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Supporting Information

for

The influence of the cationic carbenes on the initiation kinetics of ruthenium-based metathesis catalysts; a DFT study

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Mulliken partial charges, energy values and Cartesian coordinates for all investigated systems

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Table S1: Total energy values (E) and Gibbs free energy values (G; as defined in the manuscript) for carbene **1** and its complexes.

structure	M06 E, (H)	DLPNO-CCSD(T) E (H)	Solvatation E in CH_2Cl_2 (H)	Zero-point E (kcal/mol)	Entropy E (cal/mol)	Thermal correction to enthalpy (H)	M06 G (H)	DLPNO-CCSD(T) G (H)	Solvation E in H_2O (H)	D3 correction (H)
1	-1137.763	-1134.209	-0.068	352.339	198.779	0.031	-1137.332	-1133.778	-0.084	-0.016
1A	-2275.555	-2268.439	-0.168	708.671	320.706	0.061	-2274.685	-2267.570	-0.196	-0.053
1B	-2275.554	-2268.438	-0.168	708.631	320.249	0.061	-2274.684	-2267.568	-0.196	-0.053
1-GrI	-3469.236	-3461.247	-0.067	725.605	329.792	0.062	-3468.241	-3460.252	-0.085	-0.053
1-Ind	-3776.339	-3767.400	-0.067	784.641	352.794	0.068	-3775.256	-3766.317	-0.085	-0.060
1-GrII	-3347.361	-3339.302	-0.069	686.752	345.480	0.066	-3346.434	-3338.375	-0.088	-0.055
1-GrII_IMes	-3346.156	-3338.112	-0.070	672.200	350,931	0.067	-3345.255	-3337.212	-0.090	-0.054
1-Hov	-2615.468	-2609.709	-0.076	478.132	263.670	0.047	-2614.860	-2609.102	-0.095	-0.031
1-Hov-TS	-2615.425	-2609.669	-0.077	477.292	267.828	0.047	-2614.821	-2609.065	-0.098	-0.029
1-Hov-a	-2615.441	-2609.675	-0.079	477.856	264.539	0.046	-2614.838	-2609.072	-0.101	-0.030
$P(Cy)_3$	-1046.796	-1043.971	0.003	301.675	142.238	0.020	-1046.359	-1043.534	-0.005	-0.010
1-Gr_I_$P(Cy)_3$	-2422.341	-2417.178	-0.086	422.246	244.819	0.042	-2421.829	-2416.666	-0.110	-0.028
1-Ind_$P(Cy)_3$	-2729.452	-2723.339	-0.079	481.062	271.524	0.048	-2728.846	-2722.733	-0.103	-0.034
1-GrII_Imes/SIMes	-2422.347	-2417.188	-0.079	422.208	243.879	0.041	-2421.828	-2416.668	-0.101	-0.026
GrI_NC	-2331.367	-2326.935	-0.00796	371.465	198.937	0.032	-2330.846	-2326.414	-0.016	-0.019
GrII_NC_nas	-2209.493	-2204.998	-0.003	332.325	216.117	0.035	-2209.034	-2204.539	-0.024	-0.019
GrII_NC_nnas	-2208.286	-2203.802	-0.014	317.811	219.853	0.035	-2207.863	-2203.379	-0.024	-0.019
Ind_NC	-2638.464	-2633.080	-0.010	430.406	219.452	0.037	-2637.855	-2632.471	-0.019	-0.024
IMes	-923.697	-920.815	-0.005	247.943	170.480	0.025	-923.364	-920.482	-0.009	-0.009
SIMes	-924.900	-922.008	0.002	262.277	173.288	0.025	-924.537	-921.644	-0.009	-0.010

Table S2: Total energy values (E) and Gibbs free energy values (G; as defined in the manuscript) for carbene **2** and its complexes.

structure	M06 E, (H)	DLPNO-CCSD(T) E (H)	Solvatation E in CH_2Cl_2 (H)	Zero-point E (kcal/mol)	Entropy E (cal/mol)	Thermal correction to enthalpy (H)	M06 G (H)	DLPNO-CCSD(T) G (H)	Solvation E in H_2O (H)	D3 correction (H)
2	-980.606	-977.550	-0.080	281.272	180.295	0.027	-977.259	-977.241	-0.098	-0.011
2A	-1961.243	-1955.123	-0.197	567.095	276.630	0.051	-1960.617	-1954.497	-0.232	-0.042
2B	-3312.095	-1955.120	-0.200	566.868	270.669	0.050	-1960.617	-1954.495	-0.234	-0.042
2-GrI	-3312.095	-3304.602	-0.065	655.235	309.596	0.058	-3311.205	-3303.712	-0.082	-0.048
2-Ind	-3619.199	-3610.754	-0.064	714.437	323.197	0.062	-3618.216	-3609.771	-0.082	-0.055
2-GrII	-3190.207	-3182.645	-0.078	616.059	321.237	0.061	-3189.395	-3181.834	-0.100	-0.050
2-GrII_IMes	-3189.002	-3181.453	-0.079	601.417	328.031	0.062	-3188.217	-3180.667	-0.100	-0.049
2-Hov	-2458.324	-2453.062	-0.073	407.764	245.470	0.042	-2457.822	-2452.560	-0.091	-0.026
2-Hov-TS	-2458.280	-2453.020	-0.075	407.075	242.972	0.042	-2457.780	-2452.520	-0.097	-0.024
2-Hov-a	-2458.297	-2453.023	-0.078	407.597	239.583	0.042	-2457.798	-2452.524	-0.100	-0.026
2-Gr_I_P(Cy)$_3$	-2265.200	-2260.535	-0.082	351.664	222.181	0.037	-2264.790	-2260.125	-0.106	-0.023
2-Ind_P(Cy)$_3$	-2572.309	-2566.690	-0.079	410.646	247.878	0.043	-2571.809	-2566.190	-0.103	-0.028
2-GrII_Imes/SIMes	-2265.201	-2260.538	-0.079	351.750	228.839	0.038	-2264.791	-2260.128	-0.100	-0.021
P(Cy)$_3$	-1046.796	-1043.971	0.003	301.675	142.238	0.020	-1046.359	-1043.534	-0.005	-0.010
GrI_NC	-2331.367	-2326.935	-0.008	371.465	198.937	0.032	-2330.846	-2326.414	-0.016	-0.019
GrII_NC_nas	-2209.493	-980.606	-0.003	332.325	216.117	0.035	-2209.034	-2204.539	-0.024	-0.019
GrII_NC_nnas	-2208.286	-980.606	-0.014	317.811	219.853	0.035	-2207.863	-2203.379	-0.024	-0.019
Ind_NC	-2638.464	-980.606	-0.010	430.406	219.452	0.037	-2637.855	-2632.471	-0.019	-0.024
IMes	-923.697	-980.606	-0.005	247.943	170.480	0.025	-923.364	-920.482	-0.009	-0.009
SIMes	-924.900	-980.606	0.002	262.277	173.288	0.025	-924.537	-921.644	-0.009	-0.010

Table S3: Total energy values (E) and Gibbs free energy values (G; as defined in the manuscript) for carbene **3** and its complexes.

structure	M06 Gas Phase, LACV3P **++ (H)	DLPNO-CCSD(T) Gas Phase, def2-SVP (H)	Solvatation E in CH_2Cl_2 (H)	Zero-point E (kcal/mol)	Entropy E (cal/mol)	Thermal correction to enthalpy (H)	M06 G (H)	DLPNO-CCSD(T) G (H)	Solvation E in H_2O (H)	D3 correction (H)
3A	-2039.715	-2033.350	-0.171	601.078	281.659	0.053	-2039.010	-2032.645	-0.197	-0.045
3B	-2039.717	-2033.352	-0.171	600.644	285.535	0.053	-2039.013	-2032.648	-0.197	-0.046
3-GrI	-3351.326	-3343.709	-0.058	671.738	307.293	0.058	-3350.402	-3342.785	-0.074	-0.049
3-GrI_P(Cy)$_3$	-2304.436	-2299.650	-0.069	367.745	231.936	0.038	-2303.991	-2299.204	-0.088	-0.023
3-Ind	-3658.437	-3649.864	-0.054	730.091	334.512	0.064	-3657.422	-3648.850	-0.069	-0.057
3-Ind_P(Cy)$_3$	-2611.542	-2605.797	-0.068	426.682	255.519	0.045	-2611.006	-2605.262	-0.088	-0.030
3-GrII	-3229.457	-3221.770	-0.058	632.294	325.449	0.062	-3228.600	-3220.913	-0.074	-0.051
3-GrII_IMes/SIMes	-2304.436	-2299.649	-0.069	367.710	232.139	0.039	-2303.991	-2299.204	-0.088	-0.023
3-GrIIdim	-3228.253	-3220.578	-0.058	617.813	331.365	0.063	-3227.421	-3219.747	-0.074	-0.051
3-Hov	-2497.560	-2492.172	-0.065	423.666	253.732	0.044	-2497.026	-2491.638	-0.081	-0.028
3-Hov-TS	-2497.518	-2492.131	-0.067	422.791	246.817	0.043	-2496.986	-2491.599	-0.087	-0.027
3-Hov-a	-2497.531	-2492.135	-0.069	423.545	249.760	0.043	-2497.000	-2491.604	-0.088	-0.027
P(Cy)$_3$	-1046.796	-1043.971	0.003	301.675	142.238	0.020	-1046.359	-1043.534	-0.005	-0.010
GrI_NC	-2331.367	-2326.935	-0.008	371.465	198.937	0.032	-2330.846	-2326.414	-0.016	-0.019
GrII_NC_nas	-2209.493	-2204.998	-0.003	332.325	216.117	0.035	-2209.034	-2204.539	-0.024	-0.019
GrII_NC_nnas	-2208.286	-2203.802	-0.014	317.811	219.853	0.035	-2207.863	-2203.379	-0.024	-0.019
Ind_NC	-2638.464	-980.606	-0.010	430.406	219.452	0.037	-2637.855	-2632.471	-0.019	-0.024
IMes	-923.697	-980.606	-0.005	247.943	170.480	0.025	-923.364	-920.482	-0.009	-0.009
SIMes	-924.900	-980.606	0.002	262.277	173.288	0.025	-924.537	-921.644	-0.009	-0.010

Table S4: Calculated Gibbs free energies of dimerization (ΔG_1) for carbenes **1-2** using different computational approaches.

structure	**ΔG_1 [kcal/mol]**			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1A	-9.4	-8.7	-6.8	-6.0
1B	-9.0	-7.7	-6.6	-5.3
2A	-10.3	-9.8	-9.5	-9.0
2B	-10.0	-8.7	-9.1	-7.8
3A	-	-	-	-
3B	-	-	-	-

Table S5: Calculated Gibbs free energies of activation (ΔG_2-ΔG_5) for complexes **1-3-GrI** and **1-3-Ind** using different computational approaches.

structure	**ΔG_2 [kcal/mol]**			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-GrI	20.9	32.5	11.6	23.2
2-GrI	23.3	33.1	13.7	23.5
3-GrI	18.7	28.8	11.4	21.6
	ΔG_3 [kcal/mol]			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-GrI	24.0	37.7	20.1	33.8
2-GrI	23.7	35.7	18.0	30.0
3-GrI	-	-	-	-
	ΔG_4 [kcal/mol]			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-Ind	18.7	31.1	9.4	21.8
2-Ind	16.7	29.6	7.1	20.0
3-Ind	21.9	33.9	13.0	25.0
	ΔG_5 [kcal/mol]			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-Ind	25.6	37.6	20.7	37.7
2-Ind	22.5	37.3	16.4	31.2
3-Ind	-	-	-	-

Table S6: Calculated Gibbs free energies of activation (ΔG_6-ΔG_9) for complexes **1-3-GrII** and **1-3-GrII_IMES** using different computational approaches.

structure	**ΔG_6 [kcal/mol]**			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-GrII	38.0	36.5	26.8	25.3
2-GrII	35.5	33.7	24.5	22.7
3-GrII	-	-	-	-
	ΔG_7 [kcal/mol]			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-GrII	38.5	39.2	28.1	29.8
2-GrII	37.0	38.5	29.6	31.4
3-GrII	40.1	40.7	31.1	31.7
	ΔG_8 [kcal/mol]			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-GrII_IMES	33.3	34.6	30.1	31.4
2-GrII_IMES	30.9	30.3	27.4	26.7
3-GrII_IMES	-	-	-	-
	ΔG_9 [kcal/mol]			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-GrII_IMES	35.5	38.7	31.3	34.5
2-GrII_IMES	34.1	36.3	31.8	33.9
3-GrII_IMES	36.7	38.4	32.5	34.2

Table S7: Calculated Gibbs free energies of activation (ΔG_{10}-ΔG_{11}) for complexes **1-3-Hov** using different computational approaches.

structure	**ΔG_{10} [kcal/mol]**			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-GrII	24.5	22.7	23.3	21.4
2-GrII	26.3	24.7	24.0	22.4
3-GrII	24.9	24.2	23.1	22.4
	ΔG_{11} [kcal/mol]			
	M06 in CH_2Cl_2	DLPNO-CCSD(T) in CH_2Cl_2	M06 in water	DLPNO-CCSD(T) in water
1-GrII	14.2	18.5	12.7	16.9
2-GrII	15.3	22.5	13.1	20.4
3-GrII	16.4	21.4	14.8	19.7

Table S8: Mulliken partial charges of carbenes in **1-3-Hov** and **1-3-GrI** systems.

Atom No.	1-Hov	2-Hov	3-Hov	Hov	1-GrI	2-GrI	3-GrI	GrII
$C_{carbene}$	0.43	0.38	0.41	0.44	0.44	0.40	0.44	0.45
N1	-0.50	-0.47	-0.35	-0.48	-0.50	-0.48	-0.36	-0.50
N2	-0.49	-0.49	-0.51	-0.50	-0.50	-0.50	-0.51	-0.49
C1	0.15	0.25	-	0.20	0.14	0.26	-	0.20
C2	0.22	0.28	0.45	0.20	0.22	0.28	0.46	0.20
N3	0.86	0.48	0.38	-	0.85	0.47	0.38	-
Mes1	0.31	0.35	0.42	0.27	0.32	0.34	0.40	0.26
Mes2	0.33	0.35	0.37	0.30	0.33	0.34	0.37	0.28

Cartesian coordinates

1	1A
N1 0.862 5.636 5.258	N1 0.964 5.524 4.980
N2 1.082 4.866 7.249	N2 0.910 4.680 7.097
C1 1.497 4.677 5.984	C1 1.508 4.475 5.798
C2 0.128 6.625 6.089	C2 0.507 6.577 5.876
C3 -0.007 5.852 7.389	C3 -0.042 5.784 7.029
C4 1.117 5.945 3.891	C4 1.482 6.103 3.763
C5 2.428 6.223 3.460	C5 2.761 6.675 3.669
C6 2.616 6.604 2.134	C6 3.120 7.316 2.484
C7 1.556 6.714 1.234	C7 2.244 7.439 1.410
C8 0.274 6.416 1.689	C8 0.957 6.931 1.560
C9 0.033 6.020 3.004	C9 0.556 6.275 2.719
C10 3.609 6.092 4.375	C10 3.757 6.612 4.785
C11 1.799 7.103 -0.192	C11 2.674 8.065 0.120
C12 -1.360 5.653 3.425	C12 -0.862 5.800 2.834
C13 1.369 3.986 8.337	C13 0.645 3.778 8.179
C14 2.157 4.454 9.392	C14 0.915 4.258 9.481
C15 2.396 3.603 10.468	C15 0.583 3.472 10.582
C16 1.877 2.310 10.503	C16 -0.022 2.225 10.447
C17 1.097 1.876 9.431	C17 -0.311 1.787 9.158
C18 0.827 2.695 8.339	C18 0.003 2.533 8.020
C19 2.756 5.830 9.357	C19 1.544 5.595 9.744
C20 2.169 1.391 11.650	C20 -0.303 1.371 11.644
C21 -0.001 2.204 7.190	C21 -0.340 1.954 6.682
H3 3.627 6.819 1.789	H3 4.124 7.737 2.402
H4 -0.564 6.469 0.994	H4 0.242 7.042 0.743
H5 3.490 6.664 5.307	H5 3.403 7.115 5.695
H6 4.521 6.441 3.882	H6 4.692 7.101 4.493
H7 3.749 5.052 4.687	H7 3.979 5.575 5.062
H8 2.628 7.812 -0.281	H8 3.541 8.719 0.252
H9 0.911 7.556 -0.645	H9 1.869 8.653 -0.334
H10 2.060 6.226 -0.798	H10 2.955 7.291 -0.608
H11 -1.925 5.250 2.578	H11 -1.355 5.810 1.856
H12 -1.936 6.517 3.793	H12 -1.456 6.453 3.495
H13 -1.355 4.895 4.217	H13 -0.924 4.784 3.236
H14 3.013 3.953 11.295	H14 0.822 3.845 11.580
H15 0.685 0.867 9.448	H15 -0.794 0.818 9.024
H16 3.241 6.023 8.392	H16 2.087 5.981 8.877
H17 3.508 5.950 10.143	H17 2.244 5.530 10.584
H18 2.003 6.619 9.514	H18 0.796 6.350 10.031
H19 1.292 0.791 11.917	H19 -1.047 0.599 11.428
H20 2.488 1.943 12.540	H20 -0.660 1.964 12.493
H21 2.973 0.689 11.395	H21 0.612 0.862 11.974

H22 0.594 2.157 6.270 H23 -0.850 2.869 6.980 H24 -0.402 1.207 7.393 H46 -0.846 6.846 5.636 C115 1.001 7.874 6.168 H48 0.123 6.458 8.294 H49 -0.977 5.337 7.461 N118 0.271 9.198 6.324 H51 1.707 7.803 7.007 H52 1.572 7.978 5.236 C121 -0.549 9.216 7.573 H122 -1.033 10.192 7.664 H123 -1.307 8.432 7.521 H124 0.108 9.044 8.430 C125 1.302 10.281 6.400 H126 0.801 11.244 6.519 H127 1.954 10.091 7.257 H128 1.888 10.275 5.478 C129 -0.603 9.457 5.134 H130 -0.981 10.480 5.195 H131 -0.011 9.323 4.224 H132 -1.442 8.760 5.132	H22 0.549 1.862 6.051 H23 -1.050 2.564 6.109 H24 -0.787 0.961 6.796 H46 -0.232 7.208 5.368 H47 1.329 7.231 6.219 H48 -0.011 6.358 7.967 N49 3.047 2.579 6.361 N50 2.927 3.169 4.164 C51 2.411 3.513 5.462 C52 4.005 1.766 5.625 C53 3.419 1.800 4.242 C54 3.334 2.639 7.763 C55 3.976 3.729 8.389 C56 4.321 3.622 9.737 C57 4.069 2.478 10.489 C58 3.465 1.404 9.842 C59 3.096 1.458 8.501 C60 4.280 5.017 7.686 C61 4.379 2.419 11.952 C62 2.459 0.237 7.903 C63 2.389 3.421 2.848 C64 3.299 3.912 1.895 C65 2.881 4.065 0.577 C66 1.593 3.729 0.169 C67 0.732 3.185 1.118 C68 1.109 3.005 2.448 C69 4.718 4.243 2.252 C70 1.146 3.983 -1.236 C71 0.133 2.387 3.400 H72 4.800 4.476 10.219 H73 3.251 0.494 10.405 H74 5.013 4.915 6.874 H75 4.686 5.751 8.390 H76 3.383 5.440 7.225 H77 5.152 3.140 12.236 H78 4.711 1.421 12.258 H79 3.483 2.651 12.542 H80 1.773 -0.226 8.621 H81 3.205 -0.535 7.656 H82 1.899 0.460 6.991 H83 3.584 4.466 -0.155 H84 -0.272 2.885 0.815 H85 4.785 4.800 3.192 H86 5.185 4.844 1.466 H87 5.330 3.333 2.362 H88 0.306 3.341 -1.520 H89 1.956 3.823 -1.955 H90 0.816 5.024 -1.350 H91 -0.080 3.057 4.240 H92 0.503 1.446 3.830 H93 -0.809 2.158 2.891 H94 4.016 0.747 6.037 C95 5.405 2.394 5.688 H96 4.142 1.615 3.439 H97 2.612 1.051 4.148 N98 6.565 1.417 5.783 H99 5.586 3.024 4.807 H100 5.500 3.005 6.589 C101 6.544 0.432 4.660 H102 7.419 -0.219 4.742 H103 5.635 -0.171 4.715 H104 6.577 0.977 3.712 C105 7.834 2.208 5.711 H106 8.686 1.530 5.809 H107 7.877 2.725 4.749

	H108 7.843 2.936 6.526 C109 6.528 0.700 7.099 H110 7.419 0.073 7.181 H111 6.506 1.439 7.905 H112 5.635 0.076 7.156 C113 -1.457 5.254 6.758 H114 -1.552 4.231 7.135 H115 -1.668 5.258 5.680 N116 -2.591 6.002 7.439 C117 -2.517 5.804 8.923 H118 -3.392 6.271 9.382 H119 -2.500 4.732 9.138 H120 -1.609 6.267 9.313 C121 -2.562 7.459 7.112 H122 -3.421 7.945 7.584 H123 -1.639 7.904 7.490 H124 -2.619 7.579 6.026 C125 -3.880 5.420 6.947 H126 -4.714 5.919 7.448 H127 -3.949 5.573 5.867 H128 -3.895 4.351 7.173
1B	**1-GrI**
N1 1.013 5.618 5.203 N2 0.986 4.781 7.321 C1 1.539 4.547 6.011 C2 0.196 6.504 6.022 C3 -0.219 5.580 7.134 C4 1.490 6.245 4.008 C5 2.797 6.751 3.861 C6 3.118 7.466 2.707 C7 2.191 7.714 1.698 C8 0.897 7.233 1.881 C9 0.527 6.504 3.009 C10 3.874 6.524 4.879 C11 2.575 8.417 0.434 C12 -0.892 6.025 3.106 C13 0.799 3.853 8.411 C14 1.178 4.314 9.686 C15 0.953 3.503 10.793 C16 0.336 2.258 10.680 C17 -0.106 1.866 9.421 C18 0.097 2.645 8.281 C19 1.783 5.671 9.896 C20 0.189 1.369 11.875 C21 -0.434 2.151 6.972 H3 4.140 7.832 2.589 H4 0.150 7.406 1.104 H5 3.660 6.981 5.855 H6 4.824 6.943 4.531 H7 4.011 5.456 5.071 H8 3.505 8.984 0.548 H9 1.793 9.106 0.096 H10 2.731 7.691 -0.375 H11 -1.254 5.706 2.123 H12 -1.574 6.823 3.439 H13 -1.000 5.184 3.798 H14 1.274 3.851 11.776 H15 -0.633 0.917 9.315 H16 2.560 5.899 9.162 H17 2.224 5.747 10.895 H18 1.022 6.466 9.826 H19 -0.535 0.567 11.699 H20 -0.130 1.928 12.761 H21 1.150 0.898 12.124	Ru1 3.235 3.277 5.598 Cl1 1.423 1.653 5.340 Cl2 5.049 4.766 6.334 P1 4.845 1.412 5.528 N1 1.638 5.917 5.564 N2 1.373 4.830 7.441 C1 1.946 4.752 6.222 C2 0.660 6.718 6.310 C3 0.794 6.139 7.710 C4 1.722 6.122 4.149 C5 2.705 6.972 3.624 C6 2.672 7.251 2.253 C7 1.716 6.691 1.411 C8 0.764 5.830 1.964 C9 0.747 5.529 3.321 C10 3.801 7.569 4.460 C11 1.734 6.940 -0.065 C12 -0.263 4.565 3.869 C13 1.449 3.884 8.518 C14 2.457 4.002 9.482 C15 2.430 3.112 10.557 C16 1.435 2.149 10.695 C17 0.418 2.099 9.739 C18 0.391 2.968 8.655 C19 3.498 5.080 9.441 C20 1.444 1.181 11.839 C21 -0.753 2.946 7.688 C22 6.606 1.911 5.190 C23 7.635 0.781 5.295 C24 9.050 1.356 5.262 C25 9.280 2.195 4.009 C26 8.232 3.296 3.883 C27 6.820 2.717 3.905 C28 4.940 0.649 7.226 C29 5.626 1.523 8.280 C30 5.811 0.718 9.565 C31 4.484 0.179 10.088 C32 3.721 -0.601 9.022 C33 3.563 0.214 7.742 C34 4.346 -0.006 4.417 C35 4.792 -1.414 4.829 C36 4.128 -2.454 3.926

H22 0.368 2.012 6.239
H23 -1.155 2.846 6.522
H24 -0.950 1.194 7.102
H46 -0.673 6.851 5.442
C115 1.032 7.691 6.522
H48 -0.485 6.087 8.070
H49 -1.087 4.972 6.820
N118 0.317 9.030 6.587
H51 1.427 7.489 7.527
H52 1.867 7.873 5.839
C121 -0.919 8.949 7.422
H122 -1.374 9.941 7.480
H123 -1.624 8.250 6.968
H124 -0.645 8.608 8.425
C125 1.257 10.020 7.205
H126 0.775 11.000 7.237
H127 1.503 9.693 8.218
H128 2.165 10.071 6.599
C129 -0.022 9.501 5.205
H130 -0.451 10.504 5.273
H131 0.891 9.517 4.602
H132 -0.745 8.823 4.749
N65 3.040 2.587 6.442
N66 2.824 3.239 4.269
C67 2.380 3.557 5.604
C68 3.889 1.726 5.629
C69 3.224 1.838 4.285
C70 3.418 2.598 7.825
C71 4.153 3.642 8.422
C72 4.587 3.495 9.739
C73 4.335 2.346 10.485
C74 3.638 1.315 9.863
C75 3.172 1.416 8.554
C76 4.463 4.923 7.709
C77 4.744 2.244 11.922
C78 2.422 0.249 7.979
C79 2.228 3.560 2.992
C80 3.110 4.033 2.003
C81 2.625 4.272 0.720
C82 1.298 4.028 0.379
C83 0.466 3.487 1.355
C84 0.905 3.231 2.653
C85 4.569 4.253 2.274
C86 0.779 4.370 -0.983
C87 -0.053 2.622 3.629
H88 5.134 4.318 10.202
H89 3.421 0.403 10.424
H90 5.097 4.787 6.821
H91 4.988 5.615 8.375
H92 3.547 5.406 7.354
H93 5.606 2.881 12.147
H94 4.995 1.216 12.202
H95 3.923 2.565 12.578
H96 1.789 -0.211 8.746
H97 3.101 -0.544 7.628
H98 1.784 0.537 7.139
H99 3.307 4.663 -0.036
H100 -0.568 3.248 1.098
H101 4.744 4.794 3.208
H102 5.032 4.820 1.460
H103 5.115 3.298 2.343
H104 -0.079 3.749 -1.260
H105 1.549 4.251 -1.753
H106 0.448 5.417 -1.017
H107 -0.171 3.247 4.520
C37 4.419 -2.196 2.451
C38 4.022 -0.779 2.052
C39 4.712 0.244 2.949
C40 3.578 3.851 3.881
C41 3.177 3.450 2.539
C42 2.151 2.539 2.232
C43 1.867 2.224 0.912
C44 2.612 2.783 -0.126
C45 3.640 3.677 0.160
C46 3.909 4.017 1.478
H3 3.441 7.901 1.832
H4 0.032 5.354 1.309
H5 3.703 8.664 4.532
H6 4.775 7.383 3.993
H7 3.854 7.131 5.461
H8 2.330 7.821 -0.323
H9 0.724 7.075 -0.467
H10 2.172 6.076 -0.583
H11 -0.885 4.160 3.064
H12 -0.943 5.021 4.605
H13 0.223 3.716 4.373
H14 3.213 3.185 11.314
H15 -0.387 1.372 9.853
H16 3.701 5.442 8.428
H17 4.450 4.714 9.840
H18 3.194 5.927 10.074
H19 0.449 1.084 12.289
H20 2.147 1.484 12.621
H21 1.740 0.179 11.501
H22 -0.427 2.570 6.710
H23 -1.175 3.950 7.532
H24 -1.556 2.300 8.054
H25 6.782 2.623 6.014
H26 7.504 0.084 4.450
H27 7.492 0.194 6.213
H28 9.196 1.986 6.156
H29 9.788 0.546 5.327
H30 10.291 2.622 4.014
H31 9.222 1.541 3.124
H32 8.387 3.873 2.962
H33 8.334 4.006 4.720
H34 6.086 3.529 3.848
H35 6.674 2.079 3.020
H36 5.555 -0.258 7.101
H37 5.010 2.419 8.471
H38 6.601 1.890 7.932
H39 6.498 -0.120 9.360
H40 6.299 1.338 10.330
H41 3.864 1.032 10.403
H42 4.644 -0.442 10.981
H43 2.732 -0.901 9.397
H44 4.260 -1.535 8.788
H45 3.006 -0.356 6.987
H46 2.952 1.111 7.943
H47 3.245 0.033 4.489
H48 5.888 -1.500 4.749
H49 4.533 -1.628 5.874
H50 4.455 -3.461 4.213
H51 3.039 -2.420 4.093
H52 5.497 -2.329 2.267
H53 3.903 -2.935 1.824
H54 2.929 -0.657 2.147
H55 4.268 -0.583 1.000
H56 4.444 1.261 2.638
H57 5.803 0.148 2.822

H108 0.274 1.634 3.977 H109 -1.038 2.489 3.169 H110 3.852 0.696 6.012 C111 5.330 2.256 5.616 H112 3.883 1.626 3.434 H113 2.363 1.149 4.226 N114 6.424 1.201 5.595 H115 5.493 2.906 4.746 H116 5.528 2.824 6.530 C117 6.251 0.254 4.452 H118 7.083 -0.455 4.451 H119 5.310 -0.288 4.561 H120 6.250 0.824 3.518 C122 7.736 1.906 5.444 H125 8.544 1.169 5.458 H129 7.742 2.447 4.494 H133 7.857 2.607 6.272 C126 6.435 0.448 6.891 H134 7.282 -0.242 6.888 H135 6.526 1.162 7.715 H136 5.505 -0.113 7.001	H58 4.310 4.676 3.849 H59 1.597 2.077 3.046 H60 1.071 1.517 0.689 H61 2.395 2.515 -1.158 H62 4.234 4.106 -0.645 H63 4.708 4.722 1.708 H114 -0.350 6.499 5.918 C115 0.941 8.217 6.253 H116 1.483 6.735 8.333 H117 -0.161 6.049 8.243 N118 -0.110 9.064 5.551 H119 1.011 8.642 7.262 H120 1.887 8.412 5.740 C121 -1.417 8.972 6.274 H122 -2.135 9.640 5.791 H123 -1.790 7.947 6.231 H124 -1.269 9.273 7.315 C125 0.364 10.483 5.588 H126 -0.385 11.120 5.109 H127 0.503 10.790 6.627 H128 1.311 10.552 5.047 C129 -0.298 8.672 4.114 H130 -1.022 9.361 3.669 H131 0.663 8.732 3.594 H132 -0.670 7.648 4.052
1-Ind	**1-GrII**
Ru1 6.489 8.792 11.240 Cl1 6.389 6.350 11.423 Cl2 7.227 11.142 11.289 P1 7.610 8.429 9.070 N1 5.126 9.820 13.840 N2 7.097 8.962 14.220 C1 6.170 9.147 13.257 C2 5.280 9.886 15.302 C3 6.776 9.673 15.451 C4 3.796 9.959 13.326 C5 3.332 11.222 12.920 C6 1.979 11.357 12.603 C7 1.093 10.282 12.667 C8 1.592 9.036 13.047 C9 2.933 8.849 13.377 C10 4.224 12.424 12.798 C11 -0.351 10.466 12.305 C12 3.424 7.484 13.762 C13 8.332 8.233 14.160 C14 9.540 8.916 13.986 C15 10.719 8.171 14.040 C16 10.715 6.798 14.266 C17 9.492 6.164 14.492 C18 8.291 6.862 14.469 C19 9.605 10.403 13.803 C20 11.986 6.005 14.263 C21 7.006 6.169 14.801 C22 7.665 9.956 7.991 C23 8.908 10.159 7.117 C24 8.862 11.539 6.458 C25 7.587 11.744 5.648 C26 6.350 11.495 6.505 C27 6.402 10.107 7.134 C28 9.402 8.040 9.404 C29 10.050 9.084 10.317 C30 11.562 8.875 10.353 C31 11.919 7.458 10.794 C32 11.188 6.397 9.977	N1 5.675 0.685 1.585 N2 5.167 0.661 3.696 C1 4.918 1.311 2.540 C2 6.624 -0.281 2.161 C3 6.014 -0.517 3.527 C4 5.926 1.069 0.234 C5 5.158 0.461 -0.777 C6 5.550 0.651 -2.097 C7 6.656 1.438 -2.431 C8 7.373 2.050 -1.406 C9 7.030 1.879 -0.062 C10 3.943 -0.353 -0.435 C11 7.017 1.649 -3.869 C12 7.840 2.553 1.008 C13 4.592 0.773 5.008 C14 3.457 0.017 5.323 C15 3.116 -0.112 6.672 C16 3.877 0.466 7.682 C17 4.996 1.222 7.327 C18 5.384 1.377 6.002 C19 2.627 -0.677 4.288 C20 3.539 0.277 9.130 C21 6.634 2.126 5.657 H3 4.957 0.202 -2.896 H4 8.219 2.693 -1.655 H5 4.185 -1.274 0.116 H6 3.403 -0.641 -1.342 H7 3.253 0.207 0.213 H8 7.091 0.699 -4.412 H9 7.967 2.182 -3.980 H10 6.238 2.240 -4.370 H11 8.174 3.539 0.664 H12 8.756 1.994 1.261 H13 7.269 2.723 1.929 H14 2.244 -0.714 6.933 H15 5.604 1.677 8.111 H16 1.761 -0.061 4.015 H17 2.260 -1.638 4.666

C33 9.680 6.639 9.961
C34 7.052 6.954 8.077
C35 7.898 6.654 6.834
C36 7.527 5.282 6.269
C37 6.037 5.189 5.957
C38 5.193 5.536 7.180
C39 5.561 6.913 7.727
H3 1.618 12.327 12.256
H4 0.923 8.174 13.058
H5 3.957 13.205 13.529
H6 4.092 12.877 11.808
H7 5.286 12.173 12.889
H8 -0.876 11.089 13.040
H9 -0.878 9.507 12.242
H10 -0.447 10.973 11.336
H11 2.681 6.724 13.497
H12 3.612 7.386 14.844
H13 4.359 7.221 13.248
H14 11.670 8.686 13.892
H15 9.477 5.095 14.711
H16 8.734 10.800 13.271
H17 10.494 10.681 13.226
H18 9.688 10.911 14.774
H19 12.031 5.314 15.113
H20 12.868 6.653 14.300
H21 12.062 5.397 13.352
H22 6.400 6.027 13.895
H23 6.404 6.744 15.520
H24 7.199 5.184 15.237
H25 7.652 10.763 8.744
H26 8.954 9.378 6.340
H27 9.830 10.074 7.706
H28 8.917 12.305 7.249
H29 9.749 11.680 5.827
H30 7.565 12.753 5.217
H31 7.581 11.041 4.798
H32 5.432 11.605 5.913
H33 6.298 12.251 7.307
H34 5.496 9.921 7.725
H35 6.418 9.355 6.328
H36 9.893 8.102 8.417
H37 9.633 8.965 11.333
H38 9.805 10.110 10.011
H39 11.972 9.070 9.348
H40 12.030 9.611 11.023
H41 11.625 7.343 11.846
H42 13.005 7.301 10.748
H43 11.403 5.396 10.377
H44 11.561 6.403 8.939
H45 9.188 5.859 9.365
H46 9.263 6.555 10.979
H47 7.208 6.144 8.810
H48 7.714 7.427 6.068
H49 8.973 6.684 7.059
H50 8.124 5.071 5.373
H51 7.795 4.512 7.013
H52 5.795 5.894 5.145
H53 5.786 4.187 5.583
H54 5.355 4.785 7.972
H55 4.123 5.507 6.932
H56 4.956 7.139 8.611
H57 5.322 7.675 6.971
H114 4.739 9.032 15.751
C115 4.803 11.202 15.907
H116 7.319 10.635 15.484
H18 3.165 -0.847 3.346
H19 4.421 -0.027 9.705
H20 2.761 -0.480 9.274
H21 3.177 1.213 9.577
H22 6.412 3.011 5.045
H23 7.335 1.517 5.066
H24 7.157 2.449 6.563
H114 7.601 0.227 2.265
C115 6.755 -1.538 1.307
H116 5.391 -1.429 3.550
H117 6.748 -0.587 4.340
N118 8.179 -1.964 0.996
H119 6.285 -2.401 1.796
H120 6.285 -1.390 0.328
C121 8.975 -2.129 2.251
H122 9.960 -2.526 1.994
H123 9.090 -1.162 2.745
H124 8.452 -2.826 2.911
C125 8.112 -3.282 0.290
H126 9.125 -3.593 0.022
H127 7.659 -4.022 0.954
H128 7.506 -3.168 -0.612
C129 8.843 -0.974 0.084
H130 9.841 -1.348 -0.160
H131 8.240 -0.866 -0.822
H132 8.918 -0.005 0.582
Ru1 3.713 3.030 2.335
Cl1 1.765 1.608 1.932
Cl2 5.624 4.372 3.126
N68 2.453 5.915 2.085
N69 2.112 4.993 4.023
C70 2.588 4.767 2.783
C71 1.726 6.953 2.836
C72 1.761 6.405 4.250
C73 2.587 6.117 0.678
C74 3.658 6.881 0.199
C75 3.710 7.150 -1.169
C76 2.723 6.701 -2.044
C77 1.660 5.963 -1.527
C78 1.567 5.661 -0.173
C79 4.729 7.383 1.119
C80 2.792 7.003 -3.510
C81 0.425 4.840 0.346
C82 1.824 4.060 5.069
C83 2.651 3.999 6.197
C84 2.210 3.253 7.291
C85 0.991 2.584 7.284
C86 0.196 2.662 6.141
C87 0.575 3.414 5.035
C88 3.936 4.764 6.291
C89 0.518 1.806 8.474
C90 -0.363 3.585 3.881
C40 4.184 3.538 0.623
C41 3.707 3.318 -0.739
C42 2.573 2.575 -1.111
C43 2.237 2.420 -2.447
C44 3.013 3.006 -3.447
C45 4.128 3.762 -3.099
C46 4.468 3.915 -1.762
H100 4.549 7.728 -1.560
H101 0.888 5.593 -2.204
H102 4.349 8.156 1.800
H103 5.550 7.830 0.548
H104 5.134 6.579 1.748
H105 3.804 7.288 -3.816

H117 7.053 9.082 16.333 N118 3.621 11.106 16.861 H119 5.599 11.674 16.498 H120 4.508 11.905 15.123 C121 3.995 10.302 18.066 H122 3.147 10.285 18.756 H123 4.238 9.281 17.764 H124 4.860 10.764 18.549 C125 3.282 12.499 17.292 H126 2.461 12.458 18.013 H127 4.160 12.960 17.752 H128 2.975 13.072 16.412 C129 2.404 10.513 16.215 H130 1.586 10.552 16.939 H131 2.157 11.090 15.318 H132 2.600 9.479 15.929 C120 4.768 8.968 10.551 C122 4.061 10.120 9.908 C123 4.451 11.415 9.605 H125 5.451 11.755 9.861 C124 3.544 12.274 8.970 H129 3.853 13.290 8.731 C126 2.279 11.834 8.613 H133 1.595 12.505 8.098 C128 1.880 10.522 8.894 H134 0.904 10.169 8.571 C130 2.763 9.682 9.551 C131 2.627 8.269 9.957 C132 3.794 7.878 10.534 H135 4.002 6.893 10.934 C40 1.459 7.414 9.781 C41 0.154 7.918 9.844 H136 -0.002 8.979 10.022 C42 -0.941 7.073 9.721 H138 -1.948 7.482 9.780 C43 -0.751 5.710 9.520 H140 -1.607 5.048 9.413 C44 0.541 5.195 9.450 H142 0.696 4.132 9.282 C45 1.636 6.037 9.581 H144 2.647 5.638 9.505	H106 2.121 7.828 -3.780 H107 2.488 6.133 -4.106 H108 -0.265 4.584 -0.465 H109 -0.151 5.372 1.116 H110 0.771 3.901 0.801 H111 2.836 3.223 8.186 H112 -0.775 2.163 6.132 H113 4.372 4.976 5.309 H115 4.675 4.195 6.871 H118 3.787 5.718 6.816 H121 -0.572 1.845 8.570 H125 0.954 2.184 9.406 H129 0.796 0.746 8.390 H133 0.017 3.082 2.983 H134 -0.504 4.645 3.628 H135 -1.346 3.164 4.116 H58 5.078 4.187 0.622 H59 1.963 2.125 -0.332 H60 1.355 1.841 -2.713 H61 2.740 2.884 -4.493 H62 4.725 4.248 -3.869 H63 5.338 4.514 -1.489 H136 0.704 7.048 2.437 H137 2.222 7.923 2.728 H138 2.537 6.881 4.867 H139 0.803 6.479 4.777
1-GrIIdim	**1-Hov**
N1 5.818 0.833 1.612 N2 5.391 0.815 3.744 C1 5.007 1.366 2.573 C2 6.872 -0.039 2.144 C3 6.514 -0.113 3.624 C4 5.866 1.078 0.207 C5 4.979 0.372 -0.629 C6 5.195 0.426 -2.003 C7 6.244 1.165 -2.558 C8 7.080 1.877 -1.702 C9 6.910 1.852 -0.316 C10 3.826 -0.404 -0.064 C11 6.418 1.222 -4.044 C12 7.822 2.660 0.562 C13 4.724 0.778 5.015 C14 3.665 -0.129 5.174 C15 3.178 -0.349 6.463 C16 3.736 0.276 7.575 C17 4.791 1.167 7.376 C18 5.314 1.424 6.112 C19 3.114 -0.895 4.011 C20 3.274 -0.034 8.967	Ru1 13.040 5.876 5.295 Cl1 11.008 5.211 6.387 Cl2 15.330 6.424 4.843 O1 13.823 3.783 5.835 C22 12.741 4.965 3.726 H27 12.253 5.376 2.836 C23 14.211 3.284 7.146 H28 15.136 2.705 6.999 C24 14.507 4.506 7.985 H29 15.269 5.136 7.512 H30 14.870 4.194 8.971 H31 13.593 5.099 8.135 C25 13.099 2.432 7.716 H32 12.872 1.566 7.085 H33 12.188 3.035 7.809 H34 13.386 2.064 8.707 C26 13.754 2.980 4.752 C27 14.206 1.668 4.687 H35 14.655 1.183 5.548 C28 14.080 0.978 3.485 H36 14.437 -0.048 3.431 C29 13.508 1.567 2.357

C21 6.516 2.306 5.959
H3 4.509 -0.102 -2.666
H4 7.879 2.491 -2.123
H5 4.145 -1.209 0.615
H6 3.236 -0.858 -0.867
H7 3.158 0.238 0.530
H8 6.427 0.220 -4.490
H9 7.344 1.732 -4.329
H10 5.581 1.766 -4.501
H11 8.154 3.560 0.034
H12 8.741 2.115 0.838
H13 7.327 2.985 1.486
H14 2.362 -1.060 6.600
H15 5.242 1.659 8.240
H16 2.532 -0.244 3.344
H17 2.464 -1.707 4.352
H18 3.915 -1.339 3.398
H19 4.081 -0.494 9.550
H20 2.424 -0.724 8.973
H21 2.975 0.875 9.503
H22 6.462 2.920 5.052
H23 7.442 1.714 5.912
H24 6.619 2.974 6.821
H114 7.841 0.468 2.007
C115 6.877 -1.388 1.423
H116 6.200 -1.122 3.939
H117 7.339 0.196 4.280
N118 8.250 -1.887 1.006
H119 6.444 -2.179 2.049
H120 6.307 -1.326 0.489
C121 9.179 -1.936 2.177
H122 10.127 -2.378 1.859
H123 9.356 -0.925 2.550
H124 8.726 -2.549 2.961
C125 8.088 -3.271 0.461
H126 9.060 -3.635 0.119
H127 7.702 -3.924 1.247
H128 7.386 -3.239 -0.376
C129 8.821 -1.019 -0.077
H130 9.781 -1.439 -0.386
H131 8.122 -0.997 -0.918
H132 8.963 -0.003 0.297
Ru1 3.734 3.028 2.378
Cl1 1.696 1.717 2.113
Cl2 5.735 4.287 3.088
N68 2.513 5.973 2.123
N69 2.043 5.063 4.008
C70 2.626 4.796 2.806
C71 1.879 6.945 2.890
C72 1.587 6.375 4.075
C73 2.748 6.205 0.727
C74 3.881 6.918 0.325
C75 4.015 7.197 -1.035
C76 3.050 6.814 -1.964
C77 1.919 6.136 -1.514
C78 1.742 5.821 -0.172
C79 4.911 7.369 1.313
C80 3.215 7.129 -3.421
C81 0.526 5.081 0.294
C82 1.702 4.124 5.042
C83 2.545 3.979 6.147
C84 2.100 3.175 7.195
C85 0.864 2.534 7.157
C86 0.052 2.714 6.039
C87 0.436 3.523 4.976
H37 13.419 1.003 1.433
C30 13.056 2.873 2.431
H38 12.608 3.363 1.566
C31 13.174 3.602 3.624
N1 12.166 8.319 3.690
N2 12.415 8.642 5.838
C1 12.464 7.684 4.870
C2 11.681 9.682 3.926
C3 12.278 9.980 5.293
C4 11.831 7.682 2.460
C5 12.800 7.616 1.449
C6 12.421 7.080 0.215
C7 11.137 6.586 -0.009
C8 10.214 6.622 1.041
C9 10.537 7.156 2.285
C10 14.226 8.004 1.701
C11 10.760 5.986 -1.329
C12 9.557 7.084 3.420
C13 12.672 8.411 7.230
C14 13.977 8.478 7.732
C15 14.169 8.150 9.075
C16 13.108 7.810 9.908
C17 11.809 7.864 9.396
C18 11.565 8.175 8.064
C19 15.133 8.977 6.918
C20 13.346 7.389 11.326
C21 10.165 8.278 7.541
H3 13.161 7.026 -0.585
H4 9.218 6.202 0.888
H5 14.334 8.896 2.331
H6 14.768 8.162 0.763
H7 14.736 7.210 2.267
H8 11.414 6.333 -2.135
H9 9.725 6.224 -1.599
H10 10.836 4.892 -1.295
H11 8.594 6.693 3.078
H12 9.366 8.054 3.902
H13 9.925 6.419 4.218
H14 15.182 8.170 9.478
H15 10.964 7.655 10.053
H16 16.046 8.418 7.146
H17 15.324 10.032 7.157
H18 14.971 8.878 5.841
H19 12.537 7.718 11.987
H20 14.290 7.787 11.714
H21 13.397 6.295 11.400
H22 9.956 7.472 6.828
H23 9.990 9.237 7.031
H24 9.441 8.201 8.357
H114 10.578 9.655 4.012
C115 12.108 10.659 2.834
H116 13.268 10.466 5.200
H117 11.640 10.612 5.924
N118 10.974 11.342 2.086
H119 12.714 11.475 3.247
H120 12.696 10.147 2.066
C121 10.103 12.114 3.026
H122 9.355 12.659 2.445
H123 9.601 11.429 3.713
H124 10.725 12.817 3.587
C125 11.590 12.297 1.111
H126 10.795 12.794 0.551
H127 12.178 13.038 1.658
H128 12.234 11.737 0.428
C129 10.150 10.352 1.314

C88 3.846 4.716 6.238 C89 0.396 1.672 8.289 C90 -0.497 3.772 3.832 C40 4.158 3.509 0.646 C41 3.616 3.280 -0.689 C42 2.444 2.564 -0.991 C43 2.032 2.407 -2.306 C44 2.774 2.957 -3.352 C45 3.935 3.670 -3.073 C46 4.348 3.831 -1.757 H1 1.696 7.935 2.498 H2 1.095 6.751 4.962 H100 4.900 7.737 -1.375 H101 1.160 5.825 -2.234 H102 4.492 8.089 2.028 H103 5.749 7.856 0.804 H104 5.299 6.529 1.904 H105 4.272 7.231 -3.692 H106 2.719 8.071 -3.683 H107 2.775 6.345 -4.047 H108 -0.160 4.900 -0.540 H109 -0.017 5.642 1.066 H110 0.787 4.108 0.735 H111 2.733 3.070 8.078 H112 -0.928 2.237 6.009 H113 4.492 4.529 5.371 H115 4.387 4.430 7.146 H118 3.685 5.802 6.275 H121 -0.695 1.694 8.385 H125 0.827 1.987 9.246 H129 0.685 0.625 8.128 H133 -0.089 3.356 2.902 H134 -0.668 4.845 3.673 H135 -1.467 3.300 4.016 H58 5.065 4.138 0.599 H59 1.864 2.138 -0.176 H60 1.120 1.854 -2.519 H61 2.443 2.833 -4.381 H62 4.515 4.114 -3.880 H63 5.250 4.403 -1.538	H130 9.396 10.904 0.748 H131 10.806 9.793 0.640 H132 9.665 9.655 2.001
1-Hov-TS	**1-Hov-a**
Ru1 12.959 5.715 5.183 Cl1 11.265 5.283 6.747 Cl2 15.218 6.266 4.701 O1 11.527 2.731 5.062 C22 12.497 4.838 3.676 H27 11.857 5.169 2.853 C23 10.747 1.635 5.578 H28 11.411 0.977 6.160 C24 9.718 2.236 6.505 H29 10.195 2.776 7.327 H30 9.081 1.444 6.915 H31 9.085 2.945 5.957 C25 10.105 0.874 4.434 H32 10.844 0.470 3.734 H33 9.437 1.544 3.878 H34 9.509 0.039 4.818 C26 12.664 2.462 4.396 C27 13.342 1.239 4.391 H35 12.965 0.390 4.953 C28 14.515 1.107 3.659 H36 15.034 0.151 3.667 C29 15.033 2.171 2.922 H37 15.953 2.052 2.356	Ru1 13.033 5.901 5.287 Cl1 11.292 5.185 6.716 Cl2 15.278 6.360 4.658 O1 10.973 3.172 2.411 C22 12.490 4.938 3.817 H27 11.794 5.295 3.057 C23 10.079 2.330 1.670 H28 9.926 1.398 2.235 C24 8.769 3.080 1.599 H29 8.419 3.347 2.602 H30 8.003 2.470 1.109 H31 8.900 4.002 1.018 C25 10.655 2.048 0.297 H32 11.613 1.521 0.349 H33 10.823 2.998 -0.227 H34 9.963 1.442 -0.298 C26 12.048 2.640 3.025 C27 12.377 1.285 3.012 H35 11.778 0.570 2.457 C28 13.480 0.831 3.726 H36 13.716 -0.231 3.704 C29 14.283 1.706 4.452 H37 15.151 1.340 4.993

C30 14.370 3.384 2.933	C30 13.972 3.052 4.459
H38 14.769 4.241 2.391	H38 14.625 3.756 4.977
C31 13.182 3.543 3.659	C31 12.859 3.552 3.755
N1 12.165 8.198 3.720	N1 12.065 8.285 3.744
N2 12.448 8.526 5.868	N2 12.402 8.643 5.882
C1 12.447 7.566 4.909	C1 12.424 7.676 4.924
C2 11.722 9.577 3.948	C2 11.582 9.648 3.980
C3 12.332 9.864 5.308	C3 12.230 9.970 5.318
C4 11.746 7.570 2.509	C4 11.662 7.627 2.545
C5 12.654 7.476 1.443	C5 12.577 7.523 1.488
C6 12.186 6.971 0.228	C6 12.132 6.950 0.293
C7 10.870 6.538 0.067	C7 10.828 6.482 0.142
C8 10.008 6.604 1.164	C8 9.958 6.567 1.232
C9 10.423 7.105 2.397	C9 10.356 7.114 2.449
C10 14.106 7.811 1.612	C10 14.016 7.912 1.647
C11 10.403 5.969 -1.238	C11 10.366 5.897 -1.159
C12 9.504 7.047 3.583	C12 9.445 7.043 3.641
C13 12.629 8.391 7.287	C13 12.726 8.475 7.269
C14 13.905 8.430 7.850	C14 14.051 8.580 7.703
C15 14.000 8.324 9.241	C15 14.300 8.393 9.064
C16 12.878 8.220 10.051	C16 13.275 8.153 9.973
C17 11.615 8.263 9.453	C17 11.957 8.137 9.509
C18 11.465 8.358 8.078	C18 11.657 8.303 8.165
C19 15.159 8.634 7.055	C19 15.176 8.977 6.795
C20 13.005 8.073 11.537	C20 13.564 7.921 11.425
C21 10.100 8.423 7.462	C21 10.236 8.302 7.689
H3 12.879 6.892 -0.610	H3 12.835 6.849 -0.534
H4 8.988 6.232 1.062	H4 8.947 6.171 1.140
H5 14.282 8.759 2.136	H5 14.162 8.785 2.295
H6 14.618 7.849 0.645	H6 14.488 8.101 0.678
H7 14.600 7.057 2.241	H7 14.568 7.105 2.149
H8 10.958 6.388 -2.084	H8 9.916 6.662 -1.804
H9 9.336 6.151 -1.401	H9 9.605 5.123 -1.004
H10 10.552 4.883 -1.261	H10 11.197 5.451 -1.715
H11 8.518 6.673 3.292	H11 8.477 6.614 3.363
H12 9.352 8.019 4.076	H12 9.249 8.017 4.115
H13 9.904 6.374 4.357	H13 9.878 6.404 4.427
H14 14.991 8.339 9.696	H14 15.328 8.454 9.421
H15 10.725 8.219 10.081	H15 11.143 7.987 10.219
H16 15.805 7.750 7.102	H16 16.077 8.393 7.006
H17 15.725 9.481 7.461	H17 15.427 10.035 6.953
H18 14.971 8.809 5.992	H18 14.948 8.821 5.736
H19 12.229 8.639 12.064	H19 12.822 8.413 12.064
H20 13.981 8.412 11.896	H20 14.556 8.290 11.705
H21 12.892 7.023 11.832	H21 13.531 6.850 11.661
H22 9.901 7.518 6.874	H22 10.023 7.391 7.114
H23 9.981 9.290 6.795	H23 10.015 9.164 7.043
H24 9.330 8.498 8.236	H24 9.544 8.335 8.536
H114 10.620 9.579 4.036	H114 10.483 9.618 4.108
C115 12.165 10.532 2.845	C115 11.966 10.608 2.859
H116 13.331 10.327 5.218	H116 13.211 10.463 5.183
H117 11.711 10.506 5.946	H117 11.611 10.602 5.968
N118 11.041 11.299 2.167	N118 10.802 11.304 2.173
H119 12.851 11.297 3.231	H119 12.610 11.414 3.230
H120 12.670 9.989 2.040	H120 12.500 10.078 2.062
C121 10.260 12.095 3.165	C121 9.995 12.088 3.160
H122 9.519 12.697 2.633	H122 9.224 12.645 2.621
H123 9.752 11.424 3.859	H123 9.522 11.411 3.873
H124 10.947 12.747 3.712	H124 10.657 12.782 3.686
C125 11.667 12.242 1.186	C125 11.376 12.251 1.164
H126 10.877 12.794 0.671	H126 10.557 12.754 0.645
H127 12.318 12.937 1.721	H127 12.000 12.987 1.677
H128 12.250 11.664 0.464	H128 11.977 11.683 0.450
C129 10.130 10.373 1.415	C129 9.926 10.322 1.454
H130 9.379 10.976 0.899	H130 9.145 10.879 0.930

H131 10.723 9.799 0.696 H132 9.645 9.684 2.108	H131 10.536 9.755 0.744 H132 9.475 9.630 2.168
1-Gr_I_P(Cy)$_3$	**1-Ind_P(Cy)$_3$**
Ru1 3.075 3.368 5.745 Cl1 1.423 1.656 5.561 Cl2 5.045 4.572 6.408 N1 1.642 6.004 5.527 N2 1.382 4.947 7.441 C1 1.949 4.850 6.215 C2 0.675 6.813 6.280 C3 0.850 6.274 7.694 C4 1.681 6.154 4.104 C5 2.643 6.994 3.525 C6 2.578 7.221 2.147 C7 1.614 6.613 1.346 C8 0.689 5.758 1.951 C9 0.700 5.511 3.319 C10 3.771 7.598 4.314 C11 1.599 6.806 -0.138 C12 -0.283 4.547 3.914 C13 1.421 3.945 8.470 C14 2.482 3.904 9.381 C15 2.476 2.882 10.333 C16 1.441 1.957 10.413 C17 0.359 2.085 9.538 C18 0.322 3.072 8.564 C19 3.551 4.953 9.428 C20 1.468 0.845 11.416 C21 -0.858 3.193 7.648 C40 3.459 3.940 4.014 C41 3.233 3.395 2.697 C42 2.367 2.322 2.407 C43 2.154 1.933 1.095 C44 2.814 2.581 0.052 C45 3.696 3.626 0.318 C46 3.895 4.035 1.627 H3 3.331 7.862 1.684 H4 -0.047 5.247 1.330 H5 3.682 8.693 4.391 H6 4.725 7.411 3.807 H7 3.858 7.169 5.317 H8 2.201 7.665 -0.447 H9 0.580 6.942 -0.518 H10 2.007 5.915 -0.634 H11 -0.987 4.195 3.154 H12 -0.876 4.980 4.734 H13 0.223 3.664 4.334 H14 3.304 2.823 11.039 H15 -0.477 1.390 9.618 H16 3.655 5.501 8.487 H17 4.530 4.508 9.635 H18 3.339 5.666 10.237 H19 0.486 0.699 11.879 H20 2.197 1.031 12.210 H21 1.738 -0.103 10.934 H22 -0.605 2.830 6.644 H23 -1.206 4.231 7.552 H24 -1.696 2.595 8.018 H58 4.086 4.842 3.976 H59 1.864 1.815 3.227 H60 1.476 1.110 0.881 H61 2.648 2.261 -0.975 H62 4.225 4.118 -0.495 H63 4.571 4.862 1.845	Ru1 6.489 9.218 11.387 Cl1 7.147 7.055 10.763 Cl2 6.872 11.556 11.614 N1 4.852 9.577 13.909 N2 6.945 8.958 14.184 C1 5.991 9.175 13.249 C2 5.041 9.600 15.364 C3 6.542 9.337 15.526 C4 3.492 9.587 13.452 C5 2.909 10.761 12.959 C6 1.540 10.746 12.670 C7 0.750 9.619 12.863 C8 1.367 8.455 13.330 C9 2.723 8.416 13.628 C10 3.667 12.033 12.718 C11 -0.721 9.637 12.584 C12 3.329 7.131 14.115 C13 8.254 8.429 13.928 C14 9.347 9.286 13.758 C15 10.584 8.705 13.473 C16 10.750 7.327 13.394 C17 9.648 6.505 13.640 C18 8.393 7.031 13.908 C19 9.254 10.771 13.939 C20 12.076 6.726 13.044 C21 7.218 6.127 14.129 H3 1.086 11.655 12.271 H4 0.774 7.543 13.431 H5 3.167 12.880 13.208 H6 3.691 12.258 11.644 H7 4.714 11.982 13.028 H8 -1.300 9.688 13.515 H9 -1.031 8.724 12.061 H10 -1.004 10.497 11.970 H11 2.805 6.277 13.671 H12 3.239 7.010 15.206 H13 4.391 7.040 13.861 H14 11.443 9.358 13.318 H15 9.770 5.422 13.603 H16 8.229 11.143 13.869 H17 9.829 11.296 13.169 H18 9.677 11.060 14.911 H19 12.276 5.823 13.631 H20 12.897 7.431 13.207 H21 12.097 6.433 11.987 H22 6.597 6.089 13.223 H23 6.582 6.459 14.962 H24 7.548 5.106 14.347 H114 4.466 8.773 15.815 C115 4.591 10.944 15.947 H116 7.093 10.236 15.848 H117 6.765 8.535 16.243 N118 3.471 10.887 16.974 H119 5.419 11.448 16.459 H120 4.238 11.604 15.148 C121 3.891 10.073 18.155 H122 3.101 10.110 18.910 H123 4.051 9.037 17.849 H124 4.816 10.489 18.563 C125 3.206 12.292 17.422 H126 2.407 12.282 18.168

H114 -0.344 6.575 5.924 C115 0.943 8.311 6.170 H116 1.576 6.874 8.272 H117 -0.088 6.227 8.263 N118 -0.136 9.131 5.481 H119 1.049 8.765 7.164 H120 1.870 8.496 5.618 C121 -1.409 9.072 6.267 H122 -2.152 9.712 5.784 H123 -1.777 8.044 6.294 H124 -1.216 9.427 7.283 C125 0.341 10.550 5.438 H126 -0.431 11.170 4.977 H127 0.537 10.895 6.456 H128 1.259 10.594 4.845 C129 -0.390 8.681 4.072 H130 -1.123 9.360 3.629 H131 0.549 8.707 3.510 H132 -0.779 7.661 4.069	H127 4.117 12.710 17.857 H128 2.900 12.884 16.556 C129 2.201 10.336 16.396 H130 1.429 10.381 17.169 H131 1.913 10.934 15.525 H132 2.352 9.303 16.077 C31 4.790 9.119 10.645 C32 4.220 9.997 9.604 C33 4.706 11.147 9.007 H33 5.677 11.545 9.294 C34 3.917 11.787 8.040 H34 4.285 12.689 7.558 C35 2.685 11.265 7.683 H35 2.090 11.759 6.918 C36 2.189 10.098 8.287 H36 1.234 9.692 7.964 C37 2.949 9.476 9.258 C38 2.731 8.249 10.062 C39 3.824 8.069 10.859 H39 3.984 7.239 11.538 C40 1.561 7.381 10.055 C41 0.281 7.874 9.766 H41 0.152 8.927 9.530 C42 -0.832 7.046 9.842 H42 -1.818 7.447 9.617 C43 -0.688 5.712 10.209 H43 -1.560 5.063 10.264 C44 0.578 5.208 10.498 H44 0.698 4.162 10.770 C45 1.691 6.031 10.420 H45 2.683 5.624 10.609
1-GrII_Imes/SIMes	**2**
N1 6.305 0.828 1.524 N2 5.711 0.741 3.632 C1 5.360 1.259 2.424 C2 7.242 -0.119 2.135 C3 7.041 0.151 3.621 C4 6.549 1.225 0.173 C5 5.908 0.607 -0.909 C6 6.305 0.976 -2.198 C7 7.283 1.938 -2.429 C8 7.871 2.564 -1.326 C9 7.514 2.232 -0.025 C10 4.784 -0.379 -0.768 C11 7.661 2.342 -3.821 C12 8.075 2.986 1.145 C13 4.979 0.896 4.855 C14 4.106 -0.139 5.235 C15 3.387 0.018 6.413 C16 3.537 1.149 7.218 C17 4.466 2.116 6.844 C18 5.215 2.006 5.673 C19 4.007 -1.407 4.441 C20 2.716 1.302 8.460 C21 6.283 3.015 5.376 H3 5.806 0.508 -3.049 H4 8.612 3.347 -1.489 H5 4.446 -0.518 0.263 H6 5.038 -1.354 -1.214 H7 3.902 -0.018 -1.312 H8 7.415 1.565 -4.551 H9 8.731 2.563 -3.900 H10 7.125 3.252 -4.120 H11 8.778 3.756 0.814	N1 6.708 1.233 1.784 N2 5.872 0.989 3.749 C1 5.647 1.613 2.588 C2 7.507 0.198 2.362 C3 7.161 0.277 3.825 C4 6.831 1.507 0.381 C5 5.807 1.126 -0.505 C6 6.006 1.355 -1.866 C7 7.168 1.947 -2.358 C8 8.149 2.331 -1.446 C9 8.002 2.130 -0.077 C10 4.502 0.547 -0.034 C11 7.343 2.202 -3.823 C12 9.073 2.593 0.867 C13 5.009 1.059 4.890 C14 4.023 0.078 5.027 C15 3.195 0.130 6.142 C16 3.333 1.130 7.105 C17 4.318 2.100 6.923 C18 5.171 2.087 5.822 C19 3.841 -0.979 3.976 C20 2.447 1.153 8.313 C21 6.208 3.152 5.626 H3 5.220 1.069 -2.565 H4 9.054 2.817 -1.812 H5 3.997 1.231 0.656 H6 4.612 -0.407 0.506 H7 3.842 0.348 -0.882 H8 6.729 1.527 -4.427 H9 8.388 2.082 -4.129 H10 7.048 3.227 -4.076 H11 9.632 3.426 0.432

H12 8.605 2.342 1.860 H13 7.272 3.485 1.706 H14 2.697 -0.768 6.720 H15 4.619 2.986 7.484 H16 3.785 -1.215 3.385 H17 3.214 -2.050 4.835 H18 4.946 -1.981 4.503 H19 3.131 2.063 9.128 H20 2.649 0.359 9.014 H21 1.691 1.603 8.213 H22 6.545 3.054 4.314 H23 7.189 2.783 5.953 H24 5.959 4.020 5.662 H114 8.265 0.137 1.826 C115 6.887 -1.555 1.714 H116 7.076 -0.754 4.243 H117 7.786 0.862 4.013 N118 7.996 -2.315 1.009 H119 6.609 -2.171 2.579 H120 6.038 -1.547 1.024 C121 9.174 -2.477 1.916 H122 9.931 -3.081 1.410 H123 9.592 -1.498 2.157 H124 8.848 -2.979 2.832 C125 7.463 -3.672 0.660 H126 8.246 -4.242 0.154 H127 7.161 -4.184 1.577 H128 6.601 -3.552 0.000 C129 8.416 -1.634 -0.261 H130 9.186 -2.246 -0.738 H131 7.548 -1.532 -0.916 H132 8.813 -0.639 -0.045 Ru1 3.726 2.226 2.190 Cl1 2.470 0.252 1.789 Cl2 4.067 4.259 3.298 C40 4.003 2.830 0.476 C41 2.956 3.225 -0.430 C42 1.588 3.108 -0.115 C43 0.626 3.505 -1.028 C44 1.008 4.011 -2.270 C45 2.356 4.124 -2.602 C46 3.323 3.735 -1.690 H58 5.017 2.996 0.095 H59 1.286 2.688 0.844 H60 -0.428 3.415 -0.778 H61 0.248 4.318 -2.985 H62 2.648 4.519 -3.573 H63 4.382 3.820 -1.934	H12 9.813 1.807 1.081 H13 8.658 2.931 1.822 H14 2.413 -0.621 6.261 H15 4.419 2.900 7.656 H16 3.678 -0.530 2.987 H17 2.979 -1.615 4.197 H18 4.714 -1.652 3.914 H19 2.884 0.565 9.130 H20 1.462 0.727 8.097 H21 2.304 2.172 8.688 H22 6.148 3.585 4.620 H23 7.228 2.764 5.757 H24 6.078 3.960 6.350 H114 8.568 0.224 2.101 H47 7.076 -0.691 4.335 H48 7.910 0.877 4.360 N65 6.980 -1.151 1.751 H66 6.930 -1.024 0.730 H67 6.026 -1.318 2.097 H68 7.563 -1.965 1.965
2A	**2B**
N1 1.140 5.633 5.172 N2 1.052 4.655 7.219 C1 1.571 4.469 5.877 C2 0.952 6.687 6.160 C3 0.379 5.894 7.289 C4 1.435 6.121 3.848 C5 2.550 6.936 3.592 C6 2.668 7.526 2.335 C7 1.712 7.352 1.340 C8 0.595 6.573 1.636 C9 0.432 5.970 2.878 C10 3.602 7.242 4.618 C11 1.894 7.966 -0.013 C12 -0.835 5.229 3.182 C13 0.538 3.676 8.151	N1 0.973 5.582 5.186 N2 0.957 4.730 7.295 C1 1.525 4.510 5.995 C2 0.071 6.335 5.952 C3 -0.304 5.437 7.081 C4 1.435 6.274 4.002 C5 2.698 6.892 3.935 C6 3.023 7.629 2.796 C7 2.131 7.796 1.740 C8 0.870 7.219 1.861 C9 0.496 6.464 2.967 C10 3.733 6.745 5.009 C11 2.516 8.534 0.497 C12 -0.899 5.911 3.013 C13 0.822 3.805 8.400

C14 0.829 3.882 9.516	C14 1.243 4.284 9.653
C15 0.243 3.045 10.460	C15 1.012 3.506 10.781
C16 -0.640 2.023 10.110	C16 0.348 2.283 10.708
C17 -0.937 1.865 8.760	C17 -0.110 1.864 9.462
C18 -0.370 2.669 7.767	C18 0.101 2.605 8.299
C19 1.723 4.986 9.998	C19 1.889 5.629 9.814
C20 -1.232 1.128 11.152	C20 0.160 1.446 11.934
C21 -0.739 2.370 6.344	C21 -0.445 2.081 7.004
H3 3.540 8.150 2.132	H3 4.013 8.081 2.733
H4 -0.182 6.443 0.881	H4 0.147 7.349 1.054
H5 3.393 8.188 5.136	H5 3.445 7.180 5.979
H6 4.583 7.363 4.146	H6 4.665 7.240 4.718
H7 3.685 6.458 5.373	H7 3.947 5.690 5.202
H8 2.343 8.962 0.052	H8 3.433 9.114 0.631
H9 0.945 8.053 -0.551	H9 1.724 9.217 0.170
H10 2.565 7.351 -0.630	H10 2.687 7.828 -0.327
H11 -1.378 4.980 2.264	H11 -1.215 5.598 2.012
H12 -1.520 5.850 3.784	H12 -1.623 6.673 3.336
H13 -0.652 4.294 3.723	H13 -0.995 5.048 3.679
H14 0.483 3.202 11.513	H14 1.352 3.870 11.752
H15 -1.635 1.084 8.457	H15 -0.658 0.924 9.387
H16 2.442 5.305 9.236	H16 2.675 5.808 9.072
H17 2.289 4.663 10.878	H17 2.342 5.727 10.805
H18 1.145 5.866 10.314	H18 1.153 6.444 9.729
H19 -2.100 0.581 10.774	H19 -0.555 0.634 11.770
H20 -1.542 1.692 12.038	H20 -0.193 2.045 12.780
H21 -0.498 0.385 11.491	H21 1.113 0.993 12.241
H22 -0.087 1.583 5.940	H22 0.333 1.994 6.237
H23 -0.640 3.225 5.668	H23 -1.234 2.718 6.583
H24 -1.764 1.991 6.279	H24 -0.889 1.091 7.149
H46 0.289 7.468 5.768	H46 -0.747 6.783 5.380
H47 1.884 7.169 6.499	H47 -0.625 5.951 7.995
H48 0.387 6.357 8.280	H48 -1.127 4.778 6.757
N49 2.897 2.471 6.485	N49 3.054 2.564 6.424
N50 2.797 2.920 4.261	N50 2.837 3.222 4.259
C51 2.371 3.423 5.529	C51 2.382 3.538 5.584
C52 3.565 1.439 5.791	C52 3.791 1.679 5.623
C53 2.980 1.482 4.417	C53 3.181 1.802 4.269
C54 3.438 2.711 7.804	C54 3.470 2.573 7.810
C55 4.349 3.753 8.069	C55 4.273 3.597 8.347
C56 4.945 3.815 9.331	C56 4.709 3.482 9.667
C57 4.674 2.885 10.330	C57 4.397 2.380 10.458
C58 3.785 1.854 10.030	C58 3.647 1.359 9.880
C59 3.170 1.738 8.788	C59 3.179 1.424 8.571
C60 4.689 4.840 7.094	C60 4.630 4.837 7.584
C61 5.292 3.001 11.688	C61 4.811 2.307 11.894
C62 2.272 0.561 8.542	C62 2.408 0.254 8.034
C63 2.470 3.332 2.919	C63 2.268 3.591 2.980
C64 3.442 4.070 2.225	C64 3.161 4.151 2.051
C65 3.236 4.365 0.883	C65 2.713 4.409 0.760
C66 2.105 3.922 0.200	C66 1.416 4.101 0.357
C67 1.178 3.155 0.899	C67 0.574 3.489 1.282
C68 1.339 2.840 2.247	C68 0.973 3.215 2.589
C69 4.716 4.492 2.892	C69 4.595 4.435 2.396
C70 1.873 4.281 -1.234	C70 0.933 4.451 -1.015
C71 0.309 1.964 2.896	C71 0.000 2.545 3.515
H72 5.645 4.626 9.534	H72 5.309 4.288 10.090
H73 3.562 1.106 10.792	H73 3.401 0.478 10.475
H74 4.588 4.547 6.044	H74 5.210 4.653 6.667
H75 5.707 5.207 7.258	H75 5.233 5.510 8.200
H76 4.018 5.698 7.235	H76 3.729 5.372 7.267
H77 6.203 3.606 11.670	H77 5.646 2.980 12.113
H78 5.538 2.020 12.106	H78 5.104 1.292 12.180
H79 4.597 3.482 12.389	H79 3.977 2.596 12.547
H80 1.730 0.299 9.456	H80 1.782 -0.180 8.819

H81 2.846 -0.334 8.261 H82 1.533 0.754 7.758 H83 3.987 4.951 0.351 H84 0.294 2.784 0.379 H85 4.547 4.907 3.891 H86 5.238 5.252 2.302 H87 5.413 3.642 2.985 H88 1.429 3.451 -1.793 H89 2.800 4.574 -1.736 H90 1.177 5.128 -1.312 H91 0.244 2.131 3.973 H92 0.524 0.899 2.732 H93 -0.683 2.145 2.467 H94 3.562 0.474 6.307 H95 3.632 1.088 3.627 H96 2.044 0.900 4.410 N97 -1.153 5.673 6.972 H98 -1.475 4.846 7.496 H99 -1.238 5.484 5.964 H100 -1.737 6.476 7.220 N101 5.093 1.808 5.657 H102 5.422 2.158 6.569 H103 5.168 2.565 4.963 H104 5.677 1.019 5.368	H81 3.080 -0.550 7.700 H82 1.756 0.521 7.196 H83 3.401 4.861 0.043 H84 -0.436 3.210 0.977 H85 4.703 4.937 3.364 H86 5.056 5.076 1.639 H87 5.193 3.511 2.424 H88 0.504 5.464 -1.026 H89 0.151 3.767 -1.360 H90 1.746 4.439 -1.748 H91 -0.122 3.101 4.451 H92 0.303 1.525 3.788 H93 -0.983 2.460 3.040 H94 3.892 0.670 6.035 H95 3.849 1.556 3.435 H96 2.304 1.136 4.208 H97 5.607 2.432 6.473 H98 5.272 3.056 4.951 H99 5.933 1.523 5.109 N100 5.288 2.201 5.523 N101 0.835 7.585 6.565 H102 1.368 8.032 5.808 H103 1.487 7.225 7.274 H104 0.213 8.277 6.992
2-GrI	**2-Ind**
Ru1 3.180 3.223 5.590 Cl1 1.496 1.535 5.298 Cl2 4.897 4.908 6.435 P1 4.942 1.482 5.542 N1 1.761 5.916 5.577 N2 1.404 4.818 7.452 C1 1.886 4.672 6.200 C2 1.577 6.918 6.575 C3 0.889 6.168 7.690 C4 1.662 6.143 4.156 C5 2.597 6.925 3.455 C6 2.429 7.083 2.079 C7 1.382 6.485 1.384 C8 0.463 5.731 2.110 C9 0.575 5.552 3.484 C10 3.790 7.579 4.090 C11 1.268 6.601 -0.103 C12 -0.434 4.711 4.199 C13 1.211 3.797 8.452 C14 2.098 3.737 9.540 C15 1.853 2.794 10.532 C16 0.776 1.910 10.463 C17 -0.097 2.022 9.387 C18 0.080 2.974 8.383 C19 3.275 4.658 9.666 C20 0.573 0.887 11.539 C21 -0.936 3.085 7.289 C22 6.657 2.066 5.110 C23 7.733 0.976 5.188 C24 9.124 1.593 5.057 C25 9.253 2.396 3.766 C26 8.166 3.461 3.673 C27 6.775 2.844 3.797 C28 5.126 0.828 7.277 C29 5.900 1.747 8.226 C30 6.068 1.070 9.585 C31 4.724 0.675 10.188 C32 3.910 -0.187 9.229 C33 3.753 0.493 7.873	Ru1 6.418 8.753 11.320 Cl1 6.308 6.343 11.353 Cl2 6.993 11.207 11.626 P1 7.482 8.541 9.082 N1 4.985 9.584 13.903 N2 7.086 9.045 14.270 C1 6.108 8.988 13.338 C2 5.383 10.345 15.046 C3 6.609 9.616 15.533 C4 3.601 9.338 13.573 C5 2.780 10.344 13.048 C6 1.439 10.037 12.800 C7 0.903 8.782 13.063 C8 1.750 7.803 13.582 C9 3.090 8.054 13.845 C10 3.256 11.731 12.722 C11 -0.536 8.462 12.804 C12 3.960 6.956 14.371 C13 8.407 8.468 14.209 C14 9.528 9.311 14.112 C15 10.790 8.721 14.107 C16 10.966 7.344 14.204 C17 9.836 6.546 14.363 C18 8.551 7.082 14.396 C19 9.432 10.805 14.043 C20 12.332 6.730 14.146 C21 7.388 6.183 14.677 C22 7.352 9.991 7.891 C23 8.581 10.241 7.004 C24 8.391 11.498 6.155 C25 7.129 11.421 5.304 C26 5.912 11.169 6.184 C27 6.095 9.902 7.013 C28 9.313 8.378 9.396 C29 9.860 9.551 10.215 C30 11.385 9.513 10.228 C31 11.903 8.178 10.757 C32 11.273 6.984 10.047 C33 9.747 7.062 10.050

C34 4.482 -0.010 4.516
C35 5.033 -1.372 4.955
C36 4.399 -2.484 4.119
C37 4.601 -2.261 2.623
C38 4.083 -0.890 2.200
C39 4.746 0.211 3.022
C40 3.521 3.851 3.885
C41 3.155 3.456 2.540
C42 2.138 2.542 2.210
C43 1.904 2.204 0.887
C44 2.687 2.749 -0.130
C45 3.694 3.660 0.176
C46 3.912 4.024 1.496
H3 3.157 7.680 1.530
H4 -0.367 5.255 1.587
H5 3.525 8.530 4.584
H6 4.522 7.853 3.324
H7 4.307 6.913 4.794
H8 1.789 7.484 -0.486
H9 0.222 6.651 -0.425
H10 1.712 5.718 -0.584
H11 -1.292 4.503 3.554
H12 -0.810 5.203 5.106
H13 -0.004 3.745 4.505
H14 2.525 2.747 11.391
H15 -0.963 1.361 9.331
H16 3.889 4.671 8.757
H17 3.918 4.350 10.497
H18 2.963 5.693 9.882
H19 -0.301 0.259 11.344
H20 0.437 1.363 12.518
H21 1.449 0.231 11.625
H22 -0.560 2.621 6.369
H23 -1.189 4.127 7.061
H24 -1.860 2.573 7.573
H25 6.849 2.801 5.912
H26 7.578 0.253 4.370
H27 7.659 0.408 6.126
H28 9.303 2.256 5.920
H29 9.889 0.808 5.103
H30 10.248 2.852 3.695
H31 9.161 1.711 2.907
H32 8.246 4.014 2.727
H33 8.300 4.199 4.481
H34 6.014 3.632 3.759
H35 6.593 2.180 2.938
H36 5.700 -0.111 7.190
H37 5.358 2.702 8.338
H38 6.888 2.000 7.821
H39 6.692 0.170 9.458
H40 6.617 1.732 10.267
H41 4.152 1.592 10.404
H42 4.868 0.160 11.147
H43 2.919 -0.407 9.650
H44 4.412 -1.159 9.088
H45 3.158 -0.129 7.192
H46 3.177 1.429 8.001
H47 3.387 -0.038 4.647
H48 6.128 -1.396 4.834
H49 4.828 -1.560 6.018
H50 4.808 -3.456 4.423
H51 3.319 -2.518 4.338
H52 5.676 -2.325 2.389
H53 4.110 -3.056 2.049
H54 2.992 -0.839 2.351
C34 7.072 6.965 8.171
C35 7.897 6.702 6.905
C36 7.666 5.271 6.422
C37 6.185 4.997 6.182
C38 5.362 5.289 7.433
C39 5.580 6.721 7.916
H3 0.801 10.810 12.369
H4 1.353 6.806 13.780
H5 3.157 12.410 13.587
H6 2.633 12.171 11.935
H7 4.284 11.743 12.337
H8 -1.071 8.269 13.742
H9 -0.630 7.560 12.185
H10 -1.049 9.280 12.287
H11 3.358 6.094 14.673
H12 4.545 7.275 15.244
H13 4.672 6.614 13.605
H14 11.666 9.365 14.018
H15 9.956 5.470 14.491
H16 8.815 11.137 13.201
H17 10.427 11.244 13.924
H18 9.013 11.233 14.967
H19 12.502 6.050 14.989
H20 13.118 7.492 14.156
H21 12.453 6.140 13.228
H22 6.802 6.000 13.768
H23 6.716 6.608 15.433
H24 7.737 5.216 15.052
H25 7.237 10.863 8.559
H26 8.740 9.375 6.341
H27 9.492 10.349 7.606
H28 8.324 12.372 6.823
H29 9.277 11.654 5.526
H30 7.003 12.340 4.717
H31 7.229 10.597 4.578
H32 4.996 11.087 5.583
H33 5.764 12.028 6.860
H34 5.199 9.710 7.618
H35 6.200 9.051 6.324
H36 9.782 8.413 8.398
H37 9.475 9.470 11.248
H38 9.501 10.519 9.837
H39 11.755 9.680 9.202
H40 11.777 10.340 10.837
H41 11.651 8.116 11.825
H42 12.998 8.135 10.687
H43 11.602 6.047 10.517
H44 11.622 6.944 9.002
H45 9.333 6.190 9.527
H46 9.363 7.012 11.084
H47 7.362 6.216 8.925
H48 7.599 7.404 6.109
H49 8.969 6.865 7.084
H50 8.247 5.086 5.509
H51 8.049 4.572 7.184
H52 5.829 5.639 5.359
H53 6.036 3.960 5.854
H54 5.651 4.594 8.239
H55 4.294 5.120 7.240
H56 5.010 6.898 8.836
H57 5.194 7.417 7.157
H114 4.581 10.501 15.772
H102 7.369 10.256 15.995
H103 6.339 8.828 16.252
C104 4.702 9.030 10.638

H55 4.261 -0.717 1.130 H56 4.384 1.195 2.697 H57 5.832 0.190 2.833 H58 4.227 4.699 3.882 H59 1.554 2.093 3.010 H60 1.116 1.494 0.645 H61 2.510 2.461 -1.164 H62 4.306 4.087 -0.616 H63 4.695 4.744 1.740 H114 1.077 7.820 6.212 H115 1.137 6.516 8.700 H116 -0.204 6.206 7.574 N117 2.988 7.342 7.076 H118 3.407 8.009 6.422 H119 3.633 6.495 7.052 H120 2.978 7.753 8.012	C105 4.111 10.191 9.901 C106 4.591 11.445 9.555 H107 5.579 11.765 9.865 C108 3.789 12.304 8.792 H109 4.165 13.292 8.532 C110 2.546 11.897 8.338 H111 1.947 12.559 7.717 C112 2.059 10.624 8.661 H113 1.105 10.293 8.261 C114 2.825 9.796 9.462 C115 2.573 8.422 9.946 C116 3.668 8.008 10.642 H117 3.785 7.045 11.124 C118 1.388 7.619 9.673 C119 0.119 8.193 9.509 H120 -0.006 9.267 9.631 C121 -0.990 7.398 9.250 H122 -1.968 7.859 9.131 C123 -0.852 6.017 9.155 H124 -1.720 5.395 8.947 C125 0.400 5.432 9.328 H126 0.513 4.353 9.250 C127 1.509 6.224 9.582 H128 2.495 5.769 9.684 N129 5.820 11.740 14.524 H130 4.994 12.281 14.252 H131 6.373 11.611 13.626 H132 6.366 12.276 15.203
2-GrII	**2-GrIIdim**
N1 5.926 0.970 1.635 N2 5.387 0.839 3.742 C1 5.016 1.433 2.583 C2 6.822 0.010 2.167 C3 6.701 0.202 3.648 C4 5.941 1.115 0.207 C5 5.024 0.405 -0.593 C6 5.205 0.452 -1.974 C7 6.243 1.173 -2.563 C8 7.116 1.878 -1.736 C9 6.989 1.866 -0.350 C10 3.830 -0.322 -0.031 C11 6.392 1.201 -4.053 C12 7.922 2.661 0.515 C13 4.709 0.746 5.003 C14 3.664 -0.185 5.116 C15 3.156 -0.451 6.385 C16 3.688 0.145 7.526 C17 4.729 1.058 7.373 C18 5.264 1.374 6.127 C19 3.158 -0.949 3.930 C20 3.193 -0.211 8.896 C21 6.434 2.307 6.025 H3 4.485 -0.060 -2.613 H4 7.913 2.472 -2.185 H5 4.036 -1.365 0.261 H6 3.049 -0.387 -0.795 H7 3.385 0.197 0.828 H8 6.825 0.265 -4.428 H9 7.042 2.020 -4.377 H10 5.418 1.325 -4.541 H11 8.516 3.348 -0.095 H12 8.638 2.026 1.060 H13 7.377 3.247 1.268 H14 2.346 -1.175 6.485	N1 5.973 0.983 1.639 N2 5.437 0.855 3.749 C1 5.057 1.439 2.587 C2 6.885 0.041 2.176 C3 6.757 0.231 3.657 C4 5.969 1.115 0.209 C5 5.030 0.407 -0.569 C6 5.187 0.439 -1.952 C7 6.223 1.142 -2.567 C8 7.117 1.846 -1.764 C9 7.012 1.850 -0.374 C10 3.840 -0.302 0.022 C11 6.331 1.162 -4.061 C12 7.974 2.641 0.462 C13 4.765 0.771 5.015 C14 3.731 -0.170 5.145 C15 3.232 -0.426 6.420 C16 3.759 0.194 7.551 C17 4.786 1.120 7.381 C18 5.314 1.423 6.128 C19 3.227 -0.951 3.970 C20 3.274 -0.147 8.927 C21 6.472 2.369 6.014 H3 4.454 -0.075 -2.575 H4 7.915 2.423 -2.231 H5 4.068 -1.293 0.447 H6 3.094 -0.485 -0.758 H7 3.346 0.289 0.805 H8 6.464 0.151 -4.465 H9 7.171 1.775 -4.402 H10 5.412 1.565 -4.505 H11 8.516 3.361 -0.158 H12 8.734 2.006 0.940 H13 7.460 3.193 1.262 H14 2.432 -1.159 6.534

H15 5.154 1.534 8.259	H15 5.206 1.617 8.257
H16 2.766 -0.290 3.145	H16 2.812 -0.303 3.187
H17 2.357 -1.635 4.221	H17 2.446 -1.654 4.273
H18 3.959 -1.581 3.499	H18 4.037 -1.564 3.529
H19 3.964 -0.745 9.464	H19 4.050 -0.674 9.496
H20 2.305 -0.851 8.856	H20 2.388 -0.790 8.901
H21 2.937 0.685 9.475	H21 3.020 0.754 9.499
H22 6.410 2.906 5.106	H22 6.462 2.931 5.072
H23 7.386 1.758 6.060	H23 7.430 1.834 6.093
H24 6.450 2.998 6.874	H24 6.458 3.094 6.834
H114 7.832 0.054 1.748	H114 7.895 0.102 1.759
H47 6.748 -0.718 4.245	H47 6.812 -0.689 4.253
H48 7.490 0.887 3.992	H48 7.539 0.922 4.006
Ru49 3.716 3.043 2.383	Ru49 3.756 3.031 2.384
Cl50 1.699 1.702 2.154	Cl50 1.723 1.707 2.218
Cl51 5.712 4.319 3.090	Cl51 5.774 4.301 3.046
N52 2.564 5.984 2.110	N52 2.538 5.993 2.119
N53 2.115 5.059 4.028	N53 2.032 5.061 3.984
C54 2.634 4.831 2.807	C54 2.635 4.809 2.789
C55 1.852 7.045 2.846	C55 1.901 6.959 2.891
C56 1.796 6.479 4.254	C56 1.589 6.374 4.064
C57 2.722 6.177 0.703	C57 2.759 6.230 0.720
C58 3.829 6.895 0.230	C58 3.897 6.925 0.302
C59 3.904 7.154 -1.138	C59 4.019 7.195 -1.061
C60 2.907 6.745 -2.020	C60 3.038 6.819 -1.978
C61 1.807 6.058 -1.511	C61 1.901 6.161 -1.511
C62 1.690 5.764 -0.157	C62 1.736 5.858 -0.164
C63 4.909 7.360 1.158	C63 4.939 7.375 1.278
C64 3.005 7.038 -3.487	C64 3.188 7.125 -3.437
C65 0.506 4.997 0.350	C65 0.509 5.145 0.318
C66 1.725 4.100 5.016	C66 1.655 4.100 4.987
C67 2.524 3.890 6.145	C67 2.490 3.888 6.087
C68 2.037 3.046 7.142	C68 2.030 3.036 7.090
C69 0.794 2.427 7.040	C69 0.788 2.410 7.011
C70 0.011 2.688 5.918	C70 -0.020 2.668 5.907
C71 0.441 3.539 4.907	C71 0.379 3.526 4.889
C72 3.831 4.603 6.323	C72 3.797 4.609 6.223
C73 0.291 1.502 8.106	C73 0.319 1.479 8.088
C74 -0.468 3.869 3.765	C74 -0.545 3.834 3.751
C75 4.137 3.504 0.639	C75 4.155 3.487 0.635
C76 3.594 3.260 -0.689	C76 3.566 3.257 -0.676
C77 2.427 2.531 -0.981	C77 2.371 2.559 -0.928
C78 2.014 2.359 -2.293	C78 1.914 2.393 -2.226
C79 2.752 2.901 -3.346	C79 2.636 2.910 -3.303
C80 3.909 3.625 -3.079	C80 3.819 3.605 -3.074
C81 4.320 3.807 -1.766	C81 4.274 3.781 -1.775
H84 4.770 7.696 -1.523	H82 1.729 7.956 2.510
H85 1.025 5.720 -2.193	H83 1.085 6.742 4.947
H86 4.536 8.108 1.871	H84 4.906 7.722 -1.414
H87 5.727 7.822 0.598	H85 1.128 5.861 -2.219
H88 5.314 6.533 1.755	H86 4.529 8.098 1.995
H89 4.046 7.174 -3.802	H87 5.773 7.858 0.759
H90 2.463 7.955 -3.747	H88 5.331 6.536 1.866
H91 2.570 6.226 -4.082	H89 4.242 7.195 -3.728
H92 -0.171 4.746 -0.473	H90 2.716 8.082 -3.693
H93 -0.072 5.566 1.091	H91 2.712 6.354 -4.054
H94 0.806 4.057 0.834	H92 -0.185 4.965 -0.510
H95 2.643 2.887 8.036	H93 -0.022 5.724 1.085
H96 -0.980 2.238 5.841	H94 0.757 4.172 0.768
H97 4.423 4.634 5.399	H95 2.657 2.877 7.968
H98 4.429 4.118 7.102	H96 -1.006 2.205 5.847
H99 3.674 5.642 6.644	H97 4.449 4.467 5.350
H100 -0.802 1.526 8.177	H98 4.331 4.269 7.116
H101 0.701 1.751 9.091	H99 3.642 5.691 6.320
H102 0.576 0.463 7.886	H100 -0.774 1.461 8.156

H103 -0.114 3.402 2.838 H104 -0.531 4.951 3.588 H105 -1.481 3.504 3.960 H106 5.042 4.134 0.586 H107 1.852 2.108 -0.160 H108 1.103 1.800 -2.500 H109 2.420 2.762 -4.374 H110 4.489 4.058 -3.893 H111 5.219 4.387 -1.554 N112 6.289 -1.404 1.744 H113 6.153 -1.383 0.723 H115 5.367 -1.550 2.180 H116 6.914 -2.175 1.993 H117 2.551 6.924 4.918 H118 0.815 6.578 4.732 H119 0.856 7.194 2.403 H120 2.397 7.992 2.776	H101 0.716 1.757 9.070 H102 0.646 0.451 7.883 H103 -0.140 3.441 2.810 H104 -0.697 4.914 3.627 H105 -1.523 3.373 3.915 H106 5.073 4.096 0.559 H107 1.812 2.154 -0.087 H108 0.984 1.857 -2.403 H109 2.269 2.775 -4.319 H110 4.383 4.022 -3.907 H111 5.193 4.339 -1.592 N112 6.379 -1.386 1.756 H113 6.235 -1.369 0.736 H115 5.465 -1.552 2.199 H116 7.023 -2.143 2.001
2-Hov	**2-Hov-TS**
Ru1 13.081 5.835 5.304 Cl1 11.346 4.982 6.656 Cl2 15.238 6.796 4.585 O1 14.218 3.869 5.643 C22 12.669 4.914 3.762 H27 11.982 5.280 2.991 C23 14.816 3.383 6.882 H28 15.771 2.915 6.603 C24 15.079 4.613 7.719 H29 15.708 5.331 7.180 H30 15.592 4.325 8.642 H31 14.131 5.097 7.998 C25 13.883 2.400 7.552 H32 13.672 1.529 6.924 H33 12.933 2.895 7.785 H34 14.334 2.042 8.484 C26 14.068 3.068 4.562 C27 14.659 1.824 4.392 H35 15.293 1.390 5.158 C28 14.426 1.132 3.206 H36 14.891 0.158 3.071 C29 13.617 1.654 2.197 H37 13.451 1.089 1.284 C30 13.028 2.893 2.373 H38 12.392 3.330 1.604 C31 13.244 3.622 3.555 N1 12.252 8.199 3.647 N2 12.390 8.587 5.818 C1 12.375 7.585 4.899 C2 12.607 9.570 3.775 C3 12.233 9.901 5.201 C4 11.686 7.617 2.456 C5 12.465 7.364 1.316 C6 11.846 6.784 0.210 C7 10.496 6.443 0.207 C8 9.755 6.694 1.360 C9 10.321 7.281 2.488 C10 13.937 7.646 1.237 C11 9.852 5.839 -1.002 C12 9.487 7.486 3.714 C13 12.410 8.418 7.249 C14 13.616 8.576 7.951 C15 13.604 8.357 9.327 C16 12.439 8.019 10.010 C17 11.247 7.954 9.291 C18 11.203 8.159 7.916	Ru1 13.262 5.832 5.043 Cl1 12.088 5.016 6.867 Cl2 15.211 7.043 4.202 O1 12.581 2.591 5.006 C22 12.707 4.893 3.603 H27 11.826 5.084 2.980 C23 12.244 1.333 5.633 H28 13.171 0.883 6.022 C24 11.330 1.656 6.790 H29 11.828 2.296 7.523 H30 11.016 0.728 7.280 H31 10.436 2.180 6.430 C25 11.582 0.417 4.623 H32 12.218 0.223 3.752 H33 10.648 0.870 4.271 H34 11.341 -0.546 5.085 C26 13.584 2.625 4.117 C27 14.525 1.613 3.896 H35 14.490 0.686 4.461 C28 15.516 1.792 2.941 H36 16.240 0.996 2.781 C29 15.600 2.963 2.189 H37 16.382 3.086 1.447 C30 14.681 3.973 2.412 H38 14.735 4.906 1.853 C31 13.662 3.814 3.364 N1 12.050 8.142 3.652 N2 12.351 8.503 5.814 C1 12.368 7.530 4.871 C2 12.243 9.545 3.783 C3 11.977 9.799 5.248 C4 11.443 7.518 2.502 C5 12.122 7.400 1.280 C6 11.461 6.788 0.215 C7 10.169 6.284 0.331 C8 9.525 6.413 1.561 C9 10.134 7.026 2.651 C10 13.526 7.881 1.053 C11 9.496 5.600 -0.818 C12 9.406 7.107 3.958 C13 12.506 8.362 7.242 C14 13.750 8.622 7.831 C15 13.869 8.443 9.207 C16 12.792 8.042 9.994 C17 11.553 7.872 9.381 C18 11.381 8.027 8.010

C19 14.889 9.010 7.289	C19 14.935 9.100 7.047
C20 12.457 7.747 11.482	C20 12.956 7.800 11.463
C21 9.889 8.088 7.202	C21 10.033 7.790 7.404
H3 12.447 6.577 -0.676	H3 11.983 6.693 -0.737
H4 8.699 6.422 1.386	H4 8.512 6.026 1.675
H5 14.464 7.370 2.160	H5 13.556 8.956 0.803
H6 14.141 8.700 0.980	H6 13.963 7.381 0.184
H7 14.392 7.067 0.429	H7 14.183 7.669 1.905
H8 10.578 5.305 -1.624	H8 9.946 5.878 -1.775
H9 9.395 6.615 -1.630	H9 8.428 5.840 -0.857
H10 9.056 5.140 -0.725	H10 9.576 4.510 -0.722
H11 8.427 7.331 3.494	H11 8.360 6.812 3.839
H12 9.598 8.498 4.124	H12 9.420 8.122 4.376
H13 9.769 6.779 4.507	H13 9.855 6.440 4.707
H14 14.536 8.468 9.882	H14 14.834 8.628 9.678
H15 10.318 7.737 9.818	H15 10.691 7.594 9.988
H16 15.671 9.174 8.035	H16 15.353 8.318 6.404
H17 14.764 9.963 6.752	H17 15.728 9.437 7.720
H18 15.262 8.269 6.572	H18 14.683 9.956 6.401
H19 11.573 8.161 11.978	H19 12.061 8.094 12.021
H20 13.348 8.165 11.961	H20 13.811 8.346 11.872
H21 12.456 6.667 11.674	H21 13.124 6.734 11.659
H22 9.771 7.109 6.721	H22 10.003 6.802 6.926
H23 9.788 8.859 6.429	H23 9.766 8.537 6.647
H24 9.063 8.215 7.907	H24 9.257 7.809 8.174
H114 12.185 10.209 2.995	H114 11.666 10.138 3.067
H73 12.877 10.648 5.683	H73 12.572 10.605 5.693
H74 11.194 10.260 5.258	H74 10.914 10.024 5.419
N75 14.160 9.657 3.644	N75 13.752 9.831 3.502
H76 14.433 9.542 2.663	H76 13.935 9.771 2.495
H77 14.593 8.830 4.142	H77 14.331 9.058 3.928
H78 14.551 10.531 4.001	H78 14.066 10.742 3.846
2-Hov-a	**2-GrI_P(Cy)$_3$**
Ru1 13.059 5.879 5.432	Ru1 3.466 3.668 5.936
Cl1 11.613 4.992 7.026	Cl1 2.897 1.420 5.958
Cl2 15.180 6.722 4.547	Cl2 4.660 5.670 6.703
O1 11.121 3.108 2.437	N1 1.533 5.902 5.308
C22 12.458 4.879 3.996	N2 1.258 4.849 7.238
H27 11.543 5.151 3.461	C1 1.908 4.782 6.050
C23 10.309 2.288 1.578	C2 0.968 6.857 6.200
H28 10.394 1.242 1.911	C3 0.390 6.019 7.318
C24 8.894 2.771 1.797	C4 1.513 6.088 3.874
H29 8.580 2.609 2.832	C5 2.455 6.887 3.213
H30 8.200 2.245 1.134	C6 2.332 7.039 1.830
H31 8.837 3.848 1.588	C7 1.311 6.436 1.105
C25 10.772 2.441 0.144	C8 0.376 5.667 1.799
H32 11.798 2.086 -0.003	C9 0.453 5.484 3.172
H33 10.739 3.502 -0.135	C10 3.589 7.592 3.897
H34 10.117 1.884 -0.535	C11 1.214 6.575 -0.382
C26 12.344 2.718 2.813	C12 -0.577 4.653 3.872
C27 12.927 1.495 2.473	C13 1.274 3.828 8.256
H35 12.405 0.789 1.836	C14 2.033 4.021 9.422
C28 14.184 1.169 2.963	C15 2.052 2.994 10.361
H36 14.619 0.211 2.689	C16 1.331 1.815 10.181
C29 14.896 2.042 3.788	C17 0.534 1.692 9.045
H37 15.882 1.773 4.153	C18 0.485 2.683 8.071
C30 14.334 3.257 4.118	C19 2.780 5.292 9.700
H38 14.898 3.964 4.728	C20 1.407 0.704 11.182
C31 13.056 3.631 3.645	C21 -0.376 2.489 6.862
N1 12.134 8.089 3.676	C40 3.864 3.851 4.137
N2 12.454 8.646 5.799	C41 3.197 3.432 2.937
C1 12.366 7.580 4.961	C42 2.051 2.611 2.931
C2 12.498 9.462 3.671	C43 1.503 2.183 1.734
C3 12.250 9.907 5.095	C44 2.076 2.569 0.523

C4 11.475 7.447 2.565 C5 12.181 7.035 1.427 C6 11.459 6.461 0.378 C7 10.080 6.292 0.429 C8 9.413 6.683 1.591 C9 10.084 7.260 2.664 C10 13.668 7.163 1.275 C11 9.318 5.726 -0.730 C12 9.332 7.636 3.903 C13 12.592 8.580 7.233 C14 13.841 8.830 7.823 C15 13.939 8.716 9.207 C16 12.843 8.386 10.001 C17 11.605 8.218 9.385 C18 11.450 8.317 8.006 C19 15.044 9.249 7.030 C20 12.989 8.218 11.482 C21 10.096 8.132 7.397 H3 12.002 6.136 -0.510 H4 8.334 6.542 1.660 H5 14.207 7.004 2.216 H6 13.953 8.135 0.833 H7 14.042 6.415 0.569 H8 8.671 6.489 -1.180 H9 8.664 4.901 -0.419 H10 9.985 5.353 -1.514 H11 8.256 7.510 3.762 H12 9.509 8.681 4.191 H13 9.630 7.010 4.755 H14 14.904 8.898 9.680 H15 10.729 8.000 9.996 H16 15.884 9.463 7.697 H17 14.858 10.170 6.457 H18 15.369 8.472 6.329 H19 12.103 8.577 12.017 H20 13.863 8.752 11.866 H21 13.113 7.159 11.739 H22 9.995 7.115 6.996 H23 9.900 8.841 6.583 H24 9.315 8.268 8.151 H114 12.010 10.044 2.884 H73 12.939 10.680 5.457 H74 11.223 10.284 5.213 N75 14.035 9.521 3.392 H76 14.217 9.276 2.413 H77 14.513 8.767 3.951 H78 14.457 10.432 3.593	C45 3.207 3.384 0.507 C46 3.767 3.806 1.701 H3 3.068 7.648 1.306 H4 -0.433 5.187 1.247 H5 3.306 8.615 4.200 H6 4.423 7.730 3.203 H7 3.983 7.044 4.759 H8 1.920 7.315 -0.772 H9 0.205 6.870 -0.690 H10 1.428 5.615 -0.870 H11 -1.309 4.261 3.161 H12 -1.129 5.231 4.626 H13 -0.126 3.795 4.387 H14 2.644 3.123 11.267 H15 -0.064 0.791 8.907 H16 3.555 5.491 8.952 H17 3.270 5.241 10.676 H18 2.106 6.162 9.735 H19 0.443 0.195 11.292 H20 1.720 1.065 12.166 H21 2.136 -0.051 10.862 H22 0.227 2.117 6.022 H23 -0.872 3.414 6.542 H24 -1.154 1.746 7.058 H58 4.872 4.277 3.979 H59 1.633 2.282 3.880 H60 0.630 1.534 1.741 H61 1.644 2.225 -0.414 H62 3.659 3.674 -0.438 H63 4.659 4.431 1.699 H114 0.283 7.557 5.713 H64 0.442 6.485 8.311 H65 -0.661 5.763 7.116 N65 2.155 7.699 6.759 H66 2.518 8.313 6.022 H67 2.956 7.051 6.989 H68 1.910 8.266 7.575
2-Ind_P(Cy)$_3$	**2-GrII_Imes/SIMes**
Ru1 6.410 9.232 11.483 Cl1 6.999 7.104 10.760 Cl2 6.682 11.635 11.928 N1 4.821 9.610 14.012 N2 6.954 9.056 14.253 C1 5.955 9.150 13.338 C2 5.237 10.177 15.249 C3 6.505 9.427 15.591 C4 3.424 9.437 13.685 C5 2.661 10.466 13.122 C6 1.315 10.209 12.852 C7 0.717 8.988 13.139 C8 1.504 7.988 13.713 C9 2.849 8.189 13.994 C10 3.202 11.824 12.783 C11 -0.728 8.731 12.847	N1 6.286 0.643 1.476 N2 5.677 0.644 3.608 C1 5.372 1.171 2.396 C2 6.873 -0.517 2.050 C3 6.844 -0.233 3.536 C4 6.699 1.244 0.232 C5 6.339 0.698 -1.009 C6 6.723 1.380 -2.164 C7 7.435 2.575 -2.119 C8 7.790 3.081 -0.869 C9 7.440 2.437 0.312 C10 5.544 -0.565 -1.163 C11 7.788 3.317 -3.372 C12 7.805 3.048 1.629 C13 5.048 0.977 4.862 C14 4.100 0.100 5.415

C12 3.666 7.075 14.572
C13 8.252 8.485 13.999
C14 9.375 9.320 13.887
C15 10.597 8.723 13.587
C16 10.727 7.346 13.422
C17 9.603 6.546 13.618
C18 8.358 7.088 13.914
C19 9.310 10.801 14.111
C20 12.040 6.735 13.043
C21 7.181 6.186 14.118
H3 0.718 10.997 12.390
H4 1.057 7.018 13.931
H5 3.062 12.536 13.614
H6 2.644 12.254 11.944
H7 4.254 11.806 12.481
H8 -1.307 8.644 13.775
H9 -0.854 7.791 12.295
H10 -1.170 9.535 12.250
H11 3.042 6.204 14.787
H12 4.159 7.364 15.510
H13 4.458 6.753 13.882
H14 11.478 9.358 13.485
H15 9.697 5.463 13.531
H16 8.685 11.305 13.364
H17 10.311 11.240 14.055
H18 8.915 11.050 15.107
H19 12.191 5.769 13.536
H20 12.881 7.388 13.298
H21 12.080 6.555 11.962
H22 6.546 6.178 13.222
H23 6.566 6.488 14.974
H24 7.511 5.158 14.293
H114 4.453 10.182 16.011
H50 7.261 10.026 16.113
H51 6.283 8.544 16.208
C52 4.708 9.190 10.726
C53 4.265 10.096 9.646
C54 4.867 11.191 9.056
H55 5.830 11.557 9.405
C56 4.207 11.827 7.992
H57 4.666 12.689 7.515
C58 2.989 11.355 7.537
H59 2.498 11.845 6.700
C60 2.375 10.241 8.137
H61 1.436 9.863 7.741
C62 3.004 9.635 9.204
C63 2.653 8.441 10.011
C64 3.679 8.198 10.885
H65 3.727 7.376 11.589
C66 1.432 7.663 9.882
C67 0.220 8.271 9.523
H68 0.185 9.347 9.368
C69 -0.945 7.523 9.424
H70 -1.878 8.010 9.152
C71 -0.919 6.155 9.680
H72 -1.829 5.567 9.592
C73 0.276 5.540 10.050
H74 0.300 4.471 10.245
C75 1.440 6.286 10.152
H76 2.380 5.800 10.409
N77 5.591 11.668 14.956
H78 4.734 12.190 14.746
H79 6.162 11.714 14.068
H80 6.087 12.133 15.721

C15 3.490 0.472 6.610
C16 3.811 1.659 7.265
C17 4.807 2.466 6.721
C18 5.444 2.147 5.526
C19 3.758 -1.222 4.793
C20 3.107 2.057 8.525
C21 6.500 3.060 4.985
H3 6.440 0.966 -3.132
H4 8.354 4.012 -0.812
H5 4.705 -0.617 -0.459
H6 6.182 -1.462 -1.070
H7 5.116 -0.627 -2.168
H8 7.749 2.668 -4.252
H9 8.790 3.753 -3.310
H10 7.089 4.146 -3.543
H11 8.512 3.871 1.493
H12 8.268 2.321 2.308
H13 6.922 3.455 2.140
H14 2.746 -0.194 7.048
H15 5.097 3.379 7.240
H16 3.296 -1.110 3.806
H17 3.055 -1.770 5.426
H18 4.646 -1.864 4.685
H19 3.774 2.598 9.205
H20 2.703 1.190 9.056
H21 2.266 2.724 8.299
H22 6.071 3.722 4.221
H23 7.338 2.518 4.533
H24 6.904 3.694 5.780
H114 7.843 -0.779 1.619
H47 6.713 -1.118 4.170
H48 7.763 0.283 3.853
Ru49 3.668 1.937 2.043
Cl50 2.989 -0.329 1.444
Cl51 3.581 3.927 3.241
C52 3.950 2.656 0.370
C53 2.856 3.047 -0.474
C54 1.513 2.808 -0.116
C55 0.486 3.228 -0.941
C56 0.780 3.882 -2.138
C57 2.101 4.116 -2.513
C58 3.134 3.703 -1.688
H59 4.954 2.894 0.002
H60 1.276 2.284 0.812
H61 -0.547 3.047 -0.659
H62 -0.030 4.210 -2.785
H63 2.320 4.626 -3.448
H64 4.173 3.883 -1.964
N65 5.906 -1.711 1.759
H66 5.971 -1.974 0.770
H67 4.912 -1.385 1.885
H68 6.085 -2.535 2.339

3A	3B
N1 1.046 5.491 4.940	N1 1.029 5.657 5.292
N2 0.940 4.769 7.113	N2 1.159 4.768 7.396
C1 1.555 4.487 5.819	C1 1.638 4.580 6.061
C2 0.402 6.492 5.727	N4 0.551 6.657 6.275
N5 -0.187 5.706 6.835	C3 0.119 5.748 7.361
C4 1.648 6.137 3.790	C4 1.401 6.243 4.030
C5 2.861 6.832 3.878	C5 2.644 6.869 3.795
C6 3.294 7.550 2.763	C6 2.842 7.514 2.576
C7 2.546 7.623 1.594	C7 1.866 7.557 1.585
C8 1.300 6.995 1.573	C8 0.653 6.918 1.837
C9 0.824 6.267 2.656	C9 0.395 6.261 3.033
C10 3.716 6.859 5.109	C10 3.803 6.867 4.753
C11 3.057 8.345 0.387	C11 2.116 8.215 0.266
C12 -0.557 5.686 2.608	C12 -0.947 5.603 3.181
C13 0.657 3.903 8.234	C13 0.845 3.848 8.476
C14 1.107 4.347 9.501	C14 1.258 4.232 9.763
C15 0.735 3.632 10.634	C15 0.855 3.459 10.849
C16 -0.079 2.503 10.569	C16 0.025 2.351 10.704
C17 -0.501 2.081 9.311	C17 -0.442 2.053 9.424
C18 -0.146 2.746 8.139	C18 -0.062 2.790 8.306
C19 1.961 5.564 9.717	C19 2.051 5.477 10.027
C20 -0.446 1.755 11.810	C20 -0.341 1.500 11.879
C21 -0.634 2.155 6.849	C21 -0.619 2.431 6.965
H3 4.247 8.078 2.821	H3 3.806 7.990 2.392
H4 0.677 7.079 0.681	H4 -0.121 6.922 1.067
H5 3.167 6.608 6.022	H5 3.946 7.841 5.238
H6 4.159 7.851 5.246	H6 4.735 6.670 4.211
H7 4.555 6.153 5.035	H7 3.697 6.109 5.530
H8 3.846 9.059 0.642	H8 3.062 8.763 0.253
H9 2.258 8.887 -0.129	H9 1.312 8.913 0.009
H10 3.480 7.635 -0.337	H10 2.150 7.463 -0.533
H11 -0.908 5.597 1.575	H11 -1.141 4.961 2.315
H12 -1.284 6.327 3.131	H12 -1.752 6.348 3.198
H13 -0.599 4.693 3.064	H13 -1.026 4.984 4.079
H14 1.091 3.976 11.606	H14 1.194 3.744 11.846
H15 -1.130 1.193 9.231	H15 -1.138 1.224 9.292
H16 2.331 5.995 8.784	H16 2.639 5.789 9.160
H17 2.824 5.305 10.342	H17 2.732 5.335 10.873
H18 1.411 6.339 10.265	H18 1.391 6.313 10.302
H19 -1.256 1.042 11.636	H19 -1.331 1.048 11.761
H20 -0.753 2.434 12.612	H20 -0.335 2.072 12.812
H21 0.418 1.191 12.186	H21 0.376 0.677 11.998
H22 -0.154 2.603 5.980	H22 0.166 2.077 6.290
H23 -1.721 2.253 6.736	H23 -1.105 3.281 6.466
H24 -0.430 1.079 6.825	H24 -1.367 1.638 7.053
H46 -0.387 7.015 5.172	H46 0.037 6.302 8.304
H47 1.088 7.230 6.178	H47 -0.871 5.349 7.079
N48 3.040 2.480 6.324	N48 3.125 2.581 6.345
N49 2.893 3.202 4.157	N49 2.907 3.398 4.217
C50 2.403 3.476 5.471	C50 2.476 3.625 5.563
N51 4.169 1.919 5.530	N51 4.218 2.043 5.502
C52 3.563 1.941 4.179	C52 3.577 2.135 4.169
C53 3.319 2.487 7.739	C53 3.416 2.517 7.754
C54 4.118 3.466 8.370	C54 4.212 3.465 8.432
C55 4.465 3.280 9.707	C55 4.513 3.239 9.774
C56 4.039 2.182 10.447	C56 4.053 2.125 10.467
C57 3.230 1.243 9.808	C57 3.258 1.211 9.777
C58 2.868 1.362 8.471	C58 2.927 1.378 8.439
C59 4.604 4.721 7.708	C59 4.738 4.738 7.830
C60 4.390 2.027 11.892	C60 4.350 1.926 11.919
C61 2.020 0.267 7.893	C61 2.053 0.330 7.811
C62 2.276 3.358 2.854	C62 2.264 3.592 2.928
C63 3.079 3.944 1.858	C63 3.055 4.155 1.913

C64 2.583 4.006 0.562 C65 1.337 3.477 0.220 C66 0.611 2.825 1.210 C67 1.065 2.735 2.527 C68 4.460 4.451 2.149 C69 0.803 3.619 -1.170 C70 0.236 1.965 3.510 H71 5.091 4.035 10.187 H72 2.871 0.379 10.370 H73 5.690 4.714 7.555 H74 4.403 5.587 8.348 H75 4.120 4.898 6.748 H76 5.198 2.700 12.192 H77 4.694 1.000 12.124 H78 3.520 2.250 12.523 H79 1.147 0.098 8.533 H80 2.567 -0.684 7.868 H81 1.665 0.491 6.883 H82 3.190 4.480 -0.211 H83 -0.341 2.357 0.954 H84 4.516 4.965 3.112 H85 4.790 5.150 1.374 H86 5.194 3.631 2.163 H87 0.027 2.880 -1.386 H88 1.595 3.515 -1.920 H89 0.358 4.613 -1.312 H90 -0.599 2.569 3.894 H91 0.805 1.615 4.377 H92 -0.213 1.090 3.029 H93 4.343 1.870 3.412 H94 2.893 1.068 4.107 H95 -2.184 5.859 6.185 H96 -1.836 4.430 7.197 C97 -1.466 5.060 6.389 H98 -1.273 4.487 5.483 C99 -0.478 6.583 8.004 H100 -0.885 5.978 8.816 H101 0.441 7.078 8.314 H102 -1.216 7.320 7.680 H103 6.149 2.229 4.887 H104 5.213 3.728 5.168 C105 5.431 2.728 5.542 H106 5.816 2.752 6.561 C107 4.491 0.524 5.939 H108 4.906 0.531 6.949 H109 3.584 -0.077 5.898 H110 5.232 0.142 5.233	C64 2.524 4.243 0.628 C65 1.258 3.758 0.315 C66 0.535 3.125 1.325 C67 1.018 3.019 2.627 C68 4.468 4.603 2.137 C69 0.685 3.929 -1.057 C70 0.196 2.318 3.661 H71 5.119 3.978 10.300 H72 2.867 0.340 10.307 H73 5.814 4.688 7.624 H74 4.613 5.566 8.536 H75 4.225 5.002 6.904 H76 4.996 2.713 12.318 H77 4.840 0.961 12.096 H78 3.420 1.919 12.502 H79 1.176 0.152 8.443 H80 2.579 -0.631 7.736 H81 1.695 0.609 6.816 H82 3.130 4.700 -0.156 H83 -0.438 2.690 1.092 H84 4.666 4.844 3.184 H85 4.701 5.483 1.529 H86 5.180 3.823 1.833 H87 -0.037 3.143 -1.298 H88 1.465 3.925 -1.825 H89 0.157 4.889 -1.137 H90 -0.147 3.014 4.433 H91 0.750 1.522 4.178 H92 -0.686 1.856 3.210 H93 4.339 2.097 3.382 H94 2.900 1.268 4.070 H95 1.919 8.231 5.930 H96 2.427 7.044 7.186 H97 1.141 8.239 7.539 C98 4.530 0.624 5.840 H99 4.959 0.582 6.843 H100 3.614 0.037 5.789 H101 5.255 0.267 5.105 H102 6.186 2.376 4.822 H103 5.902 2.788 6.538 C104 5.491 2.835 5.530 H105 5.274 3.862 5.235 C106 -0.605 7.442 5.754 H107 -0.269 8.069 4.926 H108 -1.383 6.755 5.425 H109 -0.967 8.066 6.575 C110 1.597 7.613 6.767
3-GrI	**3-Ind**
Ru1 3.181 3.243 5.585 Cl1 1.338 1.665 5.285 Cl2 5.014 4.673 6.363 P1 4.782 1.370 5.478 N1 1.458 5.792 5.504 N2 1.377 4.829 7.463 C1 1.879 4.705 6.213 N8 0.485 6.607 6.332 C3 0.840 6.143 7.706 C4 1.585 6.128 4.122 C5 2.592 7.046 3.756 C6 2.693 7.407 2.415 C7 1.854 6.867 1.443 C8 0.908 5.918 1.832 C9 0.755 5.518 3.154 C10 3.593 7.604 4.726	Ru1 6.541 8.737 11.226 Cl1 5.952 6.382 11.708 Cl2 7.792 10.773 10.889 P1 7.603 8.003 9.110 N1 4.819 8.844 13.805 N2 6.972 8.792 14.221 C1 6.056 8.958 13.240 N8 4.985 8.337 15.252 C3 6.384 8.749 15.538 C4 3.549 9.389 13.444 C5 3.378 10.788 13.554 C6 2.131 11.325 13.277 C7 1.051 10.520 12.903 C8 1.254 9.150 12.792 C9 2.493 8.553 13.039 C10 4.514 11.692 13.923

C11 2.009 7.223 -0.002	C11 -0.274 11.141 12.590
C12 -0.222 4.418 3.458	C12 2.609 7.075 12.820
C13 1.547 3.955 8.596	C13 8.405 8.896 14.122
C14 2.580 4.198 9.509	C14 8.991 10.171 14.133
C15 2.644 3.383 10.640	C15 10.377 10.245 14.061
C16 1.713 2.378 10.881	C16 11.174 9.101 14.017
C17 0.679 2.191 9.960	C17 10.556 7.855 14.080
C18 0.559 2.979 8.823	C18 9.169 7.722 14.134
C19 3.557 5.325 9.361	C19 8.175 11.424 14.219
C20 1.792 1.516 12.105	C20 12.662 9.225 13.897
C21 -0.621 2.828 7.913	C21 8.548 6.362 14.222
C22 6.551 1.856 5.162	C22 7.723 9.310 7.794
C23 7.560 0.706 5.261	C23 8.486 8.887 6.533
C24 8.985 1.256 5.252	C24 8.737 10.104 5.643
C25 9.241 2.113 4.017	C25 7.434 10.817 5.293
C26 8.216 3.238 3.905	C26 6.660 11.203 6.550
C27 6.792 2.687 3.899	C27 6.397 9.983 7.428
C28 4.852 0.598 7.174	C28 9.384 7.561 9.442
C29 5.607 1.420 8.224	C29 10.344 8.731 9.677
C30 5.754 0.595 9.501	C30 11.776 8.202 9.733
C31 4.398 0.153 10.039	C31 11.939 7.150 10.825
C32 3.575 -0.578 8.983	C32 10.922 6.021 10.691
C33 3.457 0.244 7.703	C33 9.500 6.567 10.602
C34 4.286 -0.031 4.337	C34 6.889 6.426 8.387
C35 4.658 -1.450 4.785	C35 7.855 5.479 7.662
C36 4.047 -2.482 3.836	C36 7.145 4.165 7.331
C37 4.464 -2.243 2.389	C37 5.881 4.387 6.508
C38 4.122 -0.823 1.956	C38 4.943 5.371 7.200
C39 4.761 0.195 2.896	C39 5.665 6.681 7.500
C40 3.550 3.859 3.883	H3 1.998 12.406 13.329
C41 3.221 3.445 2.532	H4 0.431 8.513 12.465
C42 2.272 2.465 2.189	H5 4.848 11.560 14.963
C43 2.046 2.147 0.859	H6 4.225 12.741 13.811
C44 2.780 2.768 -0.151	H7 5.388 11.520 13.282
C45 3.738 3.726 0.171	H8 -0.698 11.644 13.468
C46 3.944 4.072 1.498	H9 -1.002 10.400 12.242
H3 3.471 8.111 2.120	H10 -0.162 11.907 11.811
H4 0.296 5.436 1.068	H11 2.051 6.799 11.918
H5 3.419 8.671 4.920	H12 2.150 6.509 13.644
H6 4.601 7.527 4.301	H13 3.642 6.743 12.678
H7 3.627 7.056 5.675	H14 10.851 11.227 14.045
H8 2.667 8.084 -0.144	H15 11.169 6.953 14.079
H9 1.042 7.447 -0.466	H16 7.635 11.591 13.278
H10 2.438 6.375 -0.553	H17 8.820 12.291 14.389
H11 -0.205 3.689 2.640	H18 7.445 11.395 15.038
H12 -1.255 4.784 3.523	H19 13.058 9.978 14.588
H13 0.021 3.859 4.368	H20 12.939 9.544 12.884
H14 3.451 3.547 11.356	H21 13.167 8.275 14.095
H15 -0.068 1.419 10.147	H22 7.785 6.205 13.448
H16 3.673 5.661 8.325	H23 8.073 6.192 15.201
H17 4.555 5.015 9.689	H24 9.309 5.584 14.105
H18 3.262 6.173 9.995	H25 8.318 10.079 8.314
H19 0.920 1.672 12.752	H26 7.895 8.142 5.974
H20 2.691 1.725 12.692	H27 9.442 8.406 6.786
H21 1.804 0.452 11.836	H28 9.404 10.801 6.178
H22 -0.315 2.642 6.875	H29 9.270 9.799 4.733
H23 -1.257 3.727 7.938	H30 7.637 11.701 4.675
H24 -1.248 1.988 8.228	H31 6.811 10.144 4.680
H25 6.730 2.547 6.002	H32 5.710 11.687 6.286
H26 7.428 0.022 4.406	H33 7.237 11.941 7.132
H27 7.396 0.107 6.168	H34 5.862 10.283 8.337
H28 9.134 1.866 6.159	H35 5.746 9.281 6.886
H29 9.706 0.431 5.309	H36 9.718 7.051 8.523
H30 10.260 2.520 4.038	H37 10.088 9.238 10.622
H31 9.176 1.477 3.119	H38 10.259 9.490 8.888

H32 8.392 3.831 2.998 H33 8.324 3.927 4.758 H34 6.072 3.515 3.855 H35 6.644 2.075 2.996 H36 5.410 -0.345 7.037 H37 5.053 2.353 8.429 H38 6.599 1.724 7.867 H39 6.375 -0.289 9.282 H40 6.297 1.173 10.261 H41 3.844 1.051 10.350 H42 4.521 -0.472 10.934 H43 2.573 -0.813 9.370 H44 4.050 -1.545 8.745 H45 2.860 -0.290 6.952 H46 2.901 1.176 7.911 H47 3.185 0.045 4.341 H48 5.755 -1.564 4.797 H49 4.308 -1.651 5.806 H50 4.328 -3.493 4.158 H51 2.949 -2.424 3.912 H52 5.551 -2.396 2.294 H53 3.988 -2.978 1.727 H54 3.027 -0.684 1.967 H55 4.449 -0.635 0.924 H56 4.538 1.215 2.558 H57 5.855 0.078 2.849 H58 4.228 4.730 3.887 H59 1.726 1.960 2.984 H60 1.307 1.390 0.605 H61 2.611 2.497 -1.191 H62 4.323 4.201 -0.614 H63 4.685 4.829 1.757 H114 1.595 6.830 8.119 H115 -0.052 6.124 8.344 C116 0.693 8.070 6.168 H117 -0.002 8.584 6.837 H118 1.725 8.311 6.425 H119 0.488 8.340 5.129 C120 -0.919 6.240 5.980 H121 -1.084 6.493 4.931 H122 -1.048 5.168 6.144 H123 -1.594 6.816 6.619	H39 12.039 7.766 8.755 H40 12.476 9.032 9.898 H41 11.785 7.637 11.800 H42 12.961 6.750 10.829 H43 11.007 5.325 11.538 H44 11.136 5.431 9.784 H45 8.774 5.746 10.515 H46 9.250 7.099 11.537 H47 6.533 5.903 9.290 H48 8.220 5.949 6.734 H49 8.739 5.259 8.274 H50 7.835 3.493 6.805 H51 6.880 3.663 8.276 H52 6.158 4.794 5.522 H53 5.374 3.433 6.319 H54 4.581 4.935 8.148 H55 4.058 5.562 6.578 H56 4.979 7.400 7.967 H57 5.989 7.133 6.548 H101 6.377 9.736 16.027 H102 6.868 8.011 16.187 C103 4.890 9.224 10.509 C104 4.268 10.576 10.389 C105 4.749 11.853 10.625 H106 5.755 11.997 11.008 C107 3.936 12.956 10.329 H108 4.313 13.960 10.510 C109 2.675 12.779 9.783 H110 2.064 13.644 9.533 C111 2.185 11.492 9.527 H112 1.217 11.366 9.049 C113 2.974 10.402 9.847 C114 2.750 8.953 9.658 C115 3.897 8.293 9.998 H116 4.027 7.216 10.025 C117 1.497 8.338 9.248 C118 0.263 8.927 9.564 H119 0.242 9.861 10.119 C120 -0.928 8.307 9.213 H121 -1.876 8.775 9.470 C122 -0.908 7.093 8.533 H123 -1.841 6.612 8.249 C124 0.309 6.496 8.215 H125 0.328 5.550 7.679 C126 1.500 7.109 8.572 H127 2.452 6.651 8.305 H128 2.997 8.653 15.879 H129 4.110 10.014 16.202 H130 4.214 8.519 17.189 C131 4.866 6.844 15.224 H132 3.827 6.588 15.015 H133 5.505 6.459 14.422 H134 5.164 6.460 16.204 C135 4.005 8.928 16.196
3-GrII	**3-GrIIdim**
N1 5.948 1.142 1.619 N2 5.143 0.654 3.598 C1 4.959 1.435 2.513 N4 6.973 0.200 2.294 C3 6.156 -0.357 3.398 C4 5.982 1.173 0.195 C5 5.117 0.306 -0.509 C6 5.257 0.222 -1.886 C7 6.218 0.967 -2.575	N1 5.897 1.098 1.673 N2 5.108 0.706 3.681 C1 4.923 1.448 2.565 N4 6.910 0.173 2.369 C3 6.091 -0.337 3.497 C4 5.918 1.106 0.247 C5 5.023 0.251 -0.434 C6 5.124 0.165 -1.815 C7 6.081 0.892 -2.529

C8 7.021 1.845 -1.855	C8 6.919 1.753 -1.829
C9 6.916 1.985 -0.471	C9 6.851 1.898 -0.443
C10 4.042 -0.471 0.190	C10 3.952 -0.506 0.292
C11 6.328 0.852 -4.063	C11 6.153 0.777 -4.019
C12 7.751 3.031 0.208	C12 7.722 2.931 0.210
C13 4.439 0.547 4.853	C13 4.423 0.656 4.952
C14 3.362 -0.344 4.952	C14 3.328 -0.207 5.101
C15 2.869 -0.620 6.228	C15 2.868 -0.451 6.395
C16 3.449 -0.084 7.375	C16 3.486 0.098 7.515
C17 4.517 0.800 7.230	C17 4.560 0.966 7.323
C18 5.038 1.125 5.984	C18 5.057 1.251 6.057
C19 2.778 -1.029 3.756	C19 2.687 -0.896 3.937
C20 2.996 -0.490 8.744	C20 3.066 -0.275 8.905
C21 6.241 2.012 5.881	C21 6.272 2.117 5.913
H3 4.587 -0.430 -2.446	H3 4.428 -0.476 -2.357
H4 7.736 2.472 -2.389	H4 7.633 2.366 -2.381
H5 4.435 -1.162 0.951	H5 4.349 -1.168 1.076
H6 3.473 -1.070 -0.527	H6 3.384 -1.132 -0.402
H7 3.334 0.196 0.706	H7 3.243 0.177 0.787
H8 6.476 -0.189 -4.373	H8 6.298 -0.263 -4.333
H9 7.155 1.448 -4.460	H9 6.969 1.376 -4.436
H10 5.401 1.198 -4.540	H10 5.214 1.120 -4.473
H11 7.761 3.939 -0.407	H11 7.755 3.827 -0.421
H12 8.803 2.727 0.302	H12 8.765 2.598 0.304
H13 7.362 3.313 1.193	H13 7.348 3.242 1.193
H14 2.032 -1.313 6.327	H14 2.024 -1.129 6.529
H15 4.978 1.233 8.120	H15 5.047 1.413 8.191
H16 2.315 -0.304 3.074	H16 2.149 -0.179 3.304
H17 2.015 -1.751 4.058	H17 1.977 -1.653 4.281
H18 3.537 -1.582 3.182	H18 3.422 -1.400 3.295
H19 3.728 -1.163 9.208	H19 3.805 -0.946 9.362
H20 2.035 -1.016 8.721	H20 2.101 -0.790 8.920
H21 2.896 0.377 9.408	H21 2.995 0.606 9.553
H22 6.121 2.794 5.120	H22 6.167 2.856 5.108
H23 7.148 1.438 5.633	H23 7.173 1.519 5.707
H24 6.442 2.500 6.840	H24 6.470 2.657 6.843
H46 5.724 -1.319 3.081	H46 5.633 -1.296 3.207
H47 6.773 -0.502 4.291	H47 6.716 -0.475 4.386
Ru48 3.732 3.131 2.380	Ru48 3.729 3.139 2.379
Cl49 1.676 1.870 2.150	Cl49 1.653 1.914 2.121
Cl50 5.790 4.316 3.095	Cl50 5.801 4.314 3.084
N51 2.590 6.051 2.129	N51 2.537 6.087 2.109
N52 2.235 5.168 4.086	N52 2.131 5.214 4.028
C53 2.698 4.915 2.849	C53 2.669 4.926 2.811
C54 1.922 6.594 4.292	C54 1.940 7.078 2.881
C55 2.715 6.212 0.715	C55 1.691 6.530 4.087
C56 3.819 6.909 0.205	C56 2.737 6.286 0.703
C57 3.874 7.129 -1.170	C57 3.872 6.970 0.258
C58 2.864 6.694 -2.026	C58 3.985 7.203 -1.112
C59 1.769 6.026 -1.480	C59 3.002 6.794 -2.012
C60 1.668 5.777 -0.115	C60 1.872 6.141 -1.520
C61 4.918 7.387 1.103	C61 1.712 5.878 -0.164
C62 2.943 6.935 -3.502	C62 4.928 7.431 1.215
C63 0.489 5.031 0.430	C63 3.143 7.054 -3.481
C64 1.886 4.234 5.114	C64 0.497 5.164 0.343
C65 2.735 4.044 6.209	C65 1.803 4.288 5.080
C66 2.279 3.246 7.259	C66 2.674 4.132 6.161
C67 1.014 2.668 7.247	C67 2.243 3.341 7.227
C68 0.186 2.899 6.150	C68 0.991 2.733 7.231
C69 0.588 3.694 5.084	C69 0.150 2.924 6.135
C70 4.058 4.743 6.311	C70 0.521 3.716 5.056
C71 0.521 1.831 8.386	C71 3.982 4.857 6.225
C72 -0.367 4.002 3.972	C72 0.522 1.905 8.388
C73 4.150 3.615 0.639	C73 -0.445 3.987 3.945
C74 3.651 3.301 -0.691	C74 4.166 3.616 0.641

C75 2.521 2.512 -0.979 C76 2.144 2.274 -2.291 C77 2.886 2.802 -3.348 C78 4.008 3.581 -3.086 C79 4.378 3.836 -1.773 H81 4.736 7.655 -1.586 H82 0.977 5.669 -2.140 H83 4.570 8.170 1.790 H84 5.740 7.811 0.518 H85 5.315 6.575 1.727 H86 3.977 7.087 -3.831 H87 2.373 7.827 -3.791 H88 2.525 6.090 -4.063 H89 -0.221 4.795 -0.370 H90 -0.052 5.606 1.193 H91 0.790 4.083 0.899 H92 2.925 3.101 8.127 H93 -0.820 2.477 6.142 H94 4.586 4.790 5.352 H95 4.704 4.240 7.040 H96 3.928 5.776 6.665 H97 -0.528 2.048 8.616 H98 1.107 1.996 9.298 H99 0.579 0.762 8.141 H100 -0.055 3.512 3.042 H101 -0.431 5.080 3.773 H102 -1.373 3.649 4.219 H103 5.023 4.289 0.592 H104 1.944 2.101 -0.155 H105 1.263 1.669 -2.494 H106 2.585 2.608 -4.376 H107 4.591 4.001 -3.904 H108 5.243 4.467 -1.567 H109 8.040 -0.382 0.567 H110 6.671 -1.446 0.999 H111 8.176 -1.482 1.977 C112 8.077 1.057 2.824 H113 8.641 1.452 1.980 H114 7.634 1.883 3.388 H115 8.721 0.438 3.457 C116 7.499 -0.853 1.390 C117 1.898 7.123 2.869 H117 2.710 7.058 4.901 H118 0.968 6.702 4.820 H119 0.879 7.245 2.471 H120 2.425 8.075 2.746	C75 3.658 3.332 -0.691 C76 2.514 2.568 -0.991 C77 2.130 2.360 -2.306 C78 2.881 2.891 -3.355 C79 4.020 3.642 -3.082 C80 4.395 3.868 -1.765 H81 1.748 8.062 2.478 H82 1.231 6.926 4.982 H83 4.868 7.723 -1.486 H84 1.099 5.811 -2.215 H85 4.537 8.181 1.914 H86 5.767 7.883 0.678 H87 5.311 6.602 1.826 H88 4.193 7.166 -3.771 H89 2.622 7.974 -3.773 H90 2.710 6.236 -4.069 H91 -0.217 4.993 -0.469 H92 -0.013 5.736 1.129 H93 0.755 4.186 0.777 H94 2.898 3.225 8.092 H95 -0.843 2.473 6.139 H96 4.593 4.704 5.326 H97 4.558 4.535 7.099 H98 3.827 5.941 6.314 H99 -0.525 2.118 8.631 H100 1.120 2.087 9.288 H101 0.584 0.834 8.155 H102 -0.064 3.606 2.991 H103 -0.631 5.062 3.827 H104 -1.405 3.501 4.143 H105 5.053 4.271 0.601 H106 1.931 2.151 -0.173 H107 1.238 1.775 -2.518 H108 2.575 2.720 -4.385 H109 4.612 4.061 -3.894 H110 5.274 4.477 -1.551 H111 7.957 -0.477 0.655 H112 6.577 -1.508 1.128 H113 8.088 -1.534 2.097 C114 8.031 1.028 2.869 H115 8.599 1.386 2.011 H116 7.604 1.879 3.408 H117 8.666 0.418 3.518 C118 7.416 -0.915 1.496
3-Hov	**3-Hov-TS**
Ru1 12.850 5.811 5.358 Cl1 10.558 5.379 5.970 Cl2 15.210 6.151 5.420 O1 13.298 3.664 5.970 C22 12.829 4.971 3.717 H27 12.636 5.465 2.758 C23 13.375 3.121 7.322 H28 14.247 2.450 7.337 C24 13.627 4.301 8.232 H29 14.521 4.857 7.927 H30 13.765 3.945 9.259 H31 12.763 4.981 8.229 C25 12.093 2.386 7.646 H32 11.904 1.553 6.961 H33 11.246 3.079 7.583 H34 12.145 1.983 8.663 C26 13.377 2.881 4.872	Ru1 12.739 5.690 5.597 Cl1 10.549 5.455 6.474 Cl2 15.018 6.027 6.046 O1 11.058 2.949 4.815 C22 12.883 4.811 4.023 H27 12.827 5.233 3.014 C23 9.978 2.183 4.255 H28 10.075 1.132 4.567 C24 8.709 2.756 4.836 H29 8.717 2.690 5.928 H30 7.837 2.215 4.453 H31 8.615 3.815 4.568 C25 10.050 2.285 2.744 H32 10.962 1.819 2.353 H33 10.061 3.346 2.453 H34 9.189 1.799 2.271 C26 12.313 2.482 4.656

C27 13.689 1.528 4.864	C27 12.686 1.153 4.867
H35 13.886 0.988 5.784	H35 11.946 0.421 5.178
C28 13.754 0.868 3.640	C28 14.011 0.779 4.700
H36 14.003 -0.191 3.632	H36 14.295 -0.256 4.874
C29 13.509 1.526 2.435	C29 14.982 1.711 4.328
H37 13.566 0.983 1.496	H37 16.018 1.405 4.211
C30 13.198 2.873 2.450	C30 14.620 3.029 4.121
H38 13.005 3.417 1.525	H38 15.365 3.775 3.853
C31 13.128 3.574 3.665	C31 13.280 3.426 4.269
N1 11.681 8.099 3.810	N1 11.436 7.799 4.045
N2 12.402 8.626 5.827	N2 12.410 8.607 5.858
C1 12.349 7.615 4.910	C1 12.259 7.484 5.109
N30 11.102 9.450 4.148	N30 10.836 9.157 4.292
C3 12.002 9.884 5.265	C3 11.845 9.764 5.215
C4 11.777 7.689 2.446	C4 11.440 7.250 2.725
C5 12.992 7.917 1.766	C5 12.584 7.444 1.920
C6 13.086 7.501 0.443	C6 12.601 6.867 0.656
C7 12.030 6.858 -0.205	C7 11.532 6.103 0.179
C8 10.861 6.610 0.513	C8 10.428 5.920 1.006
C9 10.709 7.001 1.842	C9 10.355 6.473 2.284
C10 14.194 8.500 2.445	C10 13.805 8.156 2.419
C11 12.165 6.401 -1.624	C11 11.602 5.466 -1.173
C12 9.463 6.609 2.577	C12 9.154 6.185 3.131
C13 13.028 8.535 7.124	C13 13.184 8.793 7.066
C14 14.400 8.799 7.244	C14 14.527 9.178 6.953
C15 14.995 8.593 8.486	C15 15.254 9.334 8.127
C16 14.261 8.168 9.591	C16 14.683 9.129 9.383
C17 12.881 8.012 9.454	C17 13.329 8.813 9.451
C18 12.236 8.202 8.236	C18 12.550 8.653 8.308
C19 15.214 9.355 6.116	C19 15.188 9.413 5.628
C20 14.930 7.884 10.900	C20 15.509 9.250 10.626
C21 10.743 8.104 8.157	C21 11.080 8.394 8.435
H3 14.018 7.671 -0.096	H3 13.481 7.002 0.027
H4 10.045 6.073 0.030	H4 9.596 5.309 0.655
H5 13.980 9.429 2.990	H5 13.588 9.125 2.890
H6 14.979 8.726 1.718	H6 14.508 8.343 1.603
H7 14.613 7.789 3.176	H7 14.327 7.550 3.174
H8 12.915 6.985 -2.167	H8 11.996 6.161 -1.923
H9 11.214 6.474 -2.162	H9 10.621 5.117 -1.508
H10 12.478 5.351 -1.663	H10 12.275 4.600 -1.156
H11 9.078 5.667 2.175	H11 8.697 5.241 2.820
H12 8.656 7.344 2.447	H12 8.373 6.950 3.010
H13 9.641 6.457 3.649	H13 9.412 6.099 4.194
H14 16.066 8.767 8.588	H14 16.305 9.617 8.060
H15 12.286 7.743 10.327	H15 12.856 8.696 10.426
H16 16.267 9.078 6.225	H16 16.228 9.718 5.770
H17 15.165 10.454 6.113	H17 14.700 10.209 5.047
H18 14.891 8.983 5.141	H18 15.195 8.496 5.029
H19 14.285 8.145 11.747	H19 14.901 9.537 11.490
H20 15.872 8.430 11.003	H20 16.311 9.986 10.508
H21 15.161 6.814 10.989	H21 15.984 8.290 10.866
H22 10.417 7.271 7.522	H22 10.782 7.444 7.977
H23 10.301 9.030 7.760	H23 10.488 9.195 7.968
H24 10.317 7.951 9.153	H24 10.787 8.362 9.488
H72 12.841 10.455 4.835	C72 10.647 9.948 3.049
H73 11.444 10.508 5.972	H73 12.579 10.326 4.617
H74 10.482 9.988 2.206	H74 11.347 10.432 5.926
H75 12.134 10.516 2.638	H75 11.605 10.062 2.539
H76 10.712 11.346 3.354	H76 9.940 9.426 2.402
C77 9.706 9.243 4.653	H77 10.247 10.923 3.338
H78 9.099 8.863 3.832	C78 9.529 8.961 5.003
H79 9.739 8.508 5.462	H79 8.835 8.478 4.316
H80 9.321 10.204 5.005	H80 9.701 8.312 5.867
C81 11.112 10.392 3.001	H81 9.153 9.942 5.307

3-Hov-a	**3-GrI_P(Cy)$_3$**
Ru1 12.486 5.818 5.511	Ru1 2.296 3.269 5.330
Cl1 10.300 5.625 6.422	Cl1 0.073 2.545 4.919
Cl2 14.846 5.741 5.438	Cl2 4.471 3.081 6.186
O1 11.023 3.244 2.036	N1 1.196 6.019 5.472
C22 12.144 4.871 3.959	N2 1.414 5.014 7.430
H27 11.835 5.303 3.005	C1 1.679 4.887 6.098
C23 10.521 2.467 0.931	N7 0.382 6.799 6.460
H28 9.995 1.589 1.334	C3 0.976 6.340 7.759
C24 9.523 3.342 0.214	C4 1.618 6.626 4.251
H29 8.742 3.689 0.899	C5 2.899 7.213 4.207
H30 9.050 2.784 -0.600	C6 3.326 7.762 3.002
H31 10.030 4.214 -0.215	C7 2.533 7.726 1.855
C25 11.672 2.055 0.036	C8 1.287 7.103 1.927
H32 12.407 1.437 0.562	C9 0.805 6.537 3.104
H33 12.186 2.953 -0.330	C10 3.848 7.162 5.366
H34 11.306 1.489 -0.828	C11 3.017 8.304 0.562
C26 11.625 2.616 3.062	C12 -0.502 5.803 3.077
C27 11.679 1.228 3.214	C13 1.772 4.074 8.466
H35 11.258 0.567 2.464	C14 3.042 4.164 9.053
C28 12.267 0.670 4.340	C15 3.372 3.224 10.024
H36 12.290 -0.413 4.436	C16 2.478 2.234 10.426
C29 12.832 1.466 5.337	C17 1.202 2.221 9.865
H37 13.303 1.016 6.205	C18 0.817 3.137 8.890
C30 12.804 2.835 5.185	C19 4.012 5.249 8.700
H38 13.301 3.456 5.934	C20 2.874 1.206 11.440
C31 12.207 3.447 4.059	C21 -0.590 3.136 8.372
N1 11.586 8.141 3.908	C40 2.755 3.792 3.625
N2 12.442 8.662 5.876	C41 3.096 2.802 2.644
C1 12.205 7.622 5.022	C42 2.908 1.424 2.876
N30 11.242 9.579 4.170	C43 3.303 0.497 1.929
C3 12.238 9.928 5.236	C44 3.879 0.928 0.733
C4 11.520 7.642 2.574	C45 4.059 2.286 0.481
C5 12.701 7.638 1.800	C46 3.670 3.219 1.428
C6 12.614 7.190 0.490	H3 4.317 8.213 2.952
C7 11.404 6.760 -0.064	H4 0.677 7.032 1.025
C8 10.274 6.729 0.747	H5 4.701 7.826 5.200
C9 10.307 7.132 2.082	H6 4.245 6.143 5.494
C10 14.034 8.014 2.375	H7 3.394 7.446 6.324
C11 11.351 6.312 -1.492	H8 3.983 8.804 0.675
C12 9.097 6.903 2.939	H9 2.301 9.030 0.161
C13 13.092 8.581 7.162	H10 3.131 7.520 -0.197
C14 14.490 8.674 7.229	H11 -0.665 5.374 2.084
C15 15.085 8.555 8.482	H12 -1.354 6.472 3.262
C16 14.334 8.379 9.642	H13 -0.531 4.976 3.796
C17 12.943 8.373 9.540	H14 4.362 3.267 10.479
C18 12.294 8.487 8.315	H15 0.478 1.481 10.204
C19 15.337 8.968 6.029	H16 4.069 5.413 7.620
C20 14.998 8.209 10.974	H17 5.020 4.987 9.034
C21 10.799 8.573 8.262	H18 3.748 6.198 9.192
H3 13.516 7.173 -0.122	H19 2.025 0.906 12.062
H4 9.335 6.351 0.343	H20 3.670 1.571 12.097
H5 14.029 8.981 2.897	H21 3.249 0.301 10.945
H6 14.793 8.074 1.591	H22 -0.634 2.931 7.295
H7 14.371 7.263 3.107	H23 -1.087 4.099 8.558
H8 11.803 7.058 -2.157	H24 -1.183 2.370 8.879
H9 10.324 6.136 -1.828	H58 2.882 4.836 3.324
H10 11.916 5.382 -1.633	H59 2.429 1.080 3.795
H11 8.662 5.929 2.687	H60 3.157 -0.564 2.113
H12 8.308 7.646 2.762	H61 4.185 0.195 -0.010
H13 9.337 6.874 4.008	H62 4.506 2.611 -0.455
H14 16.172 8.607 8.551	H63 3.809 4.285 1.248
H15 12.342 8.290 10.446	H64 1.802 7.019 8.023
H16 16.357 8.603 6.178	H65 0.212 6.349 8.544

H17 15.406 10.053 5.859 H18 14.962 8.487 5.121 H19 14.407 8.662 11.777 H20 15.998 8.653 10.988 H21 15.109 7.145 11.216 H22 10.358 7.744 7.696 H23 10.470 9.519 7.806 H24 10.379 8.545 9.272 H72 13.144 10.321 4.747 H73 11.815 10.680 5.912 H74 10.656 10.112 2.214 H75 12.390 10.366 2.574 H76 11.158 11.468 3.276 C77 9.846 9.639 4.712 H78 9.163 9.299 3.933 H79 9.786 8.979 5.581 H80 9.629 10.675 4.989 C81 11.375 10.442 2.967	H66 0.080 8.529 5.291 H67 1.534 8.573 6.333 H68 -0.098 8.744 7.063 C67 -1.047 6.354 6.351 H69 -1.419 6.642 5.368 H70 -1.078 5.267 6.460 H71 -1.621 6.848 7.141 C71 0.487 8.269 6.271
3-Ind_P(Cy)$_3$	**3-GrII_Imes/SIMes**
Ru1 6.415 9.135 11.427 Cl1 6.967 6.975 10.725 Cl2 6.774 11.485 11.718 N1 4.857 9.505 13.957 N2 6.971 8.895 14.215 C1 5.986 9.064 13.289 N7 5.280 9.935 15.331 C3 6.488 9.080 15.556 C4 3.467 9.313 13.682 C5 2.691 10.370 13.180 C6 1.339 10.123 12.935 C7 0.754 8.884 13.175 C8 1.563 7.846 13.646 C9 2.914 8.029 13.896 C10 3.248 11.723 12.852 C11 -0.698 8.634 12.915 C12 3.755 6.854 14.294 C13 8.291 8.364 13.974 C14 9.382 9.243 13.899 C15 10.636 8.695 13.637 C16 10.823 7.324 13.476 C17 9.724 6.480 13.629 C18 8.449 6.972 13.886 C19 9.248 10.716 14.134 C20 12.173 6.764 13.152 C21 7.305 6.020 14.047 H3 0.729 10.928 12.525 H4 1.127 6.856 13.786 H5 3.055 12.445 13.658 H6 2.750 12.120 11.961 H7 4.323 11.701 12.642 H8 -1.245 8.497 13.857 H9 -0.836 7.721 12.323 H10 -1.163 9.464 12.374 H11 3.157 5.939 14.304 H12 4.201 6.949 15.294 H13 4.586 6.696 13.593 H14 11.494 9.363 13.566 H15 9.863 5.402 13.545 H16 8.600 11.194 13.389 H17 10.226 11.203 14.086 H18 8.835 10.935 15.129 H19 12.339 5.802 13.648 H20 12.976 7.447 13.445 H21 12.266 6.591 12.073	N1 6.316 0.651 1.478 N2 5.718 0.691 3.608 C1 5.372 1.132 2.364 N4 7.188 -0.334 2.199 C3 7.034 0.120 3.620 C4 6.723 1.181 0.216 C5 6.352 0.526 -0.972 C6 6.732 1.111 -2.180 C7 7.434 2.312 -2.233 C8 7.754 2.954 -1.033 C9 7.404 2.418 0.200 C10 5.516 -0.718 -1.001 C11 7.796 2.940 -3.543 C12 7.651 3.212 1.447 C13 5.017 0.963 4.840 C14 4.078 0.030 5.308 C15 3.388 0.341 6.476 C16 3.625 1.519 7.183 C17 4.617 2.383 6.722 C18 5.335 2.125 5.559 C19 3.851 -1.288 4.632 C20 2.832 1.845 8.410 C21 6.429 3.055 5.130 H3 6.444 0.621 -3.110 H4 8.275 3.911 -1.063 H5 4.840 -0.784 -0.141 H6 6.131 -1.628 -1.050 H7 4.894 -0.725 -1.901 H8 7.718 2.228 -4.370 H9 8.815 3.339 -3.526 H10 7.128 3.781 -3.765 H11 8.343 4.036 1.254 H12 8.068 2.620 2.271 H13 6.711 3.651 1.817 H14 2.649 -0.366 6.852 H15 4.838 3.291 7.283 H16 3.463 -1.171 3.612 H17 3.126 -1.885 5.193 H18 4.778 -1.878 4.582 H19 3.385 2.504 9.087 H20 2.552 0.941 8.961 H21 1.902 2.362 8.142 H22 6.357 3.302 4.067 H23 7.424 2.629 5.332 H24 6.369 3.998 5.681

H22 6.702 5.989 13.130 H23 6.646 6.286 14.884 H24 7.672 5.006 14.232 H49 7.207 9.610 16.191 H50 6.171 8.143 16.040 C51 4.709 9.129 10.667 C52 4.270 10.036 9.585 C53 4.873 11.125 8.983 H54 5.848 11.474 9.313 C55 4.199 11.777 7.936 H56 4.662 12.633 7.454 C57 2.964 11.327 7.506 H58 2.461 11.826 6.681 C59 2.348 10.218 8.116 H60 1.393 9.856 7.744 C61 2.992 9.598 9.165 C62 2.635 8.408 9.974 C63 3.665 8.154 10.837 H64 3.713 7.321 11.527 C65 1.407 7.636 9.862 C66 0.189 8.254 9.546 H67 0.155 9.333 9.404 C68 -0.981 7.510 9.470 H69 -1.921 8.003 9.231 C70 -0.954 6.139 9.708 H71 -1.869 5.555 9.638 C72 0.249 5.514 10.034 H73 0.275 4.442 10.213 C74 1.418 6.255 10.112 H75 2.363 5.762 10.333 H76 4.752 11.956 15.044 H77 6.378 11.524 14.450 H78 6.074 11.680 16.230 C79 4.234 9.728 16.367 H80 3.364 10.338 16.116 H81 3.955 8.675 16.405 H82 4.657 10.047 17.323 C83 5.656 11.388 15.262	H46 7.115 -0.738 4.298 H47 7.826 0.854 3.838 Ru48 3.707 1.959 1.998 Cl49 2.715 -0.129 1.463 Cl50 3.876 3.999 3.141 C51 3.954 2.610 0.294 C52 2.841 3.153 -0.430 C53 1.516 3.045 0.044 C54 0.476 3.628 -0.655 C55 0.735 4.318 -1.840 C56 2.035 4.423 -2.330 C57 3.082 3.845 -1.632 H58 4.933 2.698 -0.187 H59 1.301 2.482 0.954 H60 -0.542 3.543 -0.286 H61 -0.086 4.772 -2.389 H62 2.226 4.959 -3.256 H63 4.106 3.922 -1.999 H64 6.664 -1.968 0.967 H65 5.556 -1.673 2.339 H66 7.178 -2.405 2.631 C67 8.601 -0.308 1.740 H68 8.636 -0.606 0.690 H69 9.005 0.699 1.857 H70 9.158 -1.019 2.355 C71 6.601 -1.704 2.022
$P(Cy)_3$	
P1 4.896 1.427 5.637 C22 6.707 1.841 5.362 C23 7.757 0.736 5.476 C24 9.168 1.319 5.432 C25 9.383 2.137 4.163 C26 8.331 3.234 4.030 C27 6.919 2.654 4.080 C28 4.943 0.711 7.371 C29 5.448 1.736 8.390 C30 5.397 1.187 9.813 C31 3.995 0.715 10.181 C32 3.491 -0.312 9.176 C33 3.535 0.245 7.756 C34 4.497 -0.119 4.633 C35 5.098 -1.470 5.032 C36 4.488 -2.599 4.202 C37 4.672 -2.352 2.708 C38 4.094 -1.000 2.302 C39 4.702 0.125 3.135 H25 6.886 2.549 6.192 H26 7.638 0.034 4.634 H27 7.615 0.150 6.395 H28 9.316 1.966 6.313 H29 9.915 0.518 5.506 H30 10.393 2.567 4.146	

H31 9.315 1.467 3.290 H32 8.479 3.799 3.100 H33 8.453 3.954 4.855 H34 6.167 3.451 4.012 H35 6.768 2.010 3.199 H36 5.619 -0.161 7.404 H37 4.828 2.647 8.321 H38 6.478 2.041 8.155 H39 6.096 0.338 9.893 H40 5.750 1.946 10.524 H41 3.312 1.580 10.184 H42 3.981 0.303 11.199 H43 2.472 -0.634 9.426 H44 4.124 -1.214 9.227 H45 3.165 -0.510 7.047 H46 2.847 1.104 7.677 H47 3.404 -0.199 4.784 H48 6.187 -1.455 4.874 H49 4.944 -1.674 6.100 H50 4.928 -3.562 4.491 H51 3.411 -2.667 4.428 H52 5.749 -2.367 2.472 H53 4.214 -3.160 2.123 H54 3.002 -1.010 2.452 H55 4.260 -0.815 1.232 H56 4.281 1.098 2.844 H57 5.783 0.174 2.921	
GrI_NC	**Ind_NC**
Ru1 2.002 1.506 3.469 Cl1 2.882 2.333 5.494 C1 3.131 2.239 2.235 Cl2 0.177 0.793 2.152 P2 2.904 -0.547 3.627 C2 2.923 3.619 1.841 H8 2.509 7.374 0.935 C3 3.974 4.330 1.240 C4 3.826 5.672 0.920 C5 2.625 6.322 1.188 C6 1.568 5.627 1.772 C7 1.710 4.288 2.093 C26 2.878 -1.509 2.035 C27 3.404 -0.771 0.801 C28 3.100 -1.577 -0.459 C29 3.672 -2.988 -0.376 C30 3.170 -3.711 0.868 C31 3.487 -2.912 2.130 C32 4.598 -0.535 4.415 C33 5.671 0.059 3.497 C34 6.979 0.267 4.255 C35 7.465 -1.032 4.883 C36 6.394 -1.627 5.790 C37 5.085 -1.852 5.035 C38 1.895 -1.606 4.787 C39 1.740 -0.933 6.156 C40 1.051 -1.870 7.143 C41 -0.305 -2.320 6.613 C42 -0.163 -2.970 5.242 C43 0.529 -2.041 4.247 H1 4.019 1.752 1.812 H2 4.914 3.817 1.039 H3 4.649 6.213 0.458 H4 0.625 6.133 1.968 H5 0.865 3.739 2.514 H39 1.790 -1.609 1.879	Ru1 6.509 8.847 10.913 Cl1 6.387 6.692 11.875 Cl2 7.327 11.062 10.809 P1 7.564 8.259 9.022 C22 7.467 9.544 7.679 C23 8.186 9.186 6.373 C24 8.384 10.451 5.541 C25 7.041 11.112 5.246 C26 6.266 11.402 6.527 C27 6.092 10.150 7.384 C28 9.399 8.152 9.415 C29 10.187 9.445 9.169 C30 11.665 9.248 9.505 C31 11.861 8.778 10.940 C32 11.068 7.504 11.200 C33 9.593 7.707 10.874 C34 7.009 6.557 8.436 C35 8.044 5.441 8.618 C36 7.370 4.083 8.430 C37 6.686 3.973 7.071 C38 5.715 5.127 6.842 C39 6.420 6.470 7.025 H25 8.033 10.352 8.171 H26 7.572 8.484 5.794 H27 9.147 8.682 6.558 H28 9.028 11.154 6.095 H29 8.910 10.212 4.608 H30 7.185 12.033 4.667 H31 6.445 10.435 4.610 H32 5.284 11.834 6.294 H33 6.804 12.157 7.123 H34 5.582 10.409 8.319 H35 5.452 9.425 6.854 H36 9.809 7.369 8.753 H37 9.767 10.249 9.793 H38 10.101 9.774 8.126

H40 4.492 -0.613 0.886 H41 2.927 0.213 0.728 H42 2.007 -1.628 -0.584 H43 3.490 -1.052 -1.340 H44 4.773 -2.930 -0.337 H45 3.423 -3.559 -1.280 H46 3.609 -4.715 0.939 H47 2.079 -3.849 0.799 H48 4.444 0.189 5.233 H49 4.582 -2.828 2.236 H50 3.123 -3.449 3.017 H51 5.331 1.019 3.091 H52 5.848 -0.618 2.643 H53 6.811 1.019 5.043 H54 7.739 0.683 3.582 H55 8.395 -0.868 5.442 H56 7.703 -1.754 4.084 H57 6.207 -0.941 6.632 H58 6.737 -2.574 6.227 H59 4.338 -2.265 5.725 H60 5.245 -2.606 4.250 H61 2.499 -2.520 4.924 H62 1.142 -0.015 6.040 H63 2.709 -0.604 6.553 H64 1.692 -2.753 7.309 H65 0.946 -1.373 8.115 H66 -0.788 -3.009 7.319 H67 -0.966 -1.442 6.529 H68 0.426 -3.898 5.340 H69 -1.144 -3.265 4.849 H70 0.630 -2.552 3.280 H71 -0.094 -1.153 4.060	H39 12.095 8.501 8.816 H40 12.208 10.185 9.325 H41 11.512 9.564 11.629 H42 12.927 8.624 11.153 H43 11.174 7.181 12.243 H44 11.465 6.686 10.575 H45 9.014 6.806 11.105 H46 9.191 8.497 11.536 H47 6.202 6.345 9.155 H48 8.852 5.562 7.875 H49 8.505 5.482 9.612 H50 8.107 3.279 8.555 H51 6.626 3.954 9.233 H52 7.454 3.993 6.279 H53 6.169 3.010 6.977 H54 4.878 5.058 7.556 H55 5.274 5.068 5.838 H56 5.725 7.296 6.819 H57 7.230 6.548 6.284 C120 4.793 8.963 10.252 C122 3.788 9.781 10.962 C123 3.921 10.719 11.971 H125 4.898 10.946 12.397 C124 2.776 11.395 12.409 H129 2.858 12.127 13.209 C126 1.544 11.158 11.816 H133 0.669 11.709 12.152 C128 1.412 10.230 10.775 H134 0.449 10.089 10.290 C130 2.533 9.528 10.366 C131 2.739 8.537 9.291 C132 4.075 8.260 9.213 H135 4.509 7.515 8.557 C40 1.705 7.923 8.468 C41 0.414 7.691 8.963 H136 0.177 7.964 9.988 C42 -0.541 7.063 8.175 H138 -1.535 6.879 8.578 C43 -0.230 6.661 6.881 H140 -0.982 6.173 6.265 C44 1.049 6.885 6.376 H142 1.298 6.576 5.363 C45 2.005 7.510 7.161 H144 2.998 7.707 6.758
GrII_NC_nnas	**GrII_NC_nas**
Ru1 2.278 3.436 5.269 Cl1 0.212 2.406 4.719 Cl2 4.341 3.544 6.411 N1 1.053 6.233 5.154 N2 0.977 5.309 7.105 C1 1.440 5.109 5.830 C2 0.368 7.107 5.993 C3 0.320 6.528 7.209 C4 1.434 6.602 3.825 C5 2.675 7.220 3.649 C6 3.059 7.542 2.348 C7 2.243 7.256 1.255 C8 1.005 6.651 1.480 C9 0.575 6.314 2.760 C10 3.602 7.441 4.806 C11 2.685 7.573 -0.143 C12 -0.735 5.626 2.992 C13 1.286 4.492 8.249 C14 2.441 4.806 8.980	Ru1 13.995 4.332 8.298 Cl2 13.721 5.355 6.177 Cl3 15.218 3.186 9.969 N4 12.301 6.152 10.021 C5 13.450 5.845 9.376 C6 8.969 5.032 8.912 H7 8.258 5.238 8.110 H8 10.593 1.440 8.357 C9 10.523 6.732 7.886 H10 11.326 6.345 7.240 H11 10.890 7.678 8.307 H12 9.658 6.956 7.253 C13 8.664 4.056 9.861 C14 15.704 6.852 9.240 C15 12.502 3.275 8.282 C16 17.464 7.350 7.696 H17 17.795 7.772 6.746 C18 10.167 5.740 8.951 C19 12.503 2.026 7.556

C15 2.746 4.010 10.078 C16 1.932 2.946 10.461 C17 0.758 2.713 9.750 C18 0.400 3.484 8.644 C19 3.316 5.963 8.609 C20 2.316 2.077 11.620 C21 -0.915 3.274 7.959 C40 2.858 3.842 3.582 C41 3.397 2.810 2.726 C42 3.396 1.452 3.097 C43 3.942 0.495 2.261 C44 4.492 0.871 1.036 C45 4.494 2.208 0.649 C46 3.951 3.171 1.486 H1 -0.005 8.052 5.623 H2 -0.107 6.851 8.148 H3 4.029 8.012 2.185 H4 0.360 6.423 0.630 H5 3.095 7.911 5.659 H6 4.445 8.076 4.516 H7 4.009 6.484 5.166 H8 3.637 8.113 -0.154 H9 1.943 8.185 -0.669 H10 2.814 6.655 -0.732 H11 -1.298 5.535 2.059 H12 -1.356 6.171 3.714 H13 -0.583 4.618 3.404 H14 3.648 4.228 10.651 H15 0.085 1.918 10.072 H16 3.847 5.758 7.671 H17 4.067 6.140 9.384 H18 2.741 6.888 8.475 H19 1.441 1.599 12.075 H20 2.836 2.650 12.396 H21 2.995 1.278 11.299 H22 -0.790 2.938 6.923 H23 -1.496 4.204 7.926 H24 -1.508 2.525 8.492 H58 2.881 4.857 3.174 H59 2.947 1.145 4.044 H60 3.936 -0.551 2.558 H61 4.917 0.115 0.379 H62 4.921 2.497 -0.309 H63 3.948 4.222 1.197	C20 9.584 3.797 10.878 H21 9.358 3.031 11.621 C22 16.221 5.906 11.539 H23 16.265 6.762 12.228 H24 16.896 5.136 11.925 H25 15.208 5.492 11.570 C26 12.428 7.362 10.844 H27 12.504 7.088 11.908 H28 11.545 7.999 10.718 C29 11.407 -0.080 7.059 H30 10.566 -0.757 7.188 C31 10.798 4.478 10.957 C32 16.111 7.421 8.026 C33 18.397 6.764 8.547 C34 16.629 6.329 10.159 C35 11.823 4.122 11.991 H36 11.446 3.346 12.665 H37 12.110 4.985 12.605 H38 12.744 3.745 11.521 C39 13.569 1.649 6.717 H40 14.408 2.329 6.561 C44 19.839 6.651 8.150 H45 20.116 7.410 7.410 H46 20.045 5.669 7.705 H47 20.502 6.758 9.015 C48 12.474 -0.441 6.241 H49 12.465 -1.401 5.729 N50 14.323 6.860 9.603 C51 11.067 5.445 9.983 C52 7.390 3.272 9.762 H53 6.567 3.887 9.380 H54 7.089 2.864 10.732 H55 7.504 2.426 9.072 C56 15.163 8.174 7.143 H57 14.127 7.843 7.263 H58 15.422 8.042 6.088 H59 15.216 9.249 7.367 C60 13.553 0.426 6.069 H61 14.381 0.143 5.424 C62 11.420 1.145 7.710 C63 17.967 6.282 9.782 H64 18.694 5.857 10.474 C70 13.711 7.984 10.310 H71 13.518 8.812 9.608 H72 14.377 8.350 11.099 H73 11.589 3.499 8.840
IMes	**SIMes**
N1 1.036 5.824 5.179 N2 0.980 5.014 7.129 C1 1.484 4.740 5.885 C2 0.296 6.723 5.944 C3 0.258 6.203 7.190 C4 1.304 6.009 3.789 C5 2.564 6.470 3.400 C6 2.800 6.658 2.040 C7 1.821 6.392 1.083 C8 0.580 5.924 1.511 C9 0.302 5.720 2.861 C10 3.625 6.732 4.424 C11 2.109 6.571 -0.378 C12 -1.024 5.186 3.310 C13 1.182 4.159 8.254 C14 2.113 4.525 9.228 C15 2.277 3.683 10.327	N1 11.616 8.487 5.656 N2 11.614 7.974 3.576 C3 11.810 7.453 4.807 C4 11.424 9.797 4.997 H5 12.344 10.397 5.080 H6 10.610 10.365 5.462 C7 11.128 9.371 3.569 H8 10.052 9.393 3.334 H9 11.648 9.974 2.815 C10 11.926 8.422 7.042 C11 10.893 8.527 7.980 C12 11.216 8.480 9.334 H13 10.415 8.547 10.072 C14 12.532 8.332 9.767 C15 13.537 8.220 8.808 H16 14.571 8.090 9.132 C17 13.259 8.265 7.444

C16 1.550 2.503 10.460 C17 0.638 2.166 9.459 C18 0.440 2.977 8.346 C19 2.924 5.776 9.080 C20 1.760 1.595 11.634 C21 -0.524 2.600 7.264 H1 -0.123 7.630 5.530 H2 -0.204 6.555 8.103 H3 3.777 7.021 1.719 H4 -0.192 5.703 0.773 H5 3.286 7.450 5.182 H6 4.535 7.125 3.959 H7 3.874 5.808 4.961 H8 2.852 7.358 -0.548 H9 1.204 6.831 -0.937 H10 2.509 5.648 -0.819 H11 -1.612 4.828 2.459 H12 -1.620 5.947 3.831 H13 -0.890 4.356 4.015 H14 3.001 3.955 11.096 H15 0.065 1.242 9.549 H16 3.328 5.862 8.063 H17 3.760 5.786 9.787 H18 2.326 6.679 9.258 H19 0.812 1.180 11.995 H20 2.240 2.118 12.468 H21 2.401 0.744 11.369 H22 0.005 2.458 6.313 H23 -1.266 3.391 7.092 H24 -1.056 1.676 7.513	C18 9.467 8.656 7.536 H19 8.779 8.391 8.345 H20 9.261 8.007 6.676 H21 9.223 9.683 7.228 C22 12.863 8.309 11.230 H23 13.754 7.705 11.430 H24 12.036 7.902 11.822 H25 13.065 9.319 11.608 C26 14.351 8.121 6.428 H27 15.331 8.057 6.910 H28 14.370 8.969 5.730 H29 14.195 7.223 5.818 C30 11.514 7.179 2.401 C31 10.435 6.296 2.256 C32 10.344 5.548 1.087 H33 9.512 4.853 0.967 C34 11.290 5.661 0.068 C35 12.356 6.538 0.247 H36 13.117 6.621 -0.530 C37 12.487 7.304 1.405 C38 9.421 6.145 3.350 H39 8.627 5.451 3.057 H40 8.955 7.105 3.608 H41 9.895 5.776 4.268 C42 11.148 4.862 -1.193 H43 10.800 3.843 -0.985 H44 12.098 4.791 -1.734 H45 10.417 5.317 -1.874 C46 13.659 8.220 1.590 H47 14.473 7.956 0.908 H48 14.036 8.175 2.618 H49 13.397 9.268 1.390