

# Exploring New Generations of Ruthenium Olefin Metathesis Catalysts: The Reactivity of a Bis-ylidene Ruthenium Complex by DFT

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## Computational details.

**DFT calculations.** All the density functional theory (DFT) calculations were performed using the Gaussian09 package.<sup>[1]</sup> The BP86 GGA functional of Becke and Perdew<sup>[2-4]</sup> was used with the standard split-valence basis set with a polarization function of Ahlrichs and coworkers for H, C, N, P, and Cl atoms (SVP keyword in Gaussian)<sup>[5]</sup> while the quasi relativistic small-core Stuttgart effective core potential (ECP) was used for Ruthenium (SDD keyword in Gaussian09), for geometry optimizations,<sup>[6-8]</sup> pointing out that the origin of energies is based on the separated reactants instead of using the pre-reactant complex approach. The reported energies have been obtained via single point energy calculations with M06<sup>[9-10]</sup> functional with the triple- $\zeta$  basis set of Ahlrichs for H, C, N, P, and Cl atoms (TZVP keyword in Gaussian09). Solvent effects, CH<sub>2</sub>Cl<sub>2</sub>, were included with the default Gaussian PCM implementation.<sup>[12-13]</sup> All geometry and energy optimizations were carried out with the keyword SCF=tight, and integral(grid=ultrafinegrid) keyword for PCM M06/TZVP calculations. Zero point energies and thermal corrections calculated at the BP86 level were added to the M06 in solvent energies to approximate free energies in solvent.

**Table S1.** xyz coordinate data sets and M06 solvent phase energies (in a.u.) for DFT optimized complexes.

<b>0•PCy<sub>3</sub></b>			<b>0•PCy<sub>3</sub>-0•14e</b>			<b>0•14e</b>			<b>0•14e-0•ClI</b>						
<b>-3257.4256315</b>			<b>-3257.3884262</b>			<b>-2210.5628234</b>			<b>-2289.1136202</b>						
Ru	-0.002929	-0.328337	-0.056133	Ru	1.104390	0.183321	-0.160134	Ru	-0.229244	0.878736	0.091096	Ru	0.223568	0.748022	0.004839
Cl	-0.293995	-0.328627	2.348918	Cl	0.473452	0.767803	-2.325842	Cl	-0.972340	1.556755	-2.007499	C	0.435735	-1.168935	0.179042
N	-0.215947	-0.536341	-2.484029	Cl	0.608213	0.021665	2.131024	N	-1.798072	-1.551861	0.152394	Cl	0.229667	1.104245	2.334231
P	-0.747209	2.069224	-0.212863	P	-3.154073	-0.670168	0.253649	C	-0.519565	-1.026598	0.092993	Cl	0.964860	1.044158	-2.209333
N	-1.015070	-3.225232	0.095517	N	2.599854	2.654828	0.165383	C	-1.805921	-2.995101	0.445091	C	-1.586639	0.865830	-0.331562
N	1.172636	-3.198198	-0.146051	N	3.993961	0.947922	0.382321	C	-3.038441	-0.830419	0.026820	H	-2.134966	0.011371	-0.780052
C	0.072168	-2.395410	-0.012679	C	2.683033	1.274729	0.099909	C	-3.601070	-0.672565	-1.271184	C	2.057359	3.390059	0.312612
C	-0.672744	-4.656519	-0.063584	C	3.832801	3.273797	0.684559	C	-4.822348	0.014823	-1.389421	C	1.207281	4.155264	-0.398787
H	-1.089000	-5.043774	-1.019609	H	3.695111	3.587036	1.744564	C	-5.506345	0.525683	-0.267297	H	1.072338	4.003443	-1.482205
H	-1.111573	-5.255509	-0.760931	H	4.096620	4.175647	0.095014	C	-4.959064	0.285203	1.006355	H	0.608249	4.950562	0.075645
C	0.859208	-4.641779	-0.050635	C	4.853169	2.139158	0.544321	C	-3.743534	0.407791	1.185730	N	1.690742	-1.728433	0.334073
H	1.286343	-5.060895	0.887833	H	5.513138	2.263155	-0.345530	C	-2.923649	-1.239000	-2.496178	N	-0.475299	-2.189696	0.334169
H	1.308994	-5.196484	-0.899853	H	5.507361	2.028628	1.433056	C	-6.787953	1.310506	-0.433667	C	1.635751	-3.132632	0.778307
C	-2.411008	-2.906315	0.275373	C	1.482168	3.500702	-1.070999	C	-3.237917	-0.745417	2.581347	C	0.171401	-3.506968	0.510666
C	-2.947684	-2.916722	1.593615	C	1.383151	3.994219	-1.501696	H	-2.099835	-3.176964	1.503966	H	2.356896	-3.753439	0.207831
C	-2.085499	-3.213649	2.795846	C	2.386261	3.613157	-2.564235	H	-2.532400	-3.524196	-0.204649	H	1.898339	-3.210859	1.857654
H	-2.684604	-3.181971	3.726942	H	2.304943	4.285335	-3.441041	H	-5.255323	0.151301	-2.394662	H	-0.296254	-4.059961	1.350950
H	-1.259367	-2.477078	2.883591	H	2.204458	2.573114	-2.910027	H	-5.500095	0.636076	1.901302	H	0.047994	-4.125528	-0.408338
H	-1.628003	-4.225025	2.728045	H	3.429988	3.660287	-2.189762	H	-2.025590	-0.639252	-2.755961	H	2.189262	3.519241	-1.397076
C	-4.235954	-2.693601	1.753974	C	0.323046	4.865421	-1.812593	H	-2.591775	-2.286893	-2.339454	C	2.967770	-1.094949	0.119608
C	-4.744665	-2.685391	2.775960	H	0.235416	5.241188	-2.846001	H	-3.608489	-1.223141	-3.366642	C	-1.899665	-2.173385	0.151842
C	-5.193603	-2.515822	0.656019	C	-0.617903	5.275886	-0.847207	H	-7.429125	0.883114	-1.232153	C	3.536518	-1.148370	-1.184293
C	-6.667866	-2.247775	0.860719	C	-1.773393	6.175103	-1.225314	H	-6.571923	2.362843	-0.721947	C	4.797137	-0.557104	-1.387890
H	-7.272237	-2.595751	-0.001482	C	-2.180841	6.713350	-0.345974	H	-7.377065	1.340618	0.504878	C	5.515031	0.056493	-0.341836
H	-6.861574	-1.158213	0.976781	H	-2.606920	5.584287	-1.665182	H	-3.598854	-1.771654	2.866124	C	4.958451	0.020570	0.950435
H	-7.051700	-2.743453	1.757355	H	-1.475326	6.926920	-1.984875	H	-3.712824	-0.050633	3.324204	C	3.703737	-0.567510	1.216054
C	-4.641036	-2.596588	-0.636652	H	0.982370	2.499389	2.433360	H	-2.172948	-0.686314	2.679736	C	-2.741509	-2.042329	1.286126
H	-5.305183	-2.516591	-1.513746	H	-1.146384	5.166283	1.256077	N	0.350653	-2.093070	0.159065	C	-4.134894	-2.097165	1.086439
C	-3.263283	-2.803305	-0.858430	C	0.598140	3.952498	0.844721	C	-0.349247	-3.394550	0.169897	C	-4.703627	-2.288492	-0.189322
C	-2.745724	-2.961987	-2.268223	C	0.792175	3.583438	2.296871	C	1.779609	-2.106671	0.029736	C	-3.835154	-2.417646	-1.291785
H	-3.552484	-2.773393	-3.003692	H	-0.103344	3.849052	2.892172	C	2.577109	-2.122157	1.202853	C	-2.433582	-2.365252	-1.149123
H	-2.375431	-3.995132	-2.450520	H	1.649826	4.138545	2.738446	C	3.975586	-2.204032	1.053357	C	2.825657	-1.828805	-2.329244
H	-1.903670	-2.269588	-2.484710	H	0.982370	2.499389	2.433360	C	4.590695	-2.277827	0.213419	H	5.234859	-0.585074	-2.399033
C	2.566720	-2.852427	-0.203595	C	4.659636	-0.323785	0.341169	C	3.765296	-2.543651	-1.356244	C	6.842879	0.730662	0.604183
C	3.220352	-2.852082	-1.465893	C	4.873567	-1.028196	1.553239	C	2.361382	-2.171552	-1.263068	H	5.525287	0.448901	1.942135
C	2.448096	-0.065053	-2.745732	C	4.314281	-0.517727	2.859736	C	1.945365	-2.014522	2.570349	C	3.218654	-0.683939	2.641785
H	3.112576	-2.976812	-3.627707	H	4.595024	-1.183920	3.698725	C	6.092686	-2.407155	-0.338621	C	-2.163064	-1.824273	2.663570
H	1.621352	-2.327464	-2.848045	H	2.205270	-0.447902	2.820977	C	1.508188	-2.088918	-2.508068	H	-4.797153	-1.985193	1.961508
H	1.981570	-4.074185	-2.782574	H	4.686868	0.501457	3.099113	H	-0.226348	-3.909345	-0.811087	C	-6.204190	-2.373239	-0.360283
C	4.612701	-2.644365	-1.490935	C	5.590486	-2.241233	1.499665	H	0.075181	-0.405797	0.951340	C	-4.259450	-2.559301	-2.300216
H	5.126749	-2.638374	-2.467315	H	5.751404	-2.802492	2.432796	C	4.630888	-2.207923	1.959992	C	-1.531554	-2.442085	-2.360021
C	5.365334	-2.460701	-0.311910	C	6.103187	-2.754129	0.288749	C	4.226818	-2.299176	-2.357163	C	3.519378	-2.002545	-3.175177
C	6.858580	-2.231408	-0.380686	C	6.904018	-4.037367	0.263287	H	1.376084	-1.065805	2.674884	C	2.394010	-2.805995	-2.029549
H	7.352057	-2.959365	-1.058093	H	6.670849	-4.683642	1.133210	H	1.224917	-2.839211	2.759639	H	1.989874	-1.192304	-2.691670
H	7.333487	-2.315739	0.617238	H	7.995836	-3.825888	0.294639	C	2.173747	-0.050263	3.367058	H	3.822032	-0.042969	3.314384
H	7.089229	-1.217705	-0.750252	H	6.714881	-4.619926	0.661510	H	6.454068	-2.060640	-1.327690	H	1.516455	-0.384615	2.749364
C	4.685612	-2.486222	0.920437	C	5.872743	-2.023149	-0.895693	H	6.411475	-3.467083	-0.225908	H	3.321147	-1.278624	3.011641
H	5.255767	-2.350788	1.854527	C	6.253651	-2.412951	-1.854793	C	6.620009	-1.826352	0.445516	H	7.456360	0.804210	0.316339
C	3.929449	-2.685887	1.006449	C	5.159937	-0.808761	-0.896772	H	0.732409	-2.883099	-2.538920	H	7.432398	0.188519	-1.371906
C	2.601006	-2.724554	2.346145	C	4.871956	-0.081537	-2.180651	H	2.126702	-2.189016	-3.421109	H	6.692950	1.765699	-0.983132
H	1.981570	-4.074185	-2.782574	H	4.686868	0.501457	3.099113	H	0.970026	-1.117812	-2.560925	H	-2.965538	-1.753112	3.423699
H	7.089229	-1.217705	-0.750252	H	3.778527	-0.039583	-2.385584	Cl	-0.390480	1.173078	2.401300	H	-1.488779	-2.655444	2.963273
C	4.685612	-2.486222	0.920437	C	1.864602	-1.467412	-0.483996	C	1.594742	1.021750	-0.147854	H	-1.555548	-0.894239	2.704378
H	5.255767	-2.350788	1.854527	C	5.859786	-3.911673	-0.847823	C	2.233667	0.150946	-0.391759	H	-2.119550	-2.613574	-3.282635
C	3.929449	-2.685887	1.006449	H	1.191117	-2.663125	-0.990405	C	2.296402	2.302119	-0.091911	H	-0.951885	-1.502089	-2.490293
C	2.601006	-2.724554	2.346145	H	1.304997	-0.988113	-3.335896	C	3.672019	2.349348	-0.463688	H	-0.787708	-3.263144	-2.280377
H	1.981570	-4.074185	-2.782574	C	0.068358	-2.654085	-1.653730	C	1.665447	3.518573	0.290405	H	-6.504478	-2.254189	-1.420522
H	7.197939	-1.959447	2.419655	C	0.062477	-0.567357	-1.997803	C	4.381194	3.558138	-0.449417	H	-6.590986	-3.837188	-0.014748
H	3.323430	-2.551399	1.673115	C	1.865996	-0.587393	-3.047096	H	4.174315	1.414792	-0.762243	C	-6.726245	-1.958811	0.235111
H	1.798257	0.029534	-0.294287	C	1.864602	-1.467412	-0.483996	C	2.377088	4.723311	0.304034	C	-2.391437	-2.083909	-0.224927
C	4.071104	0.987123	-0.187958	C	5.159937	-0.808761	-0.896772	C	3.736431	4.749047	-0.066799	C	-3.581079	2.170952	-1.005074
C	2.854285	0.688751	0.498880	H	4.871956	-0.081537	-2.180651	H	5.446619	3.574019	-0.737163	C	-2.061780	3.179690	0.621599
C	5.130685	-1.484880	0.466151	H	4.686868	0.501457	3.099113	H	1.871711	5.652806	0.610268	C	-4.387195	3.315541	-0.965993
C	2.754640	1.042637	1.862358	C	0.068358	-2.654085	-1.653730	H	4.293477	5.699435	-0.053578	H	-3.856798	1.321807	-0.615403
C	5.010631	1.974182	1.825713	C	0.062477	-0.567357	-1.997803	H	-2.883188	4.314188	0.670521	H	-1.171415	3.106589	1.262507
H	6.056811	1.863839	-0.083856	H	1.841914	-6.052108	-1.211014	H	-1.171415	3.106589	1.262507	C	-4.040725	4.392314	-0.127171
C	3.823001	1.668689	2.519212	C											

H	2.175285	-0.253957	-1.305628	H	2.926825	-1.644383	-0.225616		
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<b>0•CI1</b>		<b>0•CI1-0•MCy</b>		<b>0•MCy</b>		<b>0•MCy-0•CI2</b>					
<b>-2289.1249394</b>		<b>-2289.1274193</b>		<b>-2289.1338923</b>		<b>-2289.1205459</b>					
Ru	0.393947	0.981342	-0.468894	Ru	-0.394652	-0.970982	-0.392457	Ru	-0.209934	-0.823987	-0.472098
C	0.635354	-0.972359	0.252971	C	-0.636589	0.947431	0.271656	C	-0.708672	0.986887	0.283080
Cl	0.287400	1.503210	1.910118	Cl	-0.389761	-1.644689	1.928889	Cl	-0.029700	-1.741736	1.760236
C	0.705191	-0.033077	-2.683499	Cl	-0.830020	-0.248600	-2.674172	Cl	-0.332137	-0.004808	-2.751570
C	-1.417393	0.970789	-0.857505	C	1.418750	-0.868845	-0.821199	C	1.226952	-2.304010	-1.419977
H	-1.675790	0.338766	-1.737683	H	1.642614	-0.174456	-1.661226	H	1.616143	-1.225889	-2.244803
C	0.726680	3.217349	-0.458399	C	-0.096391	-3.335362	-0.706444	C	-1.332328	-2.227776	-1.280102
C	1.060077	2.721817	-1.719534	C	-1.326857	-2.900144	-1.161663	C	0.136012	-2.746039	-1.541792
H	2.106692	2.479759	-1.974228	H	-2.203965	-2.907826	-0.486993	H	0.186701	-2.935033	-2.629362
H	0.381004	2.807881	-2.581513	H	-1.528544	-2.755657	-2.234491	H	0.311529	-3.645709	-0.923649
N	1.869056	-1.453991	0.576040	N	-1.870796	1.450707	0.580013	N	-1.990157	1.465014	0.565488
N	-0.282939	-1.934502	0.527501	N	0.288220	1.900682	0.577987	N	0.148392	2.040745	0.544243
C	1.810882	-2.791580	1.209160	C	-1.804050	2.777152	1.231266	C	-2.009098	2.875708	1.019087
C	0.339510	-3.191871	1.011280	C	-0.322479	3.156350	1.072704	C	-0.513138	3.203453	1.181228
H	2.527662	-3.485792	0.717488	H	-2.493297	3.490883	0.734210	H	-2.506338	3.513808	0.255825
H	-2.093682	-2.714793	2.281647	H	-2.111171	2.694079	2.296737	H	-2.580786	2.970481	1.964923
H	-0.151390	-3.528254	1.947044	H	0.151932	3.467796	2.026083	H	-0.202520	3.297900	2.246850
H	0.208109	-3.993868	0.252086	H	-0.163428	3.973834	0.334819	H	-0.216061	4.144128	0.674320
H	-0.242150	3.710310	-0.275915	H	0.724818	-3.525682	-1.415802	H	-1.875143	-2.824299	-0.522774
C	3.143509	-0.793388	0.404737	C	-3.152644	0.816753	0.377796	C	-3.221618	0.721838	0.434426
C	-1.713281	-1.910829	-3.046923	C	1.709087	1.881189	0.357147	C	1.586129	1.999182	0.425457
C	3.871437	-1.012737	-0.800410	C	-3.847015	1.056916	-0.842566	C	-3.969837	0.804055	-0.771105
C	5.106564	-0.354605	-0.958972	C	-5.097368	0.436419	-1.028459	C	-5.178432	0.083046	-0.847617
C	5.655515	0.468004	0.044818	C	-5.689661	-0.373412	-0.038941	C	-5.699432	-0.679788	0.230347
C	4.961074	0.569628	1.264472	C	-5.021354	-0.503459	1.192814	C	-4.931081	-0.683042	1.429560
C	3.723817	-0.071451	1.484321	C	-3.771710	0.102343	1.440444	C	-3.714936	0.015997	1.564505
C	-2.538627	-1.551435	1.446710	C	2.568304	1.501769	1.422260	C	3.258604	1.470681	1.496010
C	-3.934450	-1.596248	1.269856	C	3.957703	1.581529	1.212475	C	3.761239	1.513631	1.380566
C	-4.524810	-0.004273	0.056923	C	4.507020	2.031878	-0.005422	C	4.406521	2.080521	0.263321
C	-3.674735	-2.399113	-0.993322	C	-3.623006	-2.416533	-1.032409	C	3.607397	2.625690	-0.759272
C	-2.269265	-2.376049	-0.873783	C	2.222675	2.360044	-0.876491	C	2.198434	2.609732	-0.700729
C	3.379865	-1.962698	1.863543	C	-3.296294	1.979685	-1.900991	C	-3.516569	1.649891	-1.936195
H	5.664832	-0.507058	-1.897923	H	-5.630921	0.606105	-1.978791	H	-5.760766	0.134686	-1.783052
C	6.955562	1.206648	-0.180049	C	-6.955563	-1.071232	-0.293089	C	-6.949050	-1.475226	0.099784
H	5.402128	1.152735	2.090384	H	-5.493641	-1.080601	2.005553	H	-5.314850	-1.241987	2.299514
C	3.119086	-0.086892	2.868155	C	-3.185278	0.055692	2.831424	C	-2.973588	0.005978	2.878572
C	-1.948614	-1.149690	2.776501	C	2.009821	1.021759	2.739104	C	1.715094	0.889599	2.731676
H	-4.580628	-1.305705	2.115102	H	4.632357	1.279655	2.031102	H	4.367552	1.096756	2.201955
C	-6.028299	-2.010766	-0.104213	C	6.005762	2.082588	-0.199300	C	5.916316	2.107507	0.180162
H	-4.115010	-2.750373	-1.941801	H	4.032955	2.781333	-1.989373	H	4.092215	3.092877	-1.632894
C	-1.400696	-2.844383	-2.016360	C	1.304395	2.773736	-2.002685	C	1.381442	3.230109	-1.807206
H	4.147161	-2.101405	-2.650120	H	-4.062628	2.192299	-2.671973	H	-4.252303	1.603176	-2.762750
H	3.146555	-2.963263	-1.440151	H	-2.967872	2.949718	-1.471097	H	-3.408982	2.719086	-1.650809
H	2.452092	-1.578193	-2.339685	H	-2.414082	1.521448	-2.398835	H	-2.530395	1.315178	-2.327729
H	3.472449	0.818412	3.445366	H	-3.466329	-0.793158	3.407584	H	-3.583575	-0.470626	3.670704
H	2.013741	-0.017222	2.842962	H	-2.084343	-0.095660	2.818525	H	-2.020583	-0.560043	2.781363
H	3.433575	-0.965659	3.432685	H	-3.441634	0.983772	3.390967	H	-2.716434	1.031022	3.220893
H	7.473627	1.427855	0.774931	H	-7.531190	-1.317301	0.652229	H	-7.440898	-1.626402	1.081963
H	7.648459	0.629124	-0.825595	H	-7.685096	-0.451762	-0.915203	H	-7.673138	-0.978910	-0.578191
H	6.775086	2.179729	-0.688125	H	-6.849617	-2.026774	-0.840528	H	-6.747337	-2.484215	-0.323270
H	-2.747218	-0.908823	3.505024	H	2.823796	0.753427	3.440419	H	2.478438	0.668719	3.502958
H	-1.334191	-1.966643	3.215096	H	1.387528	1.801220	3.230650	H	0.975577	1.586232	3.180852
H	-1.281919	-0.265996	2.675908	H	1.353501	0.134747	2.600819	H	1.168410	-0.053158	2.506169
H	-2.012741	-3.166078	-2.875204	H	1.885498	3.131033	-2.875203	H	2.037496	3.707386	-2.561213
H	-0.709593	-2.043792	-2.362937	H	0.666628	1.931129	-2.335995	H	0.758755	2.460790	-2.315224
H	-0.769992	-3.711514	-1.723671	H	0.620849	3.596176	-1.699709	H	0.688026	4.010499	-1.425842
H	-6.342638	-2.562241	-1.012751	H	6.283617	2.628585	-1.122804	H	6.269258	2.646552	-0.721376
H	-6.530155	-2.473909	0.770940	H	6.510327	2.576491	0.657441	H	6.362567	2.600643	1.069873
H	-6.421208	-0.973933	-0.187986	H	6.429451	1.057322	-0.273599	H	6.331756	1.077487	0.144848
H	1.498232	3.400501	0.306467	H	-1.493261	-3.679028	0.329258	H	-1.899633	-2.009187	-2.203867
C	-2.584760	1.708537	-0.364931	C	2.622261	-1.582366	-0.383092	C	2.544268	-2.162102	-0.547800
C	-3.790674	1.552409	-1.111715	C	3.789308	-1.428729	-1.187102	C	3.782967	-1.592450	-0.941367
C	-2.607311	2.580279	0.759400	C	2.711492	-2.402894	0.775663	C	2.558576	-3.136850	0.481487
C	-4.957797	2.244346	-0.762160	C	4.985165	-2.084691	-0.863089	C	4.988187	-1.982428	-0.337390
H	-3.790100	0.875869	-1.981492	H	3.736324	-0.785853	-2.080475	H	3.790911	-0.836294	-1.742982
C	3.779543	3.263114	1.109971	C	3.914328	-3.038648	1.107024	C	3.763688	-3.528302	1.081504
H	-1.693029	2.682823	1.363205	H	1.821047	-2.508232	1.414851	H	1.611508	-3.570422	0.832679
C	-4.955766	3.104314	0.352000	C	5.051841	-2.890701	0.288281	C	4.984553	-2.955577	0.676923
H	-5.873736	2.116040	-1.361351	H	5.870035	-1.966341	-1.508798	H	5.937354	-1.533322	-0.671195
H	-3.777130	3.930842	1.986500	H	3.967918	-3.663773	2.012829	H	3.749791	-4.289450	1.878035
H	-5.871221	3.651453	0.629602	H	5.991030	-3.405032	0.548777	H	5.928867	-3.270109	1.149522

<b>0•CI2</b>				<b>0•CI2-0•end</b>				<b>0•end</b>			
<b>-2289.1211276</b>				<b>-2289.10592</b>				<b>-1979.6085737</b>			
Ru	0.178956	-0.813456	-0.746045	Ru	-0.276896	-0.764710	-0.227876	Ru	0.079657	0.468600	-1.401147
C	0.764376	0.858245	0.349343	C	-1.080809	0.976858	0.079018	Cl	0.234259	2.758165	-0.989250
Cl	0.564547	0.587758	-2.714666	Cl	0.160829	-1.284187	2.054890	Cl	1.162148	-1.339852	-2.377836
C	0.039175	-1.971205	1.400599	Cl	-0.318001	-0.661837	-2.609735	C	-0.082662	-0.060496	0.451648
C	-1.289202	-2.575595	-1.242413	C	2.424233	-2.764168	-1.181666	C	-1.596014	0.297463	-2.059731
H	-0.702354	-3.446581	-0.908552	H	2.374740	-2.389939	-2.220607	H	-1.695233	0.630987	-3.125683
C	1.832043	-1.532649	-0.948686	C	-1.850319	-1.683238	-0.195609	H	-2.512532	-0.097116	-1.580690
C	-0.893089	-1.904475	-2.404581	C	1.383044	-3.514989	-0.729489	N	1.010283	-0.207016	1.283146
H	-0.080533	-2.298483	-3.032164	H	0.548059	-3.771286	-1.400086	N	-1.204944	-0.243198	1.227568
H	-1.561482	-1.192041	-2.912320	H	1.373914	-3.976734	0.271266	C	0.624959	-0.326957	2.701746
N	2.011911	1.211996	0.765204	N	-2.397303	1.326071	0.211116	C	-0.875739	-0.637954	2.612350
N	-0.114744	1.802338	0.777290	N	-0.324936	2.112729	0.184952	H	1.208243	-1.127624	3.200679
C	2.020276	2.492698	1.512867	C	-2.583189	2.776849	0.416840	H	0.823662	0.627222	3.240675
C	0.530074	2.867073	1.580536	C	-1.140985	3.326553	0.380545	H	-1.483821	-0.059500	3.337416
H	2.477682	2.348707	2.513797	H	-3.224224	3.204184	-0.384445	H	-1.098202	-1.718433	2.771118
H	2.631057	3.245046	0.969425	H	-3.091213	2.970485	1.386662	C	2.404480	-0.205411	0.916290
H	0.310223	3.863667	1.144090	H	-0.854571	3.838995	1.324259	C	-2.582248	-0.266255	0.823638
H	0.126538	2.857292	2.615825	H	-0.976085	4.044527	-0.451961	C	3.015678	-1.445585	0.581181
H	2.460129	-1.283051	-1.832164	H	-2.228088	-2.155684	0.739878	C	4.383375	-1.447826	0.252633
C	3.275605	0.555941	0.538719	C	-3.538049	0.457972	0.184683	C	5.159367	-0.271262	0.267779
C	-1.541937	1.870133	0.560788	C	1.113270	2.191471	0.125077	C	4.538288	0.924449	0.673642
C	3.777555	-0.339884	1.522980	C	-4.239686	0.273561	-1.038697	C	3.173117	0.984407	1.023487
C	5.040989	-0.924792	1.304449	C	-5.420158	-0.495172	-1.015047	C	-3.355341	0.917710	0.941970
C	5.821723	-0.626081	0.170439	C	-5.919875	-1.064387	0.173358	C	-4.717636	0.857177	0.590218
C	5.320836	0.317924	-0.747462	C	-5.209119	-0.842594	1.371882	C	-5.322946	-0.333327	0.135982
C	4.064862	0.935130	-0.582720	C	-4.025200	-0.082502	1.408718	C	-4.523468	-1.489283	0.036130
C	-2.035961	2.657597	-0.518295	C	1.859325	2.153406	1.336973	C	-3.154474	-1.483547	0.374552
C	-3.430969	2.787344	-0.657942	C	3.258333	2.290266	1.258109	C	2.233345	-2.737472	0.593127
C	-4.335266	2.200249	0.250144	C	3.926454	2.478108	0.031938	H	4.858597	-2.405054	-0.020148
C	-3.807725	1.476917	1.334682	C	3.150640	2.263954	-1.139796	C	6.613715	-0.296599	-0.144922
C	-2.420236	1.310537	1.527469	C	1.746203	2.439413	-1.123450	H	5.136469	1.849101	0.735625
C	2.999487	-0.653642	2.776760	C	-3.722085	0.858779	-2.329398	C	2.594186	2.271350	1.563025
H	5.428812	-1.630861	2.057881	H	-5.969684	-0.647606	-1.959071	C	-2.728294	2.210971	1.405319
C	7.154218	-1.303082	-0.058586	C	-7.178864	-1.902100	0.162827	H	-5.325183	1.774160	0.673885
H	5.931284	0.597597	-1.622531	H	-5.591496	-1.269584	2.314323	C	-6.786706	-0.355926	-0.244850
C	3.595349	1.977712	-1.567100	C	-3.280526	0.134833	2.703370	H	-4.976170	-2.429496	-0.321222
C	-1.110310	3.371372	-1.472439	C	1.190577	1.973946	2.677848	C	-2.312963	-2.728746	0.212011
H	-3.819393	3.388590	-1.497425	H	3.843101	2.255399	2.192603	H	-3.481364	3.021288	1.457219
C	-5.826865	2.379511	0.074405	C	5.434067	2.573515	-0.017989	H	-2.271310	2.110823	2.413302
H	-4.495000	1.030810	2.071906	H	3.649624	2.749883	-2.105680	H	-1.915525	2.531569	0.718241
C	1.909988	0.588696	2.749844	C	0.957072	2.585212	-2.401040	H	-2.913940	-3.562943	-0.199226
H	3.561684	-1.355369	3.423340	H	-4.440275	0.694083	-3.156161	H	-1.457844	-2.548114	-0.473707
H	2.800554	0.262187	3.375193	H	-3.541982	1.951809	-2.249066	H	-1.883728	-3.073058	1.177583
H	2.012636	-1.107167	2.535333	H	-2.747739	0.399393	-2.613303	H	-7.140073	-1.384523	-0.456488
H	4.344976	1.217413	-2.368524	H	-3.832908	-0.304523	3.556751	H	-7.422006	0.065207	0.562653
H	2.630224	1.687568	-0.037904	H	-2.266398	-0.325180	2.669635	H	-6.974411	0.257430	-1.152631
H	3.436938	2.962617	-1.075551	H	-3.131026	1.214410	2.918820	H	1.511384	-2.764427	-0.249635
H	7.854200	-0.651493	-0.620024	H	-7.820786	-1.678304	1.045312	H	2.910700	-3.607709	0.489697
H	7.638019	-1.590954	0.896719	H	-7.777557	-1.738317	-0.749779	H	1.656260	-2.864775	1.533333
H	7.028185	-2.234417	-0.653950	H	-6.935448	-2.986288	0.216268	H	3.255810	3.128102	1.328079
H	-1.687559	3.963831	-2.208859	H	1.899245	2.187944	3.501827	H	1.594997	2.492312	1.138990
H	-0.432216	4.073522	-0.940117	H	0.312749	2.641769	2.802507	H	2.500332	2.228907	2.671401
H	-0.467869	2.650608	-2.023209	H	0.827054	0.928211	2.793449	H	7.176030	0.560778	0.276574
H	-2.750940	0.278224	3.399838	H	1.601577	2.961113	-3.219587	H	7.114825	-1.232547	0.177231
H	-1.325256	-0.317256	2.467475	H	0.526266	1.607951	-2.714730	H	6.710721	-0.242069	-1.251680
H	-1.239539	1.234454	3.357915	H	0.106749	3.290569	-2.287540				
H	-6.400385	1.817301	0.837627	H	5.784912	3.077939	-0.940798				
H	-6.116133	3.449769	0.154480	H	5.838668	3.125043	0.855599				
H	-6.161139	2.035032	-0.927443	H	5.887635	1.557826	0.000461				
H	2.236116	-2.265261	-0.215346	H	-2.411954	-1.918482	-1.128193				
C	-2.617953	-2.449650	-0.599457	C	3.662581	-2.421368	-0.459535				
C	-2.954376	-3.331352	0.458422	C	4.727123	-1.822130	-1.177822				
C	-3.599864	-1.527584	-1.039561	C	3.847280	-2.677155	0.923264				
C	-4.227156	-3.301289	1.046675	C	5.940287	-1.504942	-0.546196				
H	-2.197722	-4.046433	0.815423	H	4.595083	-1.612222	-2.252020				
C	-4.873135	-1.500141	-0.451430	C	5.054379	-2.351089	1.555633				
H	-3.371704	-0.826164	-1.857111	H	3.027023	-3.116349	1.510922				
C	-5.194623	-2.387084	0.592215	C	6.107946	-1.767478	0.824992				
H	-4.467693	-4.000407	1.863596	H	6.759386	-1.052318	-1.127888				
H	-5.624361	-0.781942	-0.815756	H	5.175923	-2.551288	2.632204				
H	-6.197930	-2.368189	1.047243	H	7.057053	-1.517695	1.325780				

<b>00•PCy<sub>3</sub></b>			<b>00•PCy<sub>3</sub>•0•14e</b>			<b>00•14e</b>			<b>00•14e-00•C11</b>						
<b>-3026.4722983</b>			<b>-3026.4309605</b>			<b>-1979.6085737</b>			<b>-2058.1569993</b>						
Ru	0.360954	-0.139375	-0.021886	Ru	1.448619	0.155213	0.335516	Ru	0.079657	0.468600	-1.401147	Ru	0.083195	1.158965	0.067603
Cl	0.435171	-0.167285	2.410561	Cl	1.123985	0.994867	2.320085	Cl	0.234259	2.758165	-0.989250	C	-0.161415	-0.760277	0.093876
C	0.037615	-0.336110	-2.418272	Cl	0.809517	0.318495	-1.904929	Cl	1.162148	-1.339852	-2.377836	Cl	0.234477	1.383613	2.387043
P	-0.817789	2.052644	-0.106460	P	-3.965329	0.494448	0.132764	C	-0.082662	-0.060496	0.451648	Cl	1.174580	1.496427	-1.962260
N	0.062437	-3.209802	0.039469	N	3.795024	-1.392468	-0.433334	C	-1.596014	0.297463	-2.059731	C	-1.565592	1.817441	-0.278558
N	2.183034	-2.610552	0.024752	N	4.349843	0.742126	-0.215237	H	-1.695233	0.630987	-3.125683	H	-2.509826	1.289211	-0.513480
C	0.901225	-2.131133	0.012788	C	3.312853	-0.150578	-0.068915	H	-2.512532	-0.097116	-1.580690	C	0.759619	5.192336	-0.774763
C	0.781832	-4.498853	0.162354	C	5.149531	-1.323809	-1.011108	N	-1.010283	-0.207016	1.283146	H	1.001865	4.537383	-1.628841
H	0.429343	-5.215617	-0.607773	H	5.106411	-1.452009	-2.116480	N	-1.204944	-0.243198	1.227568	H	0.157358	6.093069	-0.984996
H	0.584362	-4.951019	1.159369	H	5.792004	-2.129484	-0.600189	C	0.624959	-0.326957	2.701746	N	0.894202	-1.644022	0.201306
C	2.249497	-4.088046	-0.020883	C	5.613190	0.083719	-0.607477	H	-1.483821	-0.059500	3.337416	C	-1.051050	-2.959071	0.186878
H	2.912864	-4.473952	0.780664	H	6.326106	0.071485	0.249328	H	-1.098202	-1.718433	2.771118	C	0.998660	-3.752786	-0.124035
H	2.671437	-4.421568	-0.955073	H	6.098217	0.653310	-1.438498	H	2.404480	-0.205411	0.916290	H	-1.673637	-3.446686	0.962528
C	-1.379564	-3.248519	0.035398	C	3.141994	2.668392	-0.288938	C	3.015678	-1.445585	0.581181	H	-1.302922	-3.427799	-0.792458
C	-2.083987	-3.272386	1.269554	C	3.282956	-3.362203	0.945349	C	4.383375	-1.447826	0.252633	H	0.930293	5.532232	1.335683
C	-1.370166	-3.176331	2.596160	C	4.072798	-2.778186	2.091939	H	5.159367	-0.271262	0.267779	C	2.300638	-1.354386	0.008025
H	-2.095358	-3.210184	3.433494	H	4.299475	-3.553760	2.849751	C	4.538288	0.924449	0.673642	C	-2.651719	-1.069900	0.005279
H	-0.778734	-2.238207	2.680363	H	3.493309	-1.971706	2.588945	C	3.173117	0.984407	1.023487	C	2.894044	-1.421493	-1.211182
H	-0.660820	-4.019792	2.740166	H	5.033016	-2.336223	1.753740	C	-3.355341	0.917710	0.941970	C	4.272166	-1.164977	-1.326379
C	-3.485686	-3.430784	1.230424	H	2.677925	-4.625376	1.073115	C	-4.717636	0.857177	0.590218	C	5.075235	-0.871314	-0.205675
H	-4.037437	-3.451095	2.185480	H	2.774239	-5.161824	2.032036	C	-5.322946	-0.333327	0.135982	C	3.093157	-1.145814	1.240259
C	-4.191926	-3.593400	0.023432	C	1.964105	-5.224592	0.015487	C	-3.154474	-1.483547	0.374552	C	-3.449415	-0.815125	1.154226
C	-5.696364	-3.748865	0.009759	C	1.279375	-6.559789	0.202307	C	2.233345	-2.737472	0.593127	C	-4.796004	-0.434019	0.989010
H	-6.021591	-4.504860	-0.734589	H	1.125062	-7.082386	-0.763234	H	4.858597	-2.405054	0.020148	C	-5.382366	-0.312220	-0.294344
H	-6.194030	-2.792648	-0.264846	H	0.278260	-6.427880	0.668900	C	6.613715	-0.296599	-0.144922	C	-5.798832	-0.576721	-1.424169
H	-6.086839	-4.050895	1.002273	H	1.869910	-7.228302	0.869865	H	1.536469	1.849101	0.735625	C	-3.229185	-0.958357	-1.307464
C	-3.454303	-3.609786	-1.177263	C	1.904147	-4.540504	-1.212604	C	2.594186	2.271350	1.563025	C	2.080727	-1.785222	-2.430824
H	-3.980340	-3.771345	-2.133343	H	1.386782	-5.009546	-0.266490	C	-2.782894	2.210971	1.405319	H	4.733234	-1.201282	-2.327683
C	-2.053424	-3.459474	-1.200262	C	2.498357	-3.274603	-1.400199	H	-1.325183	1.774160	0.673885	C	6.543059	-0.546795	-0.368077
C	-1.300557	-3.556251	-2.504022	C	2.497626	-2.642768	-2.772689	C	-6.786706	-0.359296	-0.244850	H	5.086514	-0.704318	1.954540
H	-1.992388	-3.765859	-3.343721	H	1.633463	-2.995831	-3.369503	H	-4.576170	-2.429496	-0.321222	C	2.524099	-1.262830	2.634920
H	-4.545502	-4.371914	-2.483037	H	1.869910	-7.228302	0.869865	C	-2.312963	-2.728746	0.212011	C	-2.841818	-0.916654	2.532920
H	-0.755842	-2.610058	-2.716774	H	2.443088	-1.538250	-2.725548	H	-3.481364	3.021288	1.457219	H	-5.404040	-0.221645	1.876372
C	3.423153	-1.882913	-0.018238	C	4.390601	2.134772	0.129662	C	-2.271310	2.110823	2.413302	C	-6.837786	0.068380	-0.451561
C	4.004654	-1.565907	-1.254447	C	4.198942	3.103699	-0.886443	H	-1.915525	2.531569	0.718241	C	-2.378842	-1.183944	-2.536588
C	3.308310	-1.902120	-2.571598	C	3.869655	2.694902	-2.302624	H	-1.913940	-3.562943	-0.199226	H	1.332194	-0.847072	-2.432628
H	3.913587	-1.576297	-3.440192	H	6.686124	3.583067	-2.938278	H	-1.883728	-3.073058	1.177583	H	1.535304	-2.742178	-2.291669
H	3.407668	-1.058990	-2.639522	H	2.967143	2.047918	-2.336566	H	-7.140073	-1.384523	-0.456488	H	1.332195	-0.997296	-2.653256
H	3.141049	-2.996281	-2.676240	H	4.698199	2.118442	-2.769192	C	-7.422006	0.065207	0.562653	H	3.225142	-0.840790	3.381615
C	5.259631	-0.922336	-1.281853	C	4.303313	4.465452	-0.532470	H	-6.974411	0.257430	-1.152631	H	1.558299	-0.729427	2.739060
H	5.714133	-0.665835	-2.253708	H	4.151041	5.227452	-1.315247	H	1.511384	-2.764427	-0.249635	H	2.362344	-2.329462	2.909034
C	5.947899	-0.612023	-0.094112	C	4.593478	4.878168	0.782430	H	2.910700	-3.607709	0.489697	H	7.109433	-0.723256	0.568431
C	7.280820	0.105888	-0.127022	C	4.674675	6.344438	1.145222	H	1.656260	-2.864775	1.533333	H	6.683698	0.522221	-0.641573
H	7.775792	0.008976	-1.114213	H	4.794382	6.983013	0.247622	H	3.258510	3.128102	1.328079	H	-3.588075	-0.674121	3.144410
H	7.974028	-0.283102	0.647152	H	5.523012	6.548387	1.830916	H	2.500332	2.228907	2.671401	H	-2.459041	-1.939314	2.746610
H	7.152603	1.192842	0.072107	H	3.751496	6.677597	1.668630	H	7.176030	0.560778	2.276574	H	-1.979403	-0.224486	2.640185
C	5.359217	-0.978590	1.132586	C	4.782960	3.883600	1.765384	H	7.114825	-1.232547	0.177231	H	-2.969561	-1.035263	-3.461376
H	5.892641	-0.765452	2.074457	H	5.011626	4.184283	2.801945	H	6.710721	-0.242609	-1.251680	H	-1.516515	-0.483383	-2.560661
H	4.107623	-1.620751	1.200801	C	4.687915	2.510961	1.466708	H	-1.957926	-2.211705	-2.571287	H	-6.995950	0.724893	-1.331627
C	3.512207	-2.005682	2.531704	C	4.843717	1.472324	2.553520	H	-7.471612	-0.833344	-0.602698	H	-7.222815	0.594351	0.444872
H	3.288691	-3.093017	2.586973	H	5.592629	0.696197	2.289736	H	1.779845	3.996215	0.675180	H	-1.602771	2.936806	-0.259528
H	2.551133	-1.471542	2.706967	H	3.885422	0.939387	2.735143	C	-5.092527	0.994112	0.976015				
H	4.207009	-1.764341	3.359962	H	5.162770	1.938185	3.506085	C	-6.226204	0.102242	-1.070256				
C	1.968699	0.652504	-0.171602	C	3.181378	1.875530	0.888338	C	-4.710497	-0.677830	-1.597458				
C	-2.669371	1.730218	-3.272961	C	-3.894534	-0.926112	-1.201944	C	-0.445788	3.433184	-1.292346				
C	3.168937	1.713785	-1.755016	C	3.621039	-0.424691	-2.637651	C	0.633653	4.463766	-0.882089				
C	-3.086069	4.019224	0.429124	C	-2.806809	-1.959250	-0.818081	C	-0.125011	2.906978	-2.707383				
H	-3.178673	2.578251	0.244531	H	-4.890520	-1.431778	-1.208303	H	-1.420629	3.978726	-1.326745				
H	-4.693833	1.488771	-1.792080	H	-3.568289	-1.590391	-3.645534	C	0.748325	5.606533	-1.912750				
H	-2.646810	0.902502	-2.289030	H	-2.644379	0.111376	-2.659058	H	1.617905	3.948608	-0.794586				
H	2.924591	3.666309	-2.249194	H	-4.957471	0.300585	-2.962912	H	0.414937	4.907865	0.108613				
C	-4.590645	0.190903	0.386996	C	2.742920	-3.133206	-1.813117	C	-0.027484	4.046479	-3.737444				
H	-2.564321	-0.435254	-0.096173	H	-1.822812	-1.437786	-0.803515	H	0.839562	2.356648	-2.667397				
H	-2.701378	0.384056	1.474456	H	-2.962053	-2.342396	0.210677	H	-0.861585	2.152682	-3.037337				
C	-5.118964	0.206085	-1.056350	C	-2.515894	-2.639252	-3.251037	C	1.023199	5.090353	-3.332353				
H	-5.026514	1.484488	-2.850774	H	-3.361271	-1.195998	-4.664780	H	1.542605	6.314612	-1.589870				
H	-5.209220	2.262965	-1.320897	H	-4.571356	2.072148	-3.696942	H	-0.203189	6.187603	-1.912009				
H	-4.841825	-0.768286	0.887005	H	-1.936119	-3.836383	-1.512013	H	0.207577	3.621265	-4.737433				
H	-5.092527	0.994112	0.976015	H	-3.695389	-3.710935	-1.765637	H	-1.020988	4.543668	-3.838287				
H	-6.226204	0.102242	-1.070256	H	-2.526331	-3.									

00•CI1			00•CI1-00•MCy			00•MCy			00•MCy-00•CI2						
-2058.1745202			-2058.1728689			-2058.1930081			-2058.1728689						
Ru	0.228142	1.356257	-0.081340	Ru	0.188614	1.324403	0.021309	Ru	-0.000896	1.231220	-0.009611	Ru	0.188614	1.324403	0.021309
C	-0.114903	-0.674731	0.088168	C	-0.098516	-0.697541	0.053094	C	0.000263	-0.779961	0.029645	C	-0.098516	-0.697541	0.053094
Cl	0.149636	1.377839	2.367434	Cl	0.016113	1.216715	2.443940	Cl	0.002285	1.302097	-2.418199	Cl	0.016113	1.216715	2.443940
CI	0.011659	1.065173	-2.504076	CI	0.278929	1.311152	-2.421665	CI	-0.025499	1.358434	2.397334	CI	0.278929	1.311152	-2.421665
C	-1.487558	1.947761	-0.075981	C	-1.535975	1.880753	-0.132053	C	1.348548	2.673154	-0.011816	C	-1.535975	1.880753	-0.132053
H	-1.991085	2.216104	0.877874	H	-2.166440	2.022010	0.774685	H	1.938458	2.763401	-0.942726	H	-2.166440	2.022010	0.774685
H	-2.047526	2.078327	-1.026924	H	-1.980120	2.139490	-1.118716	H	1.917427	2.789257	0.929242	H	-1.980120	2.139490	-1.118716
C	1.520944	3.117765	0.468986	C	0.860914	3.545994	0.595116	C	-1.351887	2.671441	-0.038433	C	0.860914	3.545994	0.595116
C	1.496822	3.018400	-0.221778	C	1.692238	2.963055	-0.347975	C	-0.002185	3.504847	-0.037870	C	1.692238	2.963055	-0.347975
H	2.308454	2.508612	-1.470129	H	2.574521	2.379607	-0.015731	H	-0.011359	4.118479	0.883466	H	2.574521	2.379607	-0.015731
H	0.837354	3.644575	-1.540532	H	1.668865	3.239756	-1.412664	H	0.006600	4.092674	-0.975868	H	1.668865	3.239756	-1.412664
N	0.938996	-1.529908	0.174463	N	0.960555	-1.551846	0.101668	N	-1.107115	-1.562968	0.051098	N	0.960555	-1.551846	0.101668
N	-1.266353	-1.388753	0.165921	N	-1.245755	-1.425427	0.105772	N	1.108626	-1.561565	0.055216	N	-1.245755	-1.425427	0.105772
C	0.521301	-2.941002	0.331269	C	0.548969	-2.963189	0.267460	C	-0.770218	-3.005516	0.072979	C	0.548969	-2.963189	0.267460
C	-1.017481	-2.842820	0.324196	C	-0.985257	-2.884433	0.143718	C	0.773438	-3.003148	0.119061	C	-0.985257	-2.884433	0.143718
H	0.920478	-3.555721	-0.503212	H	1.016092	-3.598920	-0.513329	H	-1.227841	-3.493864	0.959058	H	1.016092	-3.598920	-0.513329
H	0.922483	-3.358263	1.278890	H	0.879466	-3.344478	1.257903	H	-1.173379	-3.506051	-0.833535	H	0.879466	-3.344478	1.257903
H	-1.478149	-3.206747	1.266516	H	-1.512303	-3.349392	1.002126	H	1.232555	-3.542440	-0.736338	H	-1.512303	-3.349392	1.002126
H	-1.482682	-3.402476	-0.514625	H	-1.367877	-3.360942	-0.785305	H	1.176304	-3.449419	1.053492	H	-1.367877	-3.360942	-0.785305
H	0.878566	3.830217	1.009456	H	0.097438	4.277846	0.284845	H	-1.924017	2.761563	-0.980403	H	0.097438	4.277846	0.284845
C	2.336366	-1.171228	0.093812	C	2.354994	-1.181167	0.039740	C	-2.480357	-1.118726	0.018186	C	2.354994	-1.181167	0.039740
C	-2.630208	-0.925321	0.086643	C	-2.606270	-0.961213	0.013650	C	2.481571	-1.116102	0.028685	C	-2.606270	-0.961213	0.013650
C	2.978410	-1.164665	-1.177846	C	2.997802	-1.142231	-1.229028	C	-3.176034	-0.930574	1.243125	C	2.997802	-1.142231	-1.229028
C	4.342104	-0.813578	-1.228475	C	4.359052	-0.779756	-1.271751	C	-4.522332	-0.520443	1.180851	C	4.359052	-0.779756	-1.271751
C	5.085476	-0.513488	-0.069507	C	5.096969	-0.492528	-0.107025	C	-5.189614	-0.316563	-0.043584	C	5.096969	-0.492528	-0.107025
C	4.438884	-0.620543	1.176462	C	4.448319	-0.625327	1.136630	C	-4.481055	-0.565381	-1.235057	C	4.448319	-0.625327	1.136630
C	3.076998	-0.968398	1.291988	C	3.090487	-0.989066	1.243495	C	-3.132769	-0.976622	-1.235467	C	3.090487	-0.989066	1.243495
C	-3.332800	-0.616805	1.284853	C	-3.366002	-0.799245	1.203800	C	3.140824	-0.990582	-1.224740	C	-3.366002	-0.799245	1.203800
C	-4.676550	-0.211362	1.176932	C	-4.710495	-0.396367	1.080197	C	4.487245	-0.578581	-1.224330	C	-4.710495	-0.396367	1.080197
C	-5.340111	-0.127666	-0.064131	C	-5.316417	-0.173291	-0.172576	C	5.190277	-0.312087	-0.031749	C	-5.316417	-0.173291	-0.172576
C	-4.628011	-0.495579	-1.220867	C	-4.544094	-0.389464	-1.330597	C	4.517280	-0.497657	1.190749	C	-4.544094	-0.389464	-1.330597
C	-3.280683	-0.910445	-1.175437	C	-3.194996	-0.793280	-1.269159	C	3.169901	-0.909601	1.253236	C	-3.194996	-0.793280	-1.269159
C	2.252464	-1.554006	-2.441509	C	2.269005	-1.497549	-2.500493	C	-2.509136	-1.164078	2.576507	C	2.269005	-1.497549	-2.500493
H	4.841499	-0.794690	-2.211765	H	4.859496	-0.735954	-2.253579	H	-5.068337	-0.365521	2.126687	H	4.859496	-0.735954	-2.253579
C	6.538127	-0.104894	-0.166207	C	6.543852	-0.060182	-0.187493	C	-6.623733	0.162591	-0.074473	C	6.543852	-0.060182	-0.187493
H	5.015032	-0.446308	2.100539	H	5.020482	-0.459777	2.064990	H	-4.994085	-0.446592	-2.204226	H	5.020482	-0.459777	2.064990
C	2.459333	-1.160212	2.654844	C	2.474776	-1.220751	2.601910	C	-2.421638	-1.256234	-2.536674	C	2.474776	-1.220751	2.601910
C	-2.677921	-0.735198	2.639393	C	-2.764579	-1.053368	2.564589	C	2.432790	-1.287073	-2.525789	C	-2.764579	-1.053368	2.564589
H	-5.224014	0.039677	2.101181	H	-5.304265	-0.259273	1.999631	H	5.004193	-0.472157	-2.192983	H	-5.304265	-0.259273	1.999631
C	-6.777065	0.337881	-0.141177	C	-6.750699	0.296702	-0.268776	C	6.627656	0.156675	-0.072832	C	-6.750699	0.296702	-0.268776
H	-5.136343	-0.469322	-2.199314	H	-5.005801	-0.250366	-2.322606	H	5.058335	-0.326157	2.136426	H	-5.005801	-0.250366	-2.322606
C	-2.571794	-1.327231	-2.440632	C	-2.411447	-1.039916	-2.534640	C	2.499993	-1.125047	2.588328	C	-2.411447	-1.039916	-2.534640
H	2.960354	-1.633171	-3.289489	H	2.977987	-1.586657	-3.346616	H	-3.240336	-1.071240	3.403122	H	2.977987	-1.586657	-3.346616
H	1.740631	-2.534355	-2.338084	H	1.723970	-2.460972	-2.411031	H	-2.055542	-2.176315	2.641921	H	1.723970	-2.460972	-2.411031
H	1.473541	-0.803723	-2.703547	H	1.520275	-0.713608	-2.751900	H	-1.692266	-0.427555	2.747454	H	1.520275	-0.713608	-2.751900
H	3.199903	-0.954665	3.452185	H	3.177533	-0.924949	3.405243	H	-3.129534	-1.217122	-3.387488	H	3.177533	-0.924949	3.405243
H	1.590610	-0.482210	2.800860	H	1.537187	-0.639483	2.732788	H	-1.616524	-0.509222	-2.718270	H	1.537187	-0.639483	2.732788
H	2.101792	-2.203491	2.796402	H	2.236604	-2.296461	2.756156	H	-1.944461	-2.259490	-2.543322	H	2.236604	-2.296461	2.756156
H	7.058490	-0.202888	0.807494	H	7.126605	-0.411967	0.688131	H	-7.128608	-0.113326	-1.022081	H	7.126605	-0.411967	0.688131
H	7.085146	-0.715603	-0.914066	H	7.034622	-0.439246	-1.106583	H	-7.213683	-0.254678	0.767202	H	7.034622	-0.439246	-1.106583
H	6.632710	0.955964	-0.486477	H	6.625791	1.049100	-0.207442	H	-6.673594	1.270463	0.013371	H	6.625791	1.049100	-0.207442
H	-3.390985	-0.469668	3.444131	H	-3.496774	-0.832919	3.365818	H	3.144776	-1.272756	-3.371984	H	-3.496774	-0.832919	3.365818
H	-2.327260	-1.771852	2.837190	H	-2.453263	-2.114299	2.685063	H	1.942144	-2.283675	-2.512853	H	-2.453263	-2.114299	2.685063
H	-1.788498	-0.071736	2.721807	H	-1.861418	-0.425643	2.728669	H	1.638143	-0.532973	-2.721568	H	-1.861418	-0.425643	2.728669
H	-3.267701	-1.318672	-3.302058	H	-3.057804	-0.925757	-3.426623	H	3.224679	-0.996807	3.415935	H	-3.057804	-0.925757	-3.426623
H	-1.722661	-0.644043	-2.665595	H	-1.557959	-0.330973	-2.628753	H	1.666233	-0.403444	2.739836	H	-1.557959	-0.330973	-2.628753
H	-2.151273	-2.353006	-2.362093	H	-1.983211	-2.065241	-2.562023	H	2.069966	-2.145909	2.676339	H	-1.983211	-2.065241	-2.562023
H	-7.201982	0.190665	-1.153868	H	-7.216646	-0.001911	-1.229460	H	7.102251	0.115280	0.927758	H	-7.216646	-0.001911	-1.229460
H	-7.420135	-0.204091	0.583868	H	-7.370574	-0.106664	0.557787	H	7.236942	-0.456893	-0.769098	H	-7.370574	-0.106664	0.557787
H	-6.860485	1.419245	0.103172	H	-6.810080	1.405935	-0.207287	H	6.693920	1.207617	-0.429975	H	-6.810080	1.405935	-0.207287
H	2.350958	2.693940	1.057791	H	1.033980	3.441606	1.676452	H	-1.939072	2.785507	0.891571	H	1.033980	3.441606	1.676452



00•CI2				00•CI2-00•end				00•end			
-2058.1745202				-2058.1569993				-1979.6085737			
Ru	0.228142	1.356257	-0.081340	Ru	0.083195	1.158965	0.067603	Ru	0.079657	0.468600	-1.401147
C	-0.114903	-0.674731	0.088168	C	-0.161415	-0.760277	0.093876	Cl	0.234259	2.758165	-0.989250
Cl	0.149636	1.377839	2.367434	Cl	0.234477	1.383613	2.387043	Cl	1.162148	-1.339852	-2.377836
Cl	0.011659	1.065173	-2.504076	Cl	1.174580	1.496427	-1.962260	C	-0.082662	-0.060496	0.451648
C	-1.487558	1.947761	-0.075981	C	-1.565592	1.817441	-0.278558	C	-1.596014	0.297463	-2.059731
H	-1.991085	2.216104	0.877874	H	-2.509826	1.289211	-0.513480	H	-1.695233	0.630987	-3.125683
H	-2.047526	2.078327	-1.026924	C	1.174931	4.895698	0.468310	H	-2.512532	-0.097116	-1.580690
C	1.520944	3.117765	0.468986	C	0.759619	5.192336	-0.774763	N	1.010283	-0.207016	1.283146
C	1.498682	3.018400	-0.922178	H	1.001865	4.537383	-1.628841	N	-1.204944	-0.243198	1.227568
H	2.308454	2.508612	-1.470129	H	0.157358	6.093069	-0.984996	C	0.624959	-0.326957	2.701746
H	0.837354	3.644575	-1.540532	N	0.894202	-1.644022	0.201306	C	-0.875739	-0.637954	2.612350
N	0.938996	-1.529908	0.174463	N	-1.316355	-1.506447	0.144620	H	1.208243	-1.127624	3.200679
N	-1.266353	-1.388753	0.165921	C	0.450636	-3.018235	0.500782	H	0.823662	0.627222	3.240675
C	0.521301	-2.941002	0.331269	C	-1.051050	-2.959071	0.186878	H	-1.483821	-0.059500	3.337416
C	-1.017481	-2.842820	0.324196	H	0.998660	-3.752786	-0.124035	H	-1.098202	-1.718433	2.771118
H	0.920478	-3.555721	-0.503212	H	0.647381	-3.264914	1.568710	C	2.404480	-0.205411	0.916290
H	0.922483	-3.358263	1.278890	H	-1.676367	-3.446686	0.962528	C	-2.582248	-0.266255	0.823638
H	-1.478149	-3.206747	1.266516	H	-1.302922	-3.427799	-0.792458	C	3.015678	-1.445585	0.581181
H	-1.482682	-3.402476	-0.514625	H	0.930293	5.322322	1.335683	C	4.383375	-1.447826	0.252633
H	0.878566	3.830217	1.009456	C	2.300638	-1.354386	0.080025	C	5.159367	-0.271262	0.267779
C	2.336366	-1.171228	0.093812	C	-2.675179	-1.069900	-0.005279	C	4.538288	0.924449	0.673642
C	-2.630208	-0.925321	0.086643	C	2.894044	-1.421493	-1.211182	C	3.173117	0.984407	1.023487
C	2.978410	-1.164665	-1.177846	C	4.272166	-1.164977	-1.326379	C	-3.355341	0.917710	0.941970
C	4.342104	-0.813578	-1.228475	C	5.075235	-0.871314	-0.205675	C	-4.717636	0.857177	0.590218
C	5.085476	-0.513488	-0.069507	C	4.468775	-0.887012	1.064091	C	-5.322946	-0.333327	0.135982
C	4.438884	-0.620543	1.176462	C	3.093157	-1.145814	1.240259	C	-4.523468	-1.489283	0.036130
C	3.076998	-0.968398	1.291988	C	-3.449415	-0.815125	1.154226	C	-3.154474	-1.483547	0.374552
C	-3.332800	-0.618805	1.284853	C	-4.796004	-0.434019	0.980910	C	2.233345	-2.737472	0.593127
C	-4.676550	-0.211362	1.176932	C	-5.382366	-0.312220	-0.294344	H	4.858597	-2.405054	-0.020148
C	-5.340111	-0.127666	-0.064131	C	-4.579883	-0.576721	-1.424169	C	6.613715	-0.296599	-0.144922
C	-4.628011	-0.495579	-1.220867	C	-3.229185	-0.958357	-1.307464	H	5.136469	1.849101	0.735625
C	-3.280683	-0.910445	-1.175437	C	2.080727	-1.785222	-2.430824	C	2.594186	2.271350	1.563025
C	2.252464	-1.554006	-2.441509	H	4.733234	-1.201282	-2.327638	C	-2.728294	2.210971	1.405319
H	4.841499	-0.794690	-2.211765	C	6.543059	-0.546795	-0.368077	H	-5.325183	1.774160	0.673885
C	6.538127	-0.104894	-0.166207	H	5.086514	-0.704318	1.959450	C	-6.786706	-0.355926	-0.244850
H	5.015032	-0.446308	2.100539	C	2.524099	-1.262830	2.634927	H	-4.976170	-2.429496	-0.321222
C	2.459333	-1.160212	2.654844	C	-2.841818	-0.916654	2.532920	C	-2.312963	-2.728746	0.212011
C	-2.677921	-0.735198	2.639393	H	-5.404040	-0.221645	1.876372	H	-3.481364	3.021288	1.457219
H	-5.224014	0.039677	2.101181	C	-6.837786	0.068380	-0.451561	H	-2.271310	2.110823	2.413302
C	-6.777065	0.337881	-0.141177	H	-5.015631	-0.476072	-2.432628	H	-1.915525	2.531569	0.718241
H	-5.136343	-0.469322	-2.199314	C	-2.378842	-1.183944	-2.536588	H	-2.913940	-3.562943	-0.199226
C	-2.571794	-1.327231	-2.440632	H	2.733094	-1.895732	-3.319034	H	-1.457844	-2.548114	-0.473707
H	2.960354	-1.633171	-3.289489	H	1.533504	-2.742178	-2.291669	H	-1.883728	-3.073058	1.177583
H	1.740631	-2.534355	-2.338084	H	1.332195	-0.997296	-2.653526	H	-7.140073	-1.384523	-0.456488
H	1.473541	-0.803723	-2.703547	H	3.225142	-0.840790	3.381615	H	-7.422006	0.065207	0.562653
H	3.199903	-0.954965	3.452185	H	1.558299	-0.729427	2.739060	H	-6.974411	0.257430	-1.152631
H	1.590610	-0.482210	2.800860	H	2.362344	-2.329462	2.909034	H	1.511384	-2.764427	-0.249635
H	2.101792	-2.203491	2.796402	H	7.109433	-0.723256	0.568431	H	2.910700	-3.607709	0.489697
H	7.058490	-0.202888	0.807494	H	7.008838	-1.149938	-1.174446	H	1.662620	-2.864775	1.533333
H	7.085146	-0.715603	-0.914066	H	6.683698	0.522221	-0.641573	H	3.255810	3.128102	1.328079
H	6.632710	0.955964	-0.486477	H	-3.588075	-0.674121	3.314410	H	1.594997	2.492312	1.138990
H	-3.390985	-0.469668	3.444131	H	-2.459041	-1.939314	2.740610	H	2.500332	2.228907	2.671401
H	-2.327260	-1.771852	2.837190	H	-1.979403	-0.224486	2.644185	H	7.176030	0.560778	0.276574
H	-1.788498	-0.071736	2.721807	H	-2.969561	-1.035263	-3.461376	H	7.114825	-1.232547	0.177231
H	-3.267701	-1.318672	-3.302058	H	-1.516155	-0.483383	-2.560661	H	6.710721	-0.242069	-1.251680
H	-1.722661	-0.644043	-2.665595	H	-1.957926	-2.211705	-2.571287				
H	-2.151273	-2.353006	-2.362093	H	-6.995950	0.724893	-1.331627				
H	-7.201982	0.190665	-1.153868	H	-7.471612	-0.833344	-0.602698				
H	-7.420135	-0.204091	0.583868	H	-7.222815	0.594351	0.444872				
H	-6.860485	1.419245	0.103172	H	1.779845	3.996215	0.675180				
H	2.350958	2.693940	1.057791	H	-1.602771	2.936806	-0.259528				



1•PCy <sub>3</sub>			1•PCy <sub>3</sub> -1•14e			1•14e			1•14e-1•ClI						
-2602.589448			-2602.5844626			-1555.7548416			-1634.2995161						
Ru	-0.756889	-1.040781	-0.139924	Ru	1.332841	1.246441	-0.042122	Ru	0.000025	-0.334482	0.034857	Ru	-0.029798	0.888418	-0.073721
Cl	-0.788230	-1.250045	2.215798	Cl	1.168236	0.701016	2.207503	Cl	0.000328	-1.355963	-2.016924	Cl	0.174031	1.053080	2.219815
Cl	-1.115412	-0.419378	-2.500289	Cl	1.090938	0.640433	-2.275071	Cl	-0.000306	-0.994388	2.229188	Cl	0.460115	1.959210	-2.065122
P	0.697188	1.174123	-0.020694	P	-1.298514	-1.118390	-0.018135	C	-1.345946	0.925182	-0.073748	C	-1.776658	0.322088	-0.280429
C	0.360092	-2.406428	-0.712353	C	0.804603	3.019738	-0.068681	H	-1.054804	2.000967	-0.150387	H	-2.461244	1.142515	-0.602801
C	2.361059	-3.806726	-1.066510	C	-0.661202	5.010703	-0.095202	C	-2.780152	0.681559	-0.062046	C	-1.934289	3.973294	0.075102
C	1.627679	-2.932466	-0.210867	C	-0.528811	3.596500	0.021093	C	-3.669137	1.793311	-0.111764	C	-0.741848	4.151246	0.672597
C	3.584083	-4.356693	-0.661035	C	-1.915892	5.626851	-0.006744	C	-3.339754	-0.626770	-0.000752	H	-0.639141	4.154780	1.769761
C	2.161654	-2.650581	1.077065	C	-1.704616	2.824550	0.234359	C	-5.057120	1.604655	-0.096715	H	0.178386	4.300672	0.083719
C	4.094994	-4.064674	0.617808	C	-3.067029	4.845524	0.206417	H	-3.250222	2.811648	-0.160833	H	-2.030859	3.965371	-1.023581
H	4.138964	-5.023407	-1.340085	H	-1.999233	6.721179	-0.100228	C	-4.726208	-0.810381	0.012864	H	-2.858162	3.832331	0.661916
C	3.374672	-3.219278	1.485032	C	-2.955007	3.445785	0.327365	H	-2.672006	-1.502558	0.032240	C	-2.421709	-0.969172	-0.090758
H	1.584235	-2.005992	1.754819	H	-1.613858	1.729636	0.326564	C	-5.589122	0.303226	-0.034047	C	-3.670602	-1.206093	-0.737745
H	5.052590	-4.502658	0.942197	H	-4.054652	5.328004	0.281432	H	-5.730308	2.475586	-0.134322	C	-1.884824	-1.998448	0.734662
C	3.765486	-3.004192	2.492324	H	-3.856562	2.836321	0.498335	H	-5.142780	-1.828679	0.059568	C	-4.328186	-2.434304	-0.602498
C	-0.405246	2.627698	-0.581530	C	-0.402522	-2.700986	-0.621779	H	-6.680533	0.154258	-0.022821	H	-4.108916	-0.401416	-1.362065
C	-0.334405	3.035688	-0.270086	C	-0.417066	-2.949435	-2.147675	C	1.345916	0.925298	-0.073578	C	-2.556935	-3.219766	0.878173
C	-1.876315	2.357469	-0.182032	C	1.063441	-2.703755	-0.127582	H	1.054705	2.001077	-0.149957	H	-0.957916	-1.802862	1.294611
H	-0.029164	3.494883	0.012000	H	-0.942080	-3.552978	-0.141270	C	2.780105	0.681623	-0.061940	C	-3.772014	-3.446388	0.204337
C	-1.221938	4.267812	-2.340110	C	0.298311	-4.267766	-2.508057	C	3.669149	1.793368	-0.110989	H	-5.284869	-2.604592	-1.121198
H	-0.678682	2.184459	-2.695328	H	0.091687	-2.102478	-2.659287	C	3.339691	-0.626756	-0.001333	H	-2.135931	-4.000206	1.531606
H	0.709081	3.264789	-2.371074	H	-1.455472	-2.985507	-2.536746	C	5.057129	1.604670	-0.095939	H	-4.295954	-4.408523	-0.320113
C	-2.777357	3.575887	-0.461233	C	1.786839	-0.418756	-0.427874	C	3.250282	2.811752	-0.159512	C	0.793198	-0.738743	-0.411359
H	-2.238411	1.490252	-0.779726	H	1.590791	-1.859240	-0.627184	C	4.726138	-0.810407	0.012286	H	0.192393	-1.536868	-0.903311
H	-1.951927	2.065453	0.886483	H	1.119432	-2.509673	0.962530	H	2.671966	-1.502586	0.031051	C	2.195566	-1.072949	-0.215661
C	-2.683105	4.021536	-1.929718	C	1.742800	-4.304610	-1.982283	C	5.589098	0.303198	-0.033948	C	2.698189	-2.278933	-0.785977
H	-1.161632	4.539497	-3.416439	H	0.282642	-4.412194	-3.610528	H	5.730335	2.475609	-0.133041	C	3.097664	-0.242545	0.510326
H	-0.823333	5.143021	-1.775039	H	-0.271645	-5.122452	-2.074359	H	5.142662	-1.828748	0.058462	C	4.047424	-2.629189	-0.652570
H	-3.828450	3.333567	-0.192763	H	2.839186	-3.977272	-0.115787	H	6.680505	0.154195	-0.022746	H	2.009434	-2.932783	-1.365518
H	-2.472394	4.419067	0.201974	H	1.304582	-4.858838	0.079330								
H	-3.294588	4.934474	-2.099256	H	2.215277	-5.285105	-2.099928								
H	-3.115171	3.227365	-2.579983	H	2.345416	-3.534336	-2.515964								
C	2.265202	1.386335	-1.100099	C	-2.863902	-1.150386	-1.128529								
C	3.610570	1.034192	-0.424972	C	-4.177718	-0.679098	-0.466776								
C	2.148250	0.633433	-2.442970	C	-2.618919	-0.329682	-2.417732								
C	2.282886	2.482679	-1.308859	H	-3.011990	-2.206462	-1.409833								
C	4.801528	1.340161	-1.357674	C	-5.369096	-0.789952	-1.439501								
H	3.622463	-0.047823	-0.161955	H	-4.071542	0.383284	-0.147308								
H	3.744761	1.598739	0.519399	H	-4.400168	-1.264908	0.448936								
C	3.332810	0.942792	-3.376688	C	-3.801707	-0.434564	-3.399370								
H	2.122200	-0.458762	-2.229505	H	-2.467474	0.736373	-2.133625								
H	1.186539	0.850414	-2.944710	H	-1.672674	-0.635962	-2.913070								
C	4.679376	0.622308	-2.710464	C	-5.124313	-0.009699	-2.740981								
H	5.750296	1.062175	-0.848873	H	-6.297126	-0.434881	-0.939768								
H	4.852401	2.440591	-1.529556	H	-5.539068	-1.864802	-1.681309								
H	3.218044	0.372539	-4.323817	H	-3.598781	0.182578	-4.301676								
H	3.308478	2.021079	-3.659823	H	-3.889247	-1.487138	-3.756566								
H	5.525948	0.900398	-3.375456	H	-5.975174	-0.147057	-3.443490								
H	4.755347	-0.477676	-2.549392	H	-5.082978	1.080193	-2.510819								
C	1.292698	1.835854	1.674413	C	-2.013045	-1.713917	1.656455								
C	0.192439	2.471943	2.557857	C	-1.050847	-2.553683	2.527834								
C	2.060927	0.792064	2.520687	C	-2.505131	-0.495639	2.476245								
H	2.000267	2.652445	1.386052	H	-2.887833	-2.363770	1.410693								
C	0.798306	3.115517	3.822594	C	-1.718817	-2.989423	3.847913								
H	-0.534299	1.681573	2.850196	H	-0.145868	-1.947877	2.757969								
H	-0.373483	3.249157	2.005606	H	-0.707186	-3.456916	1.982503								
C	2.693605	1.438276	3.767822	C	-3.177002	-0.919544	3.795957								
H	1.335155	0.014023	2.839155	H	-1.625109	0.149702	2.695257								
H	2.838486	0.276191	1.925515	H	-3.206305	0.127226	1.883901								
C	1.630042	2.119148	4.644521	C	-2.241053	-1.787867	4.651503								
H	-0.015144	3.549995	4.443685	H	-0.998360	-3.580838	4.454477								
H	1.446254	3.970138	3.517289	H	-2.567924	-3.674808	3.617782								
H	3.242949	0.667698	4.351390	H	-3.498010	-0.018366	4.362740								
H	3.454346	2.191330	3.453752	H	-4.106734	-1.492604	3.569370								
H	2.102712	2.629817	5.511742	H	-2.758701	-2.130843	5.573886								
H	0.955547	1.340358	5.067903	H	-1.376968	-1.170074	4.987643								
H	1.951286	-0.444863	-2.061887	H	0.243454	5.619790	-0.256447								
H	0.036339	-2.912648	-1.653556	H	1.605895	3.792712	-0.170521								
C	-2.328324	-2.050873	-0.509922	C	3.112100	1.762300	-0.101468								
H	-2.281119	-2.849601	-1.282881	H	3.354516	2.836208	-0.295875								
C	-3.693389	-1.775207	-0.092488	C	4.289938	0.915074	0.007895								
C	-4.766524	-2.410487	-0.787294	C	5.550578	1.437351	-0.404059								
C	-4.019004	-0.906530	0.991382	C	4.244973	-0.415098	0.514379								
C	-6.098924	-2.178038	-0.428268	C	6.709745	0.654460	-0.339486								
H	-4.528547	-3.087024	-1.624185	H	5.601234	2.469955	-0.786489								
C	-5.353137	-0.683094	1.351174	C	5.409553	-1.187871	0.591788								
H	-3.202177	-0.444988	1.566650	H	3.288009	-0.819103	0.877904								
C	-6.395878	-1.311318	0.641819	C	6.642263	-0.660536	0.158988								
H	-6.913191	-2.673161	-0.980672	H	7.673766	1.070839	-0.671874								
H	-5.587307	-0.017794	2.197375	H	5.360886	-2.210487	0.997783								
H	-7.444397	-1.129214	0.927540	H	7.555104	-1.274468	0.218481								

<b>1•CI1</b>			<b>1•CI1-1•MCy</b>			<b>1•MCy</b>			<b>1•MCy-1•CI2</b>						
<b>-1634.3057438</b>			<b>-1634.293507</b>			<b>-1634.3075597</b>			<b>-1634.2894063</b>						
Ru	-0.038802	-1.050648	-0.021228	Ru	0.093707	0.658388	0.139361	Ru	0.096904	0.558765	0.099927	Ru	-0.070166	0.557108	-0.080860
Cl	-0.043228	-0.715518	2.308738	Cl	-0.095313	-0.529096	2.227862	Cl	-0.327303	-0.843739	1.995141	Cl	0.519389	-1.034435	-1.771941
Cl	-0.750888	-1.966374	-2.085241	Cl	0.642991	2.236831	-1.586520	Cl	0.631800	2.199731	-1.587912	Cl	-0.436975	2.273692	1.571185
C	1.742288	-0.636906	-0.398121	C	-1.658329	0.587078	-0.594779	C	-1.855695	0.966476	-0.359790	C	2.159862	1.267840	0.124121
H	2.328520	-1.442097	-0.895077	H	-1.787933	1.253975	-1.476139	H	-1.837061	1.494014	-1.332466	H	2.034825	1.814532	1.075287
C	1.006143	-3.426936	0.344647	C	-1.660086	2.167357	0.904228	C	-1.611913	1.981186	0.835874	C	1.736422	1.959856	-1.028625
C	-0.304754	-3.491301	0.715669	C	-0.284183	2.442271	1.362674	C	-0.125501	2.111349	1.354170	C	-0.593583	1.722568	-1.415313
C	-0.603529	-3.365292	1.767969	H	-0.009451	2.139613	2.386237	H	-0.005068	1.845223	2.419099	H	-0.570525	1.413537	-2.483133
H	-1.081789	-3.786578	-0.007784	H	0.277884	3.268964	0.899342	H	0.385133	3.034876	1.030063	H	-0.950805	2.747737	-1.175515
H	1.312725	-3.650016	-0.689828	H	-2.044060	2.836912	0.146627	H	-1.889053	2.973175	0.426541	H	1.468151	3.021892	-0.924730
H	1.800118	-3.235816	1.084760	H	-2.307210	1.650812	1.578664	H	-2.253449	1.679133	1.683590	H	1.997981	1.595021	-2.034152
C	2.503000	0.583208	-0.185601	C	-2.797425	-0.323242	-0.412265	C	-2.933732	-0.053923	-0.310222	C	3.069725	0.103794	0.203555
C	3.744723	0.731751	-0.874503	C	-3.866083	-0.189026	-1.345233	C	-3.475431	-0.480579	-1.551170	C	3.381165	-0.398754	1.492808
C	2.092977	1.625103	0.696832	C	-2.895110	-1.330427	0.584961	C	-3.473197	-0.604149	0.879087	C	3.681181	-0.499457	-0.923054
C	4.520354	1.885891	-0.719868	C	-4.986766	-1.028094	-1.285906	C	-4.509367	-1.427140	-1.604712	C	4.261427	-1.479416	1.652763
H	4.083115	-0.075660	-1.544645	H	-3.801652	0.586621	-2.125992	H	-3.073723	-0.053407	-2.484968	H	2.920321	0.072087	2.376976
C	2.883906	2.769944	0.859892	C	-4.023067	-2.159648	0.644737	C	-4.515133	-1.539897	0.824407	C	4.566177	-1.573098	-0.760344
H	1.171159	1.489620	1.283067	H	-2.070284	-1.439466	1.307268	H	-3.048328	-0.321790	1.853003	H	3.459778	-0.128228	-1.933692
C	4.090648	2.909672	0.147837	C	-5.068938	-2.015960	-0.287579	C	-5.035839	-1.959348	-0.414695	C	4.856216	-2.070935	0.524698
H	5.468673	1.989333	-1.270483	H	-5.800033	-0.910981	-2.019505	H	-4.911876	-1.744052	-2.579948	H	4.487682	-1.857887	2.662088
H	2.561766	3.560350	1.556168	H	-4.085284	-2.934216	1.425576	H	-4.919963	-1.955482	1.760814	H	5.034449	-2.030436	-1.646112
H	4.705989	3.814221	0.278374	H	-5.948859	-2.677259	-0.237267	H	-5.851059	-2.699431	-0.458087	H	5.551027	-2.917279	0.645028
C	-0.635787	0.674265	-0.491384	C	1.246744	-0.656825	-0.592229	C	1.387003	-0.592406	-0.590710	C	-1.453479	-0.506312	0.604647
H	0.019045	1.346614	-1.088219	H	0.724963	-1.382247	-1.252754	H	0.866006	-1.255008	-1.321342	H	-1.014797	-1.139546	1.415860
C	-1.966550	1.213062	-0.276578	C	2.663126	-0.870259	-0.435593	C	2.792507	-0.784959	-0.376415	C	-2.859560	-0.714676	0.368750
C	-2.343663	2.423354	-0.930559	C	3.293305	-1.988288	-1.058474	C	3.483913	-1.818802	-1.074824	C	-3.565848	-1.682268	1.144607
C	-3.926930	0.574504	0.562765	C	3.466250	0.017876	0.337617	C	3.523172	0.038421	0.530878	C	-3.580363	0.011945	-0.622047
C	-3.625864	2.960854	-0.767141	C	4.666859	-2.211047	-0.908980	C	4.853532	-2.019895	-0.870836	C	-4.930813	-1.910783	0.935951
H	-1.609511	2.929138	-1.578622	H	2.681516	-2.679244	-1.660514	H	2.926884	-2.458819	-1.777400	H	-3.020863	-2.251941	1.914411
C	-4.204994	1.118492	0.727826	C	4.841264	-0.206824	0.480394	C	4.890575	-0.170291	0.729119	C	-4.943476	-0.218773	-0.825896
H	-2.641200	-0.340457	1.104728	H	2.998117	0.891275	0.815479	H	2.992930	0.840338	1.067144	H	-3.039529	0.759371	-1.222055
C	-4.559420	2.309039	0.061745	C	5.442274	-1.321283	-0.140368	C	5.557699	-1.197521	0.030163	C	-5.622505	-1.179844	-0.048894
H	-3.902856	3.893124	-1.284106	H	5.140671	-3.079123	-1.393420	H	5.379194	-2.820108	-1.414728	H	-5.461948	-2.661115	1.542223
H	-4.933829	0.616865	1.383558	H	5.452973	0.487376	1.077289	H	5.447524	0.469730	1.430813	H	-5.487719	0.351131	-1.595095
H	-5.567593	2.733324	0.193976	H	6.523979	-1.495538	-0.024858	H	6.636114	-1.357056	0.188953	H	-6.697031	-1.359120	-0.213000

<b>1•CI2</b>			<b>1•CI2-1•end</b>			<b>1•end</b>			<b>1•CIisomer</b>						
<b>-1634.2902569</b>			<b>-1634.2889656</b>			<b>-1324.7935798</b>			<b>-1634.2994428</b>						
Ru	-0.276715	-1.372733	-0.000412	Ru	-0.237229	0.576281	-0.225018	Ru	1.284011	0.059005	0.080317	Ru	0.092729	-1.271252	0.062724
Cl	-0.169408	-1.625020	2.343363	Cl	0.475045	-1.372813	-1.353806	Cl	1.472831	2.151618	-0.824462	Cl	0.264280	-0.853564	2.384993
Cl	-0.159817	-2.103335	-2.254699	Cl	-0.243338	2.620798	0.978409	Cl	2.530838	-1.868881	0.093470	Cl	0.073035	-2.510492	-1.956946
C	2.389684	-0.900869	-0.608255	C	2.548281	1.292440	-0.209021	C	0.735619	0.265842	1.801292	C	0.488198	0.404359	-0.660769
H	2.286866	-1.076547	-1.692785	H	2.388339	2.011466	0.613962	H	1.438697	0.735789	2.529134	H	-0.222807	0.737538	-1.451919
C	2.137222	-1.954629	0.237826	C	1.960379	1.591726	-1.410834	H	-0.239224	-0.087697	2.202233	C	2.039128	-2.844409	0.532025
C	-1.999090	-2.032038	0.035468	C	-1.210834	1.164000	-1.647772	C	-0.292237	-0.567994	-0.660572	C	2.685931	-1.723997	0.097942
H	-2.388376	-2.545587	0.944316	H	-0.975786	0.832904	-2.686583	H	-0.137217	-1.264276	-1.520186	H	2.918001	-1.574529	-0.968940
H	-2.648742	-2.073716	-0.866774	H	-2.043629	1.895158	-1.535756	C	-1.685336	-0.318119	-0.330954	H	3.074818	-0.979094	0.806281
H	1.949943	-2.956877	-0.184784	H	1.451342	2.558729	-1.539283	C	-2.666482	-1.240876	-0.802319	H	1.894682	-3.030914	1.608568
H	2.316596	-1.903718	1.321502	H	2.085382	0.959384	-2.302888	C	-2.124716	0.810894	0.419407	H	1.755336	-3.644046	-0.170134
C	2.825331	0.448883	-0.221149	C	3.420029	0.156292	0.121707	C	-4.020443	-1.066782	-0.495153	C	1.574506	1.355467	-0.454809
C	3.184688	1.368297	-1.240594	C	3.899608	0.041874	1.451849	H	-2.341944	-2.106523	-1.402404	C	1.879957	2.255346	-1.518757
C	2.897739	0.879035	1.130612	C	3.822417	-0.818427	-0.826870	C	-3.483741	0.986209	0.709984	C	2.301168	1.478821	0.763578
C	3.623165	2.662981	-0.923554	C	4.748188	-1.010599	1.825980	H	-1.386019	1.565460	0.727631	C	2.902231	3.203305	-1.387668
H	3.124213	1.049051	-2.293934	H	3.596309	0.796612	2.196229	C	-4.432468	0.045964	0.264431	H	1.306797	2.187427	-2.457880
C	3.329372	2.174505	1.443876	C	4.670452	-1.868178	-0.452103	H	-4.763316	-1.795951	-0.854863	C	3.296918	2.454920	0.899641
H	2.594747	0.196218	1.939484	H	3.460945	-0.755131	-1.863317	H	-3.811024	1.870625	1.278920	H	2.033075	0.822288	1.606729
C	3.698603	3.070055	0.420546	C	5.135676	-1.969596	0.873528	H	-5.499963	0.188988	0.495757	C	3.612948	3.307185	-0.176329
H	3.906662	3.58742	-1.729147	H	5.109998	-1.082678	2.863829					H	3.139551	3.874865	-2.227882
H	3.376364	2.492673	2.497372	H	4.971876	-2.618731	-1.199751					H	3.835955	2.553331	1.855319
H	4.039910	4.086658	0.672551	H	5.803028	-2.797265	1.162212					H	4.408188	4.061862	-0.067274
C	-0.731524	0.420284	-0.140818	C	-1.621156	-0.221168	0.737930					C	-1.758538	-0.947624	0.035835
H	0.209619	0.992852	-0.314550	H	-1.213147	-0.506938	1.740355					H	-2.320816	-1.914149	0.029577
C	-1.939869	1.217671	-0.083437	C	-3.010884	-0.572022	0.541125					C	-2.625349	0.211740	0.063409
C	-1.904632	2.541855	-0.610455	C	-3.812437	-0.883857	1.679255					C	-3.993063	0.060458	-0.317219
C	-3.155425	0.750320	0.483925	C	-3.617576	-0.628091	-0.744461					C	-2.177581	1.504066	0.465340
C	-3.052008	3.344383	-0.606386	C	-5.169975	-1.194138	1.537416					C	-4.857899	1.159839	-0.343732
H	-0.963229	2.922761	-1.038375	H	-3.351769	-0.860742	2.680138					H	-4.357568	-0.937805	-0.609367
C	-4.296135	1.561310	0.499939	C	-4.970678	-0.956790	-0.883237					C	-3.054309	2.595974	0.459315
H	-3.175092	-0.249078	0.948258	H	-2.994544	-0.448773	-1.634952					H	-1.145801	1.620109	0.828526
C	-4.251375	2.856332	-0.053254	C	-5.778452	-1.230807	0.256124					C	-4.390099	2.431070	0.044344
H	-3.012890	4.359331	-1.032200	H	-5.778452	-1.416729	2.427964					H	-5.905625	1.028726	-0.656843
H	-5.227031	1.188389	0.955178	H	-5.421680	-1.009769	-1.886597					H	-2.698544	3.584892	0.788706
H	-5.151768	3.490891	-0.042637	H	-6.818976	-1.485563	0.143274					H	-5.074549	3.294400	0.037028

<b>2•PCy<sub>3</sub></b>			<b>2•PCy<sub>3</sub>-2•14e</b>			<b>2•14e</b>			<b>2•14e-2•Cl1</b>						
<b>-2371.6332263</b>			<b>-2371.6254903</b>			<b>-1324.7988831</b>			<b>-1403.3434239</b>						
Ru	-0.794948	-0.600892	-1.440045	Ru	1.433356	-2.005840	-0.003681	Ru	-1.316763	-0.000109	0.106435	Ru	-0.956177	0.134069	-0.486827
Cl	0.389651	0.817954	-2.923685	Cl	0.853899	-1.734687	2.227351	Cl	-1.426462	2.113449	-0.762475	Cl	-1.068244	2.243344	0.452363
Cl	-0.933595	2.598401	-0.190290	Cl	0.901162	-1.697940	-2.241250	Cl	-1.426102	-2.112758	-0.764734	Cl	-2.175195	-1.741303	-1.093793
P	1.114757	0.143350	0.401983	P	-1.182770	0.511858	0.000847	C	-2.349870	-0.000935	1.597630	C	0.475795	-0.634940	0.404495
C	-2.046856	0.512157	-0.635888	C	3.187895	-1.415150	0.010659	H	-1.942053	-0.001377	2.635437	H	0.185906	-1.437262	1.122783
C	-4.263019	1.492189	-0.123920	C	5.089621	0.168059	-0.038090	C	0.281740	-0.000509	1.036005	C	-2.216645	-0.469201	2.583292
C	-3.480412	0.341092	-0.435527	C	3.681990	-0.049500	0.014428	H	0.230914	-0.001123	2.151502	C	3.299995	-0.179184	1.837032
C	-5.646710	1.393134	0.062674	C	5.615507	1.465843	-0.048353	C	1.627498	-0.000146	0.489693	H	-3.586467	0.863810	1.624084
C	-4.137941	-0.920534	-0.511855	C	2.821332	1.083713	0.062529	C	2.733614	-0.001157	1.388086	H	-3.941130	-0.970589	1.416870
C	-6.280330	0.138112	-0.030417	C	4.748175	2.573718	-0.001311	C	1.893270	0.001168	-0.910043	H	-1.938579	-1.512736	2.809798
H	-6.237569	2.295126	0.287862	H	6.705423	1.617952	-0.092380	C	4.048666	-0.000931	0.906885	H	-1.578477	0.324614	3.005605
C	-5.521252	-1.014830	-0.308036	C	3.353400	2.377378	0.055809	H	2.541817	-0.002127	2.473443	C	1.906161	-0.389176	0.320172
H	-3.531250	-1.822151	-0.689055	H	1.729594	0.927871	0.105749	C	3.208368	0.001398	-1.385436	C	2.796629	-1.400767	0.788999
H	-7.368087	0.057922	0.125301	H	5.160074	3.595539	-0.008008	H	1.053119	0.002085	-1.622325	C	2.463915	0.821974	-0.182419
H	-6.014144	-1.998667	-0.358661	H	2.677725	3.246352	0.095236	C	4.288916	0.000338	-0.480124	C	4.183017	-1.228039	0.711752
C	5.274480	-1.084288	0.388143	H	2.631379	-0.639667	-0.491620	H	4.892904	-0.001733	1.614073	H	2.377308	-2.332321	1.200897
C	2.473776	-2.289042	1.351761	C	-2.922195	-0.742666	-2.006019	H	3.398273	0.002437	-2.470057	C	3.853131	0.994716	-0.239598
C	2.829246	-1.586655	-1.053665	C	2.388174	-2.057691	0.079892	H	5.323206	0.000522	-0.859276	H	1.785773	1.635914	-0.479724
C	3.453089	-0.477981	0.713299	H	-3.542554	-0.212236	-0.007723	H	-3.460207	-0.000989	1.500457	C	4.715194	-0.030102	0.194930
C	3.739419	-3.166975	1.272439	C	-4.116428	-1.682414	-2.282857					H	4.856537	-2.025591	1.062942
H	1.583128	-2.898607	1.084702	H	-2.020264	-1.142380	-2.524283					H	4.270432	1.941437	-0.617347
H	2.332316	-1.948662	2.398450	H	-3.134646	0.251581	-2.442722					H	5.806717	0.110417	0.145467
C	4.087913	-2.469664	-1.138292	C	-3.570290	-3.006490	-0.192344					C	-0.096452	0.480692	-2.052929
H	1.943359	-2.180188	-1.376215	H	-1.472408	-2.468616	-0.408654					H	0.913660	0.102506	-2.323214
H	2.906536	-0.740786	-1.765909	H	-2.166172	-2.023161	1.164824					H	-0.625916	1.071140	-2.837815
C	4.014924	-3.653075	-0.159700	C	-3.898040	-3.084767	-1.691935								
H	3.635139	-4.031552	1.963631	H	-4.295589	-1.746327	-3.378460								
H	4.615968	-2.581864	1.636965	H	-5.039261	-1.237656	-1.842397								
H	4.223633	-2.830652	-2.180848	H	-3.345118	-4.017128	0.213130								
H	4.986150	-1.851925	-0.904059	H	-4.465257	-2.641983	0.363893								
H	4.952886	-4.248926	-0.194817	H	-4.791185	-3.724032	-1.864935								
H	3.195602	-4.338386	-0.476415	H	-3.052605	-3.577518	-2.225109								
C	0.654389	0.229696	2.263261	C	-1.463876	1.996328	-1.179570								
C	0.132749	1.599184	2.758917	C	-1.124690	3.388878	-0.602155								
C	-0.349176	-0.872346	2.671933	C	-0.668797	1.785420	-2.490440								
H	1.623336	0.042066	2.785910	H	-2.554581	2.001699	-1.418289								
C	-0.123553	1.592903	4.280279	C	-1.415732	4.507267	-1.623030								
H	-0.820014	1.842525	2.234710	H	-0.044234	3.423445	-0.328436								
H	0.847226	2.412523	2.520834	H	-1.693404	3.587769	0.329613								
C	-0.605024	-0.885930	4.190514	C	-0.950285	2.893394	-3.522327								
H	-1.306600	-0.692893	2.133185	H	0.417243	1.774363	-2.243450								
H	-0.011825	-1.869443	2.333361	H	-0.877117	0.789595	-2.928860								
C	-1.094448	0.478482	4.698510	C	-0.664380	4.290150	-2.946504								
H	-0.507243	2.587846	4.595418	H	-1.154948	5.495226	-1.183820								
H	0.847479	1.453385	4.809714	H	-2.512001	4.536593	-1.822711								
H	-1.340464	-1.682278	4.436322	H	-0.346378	2.718360	-4.439163								
H	0.337074	-1.160109	4.720300	H	-2.017889	2.837456	-3.838997								
H	-1.222329	0.466921	5.802833	H	-0.933140	5.080778	-3.680652								
H	-2.101027	0.688675	4.268903	H	0.430851	4.392764	-2.765796								
C	2.011614	1.818095	0.179855	C	-1.804055	1.230237	1.664313								
C	3.182658	1.829586	-0.830809	C	-2.516054	0.230465	2.603957								
C	1.020300	2.955906	-0.171150	C	-0.613100	1.874737	2.415605								
H	2.446992	2.024388	1.188253	H	-2.544465	2.026601	1.408561								
C	3.885184	3.202347	-0.852392	C	-2.971233	0.915379	3.908728								
H	2.786368	1.598389	-1.843017	H	-1.816853	-0.599196	2.850572								
H	3.930456	1.047784	-0.584245	H	-3.396873	-0.225950	2.106153								
C	1.717407	4.329943	-0.189052	C	-1.050754	2.557962	3.724968								
H	0.592568	2.741519	-1.173807	H	0.124119	1.072329	2.642711								
H	0.168886	2.980814	0.538521	H	-0.084753	2.605241	1.768612								
C	2.905618	4.345531	-1.163293	C	-1.798302	1.580675	4.646690								
H	4.711903	3.184498	-1.595587	H	-3.473837	0.173044	4.566672								
H	4.362029	3.386199	0.138974	H	-3.738543	1.687455	3.666607								
H	0.982578	5.119694	-0.458346	H	-0.163744	2.982374	4.244263								
H	2.078157	4.577345	0.837130	H	-1.715010	3.421854	3.487619								
H	3.427659	5.326547	-1.128124	H	-2.157776	2.101787	5.560804								
H	2.525413	4.227817	-2.203527	H	-1.091480	0.792064	4.992712								
H	-3.763052	2.471611	-0.043808	H	5.764668	-0.702777	-0.074099								
H	-1.656092	1.493619	-0.282188	H	3.996389	-2.186181	0.002216								
C	-1.939535	-1.201173	-2.771956	C	1.950512	-3.746386	-0.010695								
H	-2.928762	-0.761827	-3.034109	H	3.010362	-4.095844	-0.003855								
H	-1.632641	-2.036780	-3.446029	H	1.179473	-4.551789	-0.023592								

<b>2•CII</b>			<b>2•CII-2•MCy</b>			<b>2•MCy</b>			<b>2•MCy-2•CII</b>						
<b>-1403.3479339</b>			<b>-1403.332098</b>			<b>-1403.3449748</b>			<b>-1403.3282399</b>						
Ru	-1.050190	0.078511	-0.318045	Ru	-1.249413	0.146601	-0.234349	Ru	-1.259981	0.179040	-0.276433	Ru	-1.271492	0.196383	-0.260166
Cl	-0.723098	2.355817	0.189501	Cl	-0.583318	2.429989	0.235766	Cl	-0.117347	2.275417	-0.395592	Cl	0.060822	2.173462	-0.332916
Cl	-2.276431	-1.912916	-0.697060	Cl	-2.359276	-1.975256	-0.293746	Cl	-2.432526	-1.894657	0.147032	Cl	-2.330895	-1.946274	0.063123
C	0.447186	-0.659600	0.519463	C	0.372809	-0.816490	0.083823	C	0.326373	-0.749515	0.669844	C	0.462111	-0.881341	1.018710
H	0.235660	-1.453997	1.270388	H	0.207698	-1.915283	0.088072	H	0.066265	-1.823590	0.636867	H	0.099559	-1.904651	0.817230
C	-2.037518	-0.154020	2.147737	C	-0.462012	-0.398483	1.951647	C	-0.378857	-0.033748	1.893426	C	-0.253681	-0.173265	2.002468
C	-3.005242	0.430420	1.387720	C	-1.790297	0.147195	1.881186	C	-1.751278	0.698338	1.598875	C	-2.208310	0.897164	1.167785
H	-3.106711	1.525878	1.341612	H	-1.936124	1.205958	2.149016	H	-1.719358	1.787334	1.779003	H	-2.017917	1.933471	1.521636
H	-3.770526	-0.179097	0.881365	H	-2.648375	-0.534698	1.992490	H	-2.637905	0.173136	1.994701	H	-2.996412	0.305613	1.681401
H	-1.994246	-1.249136	2.262436	H	-0.368073	-1.463160	2.221164	H	-0.606300	-0.847177	2.610723	H	-0.990871	-0.727574	2.602292
H	-1.324132	0.450991	2.730659	H	0.351985	0.270822	2.272803	H	0.323041	0.715467	2.302952	H	0.136410	0.770311	2.414631
C	1.862885	-0.406658	0.323835	C	1.801323	-0.470014	0.007113	C	1.750671	-0.518894	0.330792	C	1.808342	-0.590323	0.488974
C	2.794304	-1.343877	0.866107	C	2.710941	-1.565967	0.033379	C	2.406766	-1.537941	-0.409322	C	2.348867	-1.490164	-0.465100
C	2.373966	0.736344	-0.359198	C	2.329002	0.841890	-0.123363	C	2.504118	0.617042	0.719103	C	2.604245	0.501654	0.916135
C	4.171548	-1.168234	0.696602	C	4.093621	-1.359513	-0.063824	C	3.758834	-1.421543	-0.761950	C	3.635923	-1.298724	-0.988422
H	2.411793	-2.221123	1.413274	H	2.314922	-2.590400	0.127833	H	1.837034	-2.433329	-0.708103	H	1.742202	-2.349287	-0.795917
C	3.755209	0.913653	-0.509540	C	3.713211	1.041821	-0.212832	C	3.858960	0.725106	0.377735	C	3.892457	0.686213	0.398420
H	1.665565	1.498135	-0.718781	H	1.631293	1.693630	-0.151560	H	2.019902	1.434721	1.271637	H	2.210499	1.212691	1.656356
C	4.655218	-0.038757	0.006247	C	4.599065	-0.052428	-0.185195	C	4.491458	-0.287991	-0.367764	C	4.411596	-2.008011	-0.557838
H	4.875942	-1.908024	1.108298	H	4.779584	-2.221028	-0.044916	H	4.245114	-2.223244	-1.339882	H	4.036836	-2.005632	-1.731735
H	4.137523	1.807521	-1.027106	H	4.107009	2.065664	-0.313007	H	4.427199	1.615636	0.689528	H	4.499745	1.538520	0.741461
H	5.740330	0.105164	-0.119028	H	5.685512	0.113704	-0.262451	H	5.555063	-0.193631	-0.638463	H	5.424691	-0.055675	-0.962665
C	-0.271166	0.097452	-1.982083	C	-1.637054	0.585348	-1.987401	C	-2.009515	0.305401	-1.934795	C	-2.164927	0.500310	-1.841336
H	0.701654	-0.350037	-2.280079	H	-0.936216	0.363849	-2.818043	H	-1.492769	-0.155844	-2.802175	H	-1.700386	0.090297	-2.767239
H	-0.850828	0.549576	-2.821867	H	-2.574593	1.109909	-2.271577	H	-2.975485	0.822306	-2.103873	H	-3.127207	1.027803	-1.982437

<b>2•Cl2</b>				<b>2•Cl2-2•end</b>				<b>2•end</b>			
<b>-1403.336869</b>				<b>-1403.3299041</b>				<b>-1093.8398857</b>			
Ru	1.768382	-0.204042	-0.128953	Ru	1.436020	-0.188025	-0.221905	Ru	0.000085	0.105280	-0.000004
Cl	0.226008	-1.895067	-0.361032	Cl	0.180335	-2.177297	-0.096847	Cl	-2.094149	-0.803058	-0.000535
Cl	1.958360	2.076742	-0.421264	Cl	2.157193	2.065436	0.083369	Cl	2.094439	-0.802595	0.000312
C	-1.231254	1.235343	0.989962	C	-0.814791	1.035801	1.089971	C	0.000555	1.321512	-1.347387
H	-0.969763	2.215115	0.551903	H	-0.469156	2.039100	0.782307	H	0.001987	0.982439	-2.408762
C	-0.403934	0.739819	1.947085	C	-0.023926	0.362582	1.986151	H	-0.000361	2.423299	-1.178246
C	2.700708	-0.595398	1.382898	C	2.803513	-0.886113	0.755059	C	-0.001574	1.320903	1.347826
H	2.266290	-0.398256	2.387744	H	2.650080	-1.794934	1.380920	H	-0.002936	0.980715	2.408869
H	3.722041	-1.042555	1.369677	H	3.816393	-0.424206	0.778111	H	-0.001267	2.422840	1.179482
H	0.448628	1.339827	2.300392	H	0.844253	0.872386	2.430550				
H	-0.588085	-0.223235	2.449680	H	-0.290364	-0.629832	2.379920				
C	-2.454296	0.624905	0.447728	C	-2.094217	0.612385	0.506919				
C	-3.174203	1.319388	-0.556939	C	-2.709869	1.460069	-0.450261				
C	-2.956808	-0.627487	0.885015	C	-2.751344	-0.593420	0.863653				
C	-4.351674	0.788231	-1.105178	C	-3.936234	1.115328	-1.036820				
H	-2.795237	2.293390	-0.908166	H	-2.210094	2.401742	-0.731306				
C	-4.132562	-1.157783	0.338288	C	-3.976919	-0.934980	0.278550				
H	-2.418005	-1.193682	1.659608	H	-2.294179	-1.268157	1.601656				
C	-4.835796	-0.453510	-0.658392	C	-4.572904	-0.084698	-0.673472				
H	-4.894086	1.345714	-1.885279	H	-4.398780	1.785224	-1.778674				
H	-4.506211	-2.132707	0.689950	H	-4.474541	-1.874963	0.564543				
H	-5.759747	-0.874773	-1.085586	H	-5.537305	-0.358711	-1.130067				
C	3.093158	-0.791965	-1.229375	C	2.196327	-0.380367	-1.883458				
H	2.969990	-0.750855	-2.336131	H	1.537029	-0.040609	-2.717284				
H	4.061071	-1.211841	-0.867383	H	3.186010	-0.771839	-2.185470				

<b>3•PCy<sub>3</sub></b>				<b>3•PCy<sub>3</sub>-3•14e</b>				<b>3•14e</b>				<b>3•14e-3•Cl1</b>			
<b>-2371.6360586</b>				<b>-2371.6195291</b>				<b>-1324.7988831</b>				<b>-1403.3477985</b>			
Ru	0.77183	-0.109066	-1.338349	Ru	2.100624	-0.061228	-0.633665	Ru	1.316763	-0.000108	0.106434	Ru	-0.815326	0.030126	0.351384
Cl	0.862896	2.255889	-1.574506	Cl	1.932250	1.765613	0.747941	Cl	1.426458	2.113452	-0.762472	Cl	-0.911131	2.188578	-0.425701
Cl	0.841097	-2.528911	-0.868509	Cl	2.056464	-2.339999	-0.371209	Cl	1.426108	-2.112758	-0.764733	Cl	-0.976317	-2.084924	-0.531283
P	-1.232156	0.012704	0.274239	P	-2.234226	0.008095	-0.005322	C	-0.281740	-0.000511	1.036004	C	-1.651251	0.005414	1.961630
C	-0.095891	-0.438827	-2.898536	C	1.141052	0.314150	-2.125764	H	-0.230914	-0.001126	2.151500	H	-2.763491	0.025874	1.996355
C	-0.517977	-0.368574	1.993459	C	-2.455016	-1.186668	1.472980	C	-1.627498	-0.000148	0.489692	C	-4.534433	-0.443013	-0.378697
C	-0.577522	-1.840314	2.459507	C	-2.991680	-2.594283	1.128392	C	-2.733614	-0.001160	1.388086	C	-3.902668	0.272810	-1.326700
C	0.938697	0.147272	2.063830	C	-1.099577	-1.329197	2.207992	C	-1.893271	0.001167	-0.910044	H	-4.066403	1.356365	-1.444742
H	-1.145173	0.231212	2.695271	H	-3.192689	-0.071260	2.163918	C	-4.048666	-0.000934	0.906886	H	-3.197167	-0.202077	-2.028285
C	0.007717	-1.989435	3.878618	C	-3.117629	-3.473434	2.390223	H	-2.541817	-0.002130	2.473443	H	-4.360580	-1.526026	-0.263972
H	-0.000986	-2.469819	1.747005	H	-2.296303	-3.089125	0.411670	C	-3.208369	0.001397	-1.385436	H	-5.252932	0.024323	0.136696
H	-1.622817	-2.213672	2.455306	H	-3.979231	-2.532625	0.624687	H	-1.053120	0.002085	-1.622326	C	0.880989	-0.017586	1.088257
C	1.537924	-0.009998	3.473550	C	-1.213223	-2.198552	3.473633	C	-4.288917	0.000336	-0.480123	H	0.959497	-0.044742	2.202108
H	1.580564	-0.448734	1.345566	H	-0.369203	-1.793250	1.506449	H	-4.892904	-0.001736	1.614073	C	2.157104	-0.026856	0.395958
H	1.001947	1.205352	1.736690	H	-0.679354	-0.336436	2.467603	H	-3.398275	0.002437	-2.470057	C	3.357215	-0.071899	1.163278
C	1.450157	-1.463965	3.964055	C	-1.785894	-3.587883	3.150173	H	-5.323207	0.000520	-0.859275	C	2.263584	0.006581	-1.024263
H	-0.035561	-3.056731	4.185993	H	-3.493302	-4.481647	2.108656	C	2.349870	-0.000935	1.597629	C	4.609570	-0.083679	0.537087
H	-0.630616	-1.430757	4.602632	H	-3.888490	-3.031975	3.063909	H	1.942054	-0.001379	2.635436	H	3.288065	-0.097720	2.263043
H	2.592434	0.340789	3.472606	H	-0.217358	-2.291067	3.959223	H	3.460207	-0.000986	1.500454	C	3.516676	-0.004903	-1.645099
H	0.987651	0.654591	4.179734	H	-1.874448	-1.689169	4.213067	H	1.348464	0.042084	-1.635642	H	4.691799	-0.050107	-0.867886
H	1.833879	-1.547651	5.003974	H	-1.919364	-4.184944	4.078669	H	5.527955	-0.119112	1.143874	H	3.583829	0.021372	-2.743871
H	2.108950	-2.102298	3.332565	H	-1.053775	-4.145909	2.522270	H	5.676655	-0.059261	-1.361429	H	-1.114461	-0.029294	2.938540
C	-2.763811	-1.132813	0.195857	C	-3.801124	-0.359410	-1.045502								
C	-3.963933	-0.568661	-0.635379	C	-4.390687	0.852886	-1.799017								
C	-2.440299	-2.555526	-0.344459	C	-3.483954	-1.482749	-2.063785								
H	-3.080966	-1.197541	1.229308	H	-4.586455	-0.723971	-0.340372								
C	-5.189701	-1.501875	-0.547613	C	-5.633550	0.461823	-2.623868								
H	-3.672471	-0.447831	-1.703736	H	-3.619176	1.272692	-2.485900								
H	-4.257797	0.433281	-0.266164	H	-4.661838	1.665287	-1.093581								
C	-3.661640	-3.488538	-0.248281	C	-4.717039	-1.884741	-2.894819								
H	-2.107311	-2.484970	-1.403566	H	-2.681727	-1.116687	-2.746102								
H	-1.578537	-2.990198	0.193723	H	-3.061843	-2.374145	-1.556272								
C	-4.869474	-2.929423	-1.013832	C	-5.332460	-0.674302	-3.614959								
H	-6.023329	-1.069843	-1.142955	H	-6.025479	1.353875	-3.160626								
H	-5.545804	-1.531117	0.508373	H	-6.442684	0.138299	-1.928709								
H	-3.386351	-4.495151	-0.630379	H	-4.439049	-2.674380	-3.626603								
H	-3.936483	-3.629124	0.823307	H	-5.480053	-2.340654	-2.221923								
H	-5.756725	-3.587779	-0.890572	H	-6.254268	-0.969486	-4.162025								
H	-4.638188	-2.916334	-2.103880	H	-4.616880	-0.305537	-4.386136								
C	-2.059374	1.711207	0.550946	C	-2.674860	1.694825	0.787369								
C	-1.257352	2.717799	1.409016	C	-2.126408	1.911883	2.215833								
C	-2.490623	2.400292	-0.768411	C	-2.162506	2.837146	-1.025627								
H	-2.977188	1.440839	1.129884	H	-3.788963	1.749143	0.845735								
C	-2.088446	3.987178	1.688927	C	-2.514369	3.298017	2.769318								
H	-0.329189	2.992536	0.862149	H	-1.015958	1.828553	2.196811								
H	-0.952464	2.271131	2.377821	H	-2.496647	1.127814	2.908672								
C	-3.340178	3.654333	-0.488554	C	-2.544719	4.228846	0.413999								
H	-1.571493	2.689689	-1.319125	H	-1.053030	2.756816	-0.187147								
H	-3.044517	1.707227	-1.430788	H	-2.538163	2.719019	-1.163168								
C	-2.580560	4.656677	0.396002	C	-2.039385	4.435186	1.850878								
H	-1.482398	4.699708	2.289933	H	-2.095907	3.423146	3.792062								
H	-2.966674	3.717409	2.321162	H	-3.622871	3.350691	2.878373								
H	-3.632905	4.128616	-1.450122	H	-2.141625	5.018072	-0.257724								
H	-4.290933	3.360628	0.016638	H	-3.654150	4.339757	0.392992								
H	-3.219833	5.534903	0.633037	H	-2.371338	5.420320	2.245567								
H	-1.704637	5.047593	-0.169749	H	-0.925546	4.458206	1.845355								
H	-0.137121	-1.455852	-3.348337	H	1.596052	0.594537	-3.104969								
C	2.599822	-0.470047	-1.797965	C	3.743835	0.211974	-1.433468								
C	2.808963	-1.142605	-2.653104	H	3.749988	0.501606	-2.512297								
C	3.773026	-0.158208	-1.003543	C	5.061198	0.102432	-0.829966								
C	4.951667	-0.949910	-1.153813	C	6.210289	0.366194	-1.630081								
C	3.804894	0.931803	-0.083079	C	5.256296	-0.255981	0.534935								
C	6.096282	-0.685482	-0.393930	C	7.498609	0.276859	-1.088387								
H	4.942233	-1.786476	-1.870900	H	6.072690	0.644475	-2.687712								
C	4.960269	1.201600	0.660851	C	6.544918	-0.344028	1.071382								
H	2.923589	1.588342	-0.010726	H	4.382155	-0.464395	1.171441								
C	6.102587	0.390157	0.516746	C	7.668681	-0.078088	0.263199								
H	6.993668	-1.312973	-0.512985	H	8.376584	0.484667	-1.719983								
H	4.977549	2.057676	1.353812	H	6.680035	-0.621849	2.128338								
H	7.007491	0.603611	1.108117	H	8.681693	-0.148246	0.690420								
H	-0.638257	0.381697	-3.421507	H	0.030078	0.260633	-2.048372								



<b>3•CI1</b>			<b>3•CI1-3•MCy</b>			<b>3•MCy</b>			<b>3•MCy-3•CI2</b>						
<b>-1403.3533085</b>			<b>-1403.3449075</b>			<b>-1403.367965</b>			<b>-1403.3458801</b>						
Ru	-1.001776	-0.013252	0.286877	Ru	-0.975755	-0.022701	-0.204799	Ru	-0.985657	0.000277	-0.159955	Ru	1.016469	0.039390	-0.091231
Cl	-0.901452	2.251488	-0.278974	Cl	-1.004414	-2.349797	0.367688	Cl	-1.091140	-2.388179	-0.068484	Cl	1.383478	2.374135	0.196369
Cl	-0.913096	-2.220249	-0.476520	Cl	-1.076935	2.350758	-0.269393	Cl	-1.093020	2.388400	-0.065666	Cl	1.211257	-2.249662	-0.704564
C	-1.768274	-0.085742	1.945327	C	-2.134329	-0.236508	-1.601094	C	-2.844140	-0.000247	-0.902097	C	3.475631	0.021785	-0.485237
H	-2.868309	-0.089456	2.095191	H	-2.776882	0.602610	-1.951109	H	-3.119332	0.935886	-1.420293	H	3.520018	-0.777693	-1.242479
C	-3.592928	0.025380	-0.466132	C	-3.302071	0.040118	0.918155	C	-3.183794	-0.001511	0.643581	C	3.423253	-0.284598	0.848491
C	-2.902364	0.073496	-1.633734	C	-2.272106	0.250014	1.806434	C	-1.930179	-0.001356	1.611655	C	0.588424	-0.312450	1.650349
H	-2.636855	1.035982	-2.098375	H	-1.860449	-0.595248	2.382725	H	-1.810205	-0.937818	2.184098	H	-0.004493	0.404909	2.261985
H	-2.640079	-0.846913	-2.178547	H	-1.985936	1.274807	2.092111	H	-1.811140	0.934647	2.185052	H	0.926242	-1.240907	2.165316
H	-3.918478	-0.935182	-0.034602	H	-3.830317	0.890021	0.456926	H	-3.753497	0.924630	0.851309	H	3.391858	-1.333015	1.185526
H	-3.913654	0.947511	0.045378	H	-3.698520	-0.972328	0.740586	H	-3.752157	-0.928758	0.850013	H	3.502238	0.502347	1.615768
C	0.695319	-0.055678	1.083879	C	0.689214	-0.200526	-1.090183	C	0.713992	0.001029	-0.924620	C	-0.710571	0.265767	-0.782680
H	0.767261	-0.118703	2.196628	H	0.737408	-0.468393	-2.163509	H	0.583421	0.001947	-2.031270	H	-0.605904	0.634895	-1.834271
C	1.987743	-0.021854	0.431303	C	1.978353	-0.063314	-0.448509	C	2.047183	0.000552	-0.393344	C	-2.082440	0.099224	-0.358690
C	3.172176	-0.088468	1.223091	C	3.166675	-0.347494	-1.183632	C	3.164226	0.002016	-1.280569	C	-3.121418	0.716041	-1.118291
C	2.127572	0.077459	-0.984188	C	2.110191	0.344570	0.912744	C	2.288027	-0.001427	1.013095	C	-2.448271	-0.659536	0.788784
C	4.438345	-0.059085	0.627382	C	4.426547	-0.238197	-0.583058	C	4.470102	0.001569	-0.777802	C	-4.459264	0.612738	-0.720632
H	3.076937	-0.164374	2.318591	H	3.080424	-0.660656	-2.236546	H	2.987554	0.003500	-2.367861	H	-2.854393	1.293954	-2.017814
C	3.394035	0.108302	-1.575627	C	3.369512	0.453498	1.508398	C	3.595328	-0.001890	1.506031	C	-3.788689	-0.777222	1.171099
H	1.225811	0.133687	-1.612876	H	1.208232	0.590638	1.497108	H	1.429300	-0.002696	1.702156	H	-1.662009	-1.187913	1.350231
C	4.550977	0.039829	-0.772896	C	4.530470	0.161022	0.763001	C	4.687532	-0.000380	0.613659	C	-4.796432	-0.133724	0.424942
H	5.343667	-0.112378	1.252136	H	5.334703	-0.463412	-1.163802	H	5.325951	0.002710	-1.470593	H	-5.247354	1.108506	-1.308717
H	3.487361	0.186381	-2.670004	H	3.454946	0.771644	2.559012	H	3.772197	-0.003457	2.592711	H	-4.056741	-1.380159	2.052829
H	5.546987	0.064133	-1.243240	H	5.521775	0.248668	1.235423	H	5.716395	-0.000756	1.007313	H	-5.850477	-0.224520	0.732025
H	-1.160774	-0.130506	2.880061	H	-2.243962	-1.214965	-2.122311	H	-3.118502	-0.935885	-1.421602	H	3.624564	1.062250	-0.815727

<b>3•Cl2</b>			<b>3•Cl2-3•end</b>			<b>3•end</b>					
<b>-1403.3491565</b>			<b>-1403.3434155</b>			<b>-1324.793571</b>					
Ru	-1.003721	0.077741	0.015498	Ru	0.955804	0.134323	-0.487013	Ru	-1.283894	0.058847	0.080343
Cl	-0.679892	-1.957044	-1.098375	Cl	1.068855	2.242827	0.453752	Cl	-1.473902	2.151397	-0.824291
Cl	-1.937619	2.228809	-0.014009	Cl	2.174601	-1.740609	-1.095287	Cl	-2.530477	-1.869108	0.093795
C	-3.551800	-0.526635	-0.270644	C	3.301817	-0.178864	1.836910	C	0.292308	-0.567270	-0.661213
H	-4.017422	0.470477	-0.267379	H	3.945491	-0.967997	1.416355	H	0.137288	-1.262767	-1.521475
C	-3.196642	-1.146467	0.886126	C	2.218959	-0.472800	2.582348	C	-0.735067	0.265779	1.801195
C	-0.450184	-0.155735	1.749736	C	-0.475972	-0.634917	0.404395	H	-1.437716	0.735756	2.529415
H	-1.115675	-0.636766	2.497591	H	-0.185955	-1.437331	1.122547	H	0.239870	-0.088003	2.201699
H	0.532527	0.191727	2.134924	H	1.943704	-1.517364	2.807570	C	1.685430	-0.317624	-0.331347
H	-3.376013	-0.661415	1.860055	H	1.578368	0.318738	3.005275	C	2.124770	0.811116	0.419380
H	-2.799226	-2.173581	0.892800	C	0.095630	0.482168	-2.052568	C	2.666510	-1.240399	-0.802746
C	0.670324	0.753353	-0.523566	H	0.624879	1.073165	-2.837189	C	3.483775	0.986217	0.710206
H	0.602788	1.619591	-1.223306	H	3.585293	0.865179	1.625213	H	1.386083	1.565648	0.727734
C	2.031548	0.361359	-0.229809	H	-0.914598	0.104242	-2.322783	C	4.020453	-1.066545	-0.495313
C	3.095334	1.238917	-0.604234	C	-1.906369	-0.389180	0.320334	H	2.341986	-2.105884	-1.403074
C	2.365522	-0.866627	0.417106	C	-2.464197	0.822272	-0.181441	C	4.432480	0.045981	0.264592
C	4.425219	0.923718	-0.309506	C	-2.796764	-1.401101	0.788572	H	3.811050	1.870458	1.279420
H	2.849864	2.180743	-1.121543	C	-3.853424	0.995018	-0.238391	H	4.763288	-1.795726	-0.855075
C	3.701134	-1.184144	0.692824	H	-1.786090	1.636410	-0.478286	H	5.499946	0.188818	0.496168
H	1.559625	-1.576791	0.652572	C	-4.183165	-1.228374	0.711513				
C	4.730230	-0.289210	0.341171	H	-2.377389	-2.333820	1.199835				
H	5.232844	1.616556	-0.593269	C	-4.715422	-0.030113	0.195521				
H	3.947402	-2.140774	1.179813	H	-4.270780	1.941977	-0.615479				
H	5.778956	-0.543298	0.564016	H	-4.856635	-2.026184	1.062212				
H	-3.458393	-1.038257	-1.242861	H	-5.806952	0.110402	0.146231				

<b>4•PCy<sub>3</sub></b>				<b>4•PCy<sub>3</sub>-4•14e</b>				<b>4•14e</b>				<b>4•14e-4•ClI</b>			
<b>-2140.6762144</b>				<b>-2140.6627589</b>				<b>-1093.8398902</b>				<b>-1172.3906711</b>			
Ru	-0.712399	-1.151486	-1.550781	Ru	2.979628	-0.140861	-0.930679	Ru	0.000000	0.105440	0.000000	Ru	0.459144	-0.034610	0.044227
Cl	1.247040	-2.479458	-1.631443	Cl	2.925647	1.810168	0.273945	Cl	2.094041	-0.803108	0.000003	Cl	0.172441	2.175279	-0.550519
Cl	-2.587753	0.074194	-1.365173	Cl	2.743885	-2.365544	-0.432098	Cl	-2.094057	-0.803089	-0.000004	Cl	-0.203909	-2.154239	-0.581985
P	0.233602	0.334222	0.312009	P	-1.116621	0.025053	0.067504	C	-0.000007	1.321421	-1.347546	C	0.554591	-0.054095	1.861069
C	0.321304	-0.212736	-3.059329	C	1.969284	0.153167	-2.409057	H	0.000105	2.423277	-1.178992	H	-0.364832	0.024809	2.480840
C	-0.657258	-0.281335	1.870357	C	-1.138836	-0.851346	1.769025	C	-0.000013	1.321418	1.347548	C	-2.689403	0.134594	0.837847
C	-1.955503	0.464737	2.252938	C	-1.577524	-2.333249	1.763072	H	0.000059	2.423274	1.178994	C	-2.731353	0.270159	-0.502192
C	-0.944349	-1.797081	1.733318	C	0.268497	-0.743671	2.404648	H	0.000140	0.981217	-2.408405	H	-2.737039	1.262771	-0.980356
H	0.078255	-0.128972	2.695654	H	-1.867417	-0.294782	2.406432	H	0.000086	0.981213	2.408407	H	-2.761971	-0.608386	-1.166727
C	-2.563864	-0.115536	3.545754	C	-1.549253	-2.930923	3.185593	H	-2.694598	-0.859561	1.315483	H	-2.672974	1.014104	1.503761
H	-2.685795	0.371914	1.418612	H	-0.889735	-2.918982	1.110772	C	2.259066	-0.191112	-0.160115	C	2.259066	-0.191112	-0.160115
H	-1.761152	1.547893	2.396293	H	-2.596623	-2.446550	1.337019	H	2.974919	-0.258514	0.692565	H	1.516762	-0.142163	2.417580
C	-1.562182	-2.383202	3.016301	C	0.309701	-1.330317	3.827210	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-1.670350	-1.931240	0.895428	H	0.983268	-1.299883	1.756393	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-0.030205	-2.359038	1.453989	H	0.624421	0.306182	2.415560	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	-2.833510	-1.624774	3.429926	C	-0.166546	-2.791881	3.843572	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-3.501990	0.428820	3.788573	H	-1.857784	-3.998774	3.149420	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-1.867899	0.070322	4.397031	H	-2.309168	-2.409225	3.812782	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-1.778160	-3.463347	2.868517	H	1.339292	-1.251481	4.239251	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-0.810767	-2.326884	3.837826	H	-0.341249	-0.721409	4.497215	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-3.229837	-2.023536	4.388742	H	-0.190435	-3.186839	4.882674	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-3.627183	-1.796504	2.667292	H	0.566941	-3.419504	3.287129	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	0.035678	2.236177	0.385022	C	-2.705981	-0.664300	-0.748742	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	1.221922	3.050447	-0.182632	C	-3.456313	0.316411	-1.676474	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	-1.281342	2.744784	-0.239100	C	-2.355257	-1.947247	-1.542651	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	0.004879	2.421251	1.486514	H	-3.405190	-0.935110	0.078409	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	1.025322	4.564103	0.041380	C	-4.711815	-0.333527	-2.292487	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	1.313051	2.852952	-1.275159	H	-2.778161	0.641114	-2.500020	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	2.180275	2.744632	0.281232	H	-3.750362	1.235397	-1.128500	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	-1.479139	4.255765	-0.015829	C	-3.600538	-2.607501	-2.163725	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-1.259471	2.527535	-1.329672	H	-1.639186	-1.672888	-2.352011	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-2.152238	2.182446	0.144253	H	-1.818141	-2.677109	-0.903259	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	-0.295506	5.072354	-0.553973	C	-4.375318	-1.624496	-3.055982	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	1.890176	5.113681	-0.389724	H	-5.221705	0.393681	-2.961743	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	1.040479	4.772483	1.136401	H	-5.436243	-0.566423	-1.477834	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-2.428600	4.576072	-0.496082	H	-3.303071	-3.509129	-2.742334	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-1.600445	4.456610	1.074370	H	-4.268247	-2.968722	-1.347332	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-0.429377	6.154285	-0.336940	H	-5.301520	-2.097289	-3.449281	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-0.258647	4.978079	-1.663682	H	-3.753364	-1.370855	-3.945811	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	2.072533	0.121869	0.760257	C	-1.651259	1.802752	0.537876	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	2.435777	-1.171435	1.526480	C	-1.020248	2.350927	1.837788	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	3.006343	0.276707	-0.466581	C	-1.311605	2.761104	-0.630919	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	2.250170	0.980123	1.454761	H	-2.758305	1.788382	0.684240	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	3.919947	-1.161157	1.948437	C	-1.482232	3.792955	2.129830	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	2.237444	-2.043219	0.866400	H	0.088923	2.338838	1.737887	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	1.806735	-1.290211	2.432620	H	-1.271808	1.705079	2.704641	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	4.484721	0.308898	-0.036136	C	-1.767254	4.206540	-0.352591	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	2.833399	-0.589039	-1.139534	H	-0.207528	2.743903	-0.779111	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	2.761806	1.183387	-1.053432	H	-1.756286	2.403138	-1.582590	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	4.863265	-0.954750	0.752045	C	-1.174077	4.741590	0.960422	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	4.159364	-2.110419	2.475137	H	-1.002288	4.157891	3.064173	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	4.083606	-0.344448	2.690241	H	-2.580242	3.792191	2.323839	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	5.131849	0.415879	-0.933472	H	-1.484159	4.862712	-1.204565	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	4.673900	1.210108	0.594063	H	-2.880340	4.236080	-0.294206	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	5.918824	-0.900890	1.096723	H	-1.556546	5.763241	1.175297	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	4.796809	-1.837409	0.076376	H	-0.069529	4.837432	0.849511	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-1.081490	0.432012	-3.552269	H	2.396869	0.307172	-3.427335	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
C	-2.004615	-2.388851	-2.070649	C	4.578299	-0.066183	-1.785895	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-2.599544	-2.421678	-3.002799	H	4.672760	0.113241	-2.882597	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	-2.356604	-3.089257	-1.278012	H	5.532536	-0.202200	-1.226551	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208
H	0.700758	-0.252774	-3.497476	H	0.862893	0.180135	-2.284707	H	2.714972	-0.225196	-1.176208	H	2.714972	-0.225196	-1.176208

<b>4•CI1</b>			<b>4•CI1-4•MCy</b>			<b>4•MCy</b>			<b>4•MCy-4•CI2</b>						
<b>-1172.3923591</b>			<b>-1172.3873802</b>			<b>-1172.4060173</b>			<b>-1172.3873813</b>						
Ru	-0.000199	-0.367636	0.037712	Ru	-0.001031	-0.300113	-0.055678	Ru	0.000482	-0.317758	-0.000114	Ru	0.000864	-0.300223	-0.055700
Cl	2.221737	0.025341	-0.532282	Cl	2.364179	0.058467	-0.171893	Cl	2.385960	-0.129485	-0.000341	Cl	-2.364163	0.058626	-0.171767
Cl	-2.221841	0.026944	-0.532103	Cl	-2.361292	-0.090522	-0.186399	Cl	-2.385646	-0.131298	0.000051	Cl	2.361185	-0.090560	-0.186317
C	-0.000139	-0.617676	1.845723	C	-0.013962	-0.389658	1.769369	C	0.000082	1.183145	1.338657	C	0.082078	2.046375	-0.835169
H	0.000252	0.235176	2.557110	H	-0.904214	-0.065525	2.353733	H	-0.935867	1.256803	1.918981	H	1.036271	2.016067	-1.385277
C	0.001400	2.376914	0.849293	C	-0.065047	2.261363	0.519058	C	-0.002537	2.029879	0.000475	C	0.065967	2.261820	0.519032
C	0.000837	2.478111	-0.499853	C	-0.082217	2.046077	-0.835165	C	-0.001261	1.184438	-1.338093	C	0.013802	-0.389958	1.769316
H	0.942177	2.533321	-1.069075	H	0.856379	2.060709	-1.413189	H	0.934940	1.260613	-1.917691	H	-0.868601	-0.749774	2.344909
H	-0.940918	2.534691	-1.068243	H	-1.036831	2.016133	-1.384558	H	-0.937574	1.258500	-1.917746	H	0.904267	-0.066357	2.353655
H	-0.940741	2.363021	1.421980	H	-1.004611	2.372192	1.083995	H	-0.932456	2.630441	0.001214	H	1.005988	2.372446	1.083247
H	0.944084	2.361694	1.421054	H	0.884292	2.416307	1.056417	H	0.924383	2.635127	0.000438	H	-0.882917	2.417242	1.057059
C	-0.000754	-2.169574	-0.259163	C	0.148686	-2.088300	-0.472422	C	0.000773	-2.143226	0.000128	C	-0.148260	-2.088396	-0.472642
H	-0.000978	-2.943483	0.544381	H	0.254658	-2.974448	0.181512	H	0.000748	-2.705747	0.955776	H	-0.152812	-2.302482	-1.567347
H	-0.000907	-2.572478	-1.298057	H	0.868289	-0.749840	2.344962	H	0.000170	-2.706204	-0.955424	H	-0.254107	-2.974634	0.181181
H	-0.000505	-1.631443	2.310081	H	0.153567	-2.302531	-1.567125	H	0.936754	1.259697	1.917403	H	-0.856980	2.061119	-1.412434

<b>4•Cl2</b>			<b>4•Cl2-4•end</b>			<b>4•end</b>					
<b>-1172.3923626</b>			<b>-1172.3906654</b>			<b>-1172.3866941</b>					
Ru	0.000209	-0.367472	0.037684	Ru	-0.459407	-0.034333	0.044311	Ru	0.719902	-0.001817	0.107301
Cl	2.221918	0.027147	-0.531925	Cl	-0.171139	2.175216	-0.550725	Cl	0.597302	2.096837	-0.787046
Cl	-2.221759	0.025603	-0.532323	Cl	0.202318	-2.154134	-0.582410	Cl	0.569518	-2.096854	-0.791364
C	-0.001261	2.375750	0.849587	C	2.732224	0.268799	-0.502142	C	-4.437264	0.004272	0.578958
H	-0.943898	2.360026	1.421389	H	2.762326	-0.609426	-1.167147	H	-4.693391	-0.938931	1.091060
C	-0.000834	2.477860	-0.499515	C	2.690484	0.132546	0.837824	C	-3.829273	0.014784	-0.619458
C	0.000923	-2.169340	-0.259776	C	-0.554102	-0.053825	1.861176	C	2.233688	-0.013181	1.108591
H	0.001336	-2.571950	-1.298787	H	0.365725	0.024184	2.480459	H	3.233952	-0.019831	0.617799
H	0.001006	-2.943431	0.543589	H	-1.516086	-0.141085	2.418139	H	2.227477	-0.013884	2.223401
H	-0.942260	2.533195	-1.068563	H	2.695276	-0.861875	1.314905	H	-3.557216	-0.918993	-1.140140
H	0.940869	2.535081	-1.067911	H	2.674516	1.011708	1.504213	H	-3.579721	0.957612	-1.135047
C	-0.000327	-0.618341	1.845602	C	-2.259486	-0.189657	-0.159421	C	-0.433092	0.004574	1.509369
H	-0.000882	0.234263	2.557287	H	-2.715806	-0.223485	-1.175336	H	-1.531865	0.012165	1.320476
H	-0.000046	-1.632267	2.309598	H	2.738194	1.261663	-0.979788	H	-0.099236	0.001146	2.573231
H	0.940943	2.361552	1.422128	H	-2.975030	-0.256589	0.693557	H	-4.715975	0.938245	1.096171



II-III			III			III-IV			IV						
-2289.0680755			-2289.0909756			-2289.0505143			-964.259833						
C	0.954448	1.033825	0.205643	C	-0.231626	-1.580814	0.089638	C	1.157989	1.429347	0.112001	C	0.000015	0.000030	-0.202570
C	1.999279	1.268698	2.289334	C	-1.360106	-3.141520	1.420007	C	2.556079	2.453440	1.706490	C	0.761488	0.104502	2.032994
H	2.792373	2.017243	2.509921	H	-1.721291	-4.056392	0.895735	H	3.088316	3.350965	1.306427	H	1.028869	1.148048	2.335044
H	2.118834	0.415269	2.987529	H	-1.985525	-2.995455	2.321485	H	3.127903	2.085534	2.582176	H	1.285365	-0.585909	2.728070
C	0.568454	1.861342	2.360779	C	0.144171	-3.186190	1.745226	C	1.087889	2.756265	2.051166	C	-0.761529	-0.104375	2.032975
H	-0.068510	1.268282	3.045954	H	0.362448	-2.739004	2.738059	H	0.754886	2.160821	2.931814	H	-1.028916	-1.147917	2.335035
H	0.555629	2.926426	2.675374	H	0.568973	-4.208654	1.713841	H	0.907002	3.828748	2.265946	H	-1.285432	0.586049	2.728016
C	3.822325	-0.957832	0.438280	C	-3.514063	-0.701341	1.024950	C	4.184037	-0.294094	0.899141	C	3.305025	-1.193560	0.265727
C	5.076036	-1.292717	-0.120745	C	-4.768973	-0.227513	0.596499	C	5.325375	-0.932448	0.374239	C	4.651869	-1.081067	-0.132810
H	5.419885	-2.337141	-0.033581	H	-5.360602	0.384855	1.297036	H	5.788620	-1.744991	0.959485	H	5.298264	-1.973700	-0.078221
C	5.896124	-0.353459	-0.768235	C	-5.286972	-0.504022	-0.684881	C	5.884561	-0.572810	-0.867334	C	5.189641	0.131316	-0.606600
C	5.441975	0.979638	-0.830188	C	-4.514415	-1.301472	-1.549168	C	5.280967	0.481480	-1.580214	C	4.339340	1.254149	-0.664748
H	6.078275	1.746742	-1.303234	H	-4.911116	-1.555996	-2.546606	H	5.719889	0.802622	-2.540363	H	4.742620	2.217531	-1.021858
C	4.203868	1.371794	-0.290709	C	-3.247505	-1.798663	-1.180404	C	4.144393	1.160834	-1.098248	C	2.988665	1.195701	-0.269151
C	3.375794	0.386725	0.324728	C	-2.740075	-1.464233	0.103288	C	3.579283	0.747255	0.141080	C	2.471380	-0.046077	0.194562
C	3.020444	-2.041483	1.112612	C	-3.044215	-0.415171	2.431825	C	3.639216	-0.704540	2.246477	C	2.754753	-2.512115	0.759074
H	2.434934	-2.634972	0.372325	H	-3.578808	0.460358	2.847882	H	4.000775	-1.712693	2.529503	H	3.447880	-3.345900	0.530345
H	2.279085	-1.663769	1.840672	H	-1.956386	-0.194819	2.479045	H	1.765979	-0.716581	2.256446	H	1.769797	-2.730317	0.299101
C	3.690564	-2.765559	1.618802	H	-3.257385	-1.276394	3.105356	H	3.973467	-0.007302	3.047868	H	2.597903	-2.507324	1.860655
C	7.218122	-0.752389	-1.383647	C	-6.626130	0.051460	-1.113331	C	7.083972	-1.307083	-1.424533	C	6.627979	0.232317	-1.067374
H	8.001997	-0.010922	-1.189953	H	-7.006246	-0.449345	-2.025874	H	7.762809	-1.654475	-0.619123	H	7.078116	1.203944	-0.809204
H	7.126117	-0.859913	-2.486852	H	-6.550901	1.138403	-1.334757	H	7.669030	-0.669722	-2.118170	H	6.702568	0.114485	-2.172204
H	7.579166	-1.722158	-0.987226	H	-7.387700	-0.060219	-0.314034	H	6.770230	-2.209077	-1.995391	H	7.255242	-0.572543	-0.617192
C	3.788380	2.822074	-0.800305	C	-2.487076	-2.666696	-2.157755	C	3.568169	2.312721	-1.887529	C	2.118804	2.429036	-0.343552
H	4.664030	3.497228	-0.581362	H	-3.184782	-3.287276	-2.755163	H	4.289340	2.672464	-2.647676	H	2.724063	3.332330	-0.556459
H	3.305520	3.181408	0.550975	H	-1.769596	-3.343234	-1.654919	H	3.301265	3.167146	-1.232722	H	5.163873	2.601448	0.602075
H	3.061155	2.990746	-1.202244	H	-1.904035	-2.054769	-2.880631	H	6.232689	2.020016	-2.411480	H	1.348211	2.319926	-1.137620
C	-1.105940	2.430521	0.504022	C	2.111903	-2.445329	0.286305	C	-0.910071	2.812887	0.456794	C	-2.471363	0.046110	0.194497
C	-0.957206	3.522455	-0.402151	C	2.427822	-3.004237	-0.984843	C	-1.051387	3.642102	-0.691922	C	-3.305047	1.193573	0.265630
C	-2.109830	4.182578	-0.868978	C	3.782107	-3.111979	-1.354247	C	-2.336071	4.108242	-1.035884	C	-4.651904	1.081016	-0.132846
H	-1.985802	5.024652	-1.570935	H	4.026156	-3.539199	-2.341528	H	-2.442336	4.750410	-1.926824	H	-5.298339	1.973620	-0.078254
C	-3.403270	3.821022	-0.446694	C	4.826411	-2.710752	-0.498813	C	-3.475815	3.803051	-0.268435	C	-5.189659	-0.131422	-0.606531
C	-3.512573	2.783920	0.496459	C	4.478495	-2.211201	0.769906	C	-3.299552	3.005939	0.879404	C	-4.339316	-1.254217	-0.664682
H	-4.510543	2.497284	0.867961	H	5.277362	-1.906750	1.466701	H	-4.175823	2.752667	1.500109	H	-4.742567	-2.217648	-1.021691
C	-2.396362	2.078996	0.994375	C	3.140895	-2.070972	1.192843	C	-2.042030	2.499200	1.261807	C	-2.988619	-1.195699	-0.269165
C	0.397573	4.021795	-0.845707	C	1.357614	-3.501078	-1.929207	C	0.140027	4.045096	-1.526939	C	-2.754814	2.512162	0.758919
H	0.316597	5.039289	-1.275894	H	1.800493	-4.122218	-2.732221	H	-0.120842	4.869813	-2.219049	H	-3.447860	3.345954	0.529964
H	0.853321	3.372223	-1.624090	H	0.812400	-2.664627	-2.415552	H	0.520463	3.193894	-2.131839	H	-1.769759	2.730269	0.299120
H	1.115176	0.462626	-0.002221	H	0.597567	-4.115750	-1.403135	H	0.986771	4.377921	-0.891066	H	-2.598191	2.507487	1.860535
C	-4.628849	4.518138	-0.992149	C	6.271147	-2.797550	-0.935792	C	-4.848403	4.301236	-0.663712	C	-6.627986	-0.223373	-1.067323
H	-5.013583	3.995733	-1.895923	H	6.589811	-1.857735	-1.438685	H	-4.792905	5.060453	-1.469442	H	-6.702517	-0.115071	-2.172210
H	-4.408193	5.563485	-1.289598	H	6.433228	-3.623935	-1.657349	H	-5.382091	4.754742	0.197807	H	-7.255202	0.572605	-0.617485
H	-5.454125	4.535098	-0.251831	H	6.951597	-2.951274	-0.073988	H	-5.486048	3.468354	-1.032944	H	-7.078217	-1.203976	-0.808846
C	-2.615222	1.018505	2.042241	C	2.846176	-1.542889	2.575186	C	-1.920326	1.638822	2.495440	C	-2.118730	-2.429014	-0.343567
H	-2.463251	1.436315	3.063163	H	2.575616	-2.365019	3.274859	H	-1.524015	2.215077	3.360919	H	-1.563524	-2.601243	0.601932
H	-1.921925	0.158252	1.935642	H	2.009546	-0.811087	2.556761	H	-1.240647	0.777382	3.239051	H	-1.348335	-2.319981	-1.137838
H	-3.654955	0.639589	2.002163	H	3.738225	-1.041633	2.999089	H	-2.909645	1.242248	2.797532	H	-2.724004	-3.332369	-0.556161
N	2.115864	0.806378	0.893426	N	-1.461203	-1.976503	0.520070	N	2.431049	1.416324	0.674568	N	1.115602	-0.163604	0.637056
N	0.071683	1.745845	0.972556	N	0.729003	-2.349376	0.675793	N	0.389108	2.343657	0.825729	N	-1.115596	0.163708	0.637020
Ru	-0.120950	-1.559208	-0.383214	Ru	-0.712148	1.517558	-0.178542	Ru	-0.359339	-2.372600	-0.115737	C	0.000013	0.000011	-1.567367
C	-1.766135	-1.092434	-1.090222	C	0.587780	2.284746	-1.254498	C	-1.731703	-1.675340	-0.148078	H	0.940569	-0.118473	-2.119876
Ci	-0.324741	-3.862096	-0.244529	Ci	-1.625979	3.351400	1.010573	Ci	-1.021664	-4.553510	1.148078	C	-0.940552	0.118517	-2.119857
Ci	-0.231788	-1.480645	2.103783	Ci	0.295564	0.807000	2.010702	Ci	-0.001675	-1.477297	2.036602				
C	0.745048	0.605972	-1.181112	C	0.036216	-0.500808	-0.850527	C	0.717657	0.642881	-0.935612				
C	0.776955	-1.131167	-1.993164	C	-1.883282	1.516147	-1.606393	C	0.853413	-2.469709	-1.475264				
H	1.861074	-1.369325	-2.097780	H	-2.968004	1.278963	-1.434596	H	1.798424	-3.041205	-1.321187				
H	0.338055	-0.833630	-2.974668	H	-1.637372	1.668164	-2.688647	H	1.442075	0.067794	-1.520605				
H	1.668214	0.811967	-1.767386	H	-0.486118	-0.674306	-1.807837	H	-0.308517	0.761049	-1.300010				
H	-0.128210	1.148118	-1.632488	H	1.124650	-0.424285	-1.014638	H	-1.448033	-1.158174	-2.096232				
H	-1.815035	-0.302110	-1.884508	H	0.560950	2.110248	-2.361681	C	-3.162722	-1.658418	-0.873078				
C	-3.089304	-1.620139	-0.765119	C	1.706146	3.133782	-0.856959	C	-4.022223	-0.975032	-1.781872				
C	-4.193006	-1.221711	-1.574949	C	2.627129	3.550263	-1.863154	C	-5.406749	-0.935342	-1.574720				
C	-5.484235	-1.705632	-1.330002	C	3.720559	4.366900	-1.550127	C	-5.967824	-1.575358	-0.453338				
C	-5.710153	-2.587978	-0.258505	C	3.916282	4.794665	-0.222693	C	-5.135387	-2.255602	0.457368				
C	-4.636576	-2.977411	0.568060	C	3.013634	4.399925	0.784140	C	-3.751054	-2.299294	0.255217				
C	-3.340722	-2.504338	0.329225	C	1.920947	3.578496	0.479774	H	-3.581333	-0.474450	-2.659533				
H	-4.014778	-0.527805	-2.413459	H	2.465149	3.218751	-2.902595	H	-6.054418	-0.404997	-2.298010				
H	-6.320807	-1.394292	-1.976147	H	4.421837	4.677381	-2.341240	H	-7.056914	-1.545725	-0.289083				
H	-6.725691	-2.967271	-0.057438	H	4.773366	5.441155	0.026645	H	-5.573909	-2.760051	1.332845				
H	-4.812670	-3.659354	1.415267	H	3.164205	4.739470	1.821275	H	-3.106814	-2					



With C<sub>2</sub>H<sub>3</sub>X (X=Ph left):

0•I4e-I			I			I-II			II						
-2520.050358			-2520.0698969			-2520.0143709			-2520.0408247						
C	1.191732	1.037042	-0.604689	C	-0.919356	-1.204919	-0.296471	C	-0.322122	1.133914	-0.331198	C	-1.042479	0.905525	-0.062270
C	2.764644	2.258494	-1.900972	C	-2.283825	-3.106071	-0.726933	C	-0.986984	2.048094	-2.382169	C	-1.884897	1.676202	-2.137738
H	2.921621	1.839079	-2.922523	H	-3.064998	-3.301961	-1.489283	H	-1.727209	2.814200	-2.690762	H	-2.681243	2.404083	-2.398357
H	3.673248	2.835229	-1.633898	H	-2.541215	-3.687458	0.186431	H	-0.882129	1.287629	-3.185793	H	-1.800069	0.916200	-2.946887
C	1.474001	3.076075	-1.797146	C	-0.864293	-3.395960	-1.221151	C	0.386700	2.639099	-2.008678	C	-0.518655	2.337569	-1.897105
H	1.590735	3.977654	-1.152616	H	-0.444921	-4.337751	-0.814155	H	1.149273	2.410271	-2.778835	H	0.173282	2.121580	-2.732003
H	1.092491	3.412833	-2.782242	H	-0.794705	-3.446237	-2.332571	H	0.367085	3.741743	-1.849794	H	-0.596074	3.433522	-1.738375
C	4.474794	0.824957	0.519809	C	-4.194960	-0.938420	0.920993	C	-3.457683	-0.048424	-1.340809	C	-3.867656	-0.791314	-1.066637
C	5.600680	0.063345	0.876707	C	-5.401403	-0.206109	0.958964	C	-4.852635	-0.165179	-1.175150	C	-5.181638	-1.243641	-0.821743
H	6.244819	0.427514	1.694702	H	-5.973093	-0.194373	1.901986	H	-5.337051	-1.098419	-1.507471	H	-5.461383	-2.245144	-1.189227
C	5.924404	-1.147424	0.229919	C	-5.902764	0.488972	-0.156532	C	-5.640028	0.853603	-0.608761	C	-6.139720	-0.467648	-0.145487
C	5.095206	-1.574193	-0.821403	C	-5.175017	0.412010	-1.361888	C	-4.990916	2.035472	-0.204881	C	-5.757947	0.820490	0.274752
H	5.340505	-2.506605	-1.357364	H	-5.567109	0.911399	-2.263901	H	-5.585744	2.858312	0.226344	H	-6.497123	1.466134	0.778405
C	3.957053	-0.845050	-1.225905	C	-3.959781	-0.291420	-1.453573	C	-3.600815	2.211869	-0.351081	C	-4.460429	1.324333	0.061732
C	3.636313	0.345221	-0.526332	C	-3.445120	-0.923349	-0.285730	C	-2.827806	1.151136	-0.906307	C	-3.500023	0.498538	-0.588711
C	4.156167	2.102491	1.257679	C	-3.775548	-1.751311	2.120731	C	-2.691907	-1.199675	-1.933594	C	-2.911600	-1.691311	-1.803789
H	4.954285	2.348324	1.985141	H	-4.339577	-1.441152	3.022003	H	-2.300853	-1.870826	-1.134908	H	-2.200030	-2.195982	-1.114539
H	3.201025	1.985585	1.812770	H	-2.692016	-1.650211	2.338509	H	-1.812209	-0.892905	-2.532136	H	-2.276785	-1.158787	-2.539341
H	4.042000	2.972358	0.576050	H	-3.989791	-2.831428	1.957878	H	-3.349161	-1.828509	-2.566041	H	-3.461145	-2.490580	-2.338110
C	7.113987	-1.969373	0.671631	C	-7.176038	1.299021	-0.067391	C	-7.134303	0.681503	-0.455136	C	-7.527739	-1.000385	0.128360
H	7.491139	-2.618044	-0.144512	H	-7.730812	1.298316	-1.027796	H	-7.605724	1.569056	0.011554	H	-8.284750	-0.189955	0.135368
H	6.838731	-2.634945	1.519320	H	-6.951971	2.360449	0.178621	H	-7.372761	-0.202311	0.174010	H	-7.572411	-1.496623	1.123048
H	7.949468	-1.328341	1.020206	H	-7.851254	0.916837	0.724446	H	-7.622956	0.514078	-1.438715	H	-7.832945	-1.753986	-0.625278
C	3.122685	-1.365670	-2.371984	C	-3.232621	-0.370164	-2.777762	C	-2.979863	3.518212	0.090939	C	-4.140197	2.725941	0.527605
H	2.398455	-2.124721	-2.008049	H	-3.853806	0.047784	-3.593749	H	-3.758134	4.291857	2.042228	H	-5.069342	3.310916	0.674877
H	3.760165	-1.857127	-3.134309	H	-2.973711	-1.414924	-3.050076	H	-2.247127	3.914269	-0.641409	H	-3.502549	3.277019	-1.923230
H	2.541786	-0.565500	-2.870100	H	-2.280134	0.199772	-2.761075	H	-2.442672	3.412679	1.058485	H	-3.604627	2.718931	1.500735
C	-0.789287	2.593106	-0.885969	C	1.320023	-2.253572	-0.918294	C	1.904014	2.345025	-0.015673	C	0.964607	2.570179	0.080979
C	-1.743825	2.598482	-1.935280	C	1.864555	-1.790431	-2.144429	C	1.799567	3.194937	1.124843	C	0.612231	3.339354	1.225000
C	-3.027217	3.124629	-1.675983	C	3.255243	-1.910331	-2.352796	C	2.972857	3.544084	1.823639	C	1.625029	4.056126	1.899011
H	-3.776548	3.118793	-2.485742	H	3.682474	-1.537762	-3.299367	H	2.882663	4.195490	2.709622	H	1.342359	4.629884	2.798173
C	-3.372971	3.661259	-0.422241	C	4.103515	-2.505480	-1.402226	C	4.246866	3.117625	1.408355	C	2.951478	4.105149	1.443016
C	-2.388315	3.670709	0.588315	C	3.521628	-3.003373	-0.217851	C	4.325157	2.350742	0.229905	C	3.233277	3.456116	0.226099
H	-2.631966	4.101748	1.573847	H	4.163251	-3.492819	0.533834	H	5.314361	2.036161	-0.142613	H	4.244846	3.536821	-0.206262
C	-1.094255	3.156355	0.385313	C	2.143159	-2.904602	0.044310	C	1.388461	1.961564	-0.506455	C	-2.273049	2.706352	-0.480862
C	-1.401568	2.094288	-3.319101	C	1.001526	-1.236410	-3.255962	C	0.488670	3.796211	1.582302	C	-0.806538	3.560958	1.700011
H	-2.303665	1.728411	-3.849033	H	1.467557	-0.341621	-3.716022	H	0.606464	4.886129	1.754225	H	-0.997362	4.651444	1.783654
H	-0.652628	1.279669	-3.287269	H	-0.009342	-0.959533	-2.906881	H	0.138372	3.360443	2.543062	H	-0.989547	3.130058	2.707055
H	-0.973298	2.905931	-3.949609	H	0.879817	-1.985283	-4.069500	H	-0.315218	3.656390	0.838294	H	-1.560167	3.148148	1.101457
H	-4.747900	4.235794	-0.162282	C	5.593515	-2.617391	-1.634196	C	5.489005	3.470203	2.194476	C	4.026765	4.841274	2.208227
H	-5.436490	4.055497	-1.011581	H	5.943462	-3.665099	-1.518851	H	5.770296	2.643365	2.883455	H	4.621017	4.138494	2.833036
H	-4.699064	5.333887	0.003898	H	6.158724	-2.009409	-0.895180	H	5.339518	4.376781	2.814773	H	3.597474	5.602753	2.889917
H	-5.205141	3.795971	0.749023	H	5.879952	-2.270559	-2.646881	H	6.358533	3.644681	1.528506	H	4.739745	5.348953	1.526609
C	-0.066996	3.215690	1.488919	C	1.561283	-3.512881	1.295659	C	3.382552	1.209813	-1.799837	C	2.663948	2.169267	-1.841464
H	0.881812	3.676897	1.141378	H	0.984897	-4.464337	1.062241	C	3.513704	1.925492	-2.643297	C	2.475409	2.943523	-2.618392
H	0.199086	2.202967	1.861261	H	0.868390	-2.811818	1.807237	H	2.533889	0.541405	-2.054204	H	2.112762	2.757359	-2.142283
H	-0.440645	3.812445	2.343449	H	2.362637	-3.800479	2.009332	H	4.303297	0.595331	-1.759100	H	3.747485	1.941246	-1.874027
N	2.525461	1.169324	-0.934939	N	-2.213884	-1.663570	-0.406588	N	-1.424790	1.389781	-1.137903	N	-2.183171	1.039317	-0.850716
N	0.538706	2.121103	-1.160410	N	-0.105577	-2.227542	-0.720354	N	0.714400	1.972336	-0.734612	N	0.004485	1.725410	-0.627201
Ru	0.532715	-0.602379	0.313839	Ru	-0.460057	0.528041	0.705710	Ru	0.336578	-1.065772	-0.245316	Ru	0.434941	-0.586744	-0.662229
C	-1.209184	-0.090880	0.659830	C	1.389945	0.552803	0.361763	C	2.041499	-1.004491	0.441669	C	2.234642	-0.404408	-0.223991
C	0.720154	-2.944576	0.654756	C	-0.651690	2.297778	2.324340	C	0.026903	-3.344426	-0.571395	C	0.255037	-2.892483	-0.587535
C	1.556723	-0.027940	2.318375	C	-0.418438	-0.917934	2.619783	C	0.737434	-0.918953	-2.683274	C	0.304592	-0.572708	-3.099044
H	-1.779162	-1.542569	-2.325792	C	-0.432538	1.777463	-1.317340	C	-0.484986	0.714164	1.191354	C	-1.148926	0.391955	1.355659
C	-0.424063	-1.678395	-2.295150	C	-1.563493	1.987974	-0.508118	C	-0.612323	-0.776992	1.587193	C	0.136365	-0.404729	1.532549
H	0.215200	-0.910108	-2.754487	H	-2.509520	1.466701	-0.720510	H	0.116671	-1.038436	2.379654	H	0.950096	0.267251	1.871837
H	0.065311	-2.592025	-1.927142	H	-1.669725	2.934906	0.043311	H	-1.436983	1.230785	1.441133	H	-2.035498	-0.274990	1.352788
H	-2.192242	-0.615252	-2.763154	H	-0.486935	1.017995	-2.113819	H	0.341606	1.191389	1.748634	H	-1.352421	1.169191	1.256545
C	-2.014152	-0.188612	1.877263	C	2.499055	0.585437	1.307783	C	2.214826	-0.200861	1.207709	C	5.535321	0.412358	0.468756
H	-1.802388	0.241430	-0.222698	H	1.748778	0.624171	-0.684803	C	3.225247	-1.812871	0.180763	C	3.355257	-1.216150	-0.677148
C	-3.340991	0.332274	1.836620	C	3.814936	0.523813	0.754462	C	4.361541	-1.645210	1.025707	C	4.610888	-1.029039	-0.023693
C	-4.178311	0.272205	2.957810	C	4.948150	0.586063	1.572775	C	5.524592	-2.400386	0.828838	C	5.731671	-1.785962	-0.383182
C	-3.717928	-0.324130	4.147169	C	4.798801	0.729758	2.966270	C	5.887560	-3.329553	-0.227813	C	5.632812	-2.734036	-1.420622
C	-2.418464	-0.863373	4.200667	C	3.511355	0.815254	3.528831	C	4.481757	-3.493245	-1.084158	C	4.409886	-2.914892	-2.094076
C	-1.573550	-0.800692	3.084591	C	2.370922	0.744204	2.717711	C	3.311036	-2.748393	-0.889234	C	3.279416	-2.170625	-1.732343
H	-3.702881	0.790329	0.901868	H	3.927899	0.427134	-0.337274	H	4.311979	-0.914027	1.849599	H	4.685422	-0.281775	0.783714
H	-5.199244	0.683397	2.904302	H	5.953942	0.536219	1.125685	H	6.388496	-2.265638	1				

II-III		III		III-IV		IV									
-2520.0132774		-2520.0480158		-2520.0092552		-1195.2014042									
C	-0.292982	1.258449	-0.347297	C	-0.129529	1.723271	-0.180263	C	-0.336726	-2.069130	0.123594	C	0.374248	-0.394506	0.092052
C	-0.837117	2.121811	-2.458258	C	-0.624379	3.405238	-1.730161	C	-1.079712	-3.679996	1.674054	C	1.363213	-2.470122	0.647290
H	-1.550418	2.889793	-2.819712	H	-1.029443	4.360168	-1.322541	H	-1.380118	-4.642214	1.191034	H	1.713934	-2.485806	1.708812
H	-0.685550	1.346185	-3.237543	H	-0.946260	3.318817	-2.785915	H	-1.579922	-3.630676	2.662824	H	1.921383	-3.261601	0.103291
C	0.511833	2.717186	-2.013709	C	0.903524	3.281982	-1.575310	C	0.447515	-3.541170	1.783210	C	-0.155761	-2.651166	0.535758
H	1.304995	2.535523	-2.765314	H	1.362791	2.811747	-2.469949	H	0.731397	-2.989142	2.708766	H	-0.444486	-3.222287	-0.360540
H	0.460364	3.815249	-1.823197	H	1.403674	4.251143	-1.379093	H	0.969711	-4.519544	1.788479	H	-0.576013	-3.188495	1.429727
C	-3.488746	0.367942	-1.781661	C	-3.258211	1.461090	-1.908075	C	-3.624858	-1.604428	1.476798	C	3.693991	-0.809413	-1.106395
C	-4.873596	0.234340	-1.544980	C	-4.645512	1.253052	-1.757704	C	-4.983440	-1.381428	1.176865	C	5.004783	-0.291590	-1.114196
H	-5.432440	-0.500767	-2.148564	H	-5.196678	0.802862	-2.600272	H	-5.606514	-0.857738	1.921647	H	5.641659	-0.471610	-1.996970
C	-5.559971	0.994504	-0.581948	C	-5.343414	1.597519	-0.586093	C	-5.563189	-1.794727	-0.037807	C	5.518225	0.451771	-0.034274
C	-4.822618	1.906706	0.129577	C	-4.615546	2.206140	0.454328	C	-4.743801	-2.474120	-0.960465	C	4.681004	0.664154	1.080109
H	-5.342747	2.613145	0.850749	H	-5.143676	2.525841	1.368518	H	-5.811360	-2.833300	-1.907758	H	5.066762	1.235128	1.942148
C	-3.443200	2.151396	-0.074982	C	-3.230723	2.441854	0.362344	C	-3.382121	-2.732645	-0.707871	C	3.366225	0.163272	1.140268
C	-2.755551	1.305193	-0.997347	C	-2.543811	2.023082	-0.813427	C	-2.816497	-2.269255	0.513900	C	2.873672	-0.575967	0.028223
C	-2.860487	-0.446360	-2.885717	C	-2.597113	1.119547	-3.220740	C	-3.055662	-1.154053	2.800409	C	3.171508	-1.599643	-2.284702
H	-3.451584	-1.362149	-3.084841	H	-3.223054	0.413459	-3.800965	H	-3.718367	-0.409439	3.283765	H	3.852399	-1.516684	-3.154894
H	-1.811159	-0.742620	-2.679674	H	-1.595964	0.660269	-3.077478	H	-2.050978	-0.701565	2.677741	H	2.164345	-1.249207	-2.589149
H	-2.841456	0.134807	-3.834977	H	-2.472765	2.028465	-3.852239	H	-2.953251	-2.005078	3.510964	H	3.072015	-2.681618	-2.045783
C	-7.033937	0.788782	-0.318093	C	-6.822275	1.319295	-0.440993	C	-7.012689	-1.498157	-0.352380	C	6.915656	1.029921	-0.073624
H	-7.543497	1.745680	-0.074606	H	-7.335412	2.120177	0.130040	H	-7.631378	-1.453206	0.566942	H	7.418984	0.949725	0.912190
H	-7.189110	0.108991	0.548559	H	-6.992537	0.368531	0.110501	H	-7.450991	-2.262177	-1.026506	H	6.894408	2.110467	-0.337423
H	-7.547732	0.334366	-1.188878	H	-7.320525	1.222169	-1.426344	H	-7.115605	-0.514854	-0.862697	H	7.549948	0.519852	-0.826166
C	-2.753920	3.293918	0.635095	C	-2.529621	3.149994	1.498840	C	-2.564122	-3.502689	-1.717569	C	2.510788	0.425607	2.358199
H	-3.498754	4.012738	1.028991	H	-3.260334	3.694091	2.128848	H	-3.215859	-3.978609	-2.476943	H	3.120846	0.819380	3.195012
H	-2.075611	3.844841	-0.048544	H	-1.780629	3.882236	1.135752	H	-1.958960	-4.298328	-1.236111	H	1.994031	-0.490348	2.711864
H	-2.138064	2.961288	1.497648	H	-1.987461	2.440139	2.159984	H	-1.842156	-2.840555	-2.242228	H	1.711752	1.162836	2.127771
C	2.017624	2.265492	-0.031889	C	2.256902	2.285499	0.352480	C	2.094985	-2.695029	0.027986	C	-2.043832	-1.116259	0.123514
C	1.998946	3.079347	1.138270	C	2.283771	2.928263	1.669121	C	2.358787	-3.293525	-1.236279	C	-3.009783	-1.257248	1.156713
C	3.206024	3.300736	1.833430	C	3.485126	2.764486	2.400400	C	3.667287	-3.231130	-1.755046	C	-4.327585	-1.158437	0.828915
H	3.182889	3.926737	2.742045	H	3.504276	3.184809	3.420175	H	3.868732	-3.695163	-2.735691	H	-5.122456	-1.256814	1.635393
C	4.434033	2.783563	1.385948	C	4.661457	2.208497	1.861021	C	4.723091	-2.619474	-1.052711	C	-4.812376	-0.926648	-0.488921
C	4.433478	2.050017	0.183476	C	4.611310	1.723067	0.541513	C	4.443232	-2.046857	0.201519	C	-3.833092	-0.819133	-1.495520
H	5.387349	1.661438	-0.210933	H	5.521828	1.297464	0.088020	H	5.240442	-1.548174	0.765551	H	-4.151429	-0.663580	-2.540663
C	3.259270	1.784608	-0.547235	C	3.434513	1.750336	-0.235498	C	3.140712	-2.065467	0.759786	C	-2.454605	-0.920598	-1.225001
C	0.748257	3.767786	1.637583	C	1.076545	3.497409	2.285040	C	1.272342	-3.999846	-2.010228	C	-2.592767	-1.508871	2.588222
H	0.989137	4.788475	1.998039	H	1.365905	4.082920	3.179472	H	1.694346	-4.569278	-2.861658	H	-3.348121	-1.119635	3.299953
H	0.280251	3.232934	2.493292	H	0.309138	2.760375	2.603091	H	0.526274	-3.280212	-2.410598	H	-1.613917	-1.039333	2.812976
H	-0.018663	3.856164	0.847042	H	0.578666	4.185831	1.571250	H	0.708646	-4.073639	-1.363020	H	-2.485126	-2.597044	2.798502
C	5.717682	3.018712	1.249810	C	5.931590	2.125992	2.677601	C	6.129226	-2.959301	-1.610385	C	-6.281235	-0.772700	-0.815253
H	5.570449	3.717783	2.997351	H	5.997485	1.154609	3.214901	H	6.149865	-2.870096	-2.684055	H	-6.565072	0.301350	-0.874467
H	6.509271	3.437958	1.493515	H	5.978655	2.925609	3.444492	H	6.788482	-3.311008	-1.071642	H	-6.925441	-1.241054	-0.043908
H	6.117469	2.067644	2.563497	H	6.834793	2.204921	2.039132	H	6.591420	-1.591694	-1.502868	H	-6.532488	-1.226715	-1.796117
C	3.366918	1.054878	-1.862745	C	3.467189	1.242699	-1.655043	C	2.890202	-1.416084	2.100205	C	-1.465742	-0.834469	-2.363942
H	3.515771	1.779157	-2.696153	H	3.662980	2.073666	-2.369981	H	2.848371	-2.167775	2.919862	H	-0.627902	-1.550946	-2.243304
H	2.469040	0.447122	-2.100071	H	2.511715	0.756169	-1.944206	H	1.933854	-0.853515	2.115644	H	-1.004939	0.174922	-2.418629
H	4.248043	0.383705	-1.864618	H	4.282306	0.504584	-1.786597	H	3.705775	-0.709959	2.351645	H	-1.963874	-1.042778	-3.331816
N	-1.348359	1.503152	-1.219265	N	-1.128331	2.271303	-0.931545	N	-1.444400	-2.534830	0.830067	N	1.560571	-1.152733	0.040101
N	0.801149	2.011790	-0.753150	N	1.040492	2.382202	-0.411808	N	0.776048	-2.778203	0.572465	N	-0.659327	-1.267286	0.471745
Ru	0.182803	-1.213884	-0.168009	Ru	-0.014652	-1.469900	-0.161715	Ru	0.262836	2.054771	0.274639	Ru	0.341764	0.948626	-0.225767
C	1.870033	-1.095749	0.590457	C	1.683209	-1.681438	0.542097	C	1.769395	1.712407	-0.749161	H	1.292829	1.318108	-0.643932
Cl	0.003215	-3.477397	-0.619612	Cl	-0.460445	-3.461982	-1.340631	Cl	0.481665	4.294454	0.704146	C	-0.715055	1.951718	-0.099106
Cl	0.592607	-0.961781	-2.622948	Cl	0.421179	-0.399399	-2.383215	Cl	-0.038550	0.926122	2.322403	C	-0.699167	3.083159	-0.965794
C	-0.471819	0.721983	1.022243	C	-0.295033	0.596362	0.715584	C	-0.332038	-1.060422	-0.818111	C	-1.730888	1.923964	0.897215
C	-0.595269	-1.004599	1.613661	C	-0.734177	-2.039280	1.494027	C	-0.887797	2.071899	-1.185588	C	-1.655715	4.103078	-1.865415
H	0.067061	-0.932137	2.506551	H	-0.086922	-2.102356	2.406158	H	-0.545697	1.586284	-2.130576	H	0.087670	3.149360	-1.736020
H	-1.492178	0.963456	1.362209	H	-1.334812	0.546350	1.083627	H	-1.282708	-0.634040	-1.156542	C	-2.690272	2.942685	0.992766
H	0.304012	1.122655	1.694986	H	0.428188	0.637216	1.547935	H	0.598587	-0.813800	-1.339256	H	-1.743998	1.104987	1.629449
H	2.006319	-0.475906	1.516349	H	1.830334	-1.548286	1.646303	H	1.623372	1.244222	-1.752441	C	-2.667986	4.038160	0.110290
C	3.098603	-1.786536	0.213158	C	2.916110	-2.087438	-0.128922	C	3.166861	1.949565	-0.407086	H	-1.611167	4.959627	-1.558242
C	4.226790	-1.661046	1.077476	C	4.121016	-2.102340	0.633842	C	4.171380	1.568941	-1.343440	H	-3.459966	2.886029	1.780033
C	5.429766	-2.320941	0.798815	C	5.355246	-2.504414	0.063160	C	5.527723	1.802780	-1.082517	H	-3.421364	4.837855	0.190270
C	5.541557	-3.114152	-0.360105	C	5.374065	-2.914789	-1.283784	C	5.916867	2.412803	0.125126				
C	4.443797	-3.239293	-1.232726	C	4.192355	-2.918439	-2.050079	C	4.939632	2.789672	1.067603				
C	3.234031	-2.587957	-0.957047	C	2.975830	-2.508598	-1.488408	C	3.582306	2.564322	0.809349				
H	4.135963	-1.038494	1.982883	H	4.084482	-1.792151	1.691351	H	3.866144	1.088534	-2.287174				
H	6.285608	-2.220401	1.485547	H	6.255011	-2.591677	0.670045	H	6.287597	1.510601	-1.824745				
H	6.487473	-3.633882	-0.583153	H	6.325929	-3.240965	-1.733581	H	6.983220	2.597591	0.331904				

With C<sub>2</sub>H<sub>3</sub>X (X=Ph right):

0•14e-I			I			I-II			II						
-2520.047367			-2520.0744116			-2520.0176759			-2520.0478819						
C	-0.513505	-1.569948	0.139415	C	-0.789497	-1.452911	-0.379296	C	-0.755962	1.207523	-0.255149	C	-1.152000	0.807445	-0.091508
C	-0.267972	-3.925378	0.366664	C	-2.181874	-3.298790	-0.927637	C	-1.802966	2.509357	-1.895990	C	-2.287202	1.410238	-2.069258
H	0.368341	-4.533457	1.036326	H	-2.634193	-3.350207	-1.943317	H	-2.681397	3.184475	-1.942374	H	-3.139538	2.082386	-2.299085
H	-0.419772	-4.504485	-0.578268	H	-2.832970	-3.875655	-0.240565	H	-1.664512	2.016063	-2.883289	H	-2.261237	0.586756	-2.818174
C	-1.597335	-3.498122	1.002217	C	-0.717928	-3.765609	-0.899252	C	-0.507050	3.224933	-1.459906	C	-0.934456	2.140275	-2.048586
H	-2.467938	-4.067325	0.617670	H	-0.507030	-4.480748	-0.074144	H	0.173537	3.400423	-2.316668	H	-0.346031	1.921173	-2.960125
H	-1.589162	-3.601563	2.111779	H	-0.394481	-4.242082	-1.847232	H	-0.693893	4.203999	-0.959522	H	-1.042687	3.237052	-1.914868
C	2.296643	-2.816416	-1.487949	C	-3.951101	-1.336283	1.028799	C	-3.831228	-0.146735	-1.255848	C	-3.962306	-1.063232	-0.599826
C	3.691271	-2.713320	-1.675830	C	-5.094501	-0.565077	1.299241	C	-5.119135	-0.619594	-0.893694	C	-5.186862	-1.597900	-0.143733
H	4.099770	-2.914829	-2.680194	H	-5.594083	-0.694177	2.273838	H	-5.527812	-1.472382	-1.456149	H	-5.432900	-2.638120	-0.416339
C	4.570895	-2.367860	-0.633625	C	-5.615556	0.364869	0.376580	C	-5.872912	-0.042437	0.137096	C	-6.100385	-0.855528	0.623300
C	4.026239	-2.156073	0.650133	C	-4.993938	0.459064	-0.879636	C	-5.333259	1.077927	0.800077	C	-5.774561	0.484626	0.908991
H	4.700822	-1.925110	1.491828	H	-5.421414	1.130014	-1.643977	H	-5.927227	1.580999	1.581844	H	-6.490710	1.105674	1.473282
C	2.644244	-2.240322	0.892017	C	-3.845817	-0.292346	-1.208806	C	-4.063046	1.592578	0.482790	C	-4.567430	1.069899	0.484193
C	1.777592	-2.524905	-0.199268	C	-3.283871	-1.136904	-0.214899	C	-3.285793	0.945763	-0.525501	C	-3.634631	0.274779	-0.243420
C	1.407441	-3.260527	-2.623511	C	-3.502976	-2.381244	2.023026	C	-3.103236	-0.822072	-2.389117	C	-3.070459	-1.939583	-1.442326
H	1.964041	-3.262188	-3.580922	H	-3.910457	-2.162573	0.302945	H	-2.520522	-1.703457	-0.236439	H	-2.471149	-2.637961	-0.821266
H	0.527095	-2.593931	-2.737724	H	-2.400093	-2.412126	2.110327	H	-2.368591	-0.168603	-2.894456	H	-2.342974	-1.382118	-2.063066
H	1.032723	-4.295243	-2.459711	H	-3.875528	-3.390504	1.733751	H	-8.323716	-1.201993	-3.140964	H	-3.677161	-2.565733	-2.127399
C	6.054237	-2.212860	-0.880038	C	-6.802054	1.230334	0.732614	C	-7.223679	-0.599946	0.524212	C	-7.385964	-1.470374	1.127745
H	6.653125	-2.722241	-0.017880	H	-7.327027	1.602017	-0.170318	H	-7.666193	-1.205758	-0.291543	H	-8.203092	-0.722696	1.185894
H	6.315953	-1.143064	-0.034705	H	-6.473721	2.120219	1.313311	H	-7.940007	0.205643	0.786358	H	-7.251304	-1.885376	2.151070
H	6.380692	-2.765364	-1.783640	H	-7.534732	0.684703	1.361870	H	-7.138404	-1.259998	1.415463	H	-7.723837	-2.304053	0.479831
C	2.094948	-2.082043	2.291138	C	-3.320313	-0.214685	-2.625759	C	-3.575515	2.829245	1.205408	C	-4.315950	2.525762	0.804345
H	2.907188	-1.884991	3.017937	H	-4.162605	-0.261602	-3.346130	H	-4.422829	3.367945	1.673319	H	-5.268863	3.045155	1.027141
H	1.563973	-2.998665	2.627914	H	-2.625794	-1.041994	-2.866327	H	-3.055783	3.561115	0.527712	H	-3.822986	3.061510	-0.031117
H	1.364712	-1.249497	2.353308	H	-2.787695	0.739267	-2.823643	H	-2.864418	2.585773	0.202493	H	-3.665972	2.645434	1.697127
C	-2.907212	-1.368307	0.954284	C	1.466258	-2.561521	-0.692395	C	1.330413	2.603323	0.166791	C	0.765638	2.528146	-0.279555
C	-3.059920	-0.816873	2.252728	C	2.141183	-2.536893	-1.939669	C	1.304464	3.103907	1.500384	C	0.454608	3.391627	0.809877
C	-4.288609	-0.208787	2.584795	C	3.548846	-2.644909	-1.941963	C	2.525800	3.396636	2.142220	C	1.474300	4.211752	1.337781
H	-4.409564	0.227454	3.591000	H	4.080005	-2.611600	-2.908420	H	2.498787	3.777178	3.177508	H	1.226639	4.863516	2.193089
C	-5.360910	-0.154043	1.674728	C	4.287396	-2.812163	-0.757335	C	3.764811	3.248828	1.495292	C	2.767832	4.256433	0.791634
C	-5.181558	-0.727651	0.400820	C	3.577754	-2.884505	0.460109	C	3.754046	2.825358	0.151456	C	3.003201	3.488669	-0.363440
H	-6.010241	-0.698369	-0.326415	H	4.132312	-3.039438	1.400570	H	4.709323	2.734893	-0.392238	H	3.985181	3.552545	-0.861927
C	-3.976088	-1.344978	0.017965	C	2.176532	-2.772173	0.523380	C	2.568052	2.509563	-0.539261	C	2.031327	2.640167	-0.930455
C	-1.952995	-0.893789	3.279998	C	1.410962	-2.459797	-3.263219	C	0.017526	3.398309	2.239473	C	-0.935341	3.566468	1.381706
H	-2.043280	-0.081663	0.402897	H	1.907025	-1.748692	-3.955132	C	0.686789	4.398654	2.716764	H	-1.191566	4.645968	1.411724
H	-0.950706	-0.827649	2.812194	H	0.358140	-2.142573	-3.149727	H	-0.175724	2.668580	3.055544	H	-1.013444	3.191374	2.240403
H	-1.985619	-1.853798	3.842174	H	1.415031	-3.449894	-3.770426	H	-0.858430	3.388913	1.566956	H	-1.710648	3.058376	0.786039
C	-6.644511	0.525381	2.036407	C	5.795516	-2.926448	-0.777846	C	5.066172	3.542320	2.206738	C	3.856992	5.104870	1.406359
H	-7.537369	-0.107914	1.773023	H	6.136567	-3.856632	-0.275730	H	5.607776	2.602246	2.450308	H	4.493787	4.499134	2.088331
H	-6.783051	1.480950	1.480544	H	6.271136	-2.080330	-0.236627	H	4.901273	4.087378	3.157510	H	3.439406	5.939809	2.004376
H	-6.722498	0.757137	3.118606	H	6.193382	-2.931417	-1.811900	H	5.747561	4.148879	1.574675	H	4.527887	5.533004	0.633921
C	-3.830099	-1.979091	-1.346753	C	1.460124	-2.891761	1.844732	C	2.642490	2.133770	-1.996431	C	2.369796	1.969888	-2.243909
H	-3.647847	-3.065812	-1.276619	H	0.716827	-3.718395	1.831096	H	2.520234	3.036851	-2.637128	H	2.311799	2.719636	-3.064289
H	-2.967157	-1.535752	-1.897334	H	0.892201	-1.969729	2.099403	H	1.860890	1.404000	-2.295821	H	1.704260	1.128781	-2.512502
H	-4.746964	-1.822704	-1.949813	H	2.176538	-3.099612	2.662931	H	3.632795	1.701769	-2.240213	H	3.410593	1.588808	-2.232826
N	0.566085	-2.625558	0.068251	N	-2.082287	-1.889023	-0.491176	N	-1.991326	1.493838	-0.846195	N	-2.407618	0.896920	-0.699341
N	-1.699035	-2.071232	0.620638	N	0.027953	-2.504335	-0.672363	N	0.093797	2.285405	-0.496658	N	-0.232390	1.605462	-0.837878
Ru	0.012147	0.211540	-0.622850	Ru	-0.416373	0.517255	0.135993	Ru	0.021125	-0.830213	-0.691468	Ru	0.213143	-0.722217	-0.831730
C	-1.425869	1.185777	0.000510	C	1.431381	0.464547	0.358634	C	1.768369	-0.809868	-0.106143	C	1.944634	-0.424058	-0.228194
Cl	1.478079	1.770302	-1.611263	Cl	-1.082541	2.633332	1.058021	Cl	-0.232647	-3.016507	-1.490961	Cl	0.232187	-3.051091	-0.868786
Cl	-0.812609	-0.502062	-2.683004	Cl	-0.946040	-0.296514	2.350887	Cl	0.263592	-0.155018	-3.048998	Cl	0.055614	-0.664516	-3.261669
C	1.226243	1.659210	1.832838	C	0.007941	0.474414	-0.024970	C	-0.271641	0.433132	1.139844	C	-0.984835	0.447905	1.368746
C	2.559085	1.466227	2.027093	C	-0.308820	1.818458	-1.711688	C	-0.994789	-1.082430	1.093623	C	-0.444057	-0.972539	1.263764
H	2.872618	0.586261	2.615744	H	-1.362495	2.132074	-1.823273	H	-0.253612	-1.285953	0.828653	H	-1.266533	-1.700773	1.117593
H	0.495906	0.985585	2.307653	H	-0.733323	-0.133670	-2.561336	H	-1.593070	0.914814	1.630991	H	-1.933034	0.562821	1.943233
H	0.830717	2.536900	1.301408	H	2.247651	0.855469	1.504017	H	0.188880	0.710022	1.702414	H	-0.234549	1.121556	1.820573
C	-2.361439	2.079099	-0.681459	C	2.062913	0.161342	-0.508095	H	1.959620	-0.187544	0.805094	H	2.116857	0.448046	0.442006
H	-1.545653	1.214900	1.112927	C	3.654196	0.630211	1.407643	C	2.968807	-1.454015	-0.621647	C	3.163332	-1.165902	-0.526216
C	-3.404875	2.671096	0.088653	C	4.516820	0.973115	2.454960	C	4.165393	-1.362540	0.148436	C	4.312538	-0.904921	0.277161
C	-4.325823	3.550506	-0.495028	C	3.998420	1.569475	3.621311	C	5.354023	-1.958150	-0.291575	C	5.514986	-1.588000	0.059060
C	-4.220260	3.872458	-1.861707	C	2.618122	1.823697	3.725521	C	5.380308	-2.648312	-1.518923	C	5.608216	-2.528263	-0.985130
C	-3.184278	3.313318	-2.633986	C	1.746524	1.472920	2.685396	C	4.210839	-2.737101	-2.298285	C	4.492568	-2.778713	-1.806936
C	-2.262665	2.428945	-2.057607	H	4.056225	0.172806	0.488965	C	3.015268	-2.151340	-1.861871	C	3.280708	-2.112402	-1.584224
H	-3.483858	2.419505	1.158921	H	5.598685	0.785619	2.362847	H	4.143696	-0.818825	1.107301	H	4.236458	-0.167904	1.092850
H	-5.125945	3.995801	1.0118014	H	4.675470	1.847362	4.445455	H	6.266311	-1.8845					

II-III			III			III-IV			IV						
-2520.013277			-2520.045404			-2520.0026394			-1195.2014042						
C	-0.962775	1.316718	-0.344310	C	-1.102595	-1.769623	0.036189	C	-1.315482	1.696050	-0.121757	C	0.374248	-0.394506	0.092052
C	-2.005619	2.236642	-2.297333	C	-1.256238	-3.818016	-1.089493	C	-2.665020	3.085723	-1.464265	C	1.363213	-2.470122	0.647290
H	-2.809837	3.004348	-2.186874	H	-1.269710	-4.733537	-0.453779	H	-3.270780	3.809015	-0.865148	H	1.713934	-2.485806	1.708812
H	-2.109825	1.672465	-3.178920	H	-0.890047	-4.105598	-2.094077	H	-3.157691	2.969455	-2.450854	H	1.921383	-3.261601	0.103291
C	-0.584140	2.837749	-2.082553	C	-2.618032	-3.099433	-1.143711	C	-1.197763	3.529422	-1.591700	C	-0.155761	-2.651166	0.553758
H	0.063931	2.524224	-2.924345	H	-2.835132	-2.7711946	-2.161339	H	-0.775608	3.227171	-2.577293	H	-0.444486	-3.222287	-0.360540
H	-0.587288	3.946226	-2.013221	H	-3.462677	-3.737428	-0.817110	H	-1.067080	4.624564	-1.477560	H	-0.576013	-3.188495	1.429727
C	-3.798229	-0.514426	-1.267700	C	1.858671	-2.812107	-1.537068	C	-4.127965	0.158585	-1.610531	C	3.639391	-0.809413	-1.106395
C	-5.047985	-1.037966	-0.867123	C	3.249040	-2.990633	-1.396802	C	-5.301120	-0.652788	-1.383140	C	5.004783	-0.291590	-1.114196
H	-5.375073	-1.994008	-1.309445	H	3.886060	-2.829676	-2.282069	H	-5.672832	-1.280019	-2.211309	H	5.641659	-0.471610	-1.996790
C	-5.884521	-0.388866	0.056387	C	3.846474	-3.361887	-0.176504	C	-5.960111	-0.693565	-0.137818	C	5.518225	0.451771	-0.034274
C	-5.451636	0.848522	0.574766	C	3.003061	-3.586101	0.928441	C	-5.470458	0.131168	0.892362	C	4.681004	0.664154	1.080109
H	-6.101224	1.398221	1.276881	H	3.442459	-3.917063	1.884763	H	-5.987757	0.139887	1.867131	H	5.066762	1.235128	1.942148
C	-4.218438	1.418949	0.212044	C	1.660227	-3.413776	0.852401	C	-4.350949	0.970863	0.716311	C	3.366225	0.163272	1.140268
C	-3.373280	0.715946	-0.696980	C	1.044904	-2.986512	-0.381494	C	-3.684269	0.961133	-0.540251	C	2.873672	-0.575967	0.028223
C	-2.977547	-1.290224	-2.266026	C	1.276667	-2.485073	-2.891041	C	-3.512705	0.179166	-2.968083	C	3.171508	-1.599643	-2.284702
H	-2.384720	-2.093199	-1.769171	H	2.047052	-2.038945	-3.548772	H	-3.803409	-0.707591	-3.565050	H	3.852399	-1.516684	-3.154894
H	-2.240302	-0.675672	-2.814796	H	0.434906	-1.763586	-2.827699	H	-2.407265	0.197019	-2.885716	H	2.164345	-1.249207	-2.589149
H	-3.634805	-1.806139	-2.994813	H	0.910607	-3.408024	-3.395789	H	-3.817567	1.075686	-3.553891	H	3.072015	-2.681618	-2.045783
C	-7.201696	-0.992837	0.487463	C	5.347241	-3.498008	-0.058462	C	-7.151990	-1.599770	0.078116	C	6.915656	1.029921	-0.073624
H	-7.997025	-0.223428	0.569174	H	5.637434	-4.120712	0.811512	H	-7.890937	-1.505200	-0.745105	H	7.418984	0.949725	0.912190
H	-7.110949	-1.470496	1.487810	H	5.821538	-2.500744	0.072765	H	-7.671200	-1.374926	1.031214	H	6.894408	2.110467	-0.337423
H	-7.546329	-1.773044	-0.219968	H	5.789820	-3.947411	-0.970812	H	-6.843944	-2.667863	0.109655	H	7.549948	0.519852	-0.826166
C	-3.826132	2.756503	0.795968	C	0.760004	-3.693884	2.074613	C	-3.900816	1.865238	1.847636	C	2.510788	0.425607	2.358199
H	-4.712430	3.283564	1.200255	H	1.228334	-4.477628	2.702782	H	-4.697296	1.969047	2.610754	H	3.120846	0.819380	3.195012
H	-3.346520	3.419718	0.048189	H	-0.262358	-4.029228	1.812372	H	-3.631780	2.879197	1.487952	H	1.994031	-0.490348	2.711864
H	-3.103856	2.643400	1.631946	H	0.648318	-2.791046	2.714289	H	-2.993768	1.463132	2.348284	H	1.711752	1.162836	2.127771
C	1.076101	2.759642	-0.129963	C	-3.532052	-1.288992	0.418520	C	0.698414	3.185060	0.084451	C	-2.043832	-1.116259	-0.123514
C	0.907733	3.427887	1.094180	C	-3.744467	-1.461941	1.816004	C	0.739585	3.658379	1.429012	C	-3.009783	-1.257248	1.156713
C	2.048544	3.949111	1.767969	C	-4.836051	-0.805953	2.416371	C	1.977804	4.049332	1.971427	C	-4.375785	-1.158437	0.828915
H	1.909368	4.497943	2.714873	H	-4.997130	-0.936367	3.499854	H	2.004470	4.413568	3.012835	H	-5.122456	-1.256814	1.635393
C	3.348652	3.772132	1.257644	C	-5.733087	-0.011601	1.676297	C	3.171400	4.011712	1.221961	C	-4.812376	-0.926648	-0.488921
C	3.476827	3.122516	0.017226	C	-5.521043	0.096690	0.289414	C	3.096342	3.558675	-0.107581	C	-3.833092	-0.819133	-1.495520
H	4.480185	2.994409	-0.422069	H	-6.218701	0.697961	-0.317349	H	4.016769	3.513036	-0.713867	H	-4.151429	-0.663580	-2.540663
C	-2.372314	2.615364	-0.700827	C	-4.440415	-0.527887	-0.366592	C	1.884806	3.140668	-0.698038	C	-2.544605	-0.920598	-1.225001
C	-0.455938	3.771157	1.671195	C	-2.851125	-2.342142	2.659496	C	-0.514644	3.765105	2.262176	C	-2.592767	-1.508871	2.588222
H	-0.392179	4.580731	2.424479	H	-3.309684	-2.532310	3.649542	H	-0.330150	4.346537	3.186841	H	-3.348121	-1.119635	3.299953
H	-0.903452	2.887960	2.176392	H	-1.857144	-1.878363	2.833567	H	-0.896081	2.762374	2.551912	H	-1.613917	-1.039333	2.812976
H	-1.171842	0.408847	0.887057	H	-2.665381	-3.324142	2.176021	H	-1.333540	4.257342	1.696939	H	-2.485126	-2.597044	2.798502
C	4.561616	4.257186	2.018550	C	-6.874234	0.714071	2.352493	C	4.479969	4.474905	1.823846	C	-6.281235	-0.772700	-0.815253
H	4.952134	3.462187	2.691756	H	-6.562190	1.733446	2.670636	H	4.619875	4.082064	2.852665	H	-6.565072	0.301350	-0.874467
H	4.323695	5.134201	2.654280	H	-7.218534	0.180138	3.261423	H	4.518152	5.584274	1.896645	H	-6.925441	-1.241054	-0.043908
H	5.388494	4.538217	1.335372	H	-7.741713	0.837468	1.672999	H	5.347478	4.154374	1.212940	H	-6.532488	-1.226715	-1.796117
C	2.611581	1.981174	-2.046764	C	-4.285216	-0.379480	-1.859600	C	1.877674	2.660554	-2.129859	C	-1.465742	-0.834469	-2.363942
H	2.455759	2.721289	-2.864010	H	-4.652648	-1.282120	-2.397199	H	1.545666	3.461560	-2.827762	H	-0.627902	-1.550946	-2.243304
H	1.931666	1.126898	-2.246736	H	-3.221553	-0.217073	-2.139354	H	1.203408	1.791900	-2.275302	H	-1.004939	0.174922	-2.418629
H	3.657054	1.625962	-2.130660	H	-4.878195	0.479311	-2.230503	H	2.895081	2.358884	-2.447731	H	-1.963874	-1.042778	-3.331816
N	-2.118617	1.325216	-1.077563	N	-0.378379	-2.799237	-0.485511	N	-2.546224	1.798642	-0.768503	N	1.560571	-1.152733	0.040101
N	-0.089315	2.260590	-0.813963	N	-2.428721	-1.972391	-0.204883	N	-0.557902	2.808101	-0.482919	N	-0.659327	-1.267286	0.471745
Ru	0.151841	-1.305908	-0.670681	Ru	0.784100	0.664462	-0.509335	Ru	0.628334	-1.867741	-0.916947	Ru	0.341764	0.948626	-0.225767
C	1.787561	-1.086740	0.166432	C	0.269596	2.210499	0.384958	C	2.077165	-1.189201	0.015597	C	1.292829	1.318108	-0.643932
Cl	0.392323	-3.418864	-1.588092	Cl	2.203205	1.508659	-2.225727	Cl	1.400457	-3.920766	-1.626432	Cl	-0.715055	1.951718	-0.099106
Cl	0.268061	-0.378755	-2.979394	Cl	-0.881268	0.291613	-2.349551	Cl	0.131663	-0.548311	-2.801285	Cl	-0.699167	3.083159	-0.965794
C	-0.751060	0.484914	0.829058	C	-0.547113	-0.627861	0.740368	C	-0.907364	0.661656	0.695360	C	-1.730888	1.923964	0.897215
C	-0.757002	-1.467838	0.981341	C	2.244706	0.390503	0.655976	C	-0.459836	-2.452858	0.471535	C	-1.655715	4.103078	-0.865415
H	-1.678213	0.422461	1.427689	H	2.493429	-0.686224	0.838579	H	-1.463113	-2.733068	0.061149	H	0.087670	3.149360	-1.736020
H	0.113035	0.809446	1.430301	H	0.136777	-0.951690	1.544614	H	-1.634560	-0.085803	1.026828	C	-2.690272	2.942685	0.992766
H	1.821847	-0.614899	1.184030	H	-1.361853	-0.004721	1.147295	H	0.075594	0.705531	1.176469	H	-1.174398	1.104987	1.629449
C	3.119757	-1.452675	-0.309264	H	0.428839	2.280480	1.487991	H	1.806920	-0.566480	0.901440	C	-2.667986	4.038160	0.110290
C	4.214868	-1.340469	0.596755	C	-0.360278	3.409477	-0.160944	C	3.510189	-1.205848	-0.264916	H	-1.611167	4.959627	-1.558242
C	5.514223	-1.693178	0.211108	C	-0.772221	4.424260	0.753616	C	4.373066	-0.508376	0.631308	H	-3.459966	2.886029	1.780033
C	5.756905	-2.150903	-1.098497	C	-1.368823	5.607567	0.301505	C	5.759233	-0.486033	0.430799	H	-3.421364	4.837855	0.190270
C	4.691811	-2.249432	-2.014382	C	-1.559565	5.811715	-1.079063	C	6.320506	-1.151906	-0.675190				
C	3.588002	-1.907042	-1.623311	C	-1.152538	4.824784	-1.997748	C	5.844056	-1.838089	-1.577197				
H	4.023473	-0.978358	1.620773	C	-0.563086	3.634233	-1.552967	C	4.098042	-1.867819	-1.380264				
H	6.344049	-1.610424	0.931406	H	0.611435	4.264973	1.833137	C	3.932588	0.019704	1.492852				
H	6.778829	-2.425119	-1.406730	H	-1.682063	6.378153	1.024111	H	6.407392	0.055266	1.138372				
H	4.880907	-2.597355	-3.042491	H	-2.023223	6.744575	-1.439042	H	7.410397	-1.134017	-0.835996				

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