024
	37	38	39
	A	A	A
Frequencies --	1478.4911	1490.3937	1499.9898
Red. masses --	1.1292	1.0865	1.0979
Frc consts --	1.4543	1.4220	1.4554
IR Inten --	22.0507	9.6359	5.5735
	40	41	42
	A	A	A
Frequencies --	1741.5152	3036.8493	3046.5608
Red. masses --	5.9672	1.0674	1.0638
Frc consts --	10.6629	5.8000	5.8176
IR Inten --	20.6894	39.5019	42.3377
	43	44	45
	A	A	A
Frequencies --	3055.4985	3056.8701	3098.5279
Red. masses --	1.0629	1.0638	1.0963
Frc consts --	5.8465	5.8569	6.2012
IR Inten --	43.4254	23.4454	93.2327
	46	47	48
	A	A	A
Frequencies --	3103.2739	3107.5636	3111.3460
Red. masses --	1.0994	1.0911	1.1018
Frc consts --	6.2380	6.2081	6.2840
IR Inten --	50.8434	59.7266	53.6967
	49	50	51
	A	A	A
Frequencies --	3112.4408	3143.6409	3231.4614
Red. masses --	1.0990	1.0619	1.1165
Frc consts --	6.2729	6.1831	6.8690
IR Inten --	47.2604	13.7515	17.8591

25e

	1	2	3
	A	A	A
Frequencies --	113.9245	170.2063	288.5704
Red. masses --	3.3272	2.4477	3.7139
Frc consts --	0.0254	0.0418	0.1822
IR Inten --	1.8801	0.7615	3.9630
	4	5	6
	A	A	A
Frequencies --	311.5742	353.7252	389.2068
Red. masses --	1.9215	3.0512	3.6415
Frc consts --	0.1099	0.2249	0.3250
IR Inten --	1.8785	2.9756	2.2338
	7	8	9
	A	A	A
Frequencies --	426.2422	481.5325	562.7025
Red. masses --	2.5842	2.4982	2.9426
Frc consts --	0.2766	0.3413	0.5490
IR Inten --	0.8439	4.1495	18.6021
	10	11	12
	A	A	A
Frequencies --	642.6875	746.3475	788.7642
Red. masses --	2.3663	1.1571	2.0573
Frc consts --	0.5759	0.3798	0.7541
IR Inten --	10.0018	0.6875	2.0463
	13	14	15
	A	A	A
Frequencies --	843.3164	876.0761	878.9650
Red. masses --	1.7049	1.6594	2.5304
Frc consts --	0.7144	0.7504	1.1518
IR Inten --	15.0028	25.3906	0.6248
	16	17	18
	A	A	A
Frequencies --	945.5742	952.9109	960.5092
Red. masses --	1.4086	1.8140	1.7683
Frc consts --	0.7421	0.9705	0.9612
IR Inten --	73.1028	15.2529	25.8919
	19	20	21
	A	A	A
Frequencies --	1001.7785	1053.4807	1074.3170
Red. masses --	1.6556	3.1814	1.9399
Frc consts --	0.9789	2.0803	1.3192
IR Inten --	15.7925	113.2811	29.7297
	22	23	24
	A	A	A
Frequencies --	1095.3930	1121.8996	1170.3922
Red. masses --	1.8574	1.7047	1.5191
Frc consts --	1.3131	1.2642	1.2260
IR Inten --	2.9154	3.5958	3.8242
	25	26	27
	A	A	A
Frequencies --	1182.8219	1273.2714	1276.0966
Red. masses --	1.6013	1.4520	1.3550
Frc consts --	1.3199	1.3869	1.3000
IR Inten --	1.6080	0.7277	3.3930
	28	29	30
	A	A	A
Frequencies --	1291.8085	1341.7828	1362.2322
Red. masses --	1.3565	1.2087	1.3764
Frc consts --	1.3337	1.2821	1.5049
IR Inten --	0.2140	0.2867	1.2822
	31	32	33
	A	A	A

Frequencies	--	1368.9279	1381.1097	1393.8764
Red. masses	--	1.4486	1.5468	1.4763
Frc consts	--	1.5994	1.7384	1.6900
IR Inten	--	2.3334	4.6535	0.5154
		34	35	36
		A	A	A
Frequencies	--	1403.8104	1445.2560	1482.0723
Red. masses	--	1.6054	1.1792	1.1035
Frc consts	--	1.8641	1.4512	1.4282
IR Inten	--	17.5523	7.1633	13.3818
		37	38	39
		A	A	A
Frequencies	--	1485.7687	1491.7290	1502.2495
Red. masses	--	1.1017	1.0921	1.0990
Frc consts	--	1.4329	1.4318	1.4613
IR Inten	--	11.2875	13.0993	3.8027
		40	41	42
		A	A	A
Frequencies	--	1742.1081	3032.3361	3042.5620
Red. masses	--	6.3443	1.0677	1.0685
Frc consts	--	11.3446	5.7843	5.8280
IR Inten	--	40.3659	32.5326	31.3023
		43	44	45
		A	A	A
Frequencies	--	3047.3955	3051.1688	3057.9174
Red. masses	--	1.0625	1.0724	1.0729
Frc consts	--	5.8134	5.8824	5.9111
IR Inten	--	65.2767	6.6103	76.5911
		46	47	48
		A	A	A
Frequencies	--	3103.5704	3105.5678	3109.6410
Red. masses	--	1.0972	1.0982	1.0988
Frc consts	--	6.2265	6.2407	6.2605
IR Inten	--	71.2010	72.8457	41.6269
		49	50	51
		A	A	A
Frequencies	--	3115.4625	3158.7340	3252.1591
Red. masses	--	1.1035	1.0616	1.1158
Frc consts	--	6.3106	6.2406	6.9534
IR Inten	--	70.6799	11.5214	9.6845