

## How does the addition of sterical hindrance on a typical IPr NHC ligand affect catalytic activity in Olefin Metathesis?

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

1-PPh <sub>3</sub>			1-PPh <sub>3</sub> -14e1			2-Py			2-Py-14e1						
-3788.2110421			-3788.1678748			-3000.4293231			-3000.3924158						
Ru	-0.478210	0.012347	0.088286	Ru	0.306386	-0.483986	0.152910	Ru	-0.588520	0.873610	-0.176013	Ru	-0.517877	0.474239	0.109297
Cl	-0.420958	-0.268832	-2.315200	Cl	0.241040	-0.622133	-2.067179	Cl	-0.371774	0.293690	-2.485720	Cl	-1.142308	0.736502	-2.116915
Cl	-1.082896	0.052576	2.420656	Cl	-0.314088	-0.828015	2.345008	Cl	-1.427454	1.605427	1.949194	Cl	-1.028212	0.756631	2.361497
P	-1.399561	2.255159	-0.252911	P	-4.011258	0.810342	-0.189579	N	-2.585785	-1.345482	0.235150	N	-1.661222	-2.228300	0.095997
N	-1.478803	-2.885841	0.260596	N	1.653924	-3.133399	0.238801	N	-0.681452	-2.104115	0.974617	N	-4.352822	-2.403282	0.723916
N	0.619491	-2.881787	0.851898	N	3.151555	-1.669619	0.898100	N	-0.473958	2.927328	-0.837076	N	-3.220002	3.318558	0.217087
C	-0.369890	-2.051606	0.349281	C	1.864602	-1.754041	0.364001	C	-1.233580	-1.006201	0.334481	C	-0.486720	-1.466593	0.251489
C	-1.187282	-4.166475	0.734252	C	2.751388	3.852414	0.713222	C	-2.840419	-2.592226	0.807060	C	-1.462394	-3.545484	0.489471
C	0.124775	-4.164864	1.011480	C	3.681655	-2.944942	1.122426	C	-1.650673	-3.068150	1.271426	C	-0.161347	-3.661493	0.874888
C	-2.790202	-2.620986	-0.316531	C	0.526236	-3.803124	-0.389124	C	-3.638509	-0.573486	-0.407723	C	-2.927145	-1.807557	-0.488089
C	-3.872302	-2.287000	0.546572	C	-0.502190	-4.349978	0.428254	C	-3.828770	-0.718543	-1.815128	C	-3.116210	-1.997791	-1.888126
C	-5.151515	-2.150517	-0.034165	C	-1.564281	-5.014276	-0.222457	C	-4.834253	0.064533	-2.418654	C	-5.375968	-1.617802	-2.434142
C	-5.357609	-2.361628	-1.401768	C	-1.591526	-5.140173	-1.614641	C	-5.646899	0.919091	-1.662387	C	-5.375376	-1.087720	-1.629293
C	-4.283310	-2.728357	-2.223393	C	0.538395	-4.652559	-2.392293	C	-5.503180	0.970605	-0.270681	C	-5.182090	-0.957844	-0.249138
C	-2.989177	-2.883458	-1.706029	C	0.549560	-3.978634	-1.804118	C	-4.515336	0.214094	0.395574	C	-3.964071	-1.329741	0.306468
C	-3.722959	-2.168385	2.063462	C	-0.449333	-4.331449	1.956942	C	-3.080300	-1.765276	-2.645419	C	-2.068751	-2.670753	-2.779418
C	-4.165869	-3.477512	2.757325	C	0.096622	-5.676926	2.491007	C	-3.805139	-3.130745	-2.556110	C	-2.358387	-4.187230	-2.892995
C	-4.488840	-0.965750	2.648388	C	-1.809072	-4.010150	2.606846	C	-2.895267	-1.370310	-4.121497	C	-1.956617	-2.049289	-4.184404
C	-1.873236	-3.429262	-2.611444	C	1.742950	-3.554995	-2.664662	C	-4.513107	0.166262	1.925789	C	-3.844915	-1.308556	1.885155
C	1.909989	9.76524	-2.628213	C	2.777977	-7.703706	-2.744451	C	-5.538745	-0.881838	2.422967	C	-4.445870	-2.601758	2.485214
C	-1.931529	-2.884414	-4.050813	C	1.358728	-3.097613	-0.484017	C	-4.802158	1.526366	2.588680	C	-4.488678	-0.065798	2.528490
C	2.038780	-2.628546	1.034123	C	4.023258	-0.517709	1.017323	C	0.714007	-2.418228	1.197023	C	1.867073	-2.306495	0.895893
C	2.913691	-2.878977	-0.063614	C	4.971579	-0.301263	-0.022804	C	1.344606	-3.294365	0.271331	C	2.690609	-2.713643	-0.192786
C	4.296973	-2.740052	0.166937	C	5.855934	0.788460	0.117057	C	2.674474	-3.678978	0.544439	C	4.081724	-2.776312	0.027394
C	4.792400	-2.380322	1.428167	C	5.808128	1.620610	1.243024	C	3.344919	-3.213006	1.683413	C	4.632808	-2.450907	1.275027
C	3.911147	-2.160668	2.493430	C	4.888729	1.361651	2.268140	C	2.691308	-2.362409	2.586065	C	3.800073	-2.045410	2.326666
C	2.515142	-2.291165	2.329615	C	3.982480	0.283556	2.188725	C	1.357368	-1.955430	2.376575	C	2.399300	-1.970249	2.168746
C	2.405023	-3.334442	-1.437080	C	5.087639	-1.205800	-1.255173	C	0.635348	-3.855652	-0.965825	C	2.124372	-3.105462	-1.560566
C	2.251065	-4.873520	-1.496672	C	6.450633	-1.933017	-1.279441	C	0.563485	-5.398761	-0.912146	C	2.289070	-4.620317	-1.814981
C	3.294201	-2.876424	-2.609963	C	4.844059	-0.446078	-2.576478	C	1.273155	-3.370368	-2.846335	C	2.741091	-2.800070	-2.709594
C	3.888781	-2.147288	3.537991	C	5.808128	1.620610	1.243024	C	0.622023	-1.115395	3.419980	C	5.154354	-1.606311	3.358337
C	1.557677	-3.457329	4.359900	C	4.888729	1.361651	2.268140	C	-0.075426	-2.029987	4.454830	C	1.368946	-2.811956	4.314859
C	1.961854	-0.959732	4.444677	C	3.826186	-0.857060	4.429608	C	1.525435	-0.091673	1.306101	C	2.014117	-0.357704	4.110333
C	1.304374	0.581290	0.247476	C	2.214087	1.211809	3.988036	C	1.254542	0.861051	0.183471	C	1.202476	1.191477	0.025653
C	2.356139	0.261168	0.276420	C	1.146460	1.228476	0.193822	C	2.261907	0.005724	-0.441353	C	2.568499	0.768237	-0.205077
C	5.294742	0.933460	-0.438254	C	2.318654	1.791704	-0.454678	C	3.533769	0.537297	-0.276129	C	3.394403	1.896287	-0.379981
C	1.305428	1.713284	0.796320	C	2.270415	3.179235	-0.436627	C	3.418834	1.722898	0.616206	C	2.576413	3.099973	-0.198829
C	4.104475	2.615800	1.488554	C	1.037385	3.586777	0.282091	C	4.388542	2.535429	1.216587	C	2.917924	4.459014	-0.171880
C	3.644328	3.267141	2.643862	C	0.493589	4.845061	0.570814	C	3.972311	3.592970	2.061912	C	1.902921	5.415487	0.062603
C	2.332429	3.038963	3.801048	C	-0.725874	4.919483	1.286117	C	2.609566	3.818669	2.303896	C	0.575343	5.013073	0.276466
C	1.472787	2.171885	2.363936	C	-1.386205	3.752912	1.702211	C	1.626264	2.986796	1.716508	C	0.225477	3.642153	0.283140
C	1.925254	1.522518	1.220442	C	0.855143	2.477784	1.394303	C	2.028856	1.937529	0.881714	C	5.678902	0.851928	-0.166306
C	7.622538	2.647440	0.242374	C	-0.343768	2.395255	0.673710	C	4.943811	-1.301693	-1.248034	C	4.826619	1.845269	-0.714650
C	4.691783	0.840661	-2.659624	C	4.493740	0.814141	-1.040370	C	6.093045	-1.747051	-1.915134	C	7.041337	0.809347	-0.495347
C	5.856566	0.783263	-3.439143	C	0.493589	4.845061	0.570814	C	7.091988	-0.832904	-2.299641	C	5.880991	1.752880	-1.384827
C	7.122368	0.776018	-2.824300	C	-0.725874	4.919483	1.286117	C	6.924920	0.533198	-2.012248	C	6.755920	2.738915	-1.944419
C	7.210598	0.824194	-1.421593	C	-1.386205	3.752912	1.702211	C	5.772726	0.981179	-1.359093	C	5.393660	2.789355	-1.611567
C	6.046988	0.886194	-0.638782	C	0.855143	2.477784	1.394303	C	-1.440640	3.810988	-0.479934	C	-3.906865	4.011519	1.144371
C	-3.215520	2.120634	-0.648516	C	-0.343768	2.395255	0.673710	C	-0.511269	5.106272	-1.009588	C	-5.136478	1.643414	0.884569
C	-4.195036	2.956417	-0.060227	C	4.842925	4.598715	-2.849360	C	-0.542206	5.520057	-1.937954	C	-5.676306	4.547742	-0.490899
C	-5.540728	2.859019	-0.463141	C	5.226945	5.784262	-2.195373	C	-0.462930	4.609265	-2.301795	C	-4.967197	3.823758	-1.381408
C	-5.923009	1.936337	-1.451479	C	4.634590	6.118629	-0.964643	C	0.461515	3.326863	-1.738889	C	-3.744813	3.227303	-1.020075
C	-4.952264	1.105025	-0.036757	C	-0.044510	-0.646069	-0.708450	C	-3.844620	0.023707	0.827534	C	-2.271303	-2.802588	0.451415
C	-3.607881	1.187864	-1.637202	C	-6.306365	-0.967010	-0.160065	C	-1.390821	-4.007651	1.767595	C	0.431369	-4.518665	1.237348
C	-0.771475	2.389924	-1.146973	C	-7.007392	-2.103879	-0.601684	C	-4.988837	-0.006614	-3.505125	C	-4.529217	-1.739454	-3.514318
C	0.579496	3.113301	-2.100873	C	-6.461492	-2.929791	-1.599818	C	-6.818959	1.603168	0.321120	C	-6.334217	-0.787316	-2.081585
C	1.079108	3.886042	-3.163717	C	-5.203446	-2.620162	-1.248742	C	-6.181959	1.603168	0.321120	C	-5.997150	-0.567708	0.378724
C	0.232974	4.767002	-3.858604	C	-4.493740	0.814141	-1.040370	C	-2.064994	-1.871632	-2.211105	C	-1.082337	-2.545742	-2.285154
C	-1.117492	4.876279	-3.482657	C	-0.725874	4.919483	1.286117	C	-4.832869	-3.600542	-2.972806	C	-3.342143	-4.365109	-3.377603
C	-1.617895	4.112476	-2.414540	C	-5.857878	2.986894	-3.270796	C	-3.899006	-3.500302	-1.514702	C	-2.377892	-4.687944	-1.904314
C	-4.492077	3.289924	-1.146973	C	-5.358584	1.974368	-3.232665	C	-3.254941	-3.898587	-3.140291	C	-1.582066	-4.687953	-3.509611
C	-2.011377	3.250564	2.334195	C	-5.891310	2.387407	1.365431	C	-2.435140	-0.367399	-4.211427	C	-1.777903	-0.958401	-4.123781
C	-1.967087	4.186238	3.381202	C	-4.497870	0.810767	2.569378	C	-3.855480	-1.382433	-4.680760	C	-2.868637	-2.229561	-4.792464
C	-1.255703	5.390245	3.230123	C	-5.074193	1.201005	3.781339	C	-2.222167	-2.096908	-4.621671	C	-1.108763	-2.509351	-4.733706
C	-0.584812	5.652343	2.023835	C	-6.073183	2.191784	3.797011	C	-3.499817	-0.146939	2.249895	C	-2.766927	-1.279707	2.143447
C	-1.403404	4.723012	0.969824	C	-6.476050	2.785455	2.581403	C	-5.843876	1.867181	2.406761	C	-3.925689	-3.514043	2.091440
H	1.942399	3.289885	-4.457537	C	-5.891310	2.387407	1.3654								

1-14eI			1-14eI-CII			CII			1-CII-MCy1						
-2752.2157264			-2830.7694473			-2830.7833647			-2830.7781423						
Ru	0.590207	-1.204377	-0.191320	Ru	0.612716	-1.055365	-0.321396	Ru	0.567225	-0.782365	-0.957359	Ru	0.485118	-0.449227	-1.066863
Cl	0.862845	-1.242055	-2.484574	Cl	0.643485	-0.520320	-2.595469	Cl	0.222281	1.146847	-2.370662	Cl	0.233295	1.769307	-1.988582
Cl	1.264612	-2.242019	1.778031	Cl	1.366712	-2.231459	1.559972	Cl	1.360876	-2.525052	0.523614	Cl	1.250213	-2.568727	-0.188127
N	2.652898	0.841031	0.183004	N	2.553563	1.031350	0.342291	N	2.664666	0.776191	0.566496	N	2.801732	0.550688	0.695691
N	0.838949	1.536412	1.205788	N	0.677245	1.547358	1.357498	N	0.757316	1.268743	1.497688	N	0.913654	0.832529	1.753803
C	1.301738	0.518977	0.371260	C	1.210981	0.637656	0.444700	C	1.302466	0.511865	0.484341	C	1.439039	0.357062	0.575244
C	2.999924	1.982586	0.905826	C	2.826849	2.105158	1.189859	C	2.938792	1.669417	1.602404	C	3.107281	1.136897	1.926929
C	1.874409	2.417706	1.538545	C	1.663162	2.426848	1.820267	C	1.747073	1.976528	2.189263	C	1.927593	1.309294	2.591268
C	3.601673	0.196689	-0.710863	C	3.566353	0.492925	-0.551891	C	3.715529	0.244731	-0.291590	C	3.817468	0.240776	-0.300486
C	3.647183	0.629824	-2.068527	C	3.648678	1.016191	-1.877201	C	4.007621	0.919357	-1.514337	C	4.116515	1.216676	-1.295350
C	5.490330	0.014072	-2.913818	C	4.638946	0.481666	-2.725081	C	4.994477	0.351284	-2.348387	C	5.076375	0.873764	-2.271132
C	5.463902	-0.972197	-2.435120	C	5.530107	-0.502866	-2.267570	C	5.698016	-0.798281	-1.967392	C	5.738674	-0.360045	-2.239640
C	5.430137	-1.345391	-1.086622	C	5.472739	-0.949200	-0.951456	C	5.462767	-1.379637	-0.715028	C	5.485548	-1.265061	-1.200880
C	4.510844	-0.763623	-0.186993	C	4.504758	-0.454266	-0.050385	C	4.483860	-0.868293	0.162163	C	4.534412	-0.986184	-0.197238
C	2.780441	1.776824	-2.596033	C	2.779764	2.182048	-2.358570	C	3.406182	2.280294	-1.872263	C	3.539155	2.633617	-1.263093
C	3.515522	3.127854	-2.420331	C	3.429551	3.532873	-1.970100	C	3.273934	3.409696	-1.265074	C	4.455070	3.555257	-0.421373
C	2.340725	1.603023	-4.061809	C	2.491858	2.163006	-3.870838	C	3.233125	2.504814	-3.385127	C	3.313729	3.242537	-2.658719
C	4.589471	-1.107233	1.301446	C	4.574239	-0.861144	1.423218	C	4.574073	-1.438062	1.578679	C	4.393178	-1.933874	0.996108
C	5.715510	-0.292764	1.981300	C	5.636306	-0.011103	2.161413	C	5.408924	-0.754290	2.305788	C	5.453071	-1.594134	2.072064
C	4.780210	-2.612878	1.568623	C	4.859141	-2.361196	1.629545	C	4.549766	-2.967427	1.646536	C	4.490738	-3.422855	0.614030
C	-0.517925	1.893865	1.566203	C	0.703319	1.815689	1.709474	C	-0.633426	1.442952	1.867036	C	-0.486581	0.905881	2.130105
C	-1.162960	2.893812	0.782692	C	-1.349603	2.899513	1.049105	C	-1.277190	2.649808	1.480025	C	-1.163383	2.145145	1.965596
C	-2.345693	3.333014	1.202872	C	-2.648871	3.243249	1.477137	C	-2.585209	2.868660	1.962545	C	-2.504179	2.211600	2.399915
C	-3.043594	2.802744	2.349818	C	-3.284031	2.538443	2.509201	C	-3.225533	1.926402	2.778430	C	-3.140774	1.098977	2.965788
C	-2.382639	1.825666	3.105523	C	-2.620506	1.482006	3.146722	C	-2.565848	0.742917	3.138507	C	-2.441441	-0.104714	3.130319
C	-1.101064	1.357375	2.744241	C	-1.311618	1.105672	2.778286	C	-1.249752	0.476317	2.708112	C	-1.094115	-0.230816	2.732719
C	-0.520868	3.527577	-0.455441	C	-0.682167	3.723859	-0.057805	C	-0.599343	3.197006	0.617809	C	-0.477072	3.400293	1.421067
C	-0.203013	5.019748	-0.211901	C	-0.372589	5.162522	0.432946	C	-0.268946	4.975045	1.457043	C	-0.103425	4.356769	2.577607
C	-1.375588	3.343541	-1.727457	C	-1.512224	3.761993	-1.358447	C	-1.432678	4.095586	-0.623989	C	-1.315163	4.136735	0.358306
C	-0.366703	0.376392	3.655564	C	-0.569797	0.033626	3.572027	C	-0.505833	-0.767487	3.194487	C	-0.313569	-1.514947	3.017891
C	0.164651	1.105461	4.911106	C	0.011069	0.638006	4.871552	C	0.274002	-0.456451	4.494081	C	0.407268	-1.418087	4.383915
C	-1.232224	-0.838471	4.041242	C	-1.436606	-1.201727	3.877687	C	-1.419939	-1.988974	3.397024	C	-1.180608	-2.875061	2.968028
C	-1.272154	-1.203808	-0.079782	C	-1.246417	-1.088507	-0.114005	C	-1.269471	-1.062518	-0.600646	C	-1.388526	-0.898818	-1.099604
C	-2.321840	-0.228070	-0.297468	C	-2.224991	-0.093216	-0.437356	C	-2.303570	-0.030250	-0.679039	C	-2.422639	0.149492	-1.196789
C	-3.521179	-0.869167	-0.595062	C	-3.491618	-0.698555	-0.623215	C	-3.569125	-0.597255	-0.671844	C	-3.681481	-0.365734	-0.968671
C	-3.305858	-2.332258	-0.477683	C	-3.354598	-2.137960	-0.294785	C	-3.411591	-2.061289	-0.449680	C	-3.542068	-1.824979	-0.716734
C	-4.188590	-3.418106	-0.554664	C	-4.305954	-3.157610	-0.163562	C	-4.353685	-3.071808	-0.228368	C	-4.498580	-2.795876	-0.392713
C	-3.692636	-4.724074	-0.332763	C	-3.883783	-4.411875	0.256044	C	-3.903986	-4.400471	-0.026695	C	-4.090841	-4.142052	-0.247320
C	-2.341890	-4.934651	-0.013705	C	-2.536555	-4.687551	0.559949	C	-2.535100	-4.697286	-0.042820	C	-2.746010	-4.496465	-0.422652
C	-1.451022	-3.842148	0.098416	C	-1.573637	-3.655849	0.453677	C	-1.576716	-3.672860	-0.239931	C	-1.769918	-3.512114	-0.707683
C	-1.930382	-2.546930	-0.144205	C	-1.980284	-2.387170	0.019522	C	-2.011318	-2.355625	-0.428040	C	-2.159005	-2.172680	-0.833819
C	-4.773407	-0.209742	-0.996359	C	-4.704573	-0.046252	-1.147854	C	-4.833063	0.106537	-0.935972	C	-4.938124	0.400777	-1.023142
C	-5.145824	1.038429	-0.431844	C	-4.993363	1.305411	-0.824031	C	-4.997580	1.465792	-0.560274	C	-4.971011	1.753318	-0.594392
C	-6.325440	1.685241	-0.826593	C	-6.133409	1.941550	-1.334540	C	-6.184000	2.154658	-0.845335	C	-6.147897	2.509832	-0.683713
C	-7.162141	1.106706	-1.199194	C	-7.013806	1.247901	-2.185884	C	-7.236971	1.508876	-1.520485	C	-7.322267	1.937353	-1.206863
C	-6.804199	-0.125426	-2.374919	C	-6.739535	-0.089437	-2.523240	C	-6.7087329	0.166941	-1.911699	C	-7.305385	0.601233	-1.644036
C	-5.622770	-0.779242	-1.977406	C	-5.602337	-0.731287	-2.009392	C	-5.903337	-0.828074	-1.621540	C	-6.130266	-0.160775	-1.550790
H	4.019748	3.277825	0.896131	H	3.828814	2.536909	1.262896	H	3.957168	1.999718	1.823285	H	4.135991	1.374406	2.210856
H	1.699746	3.278424	2.190011	H	1.428253	3.206201	2.550505	H	1.469796	2.631108	3.029517	H	1.707899	1.724937	3.578563
H	4.640583	0.312821	-3.971398	H	4.715937	0.847308	-3.759389	H	5.227296	0.834885	-3.308511	H	5.315575	1.598402	-3.063398
H	6.186289	-1.445480	-3.119277	H	6.289436	-0.911022	-2.962776	H	6.458541	-1.227073	-2.639646	H	6.870001	-0.608308	-3.018056
H	1.637813	-2.102064	-0.715091	H	6.202499	-1.693887	-0.598939	H	6.056992	-2.251260	-0.402482	H	6.041753	-2.213514	-1.160651
H	1.856304	1.803825	-1.980523	H	1.801580	2.099809	-1.839790	H	2.392603	2.332687	-1.424229	H	2.544784	2.584118	-0.773664
H	4.456726	3.142015	-3.010037	H	4.423612	3.644799	-2.453499	H	5.301303	3.393092	-1.688145	H	5.462205	3.641664	-0.882752
H	3.778261	3.330520	-1.362820	H	3.573312	3.636549	-0.876378	H	4.365108	3.326389	-0.163265	H	4.593454	3.182054	0.613718
H	2.880519	3.966729	-2.776706	H	2.793662	4.379216	-2.306233	H	3.829521	4.402009	-1.491205	H	4.022549	4.576040	-0.356073
H	1.845699	0.624850	-4.217561	H	2.080142	1.186295	-4.189562	H	2.647881	1.687680	-3.850127	H	2.678970	2.586801	-3.285251
H	3.195092	1.688252	-4.766555	H	3.400223	2.383507	-4.471369	H	4.208077	2.596328	-3.910424	H	4.269106	3.439733	-3.190985
H	1.619898	2.401644	-4.335024	H	1.745423	2.945491	-4.120001	H	2.680319	3.450321	-3.561543	H	2.789288	4.215381	-2.562367
H	3.625589	-0.817431	1.767627	H	3.585658	-0.622801	1.880651	H	3.355401	-1.209719	1.952366	H	3.384181	-1.775150	1.428649
H	5.574186	0.800776	1.859661	H	5.433340	1.076544	2.084942	H	5.291229	0.347523	2.539230	H	5.385112	-0.543211	2.418983
H	6.708140	-0.549357	1.525999	H	6.650620	-0.189177	1.744397	H	6.445255	-0.966113	2.165658	H	6.480811	-1.747367	1.678573
H	5.748986	-0.509176	3.070055	H	5.661690	-0.273584	3.240179	H	5.308659	-1.134927	3.544252	H	5.328501	-2.249712	2.959760
H	5.774710	-2.975678	1.231796	H	5.884483	-2.640591	1.306264	H	5.592180	-3.278653	1.420680	H	5.513154	-3.702792	0.280750
H	3.997051	-3.214891	1.067390	H	4.130126	-2.988837	1.030106	H	3.861285	-3.480449	0.947263				

1-MCy1			1-MCy1-CI2			1-CI2			1-CI2-14e2						
-2830.7906759			-2830.7772062			-2830.7858702			-2830.7636218						
Ru	0.460983	-0.377301	-1.023577	Ru	-0.264900	-0.246607	-1.006140	Ru	-0.028731	-0.147225	-0.961807	Ru	-0.569784	-1.042651	-0.917498
Cl	0.151076	1.775852	-2.061418	Cl	0.530574	-2.102227	0.345152	Cl	1.258860	-0.497159	1.041507	Cl	0.832360	-1.341799	0.503764
N	1.109276	-2.465852	-0.014668	N	-1.257278	1.622205	-2.186264	N	-1.805592	0.115700	-2.630639	Cl	-0.824729	1.857947	-2.074872
C	2.791958	0.591768	0.710792	N	-2.756768	-0.428662	0.829305	N	-2.536861	-0.945084	0.778566	N	-3.041442	-0.912137	0.700301
N	0.874736	1.017439	1.672948	N	-1.338605	1.064786	1.555465	N	-2.091832	1.188838	0.890951	N	-2.167551	1.004882	1.309117
C	1.430389	0.462019	0.545201	C	-1.537622	0.151229	0.542999	C	-1.651384	0.011451	0.327008	C	-2.025257	-0.017174	0.363198
C	3.071257	1.225533	1.925189	C	-3.294132	0.115469	1.999299	C	-3.504216	-0.366620	1.602938	C	-3.761849	-0.459525	1.809994
C	1.874721	1.480219	2.532312	C	-2.402295	1.042727	2.458682	C	-3.226650	0.968551	1.671864	C	-3.212443	0.782805	2.191532
C	3.841072	1.048908	-0.196169	C	-3.463407	-1.438471	0.066039	C	-2.550780	-2.370254	0.493381	C	-3.472027	-2.106335	0.004763
C	4.195364	0.986305	-1.292501	C	-3.351075	-2.801881	0.452940	C	-1.793946	-3.241645	1.329650	C	-2.951764	-3.368370	0.407170
C	5.219907	0.531294	-2.148877	C	-4.072376	-3.752749	-0.300067	C	-1.849114	-4.621773	1.043988	C	-3.451258	-4.510943	-0.257885
C	5.883806	-0.679614	-1.912072	C	-4.881968	-3.690411	-1.376811	C	-2.639107	-5.119343	-0.000812	C	-4.464782	-1.972425	-1.005929
C	5.550901	-1.455002	-0.794663	C	-5.005563	-2.014597	-1.714895	C	-3.417483	-4.244681	-0.769747	C	-4.920160	-3.150727	-1.633502
C	4.530075	-1.062119	0.096335	C	-4.310720	-1.014304	-1.003114	C	-3.406302	-2.852981	-0.538362	C	-4.464782	-1.972425	-1.005929
C	3.585678	2.374944	-1.494404	C	-2.557338	-3.247788	1.682338	C	-1.022960	-2.744281	2.553051	C	-1.949155	-3.516139	1.548866
C	4.380352	3.427395	-0.684550	C	-3.492982	-3.388368	2.906216	C	-1.919078	-2.819555	3.812248	C	-2.664990	-3.910503	2.858541
C	3.489183	2.800485	-2.970108	C	-1.770514	-4.552348	1.456107	C	0.301741	-3.491480	2.791464	C	-0.817861	-4.509588	1.129216
C	4.268628	-1.895308	1.353592	C	-4.546865	0.462228	-1.327322	C	-4.358574	-1.949788	-1.324990	C	-5.056458	-0.619763	-1.409491
C	5.296665	-1.547636	2.456666	C	-5.753533	1.000660	-0.521871	C	-5.782372	-2.023485	-0.723900	C	-6.519243	-0.494399	-0.927208
C	4.272405	-3.415113	1.085813	C	-4.742204	0.740185	-2.829067	C	-4.394828	-2.270964	-2.831386	C	-4.945662	-0.356090	-2.925414
C	0.540441	1.137978	1.980813	C	-0.219733	1.985888	1.676060	C	-1.503488	2.514702	0.755076	C	-1.455307	2.270529	1.365361
C	-1.185343	2.380489	1.725276	C	0.965325	1.545772	2.330380	C	-0.562139	2.944597	1.734018	C	-0.244474	2.357038	2.105885
C	-2.542794	2.485788	2.091288	C	2.025748	2.470578	2.434378	C	-0.049543	4.522333	1.605947	C	0.406319	3.609034	2.140270
C	-3.226334	1.414854	2.679302	C	1.903426	3.776533	1.944643	C	-0.463069	5.100998	0.571444	C	-0.136932	4.729550	1.499701
C	-2.558788	0.210496	2.935997	C	0.706032	4.196842	1.351255	C	-1.423063	4.666739	-0.351654	C	-1.361203	4.628824	0.825601
C	-1.196752	0.042730	2.608818	C	-0.386792	3.318791	1.202640	C	-1.982473	3.373202	-0.276828	C	-2.054008	3.404605	0.746150
C	-0.451033	3.595039	1.152537	C	1.075278	0.174508	2.997952	C	-0.171398	2.093932	2.943998	C	0.298907	1.190343	2.923207
C	-0.061122	4.575168	2.283665	C	0.616599	0.265274	4.472618	C	-1.051217	2.460813	4.162926	C	-0.241737	1.267670	4.379905
C	-1.252691	4.324671	0.057449	C	2.482063	-0.442075	2.904128	C	1.321360	2.201421	3.307898	C	1.836193	1.103091	2.935228
C	-0.459420	-1.234768	3.012241	C	-1.707892	3.839626	0.631283	C	-3.136642	2.994711	-1.206511	C	-3.436944	3.358238	0.089538
C	0.065410	-1.110614	4.462259	C	-2.519865	4.565659	1.730460	C	-4.472670	3.530079	-0.639004	C	-4.510560	3.895777	1.066109
C	-1.306956	-2.508429	2.847505	C	-1.523718	4.760221	-0.589951	C	-2.936645	3.476453	-2.655471	C	-3.509436	4.115986	-1.250323
C	-1.375375	-1.153173	-1.634856	C	1.778567	-0.359835	-2.075804	C	2.117119	0.408240	-1.854685	C	3.327570	0.062129	-2.215202
C	-2.422439	-0.106677	-1.660008	C	2.714811	-1.392712	-1.597664	C	3.036847	-0.727908	-1.726195	C	0.404419	-1.066869	-1.619745
C	-3.602389	-0.563968	-1.113321	C	3.867287	-0.821639	-1.110244	C	4.135771	-0.774220	-0.970265	C	5.135083	-0.625523	-0.900414
C	-3.408486	-1.985669	-0.729958	C	3.736068	0.607339	-1.231375	C	3.982733	1.041033	-0.569245	C	5.167012	0.895755	-0.983386
C	-4.281811	-2.916312	-0.142632	C	4.611072	1.692098	-0.883417	C	4.795707	1.894665	0.195362	C	6.014461	1.166010	-0.400674
C	-3.851528	-2.429597	0.027256	C	4.238036	3.023962	-1.162950	C	4.389670	3.231065	0.389912	C	5.765091	3.184643	-0.640210
C	-2.569340	-4.643529	-0.389365	C	3.005344	3.310718	-1.773510	C	3.187610	3.710064	-0.164270	C	4.680860	3.593560	-1.437886
C	-1.671897	-3.702450	-0.940471	C	2.104132	2.274087	-2.100547	C	2.354462	2.853851	-0.914515	C	3.813000	2.638386	-2.009952
C	-2.078870	-2.369689	-1.082945	C	2.467005	0.949739	-1.822196	C	2.752298	1.525632	-1.108738	C	4.059155	1.280196	-1.780972
C	-4.846925	0.220902	-1.017494	C	5.018147	-1.569404	-0.569041	C	5.274548	-1.259367	-0.648594	C	6.088329	-1.481750	-1.695996
C	-4.793372	1.621711	-0.794153	C	4.705742	-2.731890	0.213891	C	5.053545	-2.616155	-0.300394	C	5.628764	-2.632271	0.521468
C	5.963746	2.392645	-0.750826	C	5.873203	-3.480633	0.710272	C	6.128211	-3.474334	-0.022422	C	6.534699	-3.472606	1.198466
C	7.221470	1.786458	-0.927381	C	7.196568	-3.087190	0.438207	C	7.450636	-2.997914	-0.083021	C	7.902078	-3.184973	1.203076
C	-7.293304	0.401235	-1.156455	C	7.432690	-1.937986	-0.337159	C	7.686961	-1.655046	-0.426546	C	8.374264	-2.049530	0.521305
C	-6.122880	-0.373026	-1.200559	C	6.356955	-1.184518	-0.833851	C	6.612865	-0.794218	-0.703668	C	7.479098	-1.204686	-0.154518
H	4.098186	1.432753	2.237521	H	-4.262066	-0.207910	2.391493	H	-4.296072	-0.962719	2.064219	H	-4.602985	-1.030845	2.212767
H	1.634581	1.944374	3.492841	H	-2.421661	1.686418	3.342375	H	-3.725727	1.783734	2.202914	H	-3.466159	1.411180	3.006894
H	5.511449	1.146839	-3.012869	H	-3.998094	-4.817151	-0.030363	H	-1.266056	-5.320011	1.662973	H	-3.069406	-5.036733	0.025824
H	6.679140	-1.014247	-2.597343	H	-5.431990	-4.131753	-1.951203	H	-2.662124	-6.201653	-0.206075	H	-4.785535	-5.315085	-1.772367
H	6.095434	-2.392456	-0.605320	H	-5.025282	-1.721812	-2.547688	H	-0.057910	-4.648716	-1.568434	H	-5.684626	-3.080193	-2.423424
H	2.544317	2.349932	-1.111669	H	-1.807600	-2.459052	1.897987	H	-0.573235	-1.683244	2.374088	H	-1.470189	-2.527446	1.697755
H	5.431855	3.489807	-1.038614	H	-4.257618	-4.176674	2.736569	H	-2.210179	-3.868925	4.033434	H	-3.166648	-4.897272	2.761274
H	4.405311	3.192283	0.390993	H	-4.032703	-2.446667	3.133799	H	-2.852172	-2.230911	3.698264	H	-3.437500	-3.169427	3.149796
H	3.921946	4.432270	-0.799795	H	-2.911293	-3.669401	3.809399	H	-1.377558	-2.423275	4.696866	H	-1.935429	-3.981597	3.692582
H	2.957569	2.042379	-3.578629	H	-1.100705	-4.464328	0.578518	H	0.953231	-3.453345	1.896266	H	-0.304755	-4.238189	0.275427
H	4.487148	2.983650	-3.422874	H	-2.439270	-5.428698	1.316785	H	0.144198	-4.553789	3.076366	H	-1.186748	-5.554168	1.134291
H	2.915661	3.746345	-3.048893	H	-1.135506	-4.765780	2.340872	H	0.857769	-3.009727	3.612622	H	-0.058918	-4.949192	2.028146
H	3.253541	-1.637685	1.719106	H	-3.640478	1.026494	-1.023723	H	-3.989904	-0.908211	-1.232393	H	-4.468293	0.171231	-0.900032
H	5.286119	-0.471611	2.725006	H	-5.613050	0.882507	0.571814	H	-5.802594	-1.741171	0.348684	H	-6.603144	-0.629273	0.170863
H	6.328957	-1.796177	2.129462	H	-6.687359	0.466933	-0.800418	H	-6.197595	-0.510113	-0.804031	H	-7.169582	-1.255625	-1.408528
H	5.086020	-2.126701	3.380441	H	-5.905344	2.081453	-0.726602	H	-6.467916	-1.338088	-1.265431	H	-6.929054	0.506018	-1.180083
H	5.283884	-3.789410	0.822252	H	-5.688102	0.307907	-3.220281	H	-4.822464	-3.275353	-3.038024	H	-5.538434	-1.085148	-3.517540
H	5.367365	-3.672430	0.272269	H	-3.897403	0.347192	-3.428808	H	-3.382438	-2.211153	-3.276611	H	-3.892985	-0.406291	-3.269665
H	3.953163	-3.956813	1.999281	H	-4.786303	1.834688	-3.001168	H	-5.033194	-1.531069	-3.357291	H	-5.309972	0.656242	-3.166895
H	-3.075125	3.434013	1.910206	H	2.963159	2.158785	2.918191	H	0.687521	4.609890	2.339990	H	1.354511	3.70500	

1-14e2		1-14e2-CI3		1-CI3		1-CI3-MC <sub>y</sub> 2		
-2214.1554218		-2292.70441		-2292.7253775		-2292.7222665		
Ru 0.058833	-0.410018	-1.753226	Ru -0.095415	-0.800271	1.280861	Ru 0.216418	-0.053902	1.728350
Cl 0.021942	-2.721977	-1.528723	Cl -1.361938	0.710382	2.508227	Cl -0.218762	-2.439457	1.445311
Cl 1.388736	1.314986	-2.536662	Cl -0.134234	-2.917577	0.318571	Cl 0.423009	2.371626	1.550150
N -1.177692	0.121916	0.980111	N -0.929769	0.551969	-1.230855	N 0.967491	-0.025242	-1.225227
N 1.015158	0.064008	1.018721	N 1.259306	0.544673	-1.092657	N -1.209522	0.062148	-1.101017
C -0.072338	-0.013592	1.409111	C 0.118697	0.171529	-0.384080	C -0.073870	0.011288	-0.324455
C -0.780674	0.269797	2.312872	C 0.438214	1.119376	-2.407817	C 0.488666	-0.001633	-2.535395
C 0.581789	0.226577	2.335713	C 0.922313	1.121099	-2.321115	C -0.874302	0.056536	-2.457621
C -2.573226	0.234666	0.617212	C -2.355724	0.478767	-0.959176	C 2.384316	-0.065936	-0.891742
C -3.373357	-0.938714	0.559355	C -2.997521	1.622074	-0.401662	C 3.006603	-1.333280	-0.695228
C -4.738070	-0.776459	2.402024	C -4.380995	1.531695	-0.149443	C 4.375877	-1.334159	-0.353749
C -5.284920	0.491525	-0.002321	C -5.101987	0.369492	-0.453540	C 5.101958	-1.409252	-0.247024
C -4.476492	1.633541	0.079970	C -4.457871	-0.719781	-1.053078	C 4.479452	1.085802	-0.511708
C -3.104770	1.534899	0.394836	C -3.075689	-0.689544	-1.337428	C 3.112634	1.158529	-0.852360
C -2.814204	-2.325485	0.876890	C -2.266287	2.946206	-0.163869	C 2.281261	-2.655855	-0.947078
C -3.129089	-2.713176	2.340362	C -2.436332	3.876640	-1.389566	C 2.447135	-3.078131	-2.426628
C -3.307464	-3.411357	-0.097737	C -2.709824	3.681648	1.115250	C 2.730284	-3.794088	-0.013300
C -2.256899	2.805015	0.491562	C -2.432201	-1.836749	-2.119083	C 2.502559	2.502077	-1.256534
C -2.715501	3.690132	1.671888	C -2.574155	-1.592027	-3.640472	C 2.775131	2.780876	-2.754283
C -2.243368	3.597883	-0.832497	C -2.989807	-3.225412	-1.748284	C 2.995226	3.681387	-0.397241
C 2.427561	0.066124	0.677759	C 2.641652	0.482281	-0.673570	C -2.594281	0.114491	-0.661659
C 3.131881	-1.169560	0.632812	C 3.190814	1.605960	0.003502	C -3.340763	-1.096260	-0.610854
C 4.503580	-1.121973	0.304470	C 4.556407	1.552378	0.352785	C -4.691392	-1.006271	-0.213363
C 5.152892	0.095068	0.063073	C 5.341105	0.433088	0.041618	C -5.278168	-0.225161	0.105063
C 4.447895	1.301151	0.711057	C 4.774660	-0.657848	-0.632439	C -4.528324	1.405333	0.011558
C 3.075164	1.320511	0.488177	C 3.414828	-0.661945	-1.008886	C -3.174548	1.385062	-0.383651
C 2.486316	-2.500810	1.023346	C 2.364225	2.845651	0.349694	C -2.762508	-2.447426	-1.034968
C 2.695032	-2.772155	2.532395	C 2.799698	4.057207	-0.504219	C -3.157222	-2.768822	-2.495854
C 2.987849	-3.695817	1.90527	C 2.411137	3.177179	1.855977	C -3.174157	-3.601261	-0.100854
C 2.363068	2.658569	0.705600	C 2.832558	-1.845185	-1.781629	C -2.409813	2.694948	-0.575445
C 2.605918	3.164411	2.147814	C 3.219994	-1.762487	-3.276076	C -2.618927	3.233617	-2.010724
C 2.764441	3.748443	-0.307355	C 3.234872	-3.205853	-1.181295	C -2.771427	3.775398	0.459872
H -1.513849	0.400863	3.113945	C 1.548060	-0.687338	2.031149	H -1.496244	0.150713	2.283379
H 1.289823	0.300845	3.165704	H -1.108929	1.469830	-3.196840	H 1.161284	-0.026474	-3.397019
H -5.382514	-1.664598	0.180193	H 1.691041	1.481889	-3.010557	H -1.638783	0.094245	-3.238347
H -6.353051	0.590151	-0.253641	H 4.003031	2.391099	0.297448	H 4.882666	-2.295047	-0.180618
H -4.917233	2.625864	-0.106019	H -6.180601	0.318382	-0.234653	H 6.168931	-0.168586	0.026628
H -1.712082	-2.274303	0.766129	H -5.040421	-1.615056	-1.316890	H 5.066298	2.014836	-0.457393
H -4.225237	-2.776729	2.510785	H -1.185841	2.715167	-0.053640	H 1.202994	-2.493861	-0.742500
H -2.719835	-1.976486	3.061999	H -3.505664	4.139163	-1.537159	H 3.516120	-3.253090	-2.674826
H -2.689647	-3.703586	2.582848	H -2.075654	3.410804	-2.328360	H 2.062333	-2.310668	-3.128699
H -3.098004	-3.133308	-1.149718	H -1.872319	4.822083	-1.243134	H 1.897553	-4.020412	-2.623960
H -4.396187	-3.606631	0.006639	H -2.627139	3.025395	2.002839	H 2.638583	-3.502460	1.051358
H -2.782075	-4.367005	0.105350	H -3.754470	4.051732	1.040653	H 3.775824	-4.115407	-0.209110
H -1.210650	2.498104	0.696150	H -2.065902	4.570545	1.280938	H 2.082079	-4.680794	-0.167705
H -2.687273	3.138322	2.633938	H -1.351184	-1.848996	-1.870555	H 1.406472	2.430016	-1.102979
H -3.753939	4.056979	1.526627	H -2.115471	-0.632815	-3.955431	H 2.385824	1.977643	-3.412292
H -2.058174	4.579544	1.768897	H -3.643478	-1.567175	-3.941320	H 3.865230	2.870906	-2.949352
H -3.257928	3.955509	-1.109112	H -2.078632	-2.404935	-4.212352	H 2.295298	3.732900	-3.064825
H -1.852186	2.982544	-1.667985	H -4.041583	-3.354997	-2.081478	H 4.070599	3.903638	-0.566240
H -1.590764	4.490851	-0.739055	H -2.940186	-3.403366	-0.656439	H 2.829141	3.482818	0.679284
H 5.073417	-2.061247	0.245967	H -2.391169	-4.014423	-2.245113	H 2.429947	4.599128	-0.661156
H 6.223036	0.105122	-0.198825	H 5.011842	2.404945	0.880898	H -5.293538	-1.925591	-0.154252
H 4.973719	2.253057	0.003031	H 6.405272	0.411320	0.326101	H -6.333368	0.267012	0.419531
H 1.396240	-2.415111	0.836935	H 5.401093	-1.530568	-0.873125	H -5.003518	2.369924	0.244837
H 2.274726	-1.963921	3.164899	H 1.306009	2.623847	0.101371	H -1.657557	-2.370673	-0.973323
H 3.775782	-2.860325	2.774825	H 2.720605	3.844240	-1.590347	H -2.828213	-1.981713	-3.204828
H 2.201113	-3.721755	2.828444	H 3.852980	4.341325	-0.294473	H -4.259189	-2.868121	-2.598600
H 4.050219	-3.939043	0.405624	H 2.163659	4.939944	-0.282896	H -2.699420	-3.727065	-2.820402
H 2.882350	-3.506725	-0.895976	H 3.434232	3.455118	2.187401	H -4.263171	-3.815750	-0.151032
H 2.391972	-4.599120	0.432976	H 2.069293	2.319121	2.469322	H -2.897070	-3.380572	0.948466
H 1.274039	2.479408	0.583444	H 1.746041	0.436792	2.080439	H -2.645286	-4.530773	-0.397172
H 2.062292	4.116566	2.325289	H 1.727774	-1.779263	-1.709787	H -1.330444	2.479323	-0.432816
H 3.686799	3.354379	2.320390	H 2.766862	-2.603024	-3.842662	H -2.036616	4.166716	-2.163482
H 2.269523	2.436511	2.913097	H 4.321815	-1.818955	-3.408175	H -3.689458	3.466079	-2.197726
H 2.625323	3.398427	-1.348247	H 2.875010	-0.816375	-3.741835	H -2.294663	2.506407	-2.782865
H 3.820203	4.068123	-0.176791	H 2.960481	-3.268818	-0.109537	H -2.655164	3.400300	1.496044
H 2.135608	4.651090	-0.158490	H 4.323818	-3.402678	-1.280430	H -3.808827	4.153399	0.334186
C -1.592786	0.013872	-2.360500	H 2.703840	-4.023824	-1.710156	H -2.090691	4.643662	0.346717
H -1.744226	-0.197144	-3.450920	C -0.660652	-2.062401	5.173824	C 1.269230	-0.933159	3.491977
H -2.451700	0.460619	-1.823186	C -0.874830	-3.109520	4.359110	C 1.443219	0.454924	3.526191
			H -1.077058	-1.066000	4.947792	H 2.051114	-1.591765	3.078698
			H -0.055271	-2.158174	6.091765	H 0.517213	-1.441424	4.115306
			H -1.481171	-3.015401	3.441854	H 2.363807	0.922242	3.138772
			H -0.453533	-4.108061	4.566573	H 0.833603	1.100969	4.177031
			H 2.452563	-0.151413	1.683946	H -2.158778	-0.729315	2.436896
			H 1.627306	-1.239761	3.002031	H -1.901373	1.160258	2.515303
						Ru 0.149722	-0.037473	1.661763
						Cl -0.042049	-2.446070	1.556396
						Cl 0.382291	2.382172	1.649354
						N 0.997861	-0.032263	-1.250306
						N -1.183228	0.037246	-1.162468
						C -0.059963	-0.002381	-0.364637
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						C -0.825384	0.030314	-2.514889
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						C 3.042753	-1.317329	-0.688837
						C 4.042255	-1.302168	-0.311235
						C 5.105448	-0.099234	-0.164984
						C 4.469629	1.122174	-0.422399
						C 3.111457	1.178375	-0.798617
						C 2.339363	-2.647226	-0.965576
						C 2.512968	-3.043371	-2.451382
						C 2.806164	-3.794248	-0.051287
						C 2.484572	2.518623	-1.188069
						C 2.758544	2.819310	-2.681373
						C 2.955985	3.695492	-0.313917
						C -2.568704	0.085092	-0.735400
						C -3.299327	-1.133291	-0.652591
						C -4.659142	-1.048995	-0.286876
						C -5.266394	0.185174	-0.019677
						C -4.525797	1.370745	-0.121711
						C -3.163564	1.355543	-0.487702
						C -2.680388	-2.490017	-0.993739
						C -3.021139	-2.893239	-2.447292
						C -3.091801	-3.604320	-0.012727
						C -2.396059	2.666298	-0.664327
						C -2.56		

<b>1-MCy2</b>			
<b>-2292.7405409</b>			
Ru	-0.000116	-0.000258	1.601576
Cl	0.390572	2.368368	1.640822
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C	-0.681838	0.040304	-2.584651
C	0.682064	-0.039346	-2.584609
C	-2.486239	0.123196	-0.836907
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C	-4.416365	1.426775	-0.182954
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C	-4.590261	-0.986009	-0.397719
C	-3.236488	-1.084890	-0.780742
C	-2.282657	2.703135	-0.746855
C	-2.459471	3.236604	-2.188238
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C	-2.654902	-2.441027	-1.184663
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C	2.459187	-3.235984	-2.188762
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C	1.334910	-0.210404	3.039772
H	-1.402031	0.085108	-3.406205
H	1.402337	-0.083826	-3.406111
H	-4.888626	2.394311	0.043534
H	-6.231557	0.300014	0.209562
H	-5.197346	-1.901738	-0.335751
H	-1.207403	2.482689	-0.583518
H	-3.524599	3.475096	-2.396888
H	-2.125480	2.503203	-2.950409
H	-1.868111	4.165121	-2.333890
H	-2.555901	3.411651	1.316765
H	-3.691963	4.167035	0.135669
H	-1.973276	4.653813	0.174359
H	-1.552121	-2.373507	-1.082824
H	-2.628017	-1.967759	-3.353911
H	-4.090859	-2.841442	-2.807388
H	-2.532161	-3.715849	-2.970968
H	-4.199981	-3.803206	-0.374011
H	-2.882895	-3.375090	0.788318
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H	5.197632	1.901671	-0.335344
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H	1.552396	2.373766	-1.082615
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H	2.882596	3.374827	0.789215
H	2.577039	4.526167	-0.546103
H	1.207304	-2.482417	-0.583748
H	1.867728	-4.164407	-2.334610
H	3.524277	-3.474525	-2.397548
H	2.125207	-2.502355	-2.950718
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H	1.972996	-4.653753	0.173530
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C	-1.335014	0.209753	3.039966
H	0.144366	0.917555	4.469985
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H	-1.762186	1.224065	3.152715
H	-2.053837	-0.624579	3.145662
H	2.053590	0.624032	3.145627
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3-PPh <sub>3</sub>			3-PPh <sub>3</sub> -14e1			4-Py			4-Py-14e1						
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Ru	-0.819037	0.763636	-0.530308	Ru	-0.635308	0.136814	-0.414096	Ru	0.157972	-0.427157	-1.750752	Ru	-0.393020	1.306674	-0.736000
Cl	-1.367670	1.186808	1.795149	Cl	-1.464685	0.375632	1.771472	Cl	0.657583	-2.675977	-1.019411	Cl	-0.922546	2.480007	-1.236383
Cl	0.222285	0.748658	-2.700416	Cl	0.640728	1.004891	-2.553522	Cl	-0.831465	1.600888	-2.509176	Cl	0.731771	0.166630	-2.756161
P	-2.244824	2.585495	-1.260081	P	-4.986460	1.029688	-0.818194	P	-1.786019	-0.171030	0.510702	N	1.895839	-0.103170	0.466541
N	2.035190	0.388382	0.694725	N	1.862425	1.453256	0.379626	N	0.169614	0.181447	-4.155458	N	0.104489	-1.317500	0.847984
N	1.025779	-1.550686	0.650111	N	2.066922	-0.685949	0.866022	N	0.107373	-1.203908	-3.751132	N	-0.702561	5.037832	-1.646441
C	0.862482	-0.228403	0.267459	C	1.221600	0.220708	1.215280	C	-0.431950	-0.036983	0.186663	C	0.516395	-0.160976	0.195805
C	2.872387	-0.531101	1.340295	C	3.031440	0.310285	1.136422	C	-1.989065	-0.068299	1.889990	C	2.278387	-1.159194	1.298327
C	2.245183	-1.739329	1.310892	C	3.153821	-0.011999	1.439872	C	-0.772195	0.165611	2.453688	C	1.174816	-0.921569	1.522860
C	2.497792	1.756490	0.462155	C	1.436942	2.724892	-0.184107	C	-2.893500	-0.223383	-0.433131	C	2.899936	0.741194	-0.168152
C	2.299439	2.769114	1.450844	C	0.648677	3.620970	0.593071	C	-3.301277	-1.457750	-1.015824	C	3.171945	2.048581	0.322788
C	8.223511	4.054105	1.205211	C	0.214705	4.818834	-0.011792	C	-4.297586	-1.414326	-2.016364	C	4.119003	2.832332	-0.369558
C	3.558851	4.367667	0.048858	C	0.558731	5.163905	-1.330900	C	-4.924925	-0.219551	-2.408756	C	4.809745	2.361348	-1.498941
C	3.800880	3.332750	-0.868933	C	1.423909	4.303285	-2.032012	C	-4.592584	0.957897	-1.711752	C	4.590931	1.028420	-1.893142
C	3.317267	2.022504	-0.676888	C	1.896155	3.099425	-1.481411	C	-3.609650	0.981119	-0.708277	C	3.672443	0.191543	-1.235127
C	1.662194	2.501154	2.823114	C	0.390654	3.394702	2.091412	C	-2.791406	-2.816014	-0.504108	C	2.559777	2.584113	1.625802
C	2.632241	1.827659	3.804275	C	1.645204	3.737739	2.906919	C	-3.305730	-3.147453	0.905169	C	3.148349	1.919152	2.876513
C	2.103179	1.222875	4.968290	C	2.026287	2.918666	3.991410	C	-4.493238	-2.606281	1.440965	C	4.434917	1.341800	2.910071
C	2.946204	0.668180	5.944054	C	3.151844	3.230662	4.773225	C	-4.962038	-3.006170	2.707104	C	4.957515	0.811003	4.104897
C	4.343198	0.694157	6.771791	C	3.919848	4.372117	4.485716	C	-4.255671	-3.959761	3.546051	C	4.204636	0.856954	5.289795
C	4.882168	1.286239	4.618336	C	3.551609	5.197544	3.408716	C	-2.598233	-4.011535	1.672227	C	2.919687	1.431459	5.269381
C	4.033776	1.852843	3.647440	C	2.426313	4.881197	2.626792	C	-3.098479	-3.980805	-1.462928	C	2.396433	1.949590	4.073923
C	-1.059586	3.777631	3.445683	C	-0.865584	4.124094	2.604906	C	-1.668959	-4.340055	-2.462057	C	2.626374	4.119828	1.717840
C	-0.139247	4.310743	2.919933	C	-2.124331	3.811245	2.039726	C	2.441527	-5.386380	-3.360267	C	1.830169	6.301042	0.937572
C	2.946204	0.668180	5.944054	C	3.295331	4.446166	2.481494	C	-3.653769	-6.093236	-3.280074	C	2.731033	6.957221	1.796137
C	3.800880	3.332750	-0.868933	C	3.234722	5.406920	3.508363	C	-4.589151	-5.750358	-2.285013	C	3.580110	6.194112	2.613939
C	3.317267	2.022504	-0.676888	C	-1.994001	5.721935	4.083754	C	-4.307722	-4.708442	-1.383251	C	3.526939	4.788166	2.574832
C	1.662194	2.501154	2.823114	C	0.023677	6.420891	-1.975895	C	-5.944947	-0.196414	-3.524481	C	5.759751	3.254757	-2.262331
C	2.632241	1.827659	3.804275	C	2.983696	2.304733	-2.221133	C	-3.439768	2.247000	0.152204	C	6.356983	-1.302807	-1.597189
C	2.103179	1.222875	4.968290	C	4.398488	1.032408	0.193880	C	-4.206064	2.124781	1.464476	C	5.456094	-2.120888	-0.663592
C	2.946204	0.668180	5.944054	C	3.653802	3.458599	-4.425443	C	-5.446383	1.395893	1.553381	C	5.724177	-1.585556	-0.089846
C	4.343198	0.694157	6.771791	C	5.83421	3.591159	-5.822349	C	-6.175428	1.347192	2.757075	C	6.558110	-0.277121	0.722907
C	4.882168	1.286239	4.618336	C	2.792234	2.708911	-6.578109	C	-5.708772	2.023679	3.896003	C	6.231396	-3.718723	0.979413
C	4.033776	1.852843	3.647440	C	2.070975	1.696280	-5.922192	C	-4.508213	2.753336	3.818910	C	5.064602	-4.263254	0.411746
C	-1.059586	3.777631	3.445683	C	1.174140	1.569513	-4.252551	C	-3.785344	2.804350	2.616476	C	4.236432	-3.473060	-0.400913
C	-0.139247	4.310743	2.919933	C	2.927137	2.449394	-3.752485	C	-3.788420	3.556074	-0.577854	C	3.961075	-1.588939	-0.307679
C	2.946204	0.668180	5.944054	C	9.220439	-2.784073	-0.132027	C	-2.810208	4.199132	-1.368855	C	2.956502	-1.419994	-4.056357
C	3.800880	3.332750	-0.868933	C	2.766623	-1.685556	-0.335815	C	-3.099630	5.398245	-2.041738	C	3.221337	-1.671155	-5.412929
C	3.317267	2.022504	-0.676888	C	1.814887	-4.927409	0.368975	C	-4.376114	5.979436	-1.940513	C	4.498591	-2.096082	-5.820649
C	1.662194	2.501154	2.823114	C	1.082829	-4.282909	1.384210	C	-5.357842	5.350229	-1.157032	C	5.505717	-2.027746	-4.856907
C	2.632241	1.827659	3.804275	C	1.192204	-2.901578	1.634518	C	-5.064687	4.153269	-0.478505	C	5.238063	-2.202259	-3.977572
C	2.103179	1.222875	4.968290	C	4.127585	2.04942	-0.742923	C	1.568421	0.433364	1.691769	C	-1.202679	-1.935701	0.876760
C	2.946204	0.668180	5.944054	C	5.584203	-3.177487	1.089219	C	2.119598	1.716428	1.422346	C	-1.648621	-2.704916	-0.233230
C	4.343198	0.694157	6.771791	C	6.731174	-3.200355	1.905838	C	3.483535	1.923411	1.707166	C	-2.910493	-3.325047	-0.141610
C	4.882168	1.286239	4.618336	C	7.648927	-2.138018	1.870725	C	4.296550	0.927461	2.276990	C	3.719826	-3.232721	1.005105
C	4.033776	1.852843	3.647440	C	7.409164	-1.052611	1.011438	C	3.700897	-0.308543	2.590949	C	-3.227829	-2.497118	2.100400
C	-1.059586	3.777631	3.445683	C	6.268418	-1.032408	0.193880	C	2.345467	-0.580561	2.323909	C	-1.977421	-1.849725	2.068992
C	-0.139247	4.310743	2.919933	C	4.554499	-2.504395	-2.147337	C	1.253726	2.894283	0.945282	C	0.780498	-2.043154	-1.478602
C	2.946204	0.668180	5.944054	C	4.164278	-1.753339	-3.277863	C	0.541732	3.608775	2.110518	C	0.109709	-4.194135	1.351874
C	3.800880	3.332750	-0.868933	C	4.561237	-2.123378	-4.574857	C	0.831923	3.359516	3.467843	C	0.013116	-5.114158	-0.287407
C	3.317267	2.022504	-0.676888	C	5.360929	-2.363047	-4.767573	C	0.193939	4.088992	4.902329	C	0.820561	-6.267959	-0.252648
C	1.662194	2.501154	2.823114	C	5.768732	-0.014921	-3.651733	C	-0.743515	5.084414	4.172971	C	1.737524	-6.524489	-1.283977
C	2.632241	1.827659	3.804275	C	5.791123	-6.338825	-3.526204	C	-1.045593	5.340343	2.821659	C	1.849949	-5.698055	-2.348521
C	2.103179	1.222875	4.968290	C	0.532629	-2.272751	2.869317	C	-0.412165	4.608422	1.805307	C	1.048179	-4.458453	-2.378142
C	2.946204	0.668180	5.944054	C	1.563177	-1.843314	3.929292	C	2.030088	3.909347	0.909352	C	-1.608395	-2.984900	-2.775063
C	4.343198	0.694157	6.771791	C	2.843289	-2.425330	4.041350	C	2.737721	4.987292	0.669712	C	-2.143041	-4.190337	-3.281085
C	4.882168	1.286239	4.618336	C	3.721146	-2.047033	5.073565	C	3.464172	5.884567	-0.132277	C	-2.924646	-4.197218	-4.496877
C	4.033776	1.852843	3.647440	C	3.330468	-1.083391	6.010928	C	3.488871	5.724510	-1.529155	C	-3.177566	-2.998151	-5.138730
C	-1.059586	3.777631	3.445683	C	2.054650	-0.497359	5.919179	C	2.773469	4.666703	-2.116288	C	-2.638455	-1.794696	-4.651899
C	-0.139247	4.310743	2.919933	C	1.183423	-0.872433	4.884017	C	2.048650	3.769087	-1.313030	C	-1.861202	-1.788693	-3.480784
C	2.946204	0.668180	5.944054	C	-0.537904	-3.149326	3.538228	C	5.765341	1.167942	2.534858	C	-5.085674	-3.877025	1.051340
C	3.800880	3.332750	-0.868933	C	-0.190012	-4.197953	4.420594	C	1.733990	-1.914921	2.784030	C	-1.466225	-1.121703	3.321702
C	3.317267	2.022504	-0.676888	C	-1.178860	-4.982252	5.038587	C	1.073479	-1.801013	4.168537	C	-0.606528	-2.033041	4.211788
C	1.662194	2.501154	2.823114	C	2.540002	-7.292933	8.006327	C	-0.025468	-6.232612	4.477786	C	4.020294	-1.458387	4.992856
C	2.632241	1.827659	3.804275	C	-2.899193	-3.670341	3.939172	C	-0.632026	-2.588447	5.742398	C	1.210508	-2.274422	5.843134
C	2.103179	1.222875	4.968290	C	0.532629	-2.272751	2.869317	C	-0.150519	-1.710734	6.730640	C			

H	2.865314	2.697690	-5.856182	H	1.444472	0.998184	-6.500341	H	-4.125238	3.285553	4.704370	H	4.791823	-5.313068	0.605106
H	2.238451	1.832396	-3.601486	H	1.540693	0.794353	-4.018303	H	-2.846508	3.378257	2.570775	H	3.327598	-3.912678	-0.840853
H	-0.444243	-5.124851	-1.923266	H	3.405342	-4.667039	-1.080821	H	-1.816471	3.735942	-1.474427	H	1.959611	-1.065362	-3.749804
H	-2.647737	-4.196246	1.669399	H	0.401436	-4.876515	2.011808	H	-2.317463	5.880698	-2.649795	H	2.419406	-1.533699	-6.156106
H	2.076149	-2.398719	-1.430225	H	3.855897	-0.978838	-0.845069	H	-4.602777	6.921048	-2.466022	H	4.706701	-2.295564	-6.884258
H	1.634030	-5.045557	0.730898	H	4.868091	-4.012509	1.138405	H	-6.360858	5.797138	-1.062663	H	6.510370	-2.604327	-5.160256
H	3.403202	-6.592543	1.528243	H	6.903162	-4.057836	2.576337	H	-5.838644	3.685362	0.149362	H	6.033708	-2.177877	-2.753290
H	5.523209	-6.892346	0.207653	H	8.543595	-2.153592	2.513353	H	3.923126	2.905696	1.478007	H	-3.274672	-3.901245	-1.005621
H	5.835219	-3.597045	-1.929278	H	8.113295	-0.203398	0.979098	H	4.312449	-1.098137	3.054621	H	-3.839854	-2.408857	3.011548
H	4.062115	-4.044374	-2.724090	H	6.090722	-0.170958	-0.468777	H	0.464250	2.480859	0.282040	H	-0.100809	-2.070480	-1.580263
H	1.606731	-1.450890	-3.508246	H	3.543353	-0.852442	-3.145536	H	1.573299	2.590561	3.733824	H	-0.708723	-4.937745	0.524706
H	1.395418	-1.697595	-5.972766	H	4.246810	-1.509847	-5.433963	H	0.440481	3.877230	5.543243	H	0.722753	-6.973347	0.588374
H	1.121623	-3.979832	-7.003774	H	5.676961	-3.555843	-5.781419	H	-1.235797	5.661468	4.972009	H	2.362418	-7.431503	-1.261520
H	1.105353	-6.010583	-5.519634	H	6.410813	-4.900059	-3.787397	H	-1.781168	6.116042	2.555322	H	2.570033	-5.791339	-3.162121
H	1.388185	-5.767026	-3.059183	H	5.747431	-4.205528	-1.490587	H	-0.650142	4.825640	0.751470	H	1.143900	-3.754479	-3.220575
H	-3.479094	-5.334917	-1.294596	H	0.833597	-6.499325	-0.744158	H	2.706302	5.137203	1.760969	H	-1.929760	-5.140459	-2.765427
H	-3.301361	-6.124574	0.301777	H	1.226810	-6.947312	0.941753	H	4.008735	6.719157	0.338557	H	-3.331346	-5.149174	-4.827840
H	-2.279113	-6.642158	-1.085619	H	2.523397	-6.877848	-0.304599	H	4.055276	6.430056	-2.158245	H	-3.785410	-3.004074	-6.057793
H	-0.603241	-1.328072	2.676952	H	0.016154	-1.348280	2.536671	H	2.771861	4.534137	-3.209917	H	-2.816223	-0.848360	-5.186906
H	-0.012819	-5.072575	2.675284	H	3.163384	-3.183212	3.309085	H	1.469586	2.957744	-1.782106	H	-1.427790	-0.843523	-3.117382
H	1.739514	-6.170703	4.070274	H	4.717364	-2.513327	5.140218	H	5.993828	2.248785	2.625115	H	-5.155914	-4.738561	0.357505
H	3.071877	-4.820357	5.721632	H	4.015225	-0.790969	6.831427	H	6.378364	0.767602	1.697928	H	-5.870666	-3.146937	0.755296
H	2.611038	-2.357206	5.959406	H	1.733316	0.256489	6.656186	H	6.106391	0.659182	3.459595	H	-5.337962	-4.228323	2.072592
H	0.837237	-1.274350	4.588627	H	0.182306	-0.416295	4.815316	H	0.932528	-2.171354	2.059147	H	-0.808542	-0.298475	2.971251
H	-1.990279	-4.598450	4.088942	H	0.871834	-4.392619	4.640999	H	-0.419900	-3.314465	3.707715	H	0.613617	-0.376417	4.920368
H	-4.083686	-4.663344	5.421629	H	-0.883103	-5.795462	5.720851	H	-1.497459	-3.238052	5.953070	H	2.013551	-1.775157	6.431040
H	-5.447024	-2.573245	5.747033	H	-3.516623	-5.326524	5.294760	H	-0.628585	-1.672662	7.722460	H	1.609867	-4.254839	6.597572
H	-4.690319	-0.428201	4.671488	H	-3.962143	-3.438655	3.762256	H	1.329931	-0.185431	7.201667	H	-0.214224	-5.303913	5.222557
H	-2.616823	-0.385491	3.270426	H	-2.192324	-2.064243	2.647213	H	2.399187	-0.259038	4.948527	H	-1.607237	-3.900206	3.702702
H	-3.638806	0.176255	0.900499	H	-3.024301	-1.760695	0.191120	H	3.302812	-2.982763	4.847705	H	-2.776788	-1.985201	5.649056
H	-5.359564	-3.296213	-2.493414	H	-1.594382	-6.257113	-2.939161	H	4.953613	-4.841382	4.710471	H	-4.668998	-0.877167	6.835280
H	-3.918248	-4.099330	-4.387855	H	0.524991	-5.480480	-4.270381	H	5.322063	-6.053106	2.374446	H	-5.574567	1.315923	6.005235
H	-1.581170	-3.221936	4.654644	H	2.023670	-3.487914	-4.059268	H	4.011414	-5.364213	0.501539	H	-4.551119	2.385998	3.969163
H	-0.676615	-1.532128	-3.037743	H	1.439660	-1.629430	-2.460621	H	2.370747	-3.482484	0.638452	H	-2.664264	1.269331	2.776601
H	-6.718561	-1.519546	-2.039520	H	-3.691307	-4.916826	-3.091115	H	2.976439	-0.925146	-0.166469	H	-3.103846	-4.023594	0.413084
H	-9.045864	-1.844030	-1.207141	H	-5.687346	-6.387420	-2.858109	H	5.933597	1.073552	-3.900944	H	-6.192481	1.894926	-3.003216
H	-9.497476	-1.992047	1.260700	H	-6.811562	-6.651436	-0.625989	H	4.917900	2.177762	-5.906162	H	-5.262633	3.354094	-4.817640
H	-7.584601	-1.809902	2.885263	H	-5.905015	-5.424609	1.372699	H	2.431551	2.361863	-6.129898	H	-2.793754	3.707112	-5.020566
H	-5.254865	-1.506766	2.052848	H	-3.885792	-3.976250	1.146969	H	0.923881	1.418891	-4.339404	H	-1.216244	2.618177	-3.399057
H	-2.776317	0.506007	-3.309094	H	-4.576014	-1.200588	-2.604344	H	5.026803	-2.262045	-0.305198	H	-5.233104	0.285624	1.564085
H	-3.568405	0.598405	-5.668862	H	-5.634155	-1.962841	-4.733544	H	7.270977	-2.795623	0.631378	H	-7.439508	-0.484797	2.429697
H	-3.597267	2.818607	-6.783229	H	-7.493106	-0.623832	-5.770105	H	9.192005	-1.201368	0.307927	H	-9.272195	-1.133147	0.831541
H	-3.569141	4.942400	-5.498231	H	-8.295466	1.471598	-4.641497	H	8.819161	0.952677	-0.932496	H	-8.855741	-1.019879	-1.644407
H	-2.793644	4.850679	-3.133842	H	-7.260670	2.220080	-2.496303	H	6.565407	1.503566	-1.840648	H	-6.641823	-0.271846	-2.511775
H	-5.089168	2.434374	-2.150667	H	-7.702197	-0.389682	-0.749182	H	1.944605	-2.186656	-3.591812	H	-2.046394	4.761056	-0.081364
H	-7.255366	2.714404	-0.959299	H	-8.914462	-1.546928	1.102713	H	1.769690	-3.317478	-5.831164	H	-3.442658	6.795874	-0.645216
H	-7.292443	3.311386	1.481698	H	-7.905033	-1.658848	3.400111	H	-0.316003	-2.941663	-7.237826	H	-2.762553	8.223347	-2.632163
H	-5.122661	3.609127	2.719111	H	-5.650511	-0.624825	3.821829	H	-2.118010	-1.402994	-6.313625	H	-0.709458	7.537477	-3.960662
H	-2.953246	3.282606	1.543637	H	-4.413031	0.489798	1.959607	H	-1.748061	-0.301758	-4.074659	H	0.552156	5.471716	-3.253040
H	-2.935246	5.318457	-0.102161	H	-7.122264	2.455450	0.851023								
H	-1.674608	7.469002	-0.077839	H	-7.707855	4.873394	1.074203								
H	0.624351	7.599722	-1.078829	H	-6.465153	6.604193	-0.257265								
H	1.666063	5.535694	-2.075450	H	-4.617059	5.891946	-1.805049								
H	0.423813	3.372373	-2.071426	H	-4.006146	3.478341	-2.004069								

<b>3-14e1</b>			<b>3-14e1-C11</b>			<b>3-C11</b>			<b>3-C11-MCy1</b>						
<b>-4363.960741</b>			<b>-4442.5149817</b>			<b>-4442.5289144</b>			<b>-4442.5204895</b>						
Ru	0.331682	-0.421391	-1.842406	Ru	0.238114	0.086241	-1.867097	Ru	0.205861	0.076709	-2.060943	Ru	0.396699	-0.039571	-1.899727
Cl	0.694215	-2.718559	-1.572944	Cl	0.511048	-2.28064	-2.155818	Cl	0.778201	-2.274322	-1.634972	Cl	0.772309	-2.423544	-1.694522
Cl	-0.743769	1.377651	-2.841947	Cl	-0.685651	2.196586	-2.213911	Cl	-0.614541	2.343823	-1.822088	Cl	-0.382962	2.239634	-1.981378
N	-1.813802	-0.242533	-0.170833	N	-1.77724	-0.275083	0.240505	N	-1.785323	-0.291953	0.172203	N	-1.877789	-0.257066	0.136773
N	0.085534	0.044714	1.207580	N	-0.171019	-0.064183	1.244877	N	0.149303	-0.143622	1.176220	N	0.021153	-0.193501	1.222452
C	-0.439289	-0.162120	-0.061423	C	-0.406219	-0.065133	-0.018851	C	-0.439559	-0.072838	-0.066526	C	-0.516070	-0.110337	-0.041387
C	-2.089968	-0.291552	-0.540323	C	-1.995689	-0.428294	1.611452	C	-2.019553	-0.503986	1.533075	C	-2.174623	-0.441620	1.492233
C	-0.918045	-0.037648	2.183651	C	-0.795537	-0.287292	2.236461	C	-0.813315	-0.399167	2.161868	C	-0.993110	-0.384872	2.171312
C	-2.886660	-0.319249	-0.815607	C	-2.866039	-0.139575	-0.712768	C	-2.829544	-0.182703	-0.837262	C	-2.883898	-0.082417	-0.901691
C	-3.286353	-1.504170	-1.495511	C	-3.292339	-1.247736	-1.504904	C	-3.129542	-1.286888	-1.690422	C	-3.216377	-1.155519	-1.777936
C	-4.273946	-1.389766	-2.496184	C	-4.272982	-1.010282	-2.491065	C	-4.001898	-1.050387	-2.775292	C	-4.078997	-0.871138	-2.857719
C	-4.889181	-0.166913	-2.816345	C	-4.868377	0.249548	-2.681500	C	-4.620301	0.193555	-2.993224	C	-4.466974	0.399427	-3.060528
C	-4.552812	0.959581	-2.042601	C	-4.529858	1.277591	-1.783373	C	-4.430852	1.201745	-2.028312	C	-4.409025	1.389581	-2.089432
C	-3.584286	0.907514	-1.024675	C	-3.565930	1.104879	-0.773855	C	-3.570649	1.035134	-0.929650	C	-3.559795	1.170715	-0.990655
C	-2.772565	-2.895686	-1.094119	C	-2.822276	-2.690151	-1.238339	C	-2.665980	-2.718752	-1.376348	C	-2.768818	-2.604406	-1.509331
C	-3.320355	-3.358883	0.261779	C	-3.312956	-3.233351	0.111516	C	-3.296315	-3.289349	-0.098569	C	-3.427556	-3.207462	-0.257175
C	-4.537282	-2.884756	0.801744	C	-4.480553	-2.761057	0.474085	C	-4.499094	-2.801715	0.452800	C	-4.628887	-2.718361	0.296777
C	-5.034760	-3.394669	2.016530	C	-4.944129	-3.349322	1.939010	C	-5.076372	-3.411762	1.583167	C	-5.229689	-3.356883	1.398724
C	-4.329362	-4.874264	2.708479	C	-4.252440	-4.429481	2.510894	C	-4.465056	-4.527817	2.176172	C	-4.643317	-4.502291	1.960431
C	-3.117494	-4.874264	2.179073	C	-3.088373	-4.913523	1.883625	C	-3.267375	-5.028391	1.631330	C	-3.446084	-5.002531	1.414247
C	-2.619229	-4.358374	0.971853	C	-2.622816	-4.317533	0.700345	C	-2.689928	-4.413401	0.509479	C	-2.844762	-4.359189	0.320953
C	-3.016045	-3.955996	-2.183982	C	-3.206825	-3.666579	-2.367751	C	-2.875385	-3.715144	-2.529141	C	-2.992945	-3.546142	-2.706078
C	-2.162486	-4.009585	-3.309456	C	-2.366056	-3.808879	-3.494095	C	-2.185402	-4.072532	-3.377653	C	-1.938609	-3.822213	-3.603748
C	-2.375615	-4.948246	-4.32057	C	-2.708567	-4.674852	-4.546711	C	-1.995859	-4.980347	-4.435682	C	-2.136398	-4.667426	-4.710799
C	-3.449260	-5.855392	-4.252887	C	-3.901403	-5.416699	-4.496371	C	-3.259855	-5.548905	-4.664427	C	-3.392284	-5.253750	-4.940818
C	-4.304982	-5.810388	-3.139790	C	-4.745629	-5.286884	-3.380185	C	-4.311113	-5.212055	-3.817302	C	-4.447511	-4.996189	-4.672389
C	-4.088356	-4.871596	-2.114611	C	-4.399447	-4.423292	-2.325777	C	-4.137989	-4.10312	-2.757395	C	-4.247070	-4.156140	-2.938958
C	-5.883163	-0.066555	-3.950029	C	-5.856329	0.481648	-3.800979	C	-5.483137	0.435145	-4.210256	C	-5.499952	0.688994	-4.274107
C	-3.411970	2.119626	-0.094615	C	-3.414813	2.183500	0.314746	C	-3.564589	2.076951	0.203799	C	-3.510187	2.203589	0.147681
C	-4.272161	1.970377	1.176501	C	-4.215151	1.800692	1.576083	C	-4.421682	1.604189	1.380026	C	-4.461160	1.794779	1.290636
C	-5.497000	1.268765	1.182777	C	-5.421579	1.069987	1.514628	C	-5.621193	0.850782	1.187601	C	-5.675477	1.113086	1.056459
C	-6.274886	1.190430	2.358428	C	-6.158145	0.789616	2.681553	C	-6.435249	0.488194	2.276870	C	-6.546833	0.800523	2.117377
C	-5.840162	1.810634	3.541092	C	-5.697919	1.231168	3.932921	C	-6.079753	0.865213	3.582500	C	-6.216090	1.158271	3.434816
C	-4.621803	2.514533	3.541448	C	-4.495915	1.959263	4.005994	C	-4.904744	1.611337	3.787536	C	-5.007586	1.835348	3.680647
C	-3.849323	2.594800	2.371790	C	-3.766127	2.242012	2.840661	C	-4.098596	1.978375	2.697980	C	-4.143179	2.151202	2.620143
C	-3.671627	3.473226	-0.782516	C	-3.792121	3.607351	-0.139404	C	-3.978908	3.497828	-0.224919	C	-3.791028	3.652051	-0.296529
C	-2.651813	4.069266	-1.558194	C	-2.812717	4.448620	-0.712601	C	-2.994262	4.439212	-0.597685	C	-2.725609	4.467543	-0.736509
C	-2.857950	5.304528	-2.194912	C	-3.132555	5.751697	-1.130435	C	-3.348376	5.742149	-0.987445	C	-2.950455	5.975258	-1.146168
C	-4.091165	5.969499	-0.272194	C	-4.441413	6.243145	-0.985570	C	-4.697981	6.133565	-1.013526	C	-4.249311	6.330302	-1.127191
C	-5.113550	5.386737	-1.505338	C	-5.425018	5.419096	-0.413403	C	-5.688389	5.210459	-0.637231	C	-5.318356	5.530861	-0.688922
C	-4.903735	4.152464	-0.663136	C	-5.101581	4.117448	0.007976	C	-5.330984	3.909547	-0.241042	C	-5.090140	4.206964	-0.272398
C	1.445802	0.356572	1.587801	C	1.563994	0.082664	1.604137	C	1.558096	0.008954	1.500347	C	1.428994	-0.092577	1.573903
C	1.918949	1.693584	1.488397	C	2.167619	1.370479	1.613580	C	2.109461	1.316423	1.609891	C	2.028707	1.194472	1.682537
C	3.233731	1.963531	1.918940	C	3.528910	1.457161	1.962692	C	3.483500	1.431063	1.898785	C	3.398723	1.258450	2.005680
C	4.070879	0.972404	2.461378	C	4.291422	0.331105	2.326853	C	4.306274	0.311184	2.114903	C	4.170135	0.110082	2.258147
C	3.554812	-0.333332	2.579643	C	3.964330	-0.916956	2.371098	C	3.706381	-0.960986	2.085844	C	3.524913	-1.139258	2.215235
C	2.250781	-0.666131	2.106477	C	2.284423	-1.068737	2.029672	C	2.339367	-1.144900	1.802557	C	2.160538	-1.273604	1.894851
C	1.035671	2.854225	1.658270	C	1.360533	2.650573	1.349995	C	1.236209	2.580212	1.529747	C	1.210263	2.492294	1.567299
C	0.304810	3.866065	2.160400	C	0.603263	3.133248	2.601404	C	0.434282	2.828838	2.820690	C	0.385796	2.787854	2.834121
C	0.516970	3.263785	3.521076	C	0.861239	2.644001	3.898923	C	0.727064	2.198719	4.047961	C	0.623640	2.161461	4.075117
C	-0.158331	3.972691	4.533972	C	0.188339	3.171676	5.018177	C	0.015975	3.927422	5.218492	C	-0.097068	2.536804	5.225509
C	-1.055622	5.000402	4.203655	C	-0.471392	4.202610	4.860298	C	-0.996923	3.498966	5.183879	C	-1.064233	3.552116	5.156388
C	-1.280597	5.309388	2.848519	C	-1.021047	4.697378	3.569850	C	-1.298527	4.136544	3.965210	C	-1.310763	4.186109	3.923546
C	-0.610150	4.598699	1.841118	C	-0.535814	4.164977	2.455568	C	-0.593163	3.800927	2.798853	C	-0.596832	3.808385	2.776903
C	1.813438	3.853991	0.132297	C	2.214002	3.786855	0.762253	C	2.034456	3.843313	1.163993	C	2.070027	3.719270	1.216303
C	2.459944	4.982128	0.685718	C	2.873232	4.726078	1.586695	C	2.649331	4.647388	2.150611	C	2.695466	4.497700	2.217090
C	3.196849	5.860060	-0.127851	C	3.675066	5.736641	1.027729	C	3.400386	5.760056	1.791502	C	3.501175	5.597743	1.876091
C	3.292635	5.631214	-1.511491	C	3.825048	5.830304	-0.367011	C	3.544039	6.133766	0.438136	C	3.689354	5.944620	0.526447
C	2.640164	4.520744	-0.074525	C	3.162591	4.909137	-1.196934	C	2.925419	5.348289	-0.549688	C	3.060514	5.185413	-0.475206
C	1.907807	3.640055	-1.259749	C	2.364026	3.897275	-0.636345	C	2.176614	4.214635	-0.189022	C	2.257614	4.082883	-0.133515
C	5.487180	1.288277	2.882651	C	5.764707	0.457229	2.635848	C	5.787368	0.466929	2.366808	C	5.645326	0.211607	2.567283
C	1.711920	-2.083585	2.408858	C	1.621217	-2.440372	2.187780	C	1.722781	-2.548344	1.944227	C	1.488846	-2.653095	2.017371
C	0.969154	-2.187535	3.750047	C	1.037580	-2.642897	3.600842	C	1.013280	-2.712644	3.298139	C	0.708679	-2.780068	3.335518
C	-0.125748	-3.071998	3.866276	C	-0.088278	-3.480306	3.766065	C	-0.124973	-3.543170	3.390163	C	-0.464323	-3.564474	3.377153
C	-0.809973	-3.220198	5.083211	C	-0.629334	-3.723909	5.037926	C	-0.779724						

H	-5.708067	3.718790	-0.049069	H	-5.879526	3.495684	0.479234	H	-6.118965	3.210094	0.078500	H	-5.935929	3.603177	0.091434
H	3.616752	2.990396	1.819659	H	4.012275	2.445794	1.945403	H	3.923306	2.437635	1.960662	H	3.874882	2.248062	2.070768
H	4.188810	-1.128571	3.002998	H	4.214795	-1.811603	2.664545	H	4.321693	-1.850325	2.292089	H	4.099545	-2.050284	2.443148
H	0.249072	2.422967	0.351738	H	0.600519	2.408711	0.576570	H	0.502962	2.429428	0.706866	H	0.496215	2.364337	0.723771
H	1.224252	2.467960	3.799730	H	1.605819	1.845976	4.043703	H	1.528257	1.444880	4.095354	H	1.389640	1.374006	4.149501
H	0.026942	3.718639	5.590137	H	0.409528	2.774149	6.021896	H	0.264640	2.021921	6.165527	H	0.108459	2.033602	6.184059
H	-1.577269	5.560777	4.995817	H	-1.270837	4.622216	5.736532	H	-1.346375	3.763867	6.101299	H	-1.620620	3.853800	6.058189
H	-1.986281	6.108690	2.571736	H	-1.757814	5.504069	3.428121	H	-2.087647	4.904376	3.922649	H	-2.063621	4.987606	3.853996
H	-0.790564	4.854631	0.784535	H	-0.565856	4.568705	1.452399	H	-0.826952	4.317284	1.853689	H	-0.787655	4.317491	1.820582
H	2.371196	5.187407	1.764760	H	2.746200	4.675108	2.679915	H	2.530376	4.390224	3.215269	H	2.540926	4.247479	3.278841
H	3.693325	6.734846	0.323615	H	4.179878	6.460177	1.688224	H	3.870902	6.393766	2.576784	H	3.978431	6.191884	2.672315
H	3.865538	6.322599	-2.150100	H	4.448722	6.625850	-0.805575	H	4.129399	7.023821	0.156232	H	4.316659	6.810037	0.258190
H	2.693465	4.335765	-3.159228	H	3.259770	4.977472	-2.292108	H	3.020792	5.616068	-1.614150	H	3.190129	5.447868	-1.537177
H	1.388532	2.780992	-1.713957	H	1.832993	3.191163	-1.293795	H	1.678959	3.612729	-0.964539	H	1.750704	3.503508	-0.921429
H	5.620418	2.374019	3.049770	H	6.007434	1.445529	3.075968	H	6.025478	1.452091	2.816176	H	5.903825	1.193698	3.012076
H	6.207418	0.972834	2.096292	H	6.365582	0.353309	1.705744	H	6.352273	0.394086	1.411448	H	6.247180	0.100890	1.638771
H	5.765977	0.751083	3.812459	H	6.106989	-0.332168	3.334878	H	6.175741	-0.327807	3.035553	H	5.973100	-0.586415	3.264082
H	0.967033	-2.291192	1.611451	H	0.748957	-2.464509	1.490958	H	0.954824	-2.649992	1.148129	H	0.756860	-2.735362	1.185442
H	-0.456945	-3.642378	2.983880	H	-0.556899	-3.936546	2.879761	H	-0.516580	-4.026833	2.481360	H	-0.831429	-4.038402	2.453187
H	-1.669778	-3.906169	5.142544	H	-1.514783	-4.371895	5.136812	H	-1.675790	-4.380176	4.656338	H	-2.103330	-4.336327	4.573161
H	-0.949017	-2.599512	7.169477	H	-0.477409	-3.323684	7.177091	H	-0.818326	-3.267230	6.745420	H	-1.301011	-3.242318	6.695370
H	0.999143	-1.020209	6.992363	H	1.526534	-1.829109	6.913017	H	1.214444	-1.793771	6.614102	H	0.793040	-1.851690	6.653778
H	2.203883	-0.750744	4.826169	H	2.475946	-1.388362	4.651284	H	2.365774	-1.433635	4.429371	H	2.058026	-1.550078	4.523041
H	3.088234	-3.523151	4.388962	H	3.168213	-4.151650	3.773067	H	3.153129	-4.067648	3.816894	H	2.773896	-4.197634	3.973704
H	4.898968	-5.207167	4.069232	H	4.689547	-5.975737	3.011288	H	4.811751	-5.871896	3.384314	H	4.386919	-6.062824	3.641075
H	5.647274	-5.838121	1.753642	H	4.905787	-6.504323	0.563373	H	5.340534	-6.570475	1.027020	H	5.005549	-6.806452	1.319876
H	4.552032	-4.756770	-0.238415	H	3.575068	-5.177246	-1.112202	H	4.179185	-5.424267	-0.889666	H	3.980565	-5.643092	-0.662820
H	2.745845	-3.065531	0.084749	H	2.067352	-3.343824	-0.352580	H	2.532493	-3.596268	-0.450001	H	2.376566	-3.756154	-0.322828
H	3.300188	-0.029007	-0.063122	H	3.108811	-0.676735	-0.247291	H	3.024770	-1.095216	-0.985329	H	3.193057	-1.400945	-1.443243
H	5.897660	0.060796	-4.516895	H	5.982792	1.224669	-4.088242	H	5.997269	2.180638	-3.623673	H	6.246980	2.391083	-3.129170
H	4.705790	0.184960	-6.719787	H	4.947331	2.520478	-5.967250	H	5.020023	4.111249	-4.886646	H	5.313305	4.386591	-4.321454
H	2.208543	0.309786	-6.806554	H	2.480837	2.939759	-6.011180	H	2.548419	4.520439	-4.854718	H	2.840175	4.625742	-4.693558
H	0.860224	0.305571	-4.692454	H	1.005517	2.035140	-4.186735	H	1.027154	2.987339	-3.564054	H	1.268448	2.885441	-3.723910
H	5.366029	-1.530098	0.085985	H	4.984046	-2.240406	-0.667776	H	5.023849	-2.278766	-1.635829	H	5.360193	-2.350873	-2.085234
H	7.697801	-1.672902	0.964153	H	7.213691	-3.036672	0.101699	H	7.248805	-3.198120	-0.994983	H	7.569379	-3.257968	-1.362349
H	9.523061	-0.275005	-0.057445	H	9.251498	-1.590126	-0.200966	H	9.213307	-1.657539	-0.682143	H	9.359546	-1.705433	-0.522811
H	8.980662	1.278565	-1.956323	H	9.016621	0.675141	-1.263956	H	8.905678	0.919346	-0.978404	H	8.897488	0.760541	-0.379994
H	6.647798	1.436546	-2.821976	H	6.782667	1.484002	-2.014592	H	6.672471	1.743211	-1.579086	H	6.677315	1.662810	-1.065462
C	-1.071114	-0.234281	-1.542287	C	-0.076311	-0.716930	-5.561100	C	-0.376863	0.531288	-4.157230	C	-0.245504	-0.192861	-3.883627
C	0.076311	-0.716930	-5.561100	C	0.703032	-0.168090	-6.283798	C	0.156759	-0.764192	-4.135783	C	1.175276	-0.365887	-4.051693
H	0.475930	-1.671953	-5.181892	H	-1.503455	0.730541	-5.500330	H	1.187066	-0.967215	-4.469155	H	1.720450	0.389843	-4.635560
H	-1.503455	0.730541	-5.500330	H	-1.736924	-0.785504	-4.423919	H	-0.505020	-1.643916	-4.094768	H	1.585540	-1.388161	-4.084997
H	-1.736924	-0.785504	-4.423919	H	-1.469000	0.688367	-4.121149	H	0.205747	1.384920	-4.534003	H	-0.724627	0.733613	-4.245576
H	-1.469000	0.688367	-4.121149	H	-0.877116	-1.101102	-3.904967	H	-0.877116	-1.101102	-3.904967	H	-0.877116	-1.101102	-3.904967

3-MCy1			3-MCy1-C12			3-C12			3-C12-14e2						
-4442.5310542			-4442.5227741			-4442.5255245			-4442.5035965						
Ru	-0.440497	-0.052757	-1.815723	Ru	-0.523915	-0.444750	-1.724262	Ru	-0.816071	-0.052637	-1.616819	Ru	-0.716586	0.336007	0.709411
Cl	-0.704359	2.343174	-1.855708	Cl	-0.274653	1.865658	-2.374714	Cl	-2.456814	0.061799	0.132141	Cl	-1.824059	-0.425840	-1.179944
Cl	0.085195	-2.392511	-1.669695	Cl	-0.823553	-2.662234	-0.836038	Cl	1.250356	-0.014169	-2.933320	Cl	-0.245928	2.188659	2.054791
N	1.898831	0.114823	0.120661	N	1.889243	-0.245497	0.201301	N	1.204774	1.192157	0.449602	N	2.177123	-0.614156	0.802017
N	0.013073	0.334887	1.217806	N	0.123818	0.582163	1.108097	N	0.995426	-0.981442	0.675271	N	1.131118	0.051291	0.168529
C	0.527972	0.108414	-0.036969	C	0.561847	-0.038222	-0.042025	C	0.541165	0.091757	-0.061218	C	3.384390	-0.401573	0.122452
C	2.252547	0.357240	1.459601	C	2.254775	0.078421	1.485343	C	2.054413	0.794756	1.489677	C	3.113999	0.401548	-0.943943
C	1.051668	0.471680	2.147160	C	1.150386	0.640075	2.056555	C	1.934016	-0.558036	1.621498	C	2.097568	-1.470692	1.966179
C	2.874276	-0.210664	-0.911311	C	2.811622	-0.102384	-0.693594	C	1.151602	2.560720	-0.036423	C	2.097568	-1.470692	1.966179
C	3.265879	0.768713	-1.868859	C	3.493871	-0.282404	-1.703802	C	0.092506	3.427450	0.372290	C	1.708823	-2.829590	1.808501
C	4.090806	0.346837	-2.923011	C	4.342006	-0.989761	-2.581797	C	0.055577	4.725312	-0.178888	C	1.625467	-3.633777	2.964228
C	4.565626	-0.972557	-3.046137	C	4.566992	-2.372448	-2.468545	C	1.034423	5.202551	-1.067107	C	1.922386	-3.141290	4.247208
C	4.269442	-1.871115	-2.005176	C	3.949544	-3.053655	-1.403237	C	2.219407	4.357475	-1.362253	C	2.346265	-1.802487	4.359701
C	3.453499	-1.513732	-0.916720	C	3.086487	-2.410897	-0.496235	C	2.217150	3.048833	-0.852986	C	2.457275	-0.952946	3.243296
C	2.900997	2.256962	-1.714823	C	3.405758	1.251970	-1.801845	C	-0.933627	3.037052	1.450807	C	4.119994	-3.450100	0.432113
C	3.593776	2.922977	-0.512689	C	4.221972	1.962397	-0.706659	C	-0.343198	3.086263	2.871775	C	2.661637	-4.106437	-0.201528
C	4.578091	2.406650	0.029028	C	5.228117	1.320954	0.045185	C	0.880395	3.691714	3.192935	C	3.899073	-4.228650	0.463209
C	5.402476	3.104524	1.132511	C	6.004867	2.039679	0.974455	C	1.330770	3.758637	4.525850	C	4.993281	-4.862173	-0.157601
C	4.897951	4.336552	1.578653	C	5.794684	3.415234	1.160683	C	-0.560028	3.210213	5.563174	C	4.867665	-5.387859	-1.453062
C	3.737368	4.863455	0.980602	C	4.794638	4.067554	0.414667	C	0.0644716	2.586628	5.256324	C	3.638637	-5.268196	-2.129326
C	3.091770	4.161247	-0.049423	C	4.015336	3.346669	-0.504119	C	-1.106745	2.513518	3.926080	C	2.550922	-4.632155	-1.511166
C	3.179757	3.099980	-2.972378	C	3.819088	1.798328	-3.181672	C	-2.211900	3.896979	1.406703	C	0.226668	-4.420766	0.461135
C	2.127467	3.452476	-3.844676	C	2.841907	2.056953	-4.167387	C	-3.331668	3.476535	0.656618	C	-1.078856	-3.943681	0.210497
C	2.373236	4.217956	-4.999487	C	3.210038	2.533839	-5.438611	C	-4.491502	4.269412	0.584925	C	-2.184906	-4.810678	0.268192
C	3.675998	4.646592	-5.303403	C	4.561205	2.764009	-5.747548	C	-4.554691	5.497863	1.264122	C	-2.005831	-6.170700	0.574028
C	4.731045	4.315735	-4.433295	C	5.542412	2.525040	-4.768777	C	-3.451702	5.921590	2.026725	C	-0.709000	-6.660480	0.808458
C	4.483047	3.557096	-3.277306	C	5.173687	2.053288	-3.497559	C	-2.295339	5.126311	2.100810	C	0.396473	-5.794429	0.746848
C	5.380034	-1.408302	-4.242527	C	5.449019	-3.108515	-3.451141	C	0.930052	6.579041	-1.681984	C	1.778193	-4.011194	5.475190
C	3.334651	-2.463737	0.287303	C	2.574570	-3.187177	0.728372	C	3.516926	2.259935	-1.089051	C	3.039117	0.459809	3.407771
C	4.431754	-2.057778	1.403353	C	3.388340	-2.803374	1.981810	C	4.435751	2.314548	0.140173	C	4.518844	0.502865	2.997332
C	5.570214	-1.465493	1.131529	C	4.774416	-2.563466	1.927713	C	4.531819	3.507581	0.931294	C	5.397828	-0.576117	3.237135
C	6.464868	-1.153920	2.173347	C	5.501557	-2.275856	3.098021	C	5.412562	3.566941	0.207670	C	6.756412	-0.493905	2.879198
C	6.119962	-1.423708	3.507942	C	4.853962	-2.247485	4.344981	C	6.212588	2.458667	2.354405	C	7.258617	0.669409	2.271435
C	4.873141	-2.011199	3.790999	C	3.474370	-2.514080	4.019022	C	6.126823	1.292649	1.572282	C	6.391161	1.749593	2.026208
C	3.985378	-2.326938	2.749927	C	2.752995	-2.805131	3.241845	C	5.249613	1.238344	0.476913	C	5.037508	1.665816	2.387919
C	3.504305	-3.954513	-0.061500	C	2.530900	-4.712297	0.499660	C	4.257167	2.683963	-2.376058	C	2.809888	1.036975	4.816742
C	2.377505	-4.717025	-0.440339	C	1.522500	-5.260508	-0.326218	C	3.627274	2.410194	-3.634770	C	1.523385	1.514526	5.160492
C	2.502565	-6.079103	-0.762003	C	1.461442	-6.642623	-0.566621	C	4.317290	2.781289	-4.825198	C	1.265070	2.025406	6.442604
C	3.759357	-6.707470	-0.714703	C	2.406989	-7.509365	0.011202	C	5.562020	3.463670	-4.787387	C	2.286567	2.070196	7.409021
C	4.888018	-5.961083	-0.336331	C	3.411712	-6.977044	0.834882	C	6.153186	3.712676	-3.544655	C	3.569277	1.605208	7.076476
C	4.760216	-4.599585	-0.007297	C	3.471111	-5.592012	1.078855	C	5.507390	3.388845	-2.350700	C	3.828732	1.095446	5.790403
C	-1.398655	0.435489	1.565770	C	-1.174003	1.221497	1.264272	C	0.523827	-2.359929	0.579284	C	1.061748	1.268819	-2.070093
C	-2.159398	-0.755668	1.739439	C	-2.324827	0.443219	1.585839	C	1.098468	-3.253243	-0.376522	C	0.664390	2.634825	-2.046437
C	-3.531209	-0.620635	2.031803	C	-3.572838	1.097126	1.598626	C	0.571920	-4.588215	-0.454566	C	-0.065747	3.127743	-3.147590
C	-4.150095	0.632073	2.194391	C	-3.708391	2.476512	1.353330	C	-0.445603	-5.021417	0.399547	C	-0.380791	2.332970	-4.264206
C	-3.347643	1.782344	2.088643	C	-2.535783	3.230034	1.165191	C	-0.914498	-4.146902	1.393346	C	0.124075	1.020205	-4.299852
C	-1.973859	1.719049	1.789103	C	-1.258619	2.639430	1.143769	C	-0.440368	-2.826345	1.522617	C	0.863505	0.473909	-3.253924
C	-1.049958	-2.148287	1.758672	C	-2.216542	-1.022165	2.042686	C	2.341810	-2.897937	-1.211112	C	1.101404	3.595977	-0.929611
C	-0.693319	-2.400318	3.042836	C	-1.522206	-1.167031	3.413977	C	3.634177	-2.913384	-0.377798	C	2.599099	3.931470	-0.991916
C	-0.852349	-1.641796	4.221430	C	-1.196160	-0.108195	4.338634	C	3.745654	-3.563800	0.868764	C	3.367150	3.810829	-2.168602
C	-0.149464	-1.973805	5.395950	C	0.863481	-0.317821	5.615353	C	4.978095	-3.618667	1.548496	C	4.722922	4.191060	-2.188921
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C	0.190606	-3.504026	3.073606	C	-1.074592	-2.446808	3.805166	C	4.794058	-2.319596	-0.927935	C	3.225341	4.446580	0.166684
C	-2.506626	-3.298159	1.553618	C	-3.566300	-1.761429	2.081213	C	2.510847	-3.798473	-2.450114	C	0.248634	4.876841	-0.883344
C	-3.202490	-3.875935	2.640210	C	-4.423676	-1.669684	3.202605	C	3.224870	-5.017247	-2.388654	C	0.674844	6.082121	-1.482800
C	-4.122596	-4.918192	2.435206	C	-5.651085	-2.352578	3.232906	C	3.338287	-5.846106	-3.518362	C	-0.138724	7.229136	-1.457180
C	-4.356092	-5.408621	1.138185	C	-6.039095	-3.156071	2.145627	C	2.748375	-5.467114	-4.736908	C	-1.393267	7.192828	-0.825873
C	-3.661352	-4.848424	0.052523	C	-5.191091	-3.261771	1.029999	C	2.051565	-4.249028	-4.815190	C	-1.826450	5.999503	-0.220710
C	-2.744953	-3.801067	0.257248	C	-3.968344	-2.566106	0.994248	C	1.933583	-3.423581	-3.682976	C	-1.014516	4.833228	-0.502525
C	-5.628111	0.740755	2.482852	C	-5.071146	3.125586	1.315284	C	-0.979907	-6.429438	0.267945	C	-1.233745	2.870400	-5.389727
C	-1.131666	3.005344	1.849664	C	-0.009153	3.536905	1.156852	C	-0.863699	-2.006706	2.753868	C	1.535539	-0.896227	-3.415353
C	-0.354027	3.098395	3.172216	C	0.119737	3.720088	2.593743	C	0.241083	-0.035263	3.823028	C	2.982917	-0.747100	-3.922449
C	0.912921	3.720147	3.191684	C	1.899490	3.926911	2.803324	C	0.478185	-0.891847	4.615373	C	3.932892	-1.741381	-3.597326
C	1.633809	3.858687	4.388857	C	2.411566	4.142423	4.092613	C	1.458623	-0.897390	5.621122</				

H	-4.131317	-1.534253	2.154954	H	-4.471858	0.503291	1.819474	H	0.994628	-5.244406	-1.203493	H	-0.395931	4.177050	-3.127265
H	-3.800768	2.772316	2.251353	H	-2.611074	4.320810	1.035706	H	-1.676158	-4.496660	2.106767	H	-0.063003	0.390201	-5.183729
H	-0.796530	-2.205684	0.903000	H	-1.587106	-1.565982	1.303608	H	2.210549	-1.862851	-1.596090	H	0.936476	3.083486	0.042463
H	-1.541280	-0.782744	4.227912	H	-1.772953	0.896993	4.060963	H	2.859832	-4.041843	1.315106	H	2.899910	3.415798	-3.084452
H	-0.291594	-1.366609	6.304452	H	-0.784911	0.526459	6.318957	H	5.039976	-4.132418	2.521234	H	5.303755	4.086635	-3.119425
H	1.261466	-3.342613	6.336135	H	0.007645	-1.761699	6.995586	H	7.089801	-3.082247	1.514266	H	6.390640	5.008945	-1.049906
H	1.558855	-4.714977	4.246614	H	-0.187411	-3.669503	5.365876	H	6.917351	-1.918190	-0.710343	H	5.039531	5.240049	1.060289
H	0.315993	-4.119453	2.167815	H	-1.170437	-3.288912	3.100120	H	4.727664	-1.821127	-1.908993	H	2.634113	4.558589	1.090538
H	-3.011643	-3.514416	3.663178	H	-4.119217	-1.064664	4.071568	H	3.706779	-5.318810	-1.444989	H	1.660392	6.126970	-1.971909
H	-4.652445	-5.355800	3.296899	H	-6.302095	-2.266232	4.118025	H	3.899451	-6.791878	-3.446299	H	0.215530	8.158924	-1.930987
H	-5.070351	-6.232161	0.976536	H	-6.993661	-3.706101	2.174271	H	2.842349	-6.113254	-5.624410	H	-2.028896	8.092450	-0.799694
H	-3.825565	-5.225886	-0.968827	H	-5.471670	-3.897239	0.175178	H	1.601435	-3.930084	-5.769233	H	-2.804048	5.968004	0.285560
H	-2.187063	-3.379917	-0.594917	H	-3.303803	-2.665488	0.120860	H	1.415473	-2.454122	-3.755936	H	-1.356906	3.926989	0.236404
H	-6.000430	-0.138856	3.046377	H	-5.737541	2.722370	2.105253	H	-1.469294	-6.581163	-0.718027	H	-2.301796	2.604567	-5.228860
H	-6.208946	0.791327	1.535877	H	-5.571986	4.226729	0.342755	H	-1.722697	-6.661761	1.056140	H	-0.5738254	2.443869	-6.369872
H	-5.865677	1.655322	3.062987	H	-5.005486	4.225048	1.439164	H	-0.162761	-7.178945	0.332897	H	-1.177865	3.975526	-5.456132
H	-0.386254	2.948411	1.027351	H	0.783963	3.014799	0.582787	H	-0.986016	-0.952371	2.424279	H	1.600791	-1.372118	-2.414575
H	1.350763	4.085475	2.249701	H	2.586482	3.905477	1.942856	H	-0.102177	0.025507	4.431388	H	3.634731	-2.587079	-2.957352
H	2.627010	4.333392	4.372669	H	3.494816	4.291167	4.228646	H	1.629713	0.014090	6.215005	H	5.972484	-2.452729	-3.801031
H	1.663039	3.481946	6.537614	H	1.951309	4.329765	6.217118	H	2.994115	-2.060445	6.645913	H	6.684725	-0.531315	-5.265016
H	-0.598844	2.384158	6.534886	H	-0.513965	3.973787	5.872368	H	2.579408	-4.118405	5.262170	H	5.013379	1.248969	-5.863328
H	-1.871548	2.134858	4.401599	H	-1.417698	3.576679	3.582217	H	0.840774	-4.100258	3.473798	H	2.675291	1.115633	-5.008406
H	-2.030139	4.932848	3.682531	H	-0.952525	5.986711	2.290385	H	-1.448370	-3.198264	5.228147	H	1.927928	-1.611683	-6.096017
H	-3.396435	6.961276	3.228163	H	-1.081387	8.171828	1.144332	H	-3.666460	-3.879836	6.117734	H	0.564824	-3.174414	-7.478923
H	-4.105537	7.514209	0.880035	H	-0.682730	8.377791	-1.330200	H	-5.748267	-3.514600	4.754223	H	-1.413127	-4.357946	-6.474915
H	-3.423734	5.992167	-1.005537	H	0.035179	6.350884	-2.638377	H	-5.559045	-2.453645	2.476395	H	-2.013861	-3.937399	-4.066419
H	-2.067201	3.945813	-0.541305	H	0.318357	4.150643	-1.490440	H	-3.335632	-1.774937	1.585974	H	-0.676787	-2.336115	-2.701525
H	-3.179539	1.465753	-2.163312	H	-2.957819	1.308360	-2.641558	H	-3.411868	1.150800	-3.588138	H	-7.578056	-0.863665	2.917621
H	-6.222265	-2.667767	-2.704711	H	-6.529384	-2.422886	-2.325090	H	-6.790286	-2.018548	-1.300036	H	-9.663193	1.342220	-1.278318
H	-5.344290	-4.792651	-3.690280	H	-5.977397	-4.787714	-2.942121	H	-6.110652	-4.322975	-0.589560	H	-8.662181	3.410629	-2.259870
H	-2.923757	-5.005345	-4.297437	H	-3.655210	-5.417602	-3.622477	H	-3.762026	-5.112381	-0.903084	H	-6.624924	4.452543	-1.263166
H	-1.344812	-3.097817	-3.896429	H	-1.846231	-3.682611	-3.719649	H	-2.041545	-3.611745	-1.943402	H	-5.561632	3.448424	0.778281
H	-5.453612	2.216096	-2.652120	H	-5.262846	2.189844	-3.292346	H	-5.763705	1.462446	-4.579604	H	-10.110379	-1.171830	2.955256
H	-7.623351	3.170958	-1.877366	H	-7.270934	3.512997	-2.617578	H	-7.766575	2.955569	-4.587110	H	-11.948908	-2.813597	2.548737
H	-9.245828	1.743624	-0.591652	H	-8.880224	2.588640	-0.920826	H	-9.273912	3.056148	-2.577653	H	-12.530195	-3.502026	0.201611
H	-8.646417	-0.637470	-0.053957	H	-8.427149	0.348855	0.127177	H	-8.734379	1.669468	-0.552004	H	-11.230743	-2.551302	-1.727546
H	-6.456541	-1.576733	-0.786420	H	-6.400837	-0.954043	-0.517520	H	-6.709558	0.211426	-0.530633	H	-9.372440	-0.940985	-1.318545
C	0.330476	-0.023299	-3.619407	C	0.736381	-1.068315	-2.911520	C	-0.974017	1.722155	-1.977292	C	-1.041626	-0.959692	1.926320
C	-1.216965	0.007075	-3.949858	C	-1.215591	-0.667154	-3.948145	C	-1.427662	-1.014008	-3.493720	C	-5.583688	1.238556	2.924046
H	-1.352935	-0.737919	-4.757342	H	-0.904677	-1.538785	-4.548624	H	-0.938496	-2.003968	-3.496826	H	-4.888351	2.080938	2.781822
H	-1.501576	1.027066	-4.266558	H	-0.978738	0.325450	-4.361328	H	-1.138312	-0.357128	-4.327829	H	-5.406755	0.580845	3.790061
H	0.844597	-0.951887	-3.934407	H	0.954743	-2.157099	-3.003289	H	-0.248671	2.251101	-2.633595	H	-0.390130	-1.772151	2.301166
H	0.834843	0.910918	-3.931587	H	1.331981	-0.399781	-3.572715	H	-1.829396	2.310332	-1.579980	H	-2.079889	-0.915384	2.348686

3-14e2			3-14e2-CI3			3-CI3			3-CI3-MC2						
-3825.8992412			-3904.4485411			-3904.4649785			-3904.4649793						
Ru	0.499854	0.048857	-2.463274	Ru	0.621491	0.029273	-2.269865	Ru	-0.096714	-0.159413	-2.571431	Ru	-0.196830	0.271430	-2.450526
Cl	-1.184186	-1.394095	-3.144286	Cl	-1.066333	-1.370995	-3.035639	Cl	-0.855808	-2.145664	-2.433288	Cl	-2.031610	1.816299	-2.137637
N	0.817024	1.701449	0.332765	N	2.934666	0.287465	-1.879086	N	0.878967	-2.366918	-2.218079	Cl	1.707171	-1.698728	-2.766452
N	0.268149	-0.151755	0.302730	N	-0.014867	1.171697	0.479037	N	1.147606	0.267678	0.318630	N	0.756015	0.716263	0.392455
C	0.185387	0.097343	-0.543183	N	0.145098	-1.022079	0.474352	N	-0.992333	0.241840	0.327994	N	-0.919817	-0.695395	0.419887
C	0.021856	0.733091	1.658795	C	0.166792	0.090035	-0.377920	C	0.076558	-0.016231	-0.512917	C	-0.120579	0.039379	-0.432055
C	0.189830	-0.618697	1.642167	C	-0.119450	0.740481	1.808403	C	0.724607	0.146728	1.675652	C	0.490396	0.423212	1.735400
C	-0.209302	2.557683	-0.018074	C	-0.008240	-0.617097	1.804593	C	-0.588051	-0.159085	1.663583	C	-0.543962	-0.466290	1.752387
C	-1.524634	2.991825	-0.344599	C	-0.159669	2.567061	0.122294	C	2.524255	0.488790	-0.071373	C	1.901741	1.467023	-0.096398
C	-1.711642	4.348304	-0.679016	C	-1.429958	3.052687	-0.296490	C	2.915561	1.805420	-0.458882	C	1.738803	2.794162	-0.589189
C	-0.653943	5.275528	-0.688382	C	-1.539543	4.416308	-0.636161	C	4.248713	1.999150	-0.873978	C	2.850638	3.399251	-1.214456
C	0.626549	4.818362	-0.323615	C	-0.448973	5.301799	-0.561701	C	5.200204	0.963817	-0.882677	C	4.100788	2.764429	-1.318231
C	0.767004	3.477105	0.025236	C	0.782718	4.794295	-0.106526	C	4.801285	-0.297689	-0.407536	C	4.257262	1.512411	-0.693871
C	-2.738730	2.049129	-0.104332	C	0.954543	3.442915	0.250345	C	3.484509	-0.562212	0.016813	C	3.189854	0.854368	-0.058428
C	-3.473263	2.067085	-1.034989	C	-2.680288	2.159905	-0.347344	C	1.970552	3.016104	-0.355634	C	0.450388	3.603655	-0.355409
C	-3.103807	2.908471	2.113311	C	-3.509670	2.217862	0.949769	C	1.746426	3.480449	1.093551	C	0.201157	3.916850	1.129053
C	-3.825426	2.899446	3.322946	C	-3.204770	3.074218	2.027758	C	2.598325	3.129899	2.161453	C	1.220192	3.917466	2.104115
C	-4.931074	2.049508	3.482955	C	-4.014518	3.102037	3.180064	C	2.397233	3.660445	3.50615	C	0.946654	4.289452	3.434571
C	-5.306830	1.200418	2.424558	C	-5.144835	2.274929	3.273114	C	1.344770	4.558069	3.691970	C	-0.349908	4.672327	3.810147
C	-4.584404	1.208423	1.221220	C	-5.456808	1.411319	2.205864	C	0.487468	4.916039	2.633797	C	-1.374950	4.682344	2.845039
C	-3.707757	2.301329	-1.478789	C	-4.646749	1.822228	1.060145	C	0.684643	4.378814	1.352048	C	-1.101530	4.302610	1.521527
C	-3.545636	1.602422	-2.695073	C	-3.550520	2.440504	-1.585223	C	2.426904	4.214889	-1.209358	C	0.396222	4.904688	-1.175988
C	-4.398806	1.849291	-3.785751	C	-3.319677	1.730968	-2.784422	C	1.933439	4.385631	-2.520996	C	-0.254459	4.926927	-2.429017
C	-5.431097	2.796399	-3.679767	C	-4.079111	2.001459	-3.936977	C	2.361300	5.462553	-3.318219	C	-0.291623	6.101877	-3.201377
C	-5.612337	3.487353	-2.468806	C	-5.084333	2.983439	-3.911044	C	3.290313	6.390930	-2.819050	C	0.321633	7.272236	-2.735419
C	-4.761712	3.237801	-1.376729	C	-5.334114	3.684226	-2.718101	C	3.779526	6.229796	-1.509384	C	0.964157	7.270558	-1.484471
C	-0.878593	6.711896	-1.102886	C	-4.577899	3.410705	-1.565152	C	3.347449	5.166314	-0.711985	C	0.996292	6.097261	-0.711497
C	2.272893	3.060559	5.017777	C	-0.587939	6.747969	-0.902669	C	6.605400	1.200434	-1.386527	C	5.248545	3.408357	-2.061056
C	2.335964	2.997271	2.043960	C	2.293849	2.970406	0.834929	C	3.169391	-1.922520	0.662901	C	3.468138	-0.408703	0.773232
C	1.631887	3.906523	2.864131	C	2.241287	2.890406	2.367625	C	3.145378	-1.816388	2.195386	C	3.632770	-0.054066	2.263812
C	1.737500	3.845926	2.466135	C	1.499758	3.806863	3.145290	C	4.012284	-0.957101	2.905845	C	4.200841	1.650600	2.693377
C	2.547644	2.871156	4.873155	C	1.499361	3.727385	4.550382	C	3.991327	-0.910780	4.312551	C	4.385671	1.434685	4.062837
C	3.251743	1.959210	0.066432	C	2.240579	2.727365	5.202652	C	3.100937	-1.273326	5.035136	C	3.999375	0.491395	5.029241
C	3.146917	2.024555	2.667676	C	2.982759	1.890981	4.438230	C	2.234740	-2.584973	4.379999	C	3.429828	-0.725854	4.613331
C	3.388652	3.939865	-0.083636	C	2.983094	1.892773	3.036629	C	2.260730	-2.630938	2.934840	C	3.250595	-0.994466	3.246725
C	3.769395	3.744809	-1.431083	C	3.483910	3.810432	0.335104	C	4.116710	-3.042646	0.191971	C	4.662974	-1.240105	0.267410
C	4.762331	4.543143	-2.020830	C	3.935897	3.636737	-0.993451	C	4.005066	-3.542807	-1.127565	C	4.479071	-2.134148	-0.811151
C	5.396903	5.553938	-1.275754	C	5.006755	4.394182	-1.493901	C	4.859300	-4.556232	-1.590826	C	5.547249	-2.906341	-1.297209
C	5.031814	5.752227	0.065745	C	5.649436	5.342737	-0.677220	C	5.846780	-0.506904	-0.747101	C	6.823290	-2.800555	-0.715432
C	4.037927	4.950134	0.657353	C	5.211829	5.521093	0.645118	C	5.966610	-4.613673	0.565527	C	7.018609	-1.915264	0.357472
C	0.180409	-2.412784	-0.097323	C	4.139644	4.759675	1.147331	C	5.108210	-3.599682	1.030846	C	5.947311	-1.145204	0.846664
C	1.339454	-1.142500	-0.483248	C	0.024606	-2.417812	0.079856	C	-2.367211	-0.431522	-0.118919	C	-1.996735	-1.589243	0.033504
C	1.163741	-4.464343	-0.942435	C	1.175463	-3.198713	-0.219917	C	-2.811300	-1.717685	-0.551041	C	-1.688580	-2.912098	-0.411450
C	-0.097536	-0.083279	-1.004887	C	0.976518	-4.517740	-0.677368	C	-4.100870	-1.806570	-1.118365	C	-2.755490	-3.731203	-0.826813
C	-1.204630	-3.684049	-0.512915	C	-0.302526	-5.086084	-0.815984	C	-4.969338	-0.704799	-1.206987	C	-4.097572	-3.309657	-0.782675
C	-1.091674	-3.051560	-0.032436	C	-1.409287	-4.320631	-0.405903	C	-4.550482	0.509209	-0.631772	C	-4.368407	-2.030081	-0.268686
C	2.759477	-2.580925	-0.309308	C	-1.274361	-3.003227	0.068002	C	-3.272924	0.672974	-0.066404	C	-3.347891	-1.153732	0.152464
C	3.186528	-2.506737	1.163418	C	2.601596	-2.691690	0.044980	C	-2.001511	-3.002977	-0.297734	C	-0.258914	-3.480472	-0.364127
C	2.629973	-3.236998	2.167062	C	2.934575	-2.625222	1.542965	C	-1.919674	-3.370404	1.194225	C	0.189020	-3.833895	1.065513
C	3.104983	-3.272003	3.491446	C	2.263101	-3.395495	2.515410	C	-2.806055	-2.867628	2.168811	C	0.716768	-4.033628	2.128169
C	4.150203	-2.398633	3.833436	C	2.649887	-3.347676	3.868544	C	-2.731818	-3.301303	3.06732	C	-0.264551	-4.506966	3.394918
C	4.715233	-1.576430	2.840362	C	3.719848	-2.532049	4.271192	C	-1.774939	-4.253939	3.891167	C	1.102156	-4.682496	3.618432
C	4.234825	-1.628388	1.522066	C	4.398460	-1.759513	3.309769	C	-0.887258	-4.767389	2.926330	C	2.016207	-4.866641	2.565540
C	3.802642	-3.337546	-1.152097	C	4.006315	-1.803820	1.962430	C	-0.957979	-4.326897	1.595440	C	-0.063142	-4.703534	-1.280032
C	4.632731	-4.336106	-0.597802	C	3.668351	-3.491504	-0.723447	C	-2.519351	-4.217579	-1.090825	C	-0.376553	-6.010770	-0.841939
C	5.553483	-0.507301	-1.397663	C	4.394993	-4.541032	-0.119516	C	-4.060614	-6.108890	-1.348302	C	-0.224920	-7.115115	-1.697931
C	5.664351	-4.748941	-2.768080	C	5.579542	-4.981550	-2.204635	C	-3.477485	-6.434960	-2.585891	C	0.255955	-6.935064	-3.007038
C	4.846156	-3.753084	-3.330937	C	4.866913	-3.934484	-2.815704	C	-2.409205	-5.660564	-3.068843	C	0.591122	-5.642911	-3.445963
C	3.925177	-0.056049	-2.531604	C	3.921404	-3.198302	-2.082345	C	-1.934796	-4.562472	-2.328622	C	0.434049	-4.573228	-2.590849
C	-0.256994	-6.471045	-1.581027	C	-0.481669	-6.473913	-1.386335	C	-6.317355	-0.822986	-1.879543	C	-5.207650	-4.209424	-1.276295
C	-2.298596	-2.402963	0.661819	C	-2.497687	-2.298179	0.674361	C	-2.959407	1.964936	0.710473	C	-3.727064	0.191089	0.796437
C	-2.236491	-2.607789	2.187707	C	-2.567259	-2.514659	2.198340	C	-3.072327	1.721643	2.225152	C	-3.588649	0.139922	2.323438
C	-2.834088	-1.651011	0.308551	C	-3.144412	-1.513505	3.011529	C	-2.196003	2.386609	3.109911	C	-3.181360	1.294295	3.026999
C	-2.834652	-1.821750	4.432050	C	-3.266214	-1.688777	4.399228	C	-2.308348	2.220451	4.500152	C	-0.372641	1.288073	4.426933
C	-2.237159	-2.957803	0.008340	C	-2.812868	-2.873944	0.006943	C	-3.307451	1.388492	5.037114				

H	0.660596	-7.078868	-1.447787	H	3.379581	-2.370269	-2.565083	H	-1.076261	-3.976579	-2.694757	H	0.730387	-3.529793	-2.929115
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H	-1.107811	-7.012945	-1.120753	H	-0.624211	-6.425893	-2.488465	H	-6.261130	-0.471868	-2.933564	H	-5.240842	-4.222596	-2.387788
H	-2.240263	-1.308059	0.486628	H	-1.374027	-6.979915	-0.965342	H	-7.083684	-0.200611	-1.374153	H	-6.200305	-3.869913	-0.919649
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H	-3.303106	-1.056761	5.071720	H	-3.503064	-0.580353	2.548772	H	-1.403467	3.034063	2.703124	H	-2.925994	2.207123	2.466103
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H	-1.171829	-4.814447	4.610582	H	-2.905211	-3.012016	6.096074	H	-3.396312	1.257000	6.127314	H	-3.290040	0.117430	6.254600
H	-1.165441	-4.504175	2.137937	H	-1.878437	-4.811669	4.672430	H	-4.982258	0.075215	4.574778	H	-4.036001	-1.947623	5.030183
H	-4.175233	-4.198508	1.716674	H	-1.657577	-4.493890	2.210282	H	-4.772322	0.364700	2.105889	H	-4.215127	-1.935144	2.540028
H	-6.349994	-4.899373	0.722145	H	-4.551509	-3.991909	1.559146	H	-5.039328	3.265304	2.084183	H	-6.127739	0.229127	2.254088
H	-7.105790	-3.940419	-1.475795	H	-6.672396	-4.567983	0.383692	H	-6.397303	5.204513	1.330122	H	-8.365289	1.013295	1.499010
H	-5.637738	-2.280318	-2.670423	H	-7.192379	-3.558306	-1.859401	H	-5.966571	6.263337	-0.910190	H	-8.667906	1.948173	-0.815514
H	-3.441864	-1.616437	-1.693789	H	-5.543221	-1.975278	-2.914595	H	-4.149970	5.332376	-2.384730	H	-6.686172	2.080247	-2.362208
C	-0.074142	1.659451	-3.049322	H	-3.400877	-1.441107	-1.758511	H	-2.804626	3.367555	-1.632933	H	-4.443681	1.283278	-1.603494
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H	-0.535736	2.497977	-2.493577	C	2.674302	0.320576	-5.792051	C	-0.844685	-1.266173	-4.365435	C	-0.612508	0.697135	-4.797136
				H	3.313043	0.403164	-4.896248	H	-1.485671	-2.075036	-3.977226	H	-0.598407	-0.211626	-5.421411
				H	2.845692	1.053940	-6.598761	H	0.029004	-1.599386	-4.946887	H	-1.553742	1.267063	-4.753082
				H	-0.349218	2.502817	-2.381539	H	2.406741	-0.288170	-3.142779	H	1.549193	0.765916	-4.561883
				H	0.354017	1.779227	-3.990674	H	1.733351	1.484396	-3.315128	H	0.595075	2.269216	-3.939991
				H	1.069620	-0.706499	-6.774956	H	-0.840169	0.807832	-5.069603	H	-2.432734	-0.934891	-2.947867
				H	1.548997	-1.361285	-5.087043	H	-2.337710	0.300273	-4.092146	H	-0.944441	-1.987115	-3.478850

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C	-1.506377	4.478275	3.558233
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C	3.567868	0.172136	0.889318
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