Supporting Information

for

Utilizing the σ-complex stability for quantifying reactivity in nucleophilic substitution of aromatic fluorides

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Coordinates of all optimized structures, electronic energies, *SS* values calculated with larger basis set and zero point energies.

Contents

Coordinates (in xyz-format) for entries 1–12, Table 1

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Table 1 entry 1 starting material
C1	2.690781	-2.611010	0.017279
N2	1.565374	-1.928969	0.012945
C3	1.629622	-0.615049	0.009090
C4	2.823865	0.095769	0.009785
C5	4.019064	-0.624568	0.014657
C6	3.947568	-2.018531	0.018354
Cl7	5.538821	0.182732	0.016057
F8	2.822249	1.429289	0.005930
F9	2.607309	-3.941744	0.020726
F10	0.480156	0.060782	0.004363
F11	5.052624	-2.765212	0.022806

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Table 1 entry 1 sigma-complex
C1	-2.026805	1.513136	-0.083747
C2	-0.786023	2.128619	-0.369297
C3	0.315793	1.310641	-0.328902
N4	0.313484	0.014457	-0.066359
C5	-0.876412	-0.656020	0.048354
C6	-2.072957	0.171190	0.171519
F8	1.530719	1.863850	-0.533906
Cl8	-3.476015	2.477055	-0.052029
F12	-1.066492	-1.617292	-1.061211
N12	-0.774987	-1.726555	1.165406
H13	-0.618791	-1.299834	2.082774
H14	0.018653	-2.341923	0.959917
H15	-1.619415	-2.305036	1.206435
F14	-0.700012	3.456179	-0.633470
F15	-3.237851	-0.462798	0.464880

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Table 1 entry 2 starting material
C1	2.689688	-2.600943	0.017036
N2	1.558714	-1.928344	0.012986
C3	1.642495	-0.608772	0.009084
C4	2.820713	0.125436	0.009552
C5	4.004736	-0.613673	0.014559
C6	3.947804	-2.006972	0.018265
F7	5.051333	-2.759444	0.022855
Cl8	5.550806	0.169441	0.016212
H9	2.812041	1.208159	0.006058
F10	2.612211	-3.932165	0.020439
F11	0.474862	0.042906	0.004603

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Table 1 entry 2 sigma-complex
C1	-2.007284	1.524289	-0.064552
C2	-0.772199	2.167235	-0.330615

C3	0.310135	1.316071	-0.289574
N4	0.321258	0.015307	-0.053525
C5	-0.875669	-0.649693	0.059287
C6	-2.072210	0.183535	0.168800
F7	1.541263	1.850219	-0.481417
Cl8	-3.482634	2.471311	-0.030603
F9	-1.058751	-1.608594	-1.038044
N10	-0.786403	-1.704260	1.193240
H11	-0.616362	-1.263264	2.101368
H12	-0.005809	-2.339053	0.997609
H13	-1.641799	-2.264422	1.251426
H14	-0.681639	3.228387	-0.517223
F15	-3.241339	-0.459757	0.436329

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Table 1 entry 3 starting material

C1	2.675334	-2.615783	0.017190
N2	1.546133	-1.941020	0.012756
C3	1.619545	-0.627715	0.009123
C4	2.852768	0.027177	0.010193
N5	3.981891	-0.647533	0.014882
C6	3.908448	-1.960934	0.018193
F7	5.039224	-2.659440	0.022572
F9	2.907484	1.355201	0.006323
F10	2.620499	-3.943793	0.020805
F11	0.488885	0.070940	0.004446

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Table 1 entry 3 sigma-complex

C1	-1.842205	1.508450	0.157053
C2	-0.756359	2.024727	-0.500594
N3	0.315970	1.246452	-0.709182
C4	0.258302	0.017576	-0.332542
C5	-0.943001	-0.623962	0.217477
N6	-1.924213	0.255533	0.586446
F7	-1.427079	-1.624664	-0.754229
N8	-0.637874	-1.614359	1.355658
H9	0.045890	-2.318584	1.062258
F10	1.347564	-0.775114	-0.493717
F11	-0.689728	3.316658	-0.910522
H12	-1.503172	-2.100755	1.613418
H13	-0.284341	-1.133367	2.187819
F14	-2.888736	2.306351	0.450096

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Table 1 entry 4 starting material

C1	1.065205	3.966074	4.675460
C2	0.230655	3.423245	3.704831
C3	0.479225	3.773703	2.380371
C4	1.533359	4.636814	2.085791
C5	2.290801	5.107832	3.150760
N6	2.062594	4.781894	4.406956
F7	-0.279752	3.291126	1.404445
F8	0.852576	3.649167	5.953454
F9	-0.770625	2.598771	4.018300

F10	1.792168	4.987670	0.824006
F11	3.307151	5.935301	2.903364

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Table 1 entry 4 sigma-complex

C1	-1.897057	1.527900	0.067336
N2	-0.760836	2.204329	-0.082473
C3	0.329249	1.440833	-0.077019
C4	0.355552	0.082963	0.068251
C5	-0.860426	-0.702686	0.147112
C6	-2.011215	0.175314	0.221453
F8	1.504069	2.090631	-0.212280
F11	-3.025416	2.267791	0.080936
F12	-0.969162	-1.667522	-0.941286
N12	-0.823967	-1.747666	1.296975
H13	-0.743180	-1.295019	2.211903
H14	-0.027791	-2.380422	1.173178
H15	-1.675392	-2.317358	1.287646
F14	1.530537	-0.612544	0.071713
F15	-3.227263	-0.424942	0.378615

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Table 1 entry 5 starting material

C1	2.691655	-2.613678	0.017321
N2	1.565648	-1.931113	0.013137
C3	1.629256	-0.616153	0.009348
C4	2.816516	0.113623	0.009854
C5	3.997532	-0.632236	0.014898
C6	3.947345	-2.022837	0.018503
F7	5.068002	-2.747107	0.022865
F8	5.177741	-0.028003	0.016038
Cl9	2.846551	1.841340	0.004484
F10	2.606183	-3.942511	0.020495
F11	0.468591	0.038129	0.004575

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Table 1 entry 5 sigma-complex

C1	-1.946699	1.535814	0.083443
N2	-0.808991	2.225325	-0.024428
C3	0.283652	1.475065	-0.007354
C4	0.337180	0.107511	0.127457
C5	-0.885826	-0.688376	0.175017
C6	-2.050124	0.185684	0.213882
F8	1.441732	2.151999	-0.121644
F11	-3.077610	2.268124	0.072999
F12	-0.974523	-1.642737	-0.903661
N12	-0.917612	-1.715003	1.341451
H13	-0.810412	-1.248987	2.246998
H14	-0.170409	-2.409392	1.240911
H15	-1.809253	-2.220104	1.340650
Cl14	1.872058	-0.749585	0.069147
F15	-3.261422	-0.432056	0.325617

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Table 1 entry 6 starting material

C1	1.068080	3.970436	4.655075
C2	0.212718	3.410749	3.688162
C3	0.455512	3.755040	2.378919
C4	1.533701	4.629324	2.149609
N5	2.293733	5.116353	3.094169
N6	2.055056	4.779322	4.375938
F7	-0.280044	3.293631	1.381448
F8	0.867943	3.664388	5.930439
F9	-0.772233	2.596220	4.030161
F10	1.803825	4.988017	0.900692

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Table 1 entry 6 sigma-complex

C1	-1.972740	1.389336	0.099594
N2	-0.887512	2.146914	0.205292
N3	0.276925	1.467998	0.383453
C4	0.300489	0.182742	0.428949
C5	-0.808654	-0.755636	0.246499
C6	-2.017562	0.021039	0.155426
F11	-3.124968	2.063694	-0.054739
F12	-0.577012	-1.616690	-0.891232
N12	-0.841206	-1.852563	1.330383
H13	0.038546	-2.378706	1.332386
H14	-1.599357	-2.514749	1.137553
H15	-0.987443	-1.453465	2.262622
F18	-3.195700	-0.653083	0.062013
F14	1.503365	-0.412269	0.628203

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Table 1 entry 7 starting material

C1	1.064300	3.964468	4.681431
C2	0.231856	3.423558	3.709070
C3	0.491580	3.781314	2.393591
C4	1.544961	4.647110	2.074578
C5	2.289610	5.106135	3.160505
N6	2.061820	4.779744	4.419604
F7	-0.279690	3.286669	1.432344
F8	0.848223	3.645509	5.953024
F9	-0.768894	2.600035	4.021063
F10	3.313157	5.934504	2.967593
C11	1.788978	5.007868	0.629514
F12	2.828146	5.841213	0.470835
F13	2.035703	3.902559	-0.106001
F14	0.701966	5.603557	0.093642

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Table 1 entry 7 sigma-complex

C1	-1.979735	1.241543	-0.504956
C2	-0.908863	2.122725	-0.411748
C3	0.280518	1.502054	0.072916
C4	0.339152	0.176256	0.351891
C5	-0.798921	-0.691796	0.056110
N6	-1.982418	-0.045620	-0.244320
F11	-3.185800	1.720671	-0.870482

F12	-0.439770	-1.627276	-0.991323
N12	-1.051216	-1.732935	1.169521
H13	-0.206192	-2.275932	1.371633
H14	-1.776904	-2.386169	0.856003
H15	-1.374189	-1.290146	2.034380
F15	1.373143	2.261888	0.268842
C18	-0.947898	3.581749	-0.682262
F19	0.078533	3.984180	-1.481948
F20	-2.086839	3.979935	-1.286990
F21	-0.833034	4.335103	0.450598
F18	1.475712	-0.410385	0.816086

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Table 1 entry 8 sigma-complex (the starting material for this entry is the same as for entry 7)

C1	-1.955629	1.445767	0.168643
N2	-0.823564	2.165484	0.137657
C3	0.271590	1.437880	0.197388
C4	0.385470	0.062530	0.324924
C5	-0.840192	-0.749922	0.313493
C6	-2.030871	0.096973	0.271281
F8	1.418884	2.145660	0.128839
F11	-3.095593	2.156616	0.100600
F12	-0.855497	-1.707346	-0.755210
N12	-0.959540	-1.753672	1.497372
H13	-0.984146	-1.261840	2.394827
H14	-0.167909	-2.402933	1.503511
H15	-1.818893	-2.305325	1.408724
C15	1.727865	-0.572485	0.230290
F15	1.661221	-1.917327	0.459380
F16	2.311408	-0.430475	-0.989005
F17	2.622511	-0.075013	1.119940
F18	-3.226784	-0.555020	0.301399

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Table 1 entry 9 starting material

C1	2.736800	-2.580715	0.018235
N2	1.600187	-1.917132	0.014924
C3	1.681289	-0.603559	0.011069
C4	2.862341	0.139962	0.010385
C5	4.042744	-0.613084	0.014247
C6	4.011649	-2.013021	0.018621
F7	5.211254	0.010758	0.013584
F8	2.632646	-3.906188	0.021537
F9	0.522088	0.047511	0.007528
C10	5.222463	-2.916291	0.023434
F11	6.379110	-2.237847	0.027351
F12	5.216061	-3.718710	1.109024
F13	5.223981	-3.719705	-1.061211
C14	2.785677	1.648587	0.004794
F15	3.992982	2.232346	0.009997
F16	2.123527	2.089583	-1.085615
F17	2.110911	2.096977	1.084311

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Table 1 entry 9 sigma-complex

C1	-1.931578	1.383135	-0.207962
C2	-0.782539	2.185201	-0.244878
C3	0.401946	1.444171	-0.072667
C4	0.430200	0.088709	0.176124
C5	-0.853276	-0.648081	0.160151
N6	-2.017502	0.105284	-0.002387
F8	1.578059	2.083363	-0.169179
F11	-3.110626	2.006053	-0.401289
F12	-0.808198	-1.674375	-0.829550
N12	-1.079875	-1.543552	1.410104
H13	-1.212315	-0.972984	2.249706
H14	-0.294671	-2.181283	1.566172
H15	-1.928054	-2.103693	1.271886
C15	-0.885303	3.651546	-0.477459
F15	0.290964	4.293922	-0.317501
F16	-1.326829	3.958166	-1.729176
F17	-1.770475	4.243292	0.369147
C18	1.727701	-0.643779	0.176697
F19	1.579095	-1.928034	0.615113
F20	2.299158	-0.740191	-1.052814
F21	2.663975	-0.073813	0.973074

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Table 1 entry 10 starting material

C1	2.723940	-2.545023	0.017142
N2	1.554668	-1.929105	0.012697
C3	1.614924	-0.609558	0.009071
C4	2.811687	0.098096	0.009807
C5	3.958893	-0.686983	0.014623
N6	3.930995	-2.007712	0.018633
F8	5.143628	-0.099850	0.015645
F9	2.855320	1.428949	0.006123
F10	2.680088	-3.868812	0.020548
F11	0.472021	0.055476	0.004515

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Table 1 entry 10 sigma-complex

C1	-1.928733	1.512392	0.045882
N2	-0.752915	2.136638	-0.171144
C3	0.262304	1.296134	-0.191906
N4	0.310737	-0.005215	-0.049453
C5	-0.897996	-0.682252	0.061366
C6	-2.073398	0.178316	0.207222
F8	1.461201	1.879766	-0.372970
F11	-3.003924	2.313713	0.105075
F12	-1.080623	-1.583454	-1.038712
N12	-0.790601	-1.728163	1.188568
H13	-0.582148	-1.283782	2.087235
H14	-0.028907	-2.379291	0.970447
H15	-1.655235	-2.269437	1.280852
F14	-3.277617	-0.411578	0.430010

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Table 1 entry 11 sigma-complex (the starting material for this entry is the same as for entry 9)

C1	-1.892700	1.491384	0.333497
N2	-0.764497	2.182059	0.240184
C3	0.323116	1.424592	0.196469
C4	0.409191	0.057686	0.305593
C5	-0.839670	-0.728064	0.443548
C6	-2.046720	0.131726	0.457313
F8	1.463982	2.114133	0.017695
F11	-3.003282	2.249241	0.294203
F12	-0.932064	-1.723599	-0.564776
N12	-0.790293	-1.652557	1.698072
H13	-0.716980	-1.094385	2.553381
H14	0.016749	-2.281685	1.651339
H15	-1.636837	-2.226270	1.757011
C15	1.721955	-0.613379	0.078079
F15	1.663740	-1.945701	0.368639
F16	2.152757	-0.529664	-1.206353
F17	2.720778	-0.099894	0.835255
C18	-3.415020	-0.459068	0.391974
F19	-3.402717	-1.792733	0.683585
F20	-4.284274	0.113942	1.258245
F21	-3.989338	-0.349944	-0.833007

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Table 1 entry 12 sigma-complex

C1	0.471796	2.061718	0.080562
C2	-0.275792	3.221002	0.143642
N3	-1.595262	3.180996	0.055703
C4	-2.193350	2.035453	-0.085950
C5	-1.603473	0.712986	-0.0721270
C6	-0.167891	0.833245	-0.085443
F7	1.813781	2.116652	0.153901
F8	0.320311	4.430727	0.287631
Cl9	0.795514	-0.631942	-0.137699
F11	-2.124417	-0.106951	1.068647
N12	-2.210591	-0.218536	-1.169875
H13	-1.887474	-1.183042	-1.048570
H14	-1.962431	0.097993	-2.111516
H15	-3.231542	-0.224490	-1.086128
F15	-3.555085	2.045129	-0.192173

Coordinates (in xyz-format) for entries 1–8, Table 2

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Table 2 entry 1 starting material

C1	2.757033	-2.719896	0.113556
C2	1.544948	-2.029961	0.059854
C3	1.610882	-0.639353	-0.038128
C4	2.822137	0.044526	-0.049391
C5	4.012167	-0.673818	0.021869
C6	3.982970	-2.063053	0.104099
F7	5.128834	-2.752698	0.171344
F8	5.182404	-0.029994	0.013027

F9	2.851904	1.380882	-0.129956
F10	2.759635	-4.060039	0.190142
F11	0.479982	0.080070	-0.112071
C12	0.229978	-2.757486	0.039645
H13	-0.563121	-2.132302	0.454987
F14	-0.113597	-3.077259	-1.283666
H15	0.295506	-3.688297	0.607038

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Table 2 entry 1 sigma-complex

C1	-1.848943	1.552376	-0.007084
C2	-0.680674	2.199425	-0.440760
C3	0.441291	1.357202	-0.503549
C4	0.405187	0.015877	-0.203916
C5	-0.808802	-0.695651	0.108930
C6	-1.911452	0.213036	0.297343
F8	1.633444	1.883500	-0.872268
F11	-2.984948	2.277456	0.128386
F12	-1.120863	-1.752157	-0.911337
N12	-0.639846	-1.706286	1.277006
H13	-0.413567	-1.235162	2.157533
H14	0.107804	-2.372338	1.061881
H15	-1.501609	-2.244349	1.406045
F14	1.540176	-0.744785	-0.291130
F15	-3.088868	-0.348376	0.712447
C16	-0.614314	3.656866	-0.705784
F17	-0.301692	4.398750	0.470526
H18	0.164038	3.891922	-1.436271
H19	-1.572842	4.038521	-1.066747

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Table 2 entry 2 starting material

C1	1.019027	0.920757	0.000000
C2	-0.295339	1.388924	0.000000
C3	-1.317995	0.438781	0.000000
C4	-1.018964	-0.920848	0.000000
C5	0.295329	-1.388945	0.000000
C6	1.318297	-0.438859	0.000000
F7	2.607325	-0.787328	0.000000
F9	-2.035435	-1.790540	0.000000
F10	2.035262	1.790752	0.000000
F11	-2.606884	0.786987	0.000000
C12	-0.525218	2.885563	0.000000
F13	-1.825837	3.211395	0.000000
F14	0.038280	3.454442	1.085969
F15	0.038280	3.454442	-1.085969
C15	0.525220	-2.885447	0.000000
F16	1.825734	-3.211598	0.000000
F17	-0.038475	-3.454252	1.085678
F18	-0.038475	-3.454252	-1.085678

22

Table 2 entry 2 sigma-complex

C1	-2.054128	1.462652	-0.024685

C2	-0.815814	2.140861	-0.108046
C3	0.347316	1.418684	-0.005099
C4	0.382979	0.031702	0.218594
C5	-0.851621	-0.731778	0.276505
C6	-2.047427	0.107969	0.196957
F8	1.521909	2.075805	-0.118733
F12	-0.922786	-1.785639	-0.733846
N12	-0.972399	-1.704027	1.516795
H13	-0.983536	-1.181323	2.396575
H14	-0.181256	-2.352666	1.535267
H15	-1.831812	-2.257820	1.454200
F15	-3.199618	-0.608453	0.304915
F14	-0.780935	3.488392	-0.286350
C16	1.701911	-0.655887	0.153214
F16	1.600461	-1.985254	0.447151
F17	2.289912	-0.593911	-1.072637
F18	2.619268	-0.145889	1.016299
C19	-3.317186	2.282168	-0.151958
F20	-4.439552	1.543320	-0.210532
F21	-3.456717	3.131013	0.893787
F22	-3.290392	3.044506	-1.269371

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Table 2 entry 3 starting material

C1	2.751809	-2.704362	0.132170
C2	1.551034	-2.020917	-0.049669
C3	1.609301	-0.634454	-0.213002
C4	2.819376	0.048649	-0.192638
C5	4.005634	-0.659646	-0.009987
C6	3.975135	-2.040271	0.155481
F7	5.113331	-2.720697	0.331560
F9	2.855471	1.376729	-0.349419
F10	2.752045	-4.036273	0.294658
F11	0.483896	0.069259	-0.388625
C12	0.237696	-2.754762	-0.071229
F13	-0.576788	-2.284142	0.926903
F14	-0.409771	-2.516034	-1.255497
H14	0.353253	-3.833633	0.051936
F15	5.170881	-0.010109	0.010533

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Table 2 entry 3 sigma-complex

C1	-1.986329	1.484382	-0.096320
C2	-0.791407	2.196736	-0.306098
C3	0.370768	1.414834	-0.215625
C4	0.357966	0.071476	0.070621
C5	-0.851288	-0.709395	0.175157
C6	-2.019539	0.142075	0.188103
F7	1.576377	2.007226	-0.385242
F8	-0.937446	-1.754484	-0.877051
N9	-0.821782	-1.714097	1.361638
H10	-0.760195	-1.233552	2.263706
H11	-0.017970	-2.342558	1.270586
H12	-1.666183	-2.294013	1.357216
F13	1.531699	-0.626686	0.156328

F14	-3.213937	-0.491400	0.393672
F15	-3.162891	2.146082	-0.145038
C16	-0.744849	3.643919	-0.606393
H17	0.276365	4.011070	-0.735040
F18	-1.454706	3.959174	-1.754954
F19	-1.342733	4.397972	0.391745

14
Table 2 entry 4 starting material

C1	2.709086	-2.697123	0.017421
C2	1.523960	-1.947314	0.012410
C3	1.571937	-0.560834	0.008770
C4	2.805729	0.106256	0.009703
C5	3.990093	-0.642840	0.014415
C6	3.942339	-2.030763	0.018305
F7	5.075306	-2.728644	0.023036
F15	5.168339	-0.024077	0.015399
F11	0.346929	-2.567278	0.011251
F10	0.439870	0.138136	0.004410
N11	2.891845	2.692131	0.002973
C13	2.852904	1.531239	0.005984
N13	2.612593	-5.282059	0.025029
C15	2.657786	-4.121256	0.021631

18
Table 2 entry 4 sigma-complex

C1	-1.991689	1.478252	-0.062541
C2	-0.757110	2.167319	-0.187606
C3	0.397783	1.439870	-0.096645
C4	0.405883	0.043587	0.128704
C5	-0.832240	-0.737696	0.187073
C6	-2.014009	0.119685	0.153332
F8	1.583393	2.061338	-0.215940
F12	-0.906237	-1.737197	-0.862187
N12	-0.897312	-1.733942	1.382975
H13	-0.813209	-1.253133	2.283662
H14	-0.147278	-2.430167	1.313237
H15	-1.784393	-2.249085	1.371942
F15	-3.197690	-0.525939	0.278959
F16	-0.748106	3.503991	-0.392755
N15	-4.207341	2.807206	-0.232375
C17	-3.216846	2.204328	-0.153293
N17	2.652701	-1.222055	0.176369
C19	1.641540	-0.637061	0.148045

18
Table 2 entry 5 starting material

C1	2.691445	-2.658027	0.018627
C2	1.501977	-1.929882	0.013033
C3	1.560453	-0.512461	0.009180
C4	2.822758	0.089814	0.009012
C5	3.999426	-0.660605	0.013786
C6	3.938766	-2.041506	0.018986
F7	5.051800	-2.770532	0.023914
F8	2.997133	1.415337	0.004260

F9	2.671916	-3.995859	0.023524
C10	0.249315	-2.800843	0.011016
F11	-0.908241	-2.127612	0.003566
F12	0.245150	-3.606161	-1.073697
F13	0.235778	-3.597957	1.101370
F14	5.177237	-0.039581	0.013182
C15	0.307747	0.357353	0.004850
F16	0.585798	1.670929	0.002622
F17	-0.446434	0.123044	-1.088991
F18	-0.451458	0.127877	1.096373

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Table 2 entry 5 sigma-complex

C1	-2.021212	1.518711	-0.093790
C2	-0.793549	2.198889	-0.368949
C3	0.350011	1.381380	-0.387038
C4	0.331924	0.038218	-0.097852
C5	-0.860557	-0.702916	0.195226
C6	-2.012004	0.179055	0.232402
F8	1.560113	1.891808	-0.696586
F12	-1.077309	-1.813238	-0.745229
N12	-0.737193	-1.608228	1.462692
H13	-0.570023	-1.055937	2.308529
H14	0.037336	-2.269364	1.349640
H15	-1.592527	-2.156551	1.593865
F14	1.493179	-0.676338	-0.128524
F15	-3.153195	-0.486622	0.576397
C16	-3.360329	2.232414	-0.153955
F16	-4.382339	1.400875	-0.446748
F17	-3.674705	2.834939	1.016238
F18	-3.377677	3.183129	-1.114975
C19	-0.672713	3.674816	-0.575589
F20	0.565538	4.137407	-0.278285
F21	-0.918757	4.085507	-1.852371
F22	-1.526631	4.378265	0.214965

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Table 2 entry 6 starting material

C1	2.738850	-2.689790	0.017512
C2	1.534640	-1.971522	0.012750
C3	1.589605	-0.570739	0.008854
C4	2.806509	0.094680	0.009811
C5	3.991106	-0.639191	0.014688
C6	3.960166	-2.032558	0.018475
F7	5.100384	-2.725265	0.022950
F8	5.159727	-0.005518	0.015680
F9	2.846922	1.428229	0.006025
F10	2.716687	-4.022993	0.021214
F11	0.460476	0.137982	0.004178
N12	-0.736477	-3.204402	0.011038
C13	0.284693	-2.649638	0.011838

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Table 2 entry 6 sigma complex

C1	-1.987144	1.491034	-0.077518

C2	-0.771709	2.196192	-0.259377
C3	0.401793	1.406986	-0.171087
C4	0.370640	0.066709	0.083777
C5	-0.857123	-0.709638	0.168415
C6	-2.030655	0.150474	0.174622
F8	1.595064	2.011392	-0.319168
F11	-3.142960	2.178047	-0.132608
F12	-0.932670	-1.713909	-0.884672
N12	-0.845823	-1.699001	1.357791
H13	-0.799121	-1.210768	2.257134
H14	-0.039103	-2.328149	1.287662
H15	-1.690371	-2.279800	1.345042
F14	1.526514	-0.650428	0.173132
F15	-3.223952	-0.483542	0.354298
N16	-0.700840	4.724081	-0.741143
C17	-0.733188	3.575665	-0.523936

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Table 2 entry 7 starting material

C1	2.721619	-2.709361	0.017554
C2	1.517632	-1.959516	0.012632
C3	1.583121	-0.568116	0.008896
C4	2.811208	0.090309	0.009835
C5	3.991048	-0.644499	0.014595
C6	3.941822	-2.037222	0.018435
F7	5.084245	-2.719492	0.023024
F8	5.162217	-0.021188	0.015481
F9	2.853646	1.416356	0.006132
F11	0.467453	0.156477	0.004370
N11	-0.798253	-3.113120	0.010476
C13	0.243113	-2.597796	0.011431
N13	2.704753	-5.296584	0.024882
C15	2.710204	-4.134700	0.021602

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Table 2 entry 7 sigma complex

C1	-2.005186	1.503587	-0.076864
C2	-0.770472	2.198035	-0.272168
C3	0.393346	1.407705	-0.181026
C4	0.362188	0.062904	0.072063
C5	-0.856635	-0.719348	0.166439
C6	-2.026628	0.151226	0.167920
F8	1.590193	2.000036	-0.330207
F12	-0.948872	-1.715350	-0.886359
N12	-0.841469	-1.705430	1.355156
H13	-0.781171	-1.221878	2.256816
H14	-0.040158	-2.340587	1.276097
H15	-1.688758	-2.283250	1.351291
F14	1.521601	-0.639472	0.167410
F15	-3.207047	-0.487613	0.365223
N15	-0.633222	4.730276	-0.728488
C17	-0.697633	3.582058	-0.521466
N17	-4.251149	2.792422	-0.180669
C19	-3.246236	2.209426	-0.132063

Table 2 entry 8 is the same as Table 1 entry 4, only the temperature and thus the experimental rate constants are different.

Coordinates (in xyz-format) for entries 1–13, Table 3

12
Table 3 entry 1 starting material
C17 0.000000 1.194218 -0.696663
C18 0.000000 1.194218 0.696663
C19 0.000000 0.000000 1.406348
C20 0.000000 -1.194218 0.696663
C21 0.000000 -1.194218 -0.696663
C22 0.000000 0.000000 -1.406348
F7 0.000000 2.369877 -1.352108
F8 0.000000 2.369877 1.352108
H9 0.000000 0.000000 2.492150
F10 0.000000 -2.369877 -1.352108
H11 0.000000 0.000000 -2.492150
F12 0.000000 -2.369877 1.352108

17
Table 3 entry 1 sigma-complex
C1 -0.712940 1.231592 -0.489781
C2 -1.894786 2.045837 -0.291144
C3 -3.062160 1.241251 0.001200
C4 -2.952714 -0.103608 0.317718
C5 -1.756295 -0.800374 0.237218
C6 -0.616730 -0.105898 -0.185614
H7 -4.039244 1.707322 0.066267
F8 -1.695404 -2.135619 0.549519
F9 -1.596799 3.008533 0.995258
O10 -1.998279 3.045097 -1.282672
C11 -3.052319 3.987020 -1.118610
H12 -2.898663 4.767299 -1.869614
H13 -4.039173 3.534482 -1.288397
H14 -3.021257 4.424630 -0.117741
H15 0.334084 -0.619577 -0.298516
F16 -4.081121 -0.789237 0.670889
F17 0.409443 1.887197 -0.936537

12
Table 3 entry 2 starting material
C17 3.266860 -1.609794 -0.089956
C18 2.163657 -2.351187 0.319141
C19 0.900372 -1.763166 0.316467
C20 0.727389 -0.446206 -0.088950
C21 1.836589 0.299228 -0.499908
C22 3.094931 -0.288308 -0.497120
F7 4.484786 -2.173528 -0.088587
F8 2.326187 -3.624135 0.712047
F9 -0.147588 -2.506589 0.717903
H10 1.731846 1.330843 -0.821423
F11 4.181946 0.403111 -0.887501

H12	-0.268273	-0.013609	-0.080579

17

Table 3 entry 2 sigma-complex

C1	-0.779595	1.283502	-0.440205
C2	-1.998176	2.047794	-0.282560
C3	-3.101432	1.136792	-0.008235
C4	-2.993207	-0.206049	0.258040
C5	-1.747643	-0.866227	0.194435
C6	-0.666200	-0.063953	-0.160645
F7	-4.355724	1.720737	0.034127
H8	-1.623858	-1.924009	0.391985
F10	-1.853025	3.033144	0.913805
O11	-2.171448	2.963082	-1.360747
C12	-2.983109	4.119960	-1.148379
H13	-3.071101	4.606273	-2.124907
H14	-3.982239	3.859744	-0.789423
H15	-2.519912	4.811885	-0.440322
F15	0.575796	-0.622645	-0.279561
H16	-3.903526	-0.753647	0.491763
F17	0.348122	1.978756	-0.807498

12

Table 3 entry 3 starting material

C17	3.266972	-1.611540	-0.089420
C18	2.153839	-2.342049	0.317476
C19	0.880400	-1.786449	0.327166
C20	0.757158	-0.464173	-0.087523
C21	1.837279	0.307979	-0.503105
C22	3.090628	-0.291529	-0.495349
F7	4.488720	-2.170130	-0.090268
F8	2.337740	-3.614450	0.706622
H9	0.021736	-2.366815	0.646908
H10	1.713892	1.337412	-0.821545
F11	4.172708	0.402123	-0.885340
F12	-0.468742	0.096378	-0.086262

17

Table 3 entry 3 sigma-complex

C1	-0.711565	1.269426	-0.410412
C2	-1.900318	2.089866	-0.206079
C3	-3.078838	1.271179	0.083928
C4	-2.974274	-0.087351	0.284844
C5	-1.805950	-0.841546	0.167232
C6	-0.680653	-0.082654	-0.192325
H7	-4.043618	1.750212	0.205331
H8	-1.760449	-1.908559	0.340201
F10	-1.645616	3.028456	0.980349
O11	-2.007844	3.038554	-1.265423
C12	-3.079431	3.968875	-1.167451
H13	-2.956351	4.679957	-1.989504
H14	-4.058692	3.482123	-1.275734
H15	-3.050533	4.505976	-0.214763
F15	0.511474	-0.725192	-0.358571
F16	-4.122963	-0.762688	0.610620

F17	0.441603	1.917543	-0.783166

12

Table 3 entry 4 starting material

C17	3.257665	-1.617397	-0.086089
C18	2.168197	-2.374995	0.326213
C19	0.912961	-1.778996	0.319827
C20	0.737109	-0.458583	-0.086191
C21	1.842934	0.281511	-0.495079
C22	3.109961	-0.295034	-0.496997
F7	4.488889	-2.152925	-0.096134
H8	2.294396	-3.404458	0.644828
F9	-0.167619	-2.473871	0.710084
F10	1.687431	1.551231	-0.887488
F11	4.170107	0.423887	-0.892292
F12	-0.479896	0.103500	-0.086933

17

Table 3 entry 4 sigma-complex

C1	-0.702686	1.295385	-0.412257
C2	-1.939796	2.043396	-0.237392
C3	-3.067247	1.156219	0.019991
C4	-2.935332	-0.183674	0.295610
C5	-1.696775	-0.834671	0.236342
C6	-0.607081	-0.053156	-0.129030
F7	-4.332915	1.695932	0.048485
F8	-1.585262	-2.165913	0.529797
F10	-1.817263	3.008118	0.968988
O11	-2.103958	2.970897	-1.308879
C12	-2.949622	4.107157	-1.105104
H13	-3.003665	4.616985	-2.071692
H14	-3.958123	3.818856	-0.797897
H15	-2.530607	4.787253	-0.359178
F15	0.603495	-0.669712	-0.244870
F16	-4.040243	-0.912153	0.598720
H17	0.176949	1.833585	-0.748665

12

Table 3 entry 5 starting material

C17	3.269934	-1.611265	-0.090017
C18	2.165510	-2.352486	0.319234
C19	0.899612	-1.774483	0.320389
C20	0.739510	-0.453589	-0.088295
C21	1.840758	0.298914	-0.500462
C22	3.106340	-0.290500	-0.497977
F7	4.485634	-2.169484	-0.090378
F8	2.320477	-3.619998	0.711364
F9	-0.160200	-2.489505	0.714267
Cl10	1.639310	1.944936	-1.009064
F11	4.177838	0.404826	-0.887332
F12	-0.483190	0.083348	-0.080308

17

Table 3 entry 5 sigma-complex

C1	-0.742476	1.309835	-0.421370

C2	-1.969327	2.070108	-0.253247
C3	-3.077074	1.164832	-0.008018
C4	-2.942574	-0.175214	0.287836
C5	-1.704539	-0.813698	0.236552
C6	-0.603119	-0.035228	-0.126473
F7	-4.343676	1.693185	-0.017897
F8	-1.583973	-2.125411	0.584212
F10	-1.817790	3.033640	0.960500
O11	-2.137794	2.991393	-1.318477
C12	-2.949591	4.148219	-1.092506
H13	-3.033354	4.644314	-2.063700
H14	-3.949821	3.883004	-0.740476
H15	-2.486353	4.828022	-0.373991
Cl15	0.978380	-0.792120	-0.236370
F16	-4.047166	-0.901011	0.592338
F17	0.351215	2.017587	-0.831694

12

Table 3 entry 6 starting material

C17	0.696271	1.205977	0.000000
C18	1.392543	0.000000	0.000000
C19	0.696271	-1.205977	0.000000
C20	-0.696271	-1.205977	0.000000
C21	-1.392543	0.000000	0.000000
C22	-0.696271	1.205977	0.000000
F7	1.365224	2.364637	0.000000
F8	2.730448	0.000000	0.000000
F9	1.365224	-2.364637	0.000000
F10	-2.730448	0.000000	0.000000
F11	-1.365224	2.364637	0.000000
F12	-1.365224	-2.364637	0.000000

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Table 3 entry 6 sigma-complex

C1	-0.745441	1.289458	-0.438493
C2	-1.965522	2.053762	-0.266653
C3	-3.076962	1.152431	-0.013897
C4	-2.946664	-0.189075	0.278526
C5	-1.711930	-0.834988	0.214173
C6	-0.615099	-0.053306	-0.145169
F7	-4.342938	1.687686	-0.008658
F8	-1.575184	-2.150140	0.554096
F10	-1.809580	3.022802	0.948805
O11	-2.132509	2.978527	-1.330589
C12	-2.954452	4.127851	-1.106275
H13	-3.036709	4.627380	-2.075954
H14	-3.954479	3.854153	-0.760359
H15	-2.500454	4.808691	-0.382771
F15	0.606876	-0.635003	-0.240960
F16	-4.052918	-0.911073	0.588365
F17	0.371144	1.974377	-0.839495

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Table 3 entry 7 sigma-complex (the starting material for this entry is the same as for entry 4)

C1	-0.757578	1.271425	-0.439096

C2	-1.981463	2.038641	-0.273099
C3	-3.094870	1.136137	-0.010695
C4	-2.953234	-0.205508	0.254777
C5	-1.729426	-0.880913	0.194109
C6	-0.647025	-0.072284	-0.165184
F7	-4.355826	1.689358	0.035227
H8	-1.629176	-1.936095	0.410845
F10	-1.827412	3.002773	0.916828
O11	-2.148892	2.950498	-1.352565
C12	-2.971102	4.101581	-1.144197
H13	-3.042906	4.596454	-2.117229
H14	-3.975596	3.832912	-0.806356
H15	-2.522716	4.787736	-0.421048
F15	0.586478	-0.641230	-0.283027
F16	-4.079487	-0.913225	0.555455
F17	0.363480	1.971782	-0.809241

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Table 3 entry 8 sigma-complex (the starting material for this entry is the same as for entry 5)

C1	-0.742503	1.306011	-0.461058
C2	-1.974559	2.068864	-0.279313
C3	-3.087751	1.156348	-0.011298
C4	-2.954551	-0.181277	0.261595
C5	-1.711706	-0.824681	0.193988
C6	-0.621688	-0.047519	-0.169681
F7	-4.347951	1.698380	-0.002468
F8	-1.581470	-2.144786	0.515869
F10	-1.835521	3.023055	0.898450
O11	-2.195801	2.959907	-1.362508
C12	-2.969685	4.140226	-1.129285
H13	-3.109798	4.599006	-2.112432
H14	-3.949006	3.911080	-0.701086
H15	-2.447060	4.841275	-0.474054
F15	0.589170	-0.647314	-0.258401
F16	-4.053799	-0.915486	0.560756
Cl17	0.702895	2.190634	-0.957936

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Table 3 entry 9 sigma-complex (the starting material for this entry is the same as for entry 5)

C1	-0.723545	1.311499	-0.407177
C2	-1.948321	2.080394	-0.234214
C3	-3.060945	1.172124	0.025974
C4	-2.929846	-0.169964	0.289487
C5	-1.694147	-0.829225	0.217292
C6	-0.598469	-0.031134	-0.138707
F7	-4.322386	1.716597	0.058039
Cl8	-1.520917	-2.527562	0.609357
F10	-1.794483	3.032275	0.946256
O11	-2.119035	2.980782	-1.319155
C12	-2.946203	4.131804	-1.119270
H13	-3.024375	4.614617	-2.097488
H14	-3.947249	3.861119	-0.773896
H15	-2.497616	4.827868	-0.406279
F15	0.625913	-0.599584	-0.253056
F16	-4.043771	-0.881540	0.587750

F17	0.392106	2.007707	-0.789360

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Table 3 entry 10 starting material

C17	-0.149526	-0.478079	1.218835
C18	0.268586	0.859422	1.216285
C19	0.471535	1.508431	0.000000
C20	0.268586	0.859422	-1.216285
C21	-0.149526	-0.478079	-1.218835
C22	-0.358736	-1.147682	0.000000
Cl7	-0.404753	-1.294156	2.727416
Cl8	0.546764	1.749005	2.678933
F9	0.869289	2.779679	0.000000
Cl10	-0.404753	-1.294156	-2.727416
Cl11	-0.876723	-2.805404	0.000000
Cl12	0.546764	1.749005	-2.678933

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Table 3 entry 10 sigma-complex

C1	-0.765066	1.381368	-0.399929
C2	-2.088215	2.016847	-0.246915
C3	-3.126860	0.996070	-0.005401
C4	-2.857257	-0.335504	0.250595
C5	-1.545836	-0.851875	0.199410
C6	-0.514088	0.047195	-0.139254
Cl7	-4.774151	1.620670	0.018595
Cl8	-1.206896	-2.530952	0.589202
F10	-2.051142	2.950404	0.883971
O11	-2.405644	2.832765	-1.371063
C12	-2.629716	4.233134	-1.189198
H13	-2.860797	4.618172	-2.186889
H14	-3.476470	4.433010	-0.526102
H15	-1.742182	4.745552	-0.806682
Cl15	1.131054	-0.563667	-0.266773
Cl16	-4.183471	-1.432512	0.615099
Cl17	0.527671	2.486819	-0.861617

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Table 3 entry 11 starting material

C17	3.260610	-1.597362	-0.093242
C18	2.165594	-2.353585	0.319373
C19	0.905272	-1.759673	0.314665
C20	0.727722	-0.436090	-0.092256
C21	1.838640	0.316315	-0.506007
C22	3.113735	-0.271590	-0.505219
F7	4.470729	-2.154266	-0.093154
Cl8	2.366622	-3.996464	0.827407
F9	-0.149206	-2.472601	0.707408
Cl10	1.637268	1.960713	-1.014539
Cl11	4.532511	0.594955	-1.002319
Cl12	-0.877687	0.221946	-0.065956

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Table 3 entry 11 sigma-complex

C1	-0.761196	1.393452	-0.394307

C2	-2.096110	2.017920	-0.247185
C3	-3.115348	0.985834	-0.001215
C4	-2.821306	-0.334749	0.241483
C5	-1.518543	-0.848566	0.187138
C6	-0.493752	0.058364	-0.146146
Cl7	-4.794013	1.517301	0.061312
Cl8	-1.242369	-2.543215	0.547554
F10	-2.068886	2.958215	0.879849
O11	-2.433310	2.827334	-1.371990
C12	-2.592513	4.238840	-1.207613
H13	-2.833126	4.617563	-2.205483
H14	-3.412279	4.484656	-0.526305
H15	-1.675301	4.721020	-0.856806
Cl15	1.152088	-0.546700	-0.275178
F16	-3.829232	-1.188237	0.524331
Cl17	0.524850	2.512921	-0.848786

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Table 3 entry 12 starting material

C17	3.268970	-1.612686	-0.090053
C18	2.169087	-2.366690	0.322816
C19	0.904628	-1.776577	0.320158
C20	0.740795	-0.456725	-0.087608
C21	1.845566	0.283069	-0.496651
C22	3.119047	-0.287209	-0.501434
F7	4.481355	-2.166672	-0.090562
Cl8	2.367027	-4.012828	0.832787
F9	-0.165798	-2.470041	0.709165
F10	1.669334	1.546765	-0.883960
Cl11	4.492921	0.640893	-1.010963
F12	-0.475686	0.099552	-0.086205

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Table 3 entry 12 sigma-complex

C1	-0.900996	1.512974	-0.356062
C2	-2.267787	2.022134	-0.185791
C3	-3.192065	0.901912	0.019199
C4	-2.784074	-0.403160	0.231962
C5	-1.448935	-0.799555	0.149516
C6	-0.521845	0.214104	-0.160433
Cl7	-4.916047	1.276623	0.086192
Cl8	-0.936558	-2.434640	0.519253
F10	-2.298224	2.937929	0.997577
O11	-2.706464	2.857853	-1.246495
C12	-2.321109	4.235716	-1.229806
H13	-2.656096	4.646523	-2.186593
H14	-2.805944	4.779243	-0.414691
H15	-1.237950	4.359280	-1.149561
F15	0.784214	-0.111920	-0.305753
F16	-3.714892	-1.341580	0.516657
F17	0.050616	2.421574	-0.743175

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Table 3 entry 13 starting material

C17	3.266126	-1.611021	-0.088996

C18	2.167084	-2.365242	0.323187
C19	0.903406	-1.773933	0.319522
C20	0.728348	-0.450877	-0.087287
C21	1.842779	0.282533	-0.495619
C22	3.116692	-0.286404	-0.500860
F7	4.476775	-2.164210	-0.089755
Cl8	2.368341	-4.011567	0.831642
F9	-0.152429	-2.483637	0.710893
F10	1.688261	1.545473	-0.886356
Cl11	4.492539	0.638468	-1.011449
Cl12	-0.849138	0.270540	-0.085375

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Table 3 entry 13 sigma-complex

C1	-0.748644	1.378994	-0.410019
C2	-2.061072	2.035056	-0.261515
C3	-3.103733	1.022307	-0.003791
C4	-2.840649	-0.306712	0.238047
C5	-1.549028	-0.845927	0.176635
C6	-0.521595	0.044565	-0.159908
Cl7	-4.772406	1.587031	0.058410
Cl8	-1.236771	-2.538597	0.504382
F10	-2.011476	2.984831	0.858438
O11	-2.363815	2.850581	-1.394286
C12	-2.671772	4.233788	-1.208436
H13	-2.898233	4.614093	-2.209009
H14	-3.545121	4.383935	-0.566566
H15	-1.825640	4.793216	-0.798592
F15	0.733673	-0.442192	-0.262907
F16	-3.864154	-1.141302	0.522031
Cl17	0.611760	2.410948	-0.851271

In vacuo Energies for entries 1–12, Table 1

All energies are given in Hartrees

Table 1 entry 1 starting material −1104.786684
Table 1 entry 1 sigma-complex −1161.285384

Table 1 entry 2 starting material −1005.568989
Table 1 entry 2 sigma-complex −1062.071964

Table 1 entry 3 starting material −661.245519
Table 1 entry 3 sigma-complex −717.744772

Table 1 entry 4 starting material −744.412362
Table 1 entry 4 sigma-complex −800.921545

Table 1 entry 5 starting material −1104.788167
Table 1 entry 5 sigma-complex −1161.292582

Table 1 entry 6 starting material −661.175833

Table 1 entry 6 sigma-complex −717.700012

Table 1 entry 7 starting material −982.215014
Table 1 entry 7 sigma-complex −1038.733528

Table 1 entry 8 sigma-complex −1038.736332 (the energy for the starting material for this entry is the same as for entry 7)

Table 1 entry 9 starting material −1220.036013
Table 1 entry 9 sigma-complex −1276.546771

Table 1 entry 10 starting material −661.252215
Table 1 entry 10 sigma-complex −717.759747

Table 1 entry 11 sigma-complex −1276.569941 (the energy for the starting material for this entry is the same as for entry 9)

Table 1 entry 12 sigma-complex −1161.283261

In vacuo Energies for entries 1-8, Table 2

All energies are given in Hartrees

Table 2 entry 1 starting material −866.913343
Table 2 entry 1 sigma-complex −923.412125

Table 2 entry 2 starting material −1303.199890
Table 2 entry 2 sigma-complex −1359.666449

Table 2 entry 3 starting material −966.137849
Table 2 entry 3 sigma-complex −1022.647704

Table 2 entry 4 starting material −813.604666
Table 2 entry 4 sigma-complex -870.112817

Table 2 entry 5 starting material −1303.145967
Table 2 entry 5 sigma-complex −1359.666774

Table 2 entry 6 starting material −820.603745
Table 2 entry 6 sigma-complex −877.107671

Table 2 entry 7 starting material −813.610950
Table 2 entry 7 sigma-complex −870.116320

Table 2 entry 8 is the same as Table 1 entry 4, only the temperature and thus the experimental rate constants are different.

In vacuo Energies for entries 1-13, Table 3

All energies are given in Hartrees

Table 3 entry 1 starting material −629.158798
Table 3 entry 1 sigma-complex −744.284959

Table 3 entry 2 starting material −629.153522
Table 3 entry 2 sigma-complex −744.286826

Table 3 entry 3 starting material −629.159471
Table 3 entry 3 sigma complex −744.293485

Table 3 entry 4 starting material −728.374142
Table 3 entry 4 sigma complex −843.512456

Table 3 entry 5 starting material −1187.954958
Table 3 entry 5 sigma-complex −1303.102151

Table 3 entry 6 starting material −827.587708
Table 3 entry 6 sigma-complex −942.732321

Table 3 entry 7 sigma-complex -843.516875 (the energy for the starting material for this entry is the same as for entry 4)

Table 3 entry 8 sigma-complex -1303.105423 (the energy for the starting material for this entry is the same as for entry 5)

Table 3 entry 9 sigma-complex -1303.108509 (the energy for the starting material for this entry is the same as for entry 5)

Table 3 entry 10 starting material −2629.402554
Table 3 entry 10 sigma-complex −2744.566854

Table 3 entry 11 starting material −2269.046333
Table 3 entry 11 sigma-complex −2384.209046

Table 3 entry 12 starting material −1548.321946
Table 3 entry 12 sigma-complex −1663.480767

Table 3 entry 13 starting material −1908.688704
Table 3 entry 13 sigma-complex −2023.850269

Sigma Stability values for reaction series A calculated with a larger basis set

Reaction series A. Sigma Stability (SS) values for the same entries as in Table 1. in the main text, but calculated with a larger basis set including diffuse functions (6-31+G(d,p) with effective core potential on heavy atoms).

Entry	Reactant (Fig 1.)	Position of amination	SS (kcal mol^{-1}) water
1	**1**	2	10.73
2	**2**	2	10.38
3	**3**	Equal	7.27
4	**4**	4	5.38
5	**5**	4	6.35
6	**6**	4	1.04
7	**7**	2	3.04
8	**7**	4	2.19
9	**8**	2	0.09
10	**9**	4	−1.71
11	**8**	4	−0.28

Zero point energies for entries 1–11, Table 1

Entry	Reactant (Fig 1.)	Zero point energy for the sigma-complex (kcal/mol)	Zero point energy for the aromatic starting material (kcal/mol)	Difference between zero point energies for the sigma-complex and the corresponding starting material (kcal/mol)
1	**1**	53.942	29.620	24.322
2	**2**	59.042	34.685	24.357
3	**3**	52.541	28.175	24.366
4	**4**	55.088	30.511	24.577
5	**5**	54.379	29.655	24.724
6	**6**	52.305	27.771	24.534
7	**7**	63.111	38.524	24.587
8	**7**	63.430	38.524	24.906
9	**8**	71.429	46.566	24.863
10	**9**	53.319	28.503	24.816
11	**8**	71.756	46.566	25.190