

Supporting Information For

Comparing Ru and Fe-Catalyzed Olefin Metathesis

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xyz coordinates

Fe-I			Fe-I-II			Fe-II					
Fe	0.011908	-0.264036	-0.158900	Fe	-0.773275	-0.294035	-0.083768	Fe	0.215176	-1.187267	-0.160795
Cl	-0.526441	-0.335252	2.060674	Cl	-0.282889	-0.491288	-2.230978	Cl	0.310198	-1.996494	1.946812
Cl	-0.293414	-0.339639	-2.467466	Cl	-0.314190	-0.267695	2.104265	Cl	1.658583	-2.108540	-1.604486
N	-0.834007	-3.120511	-0.289843	P	2.490478	0.928650	0.166048	N	2.026413	1.369243	0.171030
N	1.328673	-2.912078	-0.605801	N	-1.672404	-2.986430	0.042250	N	-0.097261	1.888564	0.223234
C	0.195138	-2.223933	-0.289390	N	-3.392618	-1.645951	0.335915	C	0.778550	0.872289	0.067896
C	-0.426270	-4.462747	-0.779121	C	-2.049983	-1.668606	0.077998	C	2.055126	2.842529	0.402713
H	-0.833996	-4.626478	-1.790017	C	-2.759832	-3.906567	0.446255	H	2.576454	3.340472	-0.429255
H	-0.818999	-5.245108	-0.113888	H	-2.569527	-4.286179	1.464442	H	2.602785	3.063613	1.330557
C	1.100000	-4.369732	-0.771828	H	-2.812562	-4.763598	-0.240101	C	0.562542	3.200888	0.481742
H	1.559320	-4.919132	0.067763	C	-3.991562	-3.003269	0.379842	H	0.262649	3.582618	1.469743
H	1.556405	-4.725340	-1.706103	H	-4.595287	-3.174286	-0.528119	H	0.253334	3.934658	-0.277167
C	-2.208927	-2.972334	0.121904	H	-4.649445	-3.103166	1.254503	C	3.280048	0.663043	0.075072
C	-2.532470	-3.251746	1.473490	C	-0.372906	-3.551224	-0.226337	C	3.882941	0.174499	1.252254
C	-1.474774	-3.618845	2.483072	C	-0.082272	-3.957239	-1.351770	C	3.207059	0.285111	2.596310
H	-1.937798	-3.905603	3.436570	C	-1.082450	-3.792867	-2.667740	H	3.885125	-0.044964	3.395236
H	-0.800204	-2.768148	2.620704	H	-0.710323	-4.264508	-3.587809	H	3.902245	-0.342269	2.636047
H	-0.860638	-4.466912	2.137406	H	-1.267854	-2.728675	-2.874510	H	2.900292	1.318801	2.823798
C	-3.877007	-3.213052	1.858811	H	-2.049294	-4.259553	-2.417791	C	5.137281	-0.441450	1.140122
C	-4.126527	-3.414666	2.905018	C	1.155908	-4.556978	-1.806606	H	5.610245	-0.833249	2.045430
C	-0.966730	-2.950363	0.942487	H	1.390781	-4.857416	-2.832049	C	5.797128	-0.567510	-0.089279
H	-6.348047	-2.905590	1.394277	C	2.090628	-4.797541	-0.788563	C	7.129997	-1.271153	-0.185457
H	-7.034200	-2.822578	0.539345	C	3.438039	-5.402552	-1.102543	H	7.748426	-0.854587	-0.994182
H	-6.531829	-2.044852	2.058353	H	3.880542	-5.882821	-0.217792	H	6.990027	-2.344023	-0.398737
H	-6.19738	-3.810418	1.960530	H	4.144103	-6.28810	-1.447149	H	7.695126	-1.194186	0.754852
C	-4.557602	-2.746444	-0.395423	H	3.365065	-6.155066	-1.902038	C	5.174995	-0.047531	-1.232253
H	-5.345028	-2.574216	-1.135286	C	1.735303	-4.461087	0.521713	H	5.675208	-0.132776	-2.201450
C	-3.223240	-2.771430	-0.837377	H	2.425094	-4.688878	1.340113	C	3.919834	0.571468	-1.177014
C	-2.934579	-2.655236	-2.312755	C	0.503941	-3.861334	0.835536	C	3.263711	1.073594	-2.438777
H	-3.723190	-2.077118	-2.815088	H	1.036086	-3.657231	2.284401	H	3.979687	1.076521	-3.272135
H	-2.917405	-3.655072	-2.781821	H	1.025061	-3.403247	2.878683	H	2.865513	2.094535	-2.331284
H	-1.974604	-2.161074	-2.512665	H	-0.283552	-4.588732	2.703637	H	2.424498	0.414775	-2.714046
C	2.698990	-2.488953	-0.510208	H	-0.587731	-2.846068	2.422643	C	-1.532586	1.831312	0.149057
C	3.435478	-2.264335	-1.692778	C	-4.315721	-0.545226	0.328753	C	-2.159769	2.075494	-1.089762
C	2.784524	-2.332740	-3.051793	C	-4.766949	-0.034959	1.564600	C	-1.354092	2.289641	-2.348246
H	3.455577	-1.927138	-3.822171	C	-4.187525	-0.524817	2.868732	H	-2.016192	2.397971	-3.218149
H	1.835660	-1.774071	-3.076509	H	-4.615575	0.030411	3.714731	H	-0.672842	1.446177	-2.537140
H	2.556467	-3.374621	-3.336330	H	-3.92036	-0.405034	2.888746	H	-0.732074	3.198048	-2.291180
C	4.805080	-1.981331	-1.574989	H	-4.394772	-1.594915	3.034101	C	-3.560723	2.094926	-1.130071
H	5.381095	-1.794776	-2.486559	C	-5.735928	0.978924	1.546925	H	-4.056829	2.274200	-2.088563
C	5.453953	-1.945536	-0.334314	H	-6.083095	1.389766	2.499780	C	-4.338183	1.889050	0.017172
C	6.924921	-1.619617	-0.231764	C	-6.266244	1.478055	0.348684	C	-5.846270	1.941532	-0.043295
H	7.435841	-2.286709	0.479916	C	-7.338611	2.542240	0.358802	H	-6.226110	2.890297	0.371056
H	7.073757	-0.587348	0.126326	H	-7.286193	3.159123	1.266984	H	-6.297955	1.125975	0.540833
H	7.426765	-1.710158	-1.205898	H	-8.343718	2.088900	0.326967	H	-6.209083	1.861987	-1.077266
C	4.696213	-2.202372	0.817548	H	-7.254238	3.207102	-0.514092	C	-3.678113	1.649483	1.230892
H	5.184835	-2.186410	1.796240	C	-5.793808	0.944538	-0.859264	H	-4.267303	1.476282	2.136274
C	3.325772	-2.481461	0.757596	H	-6.186544	1.329440	-1.805130	C	-2.280455	1.620182	1.326193
C	2.549802	-2.762538	2.019075	C	-4.826519	-0.069412	-0.898103	C	-1.607676	1.334865	2.645743
H	2.103331	-3.770464	2.007367	C	-4.325599	-0.601681	-2.217668	H	-0.870934	2.109647	2.910734
H	1.721979	-2.048490	2.154026	H	-4.486954	-1.688029	-2.309618	H	-1.068028	0.373968	2.619140
H	3.206886	-2.700111	2.897296	H	-3.244575	-0.426757	-2.336175	H	-2.349361	1.287898	3.454830
C	1.679168	0.289834	-0.237426	C	-4.847575	-0.115428	-3.053100	C	-1.514299	-1.331763	-0.979596
C	3.839330	1.419265	0.067495	C	-1.793920	1.130146	-0.096490	C	-3.887656	-1.816435	-1.555943
C	2.671505	0.870353	0.662404	C	-2.559630	3.446749	-0.357410	C	-2.832649	-1.754861	-0.599536
C	4.842686	2.002290	0.840438	C	-1.609915	2.439104	-0.687841	C	-5.161541	-2.248899	-1.199400
C	2.563142	0.926594	2.073443	C	-2.466817	4.729179	-0.891228	C	-3.127500	-2.152823	0.734996
C	4.718228	2.036097	2.235292	C	-0.560557	2.787211	-1.576679	C	-5.422494	-2.637439	0.123358
H	5.724302	2.429821	0.356824	H	-1.420710	5.047111	-1.768817	H	-5.955237	-2.294502	-1.948805
C	3.577924	1.492908	2.843834	C	-3.208766	5.485823	-0.625360	C	-4.400974	-2.590374	1.085038
H	1.663227	0.525036	2.541694	H	-0.473342	4.071671	-2.107723	H	-2.320303	-2.130550	1.470635
H	5.505271	2.486075	2.845361	H	0.168208	2.025494	-1.850872	H	-6.419704	-2.986244	0.402238
C	3.475732	1.521093	3.931329	H	-1.344237	6.053446	-2.187175	H	-4.605204	-2.904713	2.111166
C	-2.627286	1.840166	-0.734174	H	0.343231	4.319631	-2.789075	H	-3.675956	-1.522471	-2.587360
C	-3.141694	2.568234	-1.818868	C	3.466103	0.212952	1.585113	H	-1.455139	-1.132053	-2.067470
C	-3.476588	0.973808	-0.021052	C	4.020586	0.977116	2.624303				
C	-4.491719	2.454635	-2.166712	C	3.629262	-1.184665	1.608859				
H	-2.489090	3.224088	-2.396358	C	4.734406	0.358677	3.658413				
C	-4.828572	0.876335	-0.364936	H	3.894772	2.061428	2.628725				
H	-3.078649	0.374589	0.802504	C	4.354177	-1.798103	2.633813				
C	-5.340317	1.616980	-1.435794	H	3.182740	-1.796923	0.820673				
H	-4.879529	3.025448	-0.313737	C	4.908025	-1.028575	3.664536				
H	-5.477987	0.206223	0.201371	H	5.159125	0.967787	4.460214				
H	-6.395816	1.534861	-1.705687	H	4.480348	-2.883602	2.633694				
C	-0.121969	3.227921	-1.373546	H	5.467203	-1.509498	4.470457				
C	-0.439762	4.587430	-1.188346	C	2.434106	2.739019	0.604494				
C	0.734960	2.865896	-2.423755	C	3.237871	3.718735	-0.001513				
C	0.092361	5.561777	-0.037921	C	1.478003	3.138100	1.559692				
H	-1.098340	4.888047	-0.371507	C	3.099199	5.067430	0.349194				
H	1.267266	3.845155	-3.271035	H	3.977201	3.429520	-0.750865				
H	0.953164	1.810642	-2.594195	C	1.353812	4.483082	1.918315				
C	0.950441	5.193349	-3.080653	H	0.828891	2.387127	2.019513				
H	-0.161956	6.612466	-1.879906	C	2.162143	5.453126	1.312657				
H	1.931276	3.547139	-4.085828	H	3.731555	5.817721	-0.132186				
H	1.368324	5.955834	-3.742237	H	0.611610	4.775811	2.664714				
C	-0.885795	2.911783	1.366722	H	2.056927	6.505424	1.586845				
C	-2.057840	3.102612	2.113195	C	3.766990	0.878990	-1.195249				
C	0.321067	3.453920	1.843570	C	5.153366	0.950543	-0.067503				
C	2.024439	3.823893	3.312237	C	3.299312	0.742541	-2.514372				
H	-3.005695	2.696314	1.758871	C	6.050964	0.903913	-2.039237				
C	0.351179	4.174101	3.040600	H	5.530914	1.036568	0.053791				
H	1.243368	3.322937	1.275490	C	4.199139	0.703133	-3.586111				
C	-0.821851	4.360701	3.780482	H	2.226165	0.639381	-2.695819				
H	-2.947097	3.966002	3.879842	C	5.575741	0.784242	-3.351223				
H	1.297431	4.589460	3.394597	H	7.125733	0.958707	-1.848810				
H	-0.798181	4.924153	4.716086	H	3.821712	0.59450					

Fe-II-IV			Fe-IV			Fe-IV-VI			Fe-VI						
Fe	-0.301091	0.845607	-0.193758	Fe	-0.241457	0.831205	-0.541457	Fe	0.290134	-0.572289	-0.342434	Fe	0.094617	1.450737	-0.743044
Cl	-0.391923	1.435486	1.955108	Cl	-0.106900	1.656306	1.538647	Cl	-0.449146	-1.200674	1.653788	Cl	-1.452049	1.510903	-2.346161
Cl	-0.885405	0.708923	-2.368544	Cl	-0.334734	-0.047823	-2.622133	Cl	0.131317	-0.301171	-2.537476	Cl	-0.219173	2.862780	0.971341
N	-1.776250	-1.513340	0.403979	N	-1.951759	-1.506183	0.473241	N	2.609451	1.034107	0.404583	N	1.166883	-1.162383	0.551353
N	0.373205	-1.983962	0.396407	N	0.156629	-2.094018	0.437980	N	0.703442	2.142404	0.349739	N	-1.021948	-1.187228	0.512129
C	-0.532161	-0.988995	0.174582	C	-0.699076	-1.076315	0.198795	C	1.276732	0.922416	0.148647	C	0.054486	-0.474794	0.173243
C	-1.727912	-2.888979	0.950011	C	-2.004593	-2.936256	0.887172	C	3.015251	2.423310	0.720990	C	0.870299	-2.442538	1.216098
H	-2.439537	-3.536115	0.417610	H	-2.558520	-3.522844	0.137808	H	3.613906	2.842309	-0.105207	H	1.280196	-2.410249	2.237398
H	-1.999323	-2.878634	2.018751	H	-2.522232	-3.033269	1.852751	H	3.626831	2.446926	1.634571	H	1.338655	-3.284264	0.685259
C	-0.265064	-3.283699	0.721159	C	-0.517661	-3.316612	0.959442	C	1.662848	3.135801	0.887241	C	-0.667005	-2.489532	1.186624
H	0.206673	-3.725015	1.610578	H	-0.176872	-3.521154	1.986665	H	1.429605	3.350723	1.942912	H	-1.061237	-3.319217	0.580034
H	-0.140760	-3.986832	-0.119615	H	-0.265290	-4.184569	0.333651	H	1.598614	4.074657	0.318765	H	-1.117743	-2.552415	2.187718
C	-3.061788	-0.879466	0.237112	C	-3.174670	-0.749459	0.369279	C	3.610025	0.017462	0.257865	C	2.536405	-0.772108	0.310930
C	-3.706770	-0.274584	1.338866	C	-3.654054	-0.067140	1.509363	C	4.011895	-0.712284	1.402534	C	3.211006	-1.216483	-0.846141
C	-3.148244	-0.326626	2.739655	C	-2.919087	-0.108960	2.825347	C	3.302592	-0.539751	2.721026	C	2.493963	-1.998696	-1.919631
H	-3.446911	0.563221	3.311496	H	-3.481734	0.434549	3.596933	H	3.746707	-1.188570	3.488198	H	3.166396	-2.204034	-2.763527
H	-2.053325	-0.371463	2.753309	H	-1.921434	0.348018	2.737259	H	2.231982	-0.788061	2.631786	H	1.622287	-1.445422	-2.300851
H	-3.854910	-1.206593	3.272674	H	-2.779983	-1.143274	3.180152	H	3.360686	0.499077	3.084343	H	2.123462	-2.967591	-1.546851
C	-4.962466	0.317416	1.127017	C	-4.854024	0.649246	1.396222	C	5.068252	-1.621930	1.269150	C	4.566753	-0.888596	-0.988313
H	-5.452367	0.812326	1.970395	H	-5.223764	1.190936	2.271942	H	5.380033	-2.197301	2.145827	H	5.059269	-1.217632	-1.887844
C	-6.609019	0.272083	-0.112622	C	-5.592915	0.680818	0.206118	C	5.736492	-1.810218	0.049892	C	5.257237	-0.151825	-0.016250
C	-6.938300	0.956409	-0.325187	C	-6.857602	1.499244	0.097289	C	6.851241	-2.821026	-0.073092	C	6.567237	0.160046	-0.174921
H	-7.584904	0.379507	-1.003202	H	-7.581551	1.033689	-0.587721	H	7.409646	-2.922022	0.689852	H	7.345991	-0.577826	0.361947
H	-6.798102	1.952325	-0.777730	H	-6.640152	2.507608	-0.293121	H	7.559609	-2.543854	-0.867039	H	6.972785	-1.151116	0.233636
H	-7.475015	1.099228	0.623950	H	-7.341844	1.625063	0.766628	H	6.449880	-3.817152	-0.324244	H	7.030826	0.138756	-1.231123
C	-4.988073	-0.433023	-1.153877	C	-5.119673	-0.061062	-0.884434	C	5.326586	-1.055447	-1.058768	C	4.552300	0.273071	-1.119434
H	-5.501299	-0.532777	-1.214908	H	-5.699326	-0.080118	-1.812261	H	5.841612	-1.185693	-2.015095	H	5.070894	0.860405	1.883019
C	-3.731126	-1.030828	-1.002058	C	-3.927014	-0.796281	-0.825785	C	4.276320	-0.131288	-0.982475	C	3.196458	-0.025930	1.310661
C	-3.145497	-1.841602	-1.229621	C	-3.497959	-1.632856	-2.003565	C	3.852727	0.651574	-2.198778	C	2.462693	0.481870	2.526220
H	-3.893348	-1.991616	-2.920815	H	-4.131015	-1.420356	-2.877949	H	4.471590	0.382875	-3.065665	H	3.159141	-0.067038	3.223464
H	-2.812679	-1.834259	-1.786469	H	-3.595088	-2.709848	-1.785916	H	3.951393	1.738147	-0.043482	H	1.950490	-0.326966	3.071015
H	-2.273784	-1.330235	-2.565453	H	-2.452356	-1.438615	-2.284031	H	2.797614	0.455263	-2.452600	H	1.693758	1.219461	2.202765
C	1.798767	-1.982883	0.215370	C	1.593694	-2.087321	0.316281	C	-0.691878	2.481276	0.216490	C	-2.413086	-0.839855	0.393743
C	2.332855	-2.333293	-1.043774	C	2.186900	-2.619171	-0.849042	C	-1.149710	2.994837	-1.018914	C	-3.096664	-0.152367	1.434532
C	1.442213	-2.555642	-2.242153	C	1.359618	-3.152753	-1.991723	C	-0.022914	3.189529	-2.191901	C	-2.357010	0.309072	2.668786
H	2.044118	-2.783694	-3.132562	H	2.006982	-3.448727	-2.828779	H	-0.721695	3.768728	-2.981318	H	-3.040980	0.720054	3.403961
H	0.825968	-1.667365	-2.461342	H	0.646341	-2.397902	-2.355157	H	0.084280	2.220264	-2.615484	H	-1.606736	1.096538	2.418218
H	0.745658	-3.395805	-2.089187	H	0.781419	-4.043473	-1.693125	H	0.693465	3.728724	-1.903640	H	-1.783627	-0.510574	3.156279
C	3.726792	-2.421140	-1.167944	C	3.587637	-2.658811	-0.918713	C	-2.502395	3.343524	-1.128713	C	-4.437190	0.116315	1.282273
C	4.151410	-2.680610	-2.142563	C	4.054682	-3.060047	-1.823100	C	-2.866868	3.727916	-2.085897	C	-4.955458	0.658424	2.078635
C	4.585717	-2.183913	-0.085089	C	4.398144	-2.216312	0.134055	C	-3.392101	3.222513	-0.052735	C	-5.152158	-0.284418	0.146133
C	6.082601	-2.317894	-0.237562	C	5.904249	-2.245252	0.023955	C	-4.856836	3.549745	-0.216407	C	-6.614502	0.085896	-0.010841
H	6.392275	-2.197706	-1.285605	H	6.370187	-2.582607	0.962216	H	-5.300289	3.899233	0.727412	H	-7.149480	-0.709643	-0.588363
H	6.425394	-3.312113	0.094961	H	6.302514	-1.239965	-0.191844	H	-5.421249	2.657022	-0.533305	H	-6.734358	1.014683	-0.547168
H	6.616693	-1.569846	0.366746	H	6.236160	-2.913313	-0.783666	H	-5.013658	4.325623	-0.980093	H	-7.110751	0.164621	0.964795
C	4.017611	-1.841980	1.150001	C	3.773246	-1.738302	1.293852	C	-2.886620	2.778295	1.175491	C	-4.467395	-0.985485	-0.855785
C	4.671572	-1.643469	2.004327	C	4.386913	-1.410173	2.137930	C	-1.035865	2.710119	2.037859	C	-5.008388	-1.309602	-1.749635
C	2.630459	-1.744703	1.329695	C	2.378750	-1.675257	1.416977	C	-1.541369	2.421398	1.344344	C	-3.101112	-1.276884	-0.756205
C	2.049927	-1.382147	2.627986	C	1.754733	-1.195131	2.702542	C	-1.038865	2.048110	2.715940	C	-2.393355	-1.999060	-1.875680
H	1.443019	-2.205517	0.380620	H	1.065379	-1.943665	3.216441	H	-0.577845	2.920881	3.213972	H	-1.825059	-2.873607	-1.520847
H	1.391805	-0.502014	2.601841	H	1.176575	-0.271101	2.547032	H	-0.297539	1.237292	2.677127	H	-1.687250	-1.320247	-2.379097
H	2.849661	-1.165277	3.394424	H	2.530856	-0.993731	3.453631	H	-1.864882	1.709075	3.352052	H	-3.116139	-2.350492	-2.624533
C	1.421310	0.898666	-0.521247	C	1.057989	2.295581	-1.267880	C	-3.002899	-2.729502	-1.433151	C	1.810665	1.650604	-1.473562
C	3.658966	1.808600	-0.960727	C	3.480857	1.908168	-0.944001	C	-5.456751	-2.447756	-1.144039	H	2.080713	1.392511	-2.511850
C	2.430763	1.904859	-0.249035	C	2.303225	2.588147	-0.547195	C	-4.183563	-2.624351	-0.563427	H	2.677022	2.065667	-0.931766
C	4.680574	2.735584	-0.769605	C	4.711864	2.180607	-0.349413	C	-6.065527	-2.369203	-0.354059				
C	2.285144	2.970841	0.675617	C	2.417598	3.545105	0.487673	C	-4.097151	-2.686972	0.843773				
C	4.513386	3.779573	0.150157	C	4.804867	3.138498	0.668223	C	-6.505994	-2.450782	1.039188				
H	5.611620	2.645451	-1.333997	H	5.605514	1.648967	-0.684731	H	-7.583246	-2.240959	-0.826844				
C	3.317149	3.885614	0.874058	C	3.650547	3.817043	1.080458	C	-5.245084	-2.603519	1.632227				
H	1.358579	3.044638	1.245277	H	1.530224	4.072155	0.838610	H	-3.117187	-2.766001	1.319264				
H	5.314417	4.506153	0.305411	H	5.768210	3.357000	1.134529	H	-7.402052	-2.385756	1.660644				
H	3.190236	4.693971	1.598106	H	3.712528	4.564950	1.874628	H	-5.156051	-2.646555	2.720449				
C	-0.651770	3.844161	-1.069960	C	-0.148340	3.242797	-1.274853	C	-1.800572	-3.233789	-1.099267				
C	-1.719333	3.387060	-0.398525	C	-1.380163	2.348826	-1.084660	C	1.611558	-1.674291	-0.392406				
H	-2.451344	2.732075	-0.877549	H	-0.082226	3.961772	-0.448454	H	-1.588106	-3.632834	-0.105716				
H	-0.911822	3.672353	0.637046	H	-0.191371	3.975504	-2.229097	H	-0.992369	-3.269561	-1.830986				
H	-0.461438	3.547688	-2.102967	H	-2.025235	2.595548	-0.235714	H	1.888835	-2.279073	0.484546				
H	3.791004	0.984664	-1.667122	H	3.414974	1.163432	-1.741894	H	-5.539053	-2.383102	-2.232726				
H	1.793670	0.105985	-1.185662	H	1.250602	1.857601	-2.251513	H	-3.146087	-2.371177	-2.459084				
H	0.066681														

Ru-I			Ru-I-II			Ru-II					
Ru	0.030857	-0.298599	-0.073068	Ru	-0.927617	-0.167812	-0.091135	Ru	-0.228253	0.906791	0.085788
Cl	-0.257592	-0.346407	2.322858	Cl	-0.380406	-0.486282	-2.347989	Cl	-0.376060	1.238734	2.387216
Cl	-0.182789	-0.446325	-2.507387	Cl	-0.421952	-0.039715	2.198125	Cl	-0.998424	1.565050	-2.004403
P	-1.181151	1.858174	-0.180370	P	2.853973	0.722765	0.156837	N	-1.804914	-1.517052	0.204079
N	-0.371079	-3.319889	-0.097146	N	-2.004933	-2.842619	0.200587	N	0.334620	-2.068650	0.217082
N	1.756614	-2.857062	-0.382767	N	-3.664612	-1.402892	0.412010	C	-0.528071	-1.002684	0.126511
C	0.535895	-2.299634	-0.138810	C	-2.317963	-1.499598	0.147348	C	-1.823439	-2.957524	0.522647
C	0.216616	-4.631016	-0.463974	C	-3.123485	-3.671982	0.690847	H	-2.544065	-3.483359	-0.121523
H	-0.125733	-4.925800	-1.469651	H	-2.953997	-3.958136	1.743286	H	-2.120261	-3.113781	1.574449
H	-0.097242	-5.404350	0.251753	H	-3.214735	-4.588217	0.090257	C	-0.371512	-3.370035	0.260440
C	1.718355	-4.341017	-0.421907	C	-4.316159	-2.727980	0.533446	H	0.046231	-4.002030	1.057194
H	2.207040	-4.751358	0.478395	H	-4.908554	-2.943753	-0.373411	H	-0.251002	-3.902190	-0.699508
H	2.254156	-4.715963	-1.305179	H	-4.994452	-2.741084	1.398304	C	-3.044297	-0.801887	0.044972
C	-1.781461	-3.268681	0.197357	C	-0.745908	-3.473037	-0.101280	C	-3.761946	-0.354941	1.176589
C	-2.193154	-3.450501	1.540620	C	-0.521975	-3.916216	-1.427116	C	-3.307058	-0.638474	2.586652
C	-1.198490	-3.650082	2.654160	C	-1.554894	-3.721661	-2.507841	H	-3.715810	0.107377	3.282479
H	-1.713338	-3.939498	3.580886	H	-1.240713	-4.223580	-3.433453	H	-2.214668	-0.619331	2.685129
H	-0.634593	-2.722742	2.842334	H	-1.696945	-2.653953	-2.728618	H	-3.671989	-1.627076	2.916677
H	-0.469240	-4.438809	2.409188	H	-2.531930	-4.138126	-2.212524	C	-4.976476	0.316977	0.965334
C	-3.565843	-3.475866	1.817351	C	0.675132	-4.582776	-1.713147	H	-5.524604	0.689156	1.836121
H	-3.887508	-3.599456	2.855727	H	0.858937	-4.912325	-2.739926	C	-5.509897	0.508694	-0.313890
C	-4.531261	-3.375757	0.805271	C	1.630995	-4.853823	-0.722846	C	-6.794815	1.275731	-0.515781
C	-6.004695	-3.380767	1.139031	C	2.933463	-5.533578	-1.067963	H	-7.392253	0.852165	-1.336984
H	-6.616414	-3.618243	0.256648	H	3.337386	-6.091080	-0.210221	H	-6.585089	2.327276	-0.773769
H	-6.328850	-2.395636	1.514282	H	3.693559	-4.792658	-1.366748	H	-7.411844	1.276834	0.394442
H	-6.236902	-4.116393	1.924053	H	2.812476	-6.233477	-1.907971	C	-4.813835	-0.026617	-1.407827
C	-4.088746	-3.277056	-0.518601	C	1.339940	-4.474000	0.592912	H	-5.234156	0.074461	-2.412761
H	-4.822745	-3.245651	-1.329451	C	2.046273	-4.723540	1.396030	C	-3.593101	-0.693203	-1.255449
C	-2.724922	-3.240244	-0.853864	C	0.155055	-3.803001	0.936016	C	-2.902973	-1.292531	-2.454802
C	-2.317912	-3.241492	-2.305812	C	-0.148646	-3.527877	2.387370	H	-3.557814	-1.247454	-3.336037
H	-3.140087	-2.874637	-2.935992	H	0.778330	-3.491379	2.976343	H	-2.633840	-2.347496	-2.285511
H	-2.085612	-4.267750	-2.641003	H	-0.772973	-4.334332	2.810379	H	-1.978990	-0.742680	-2.688944
H	-1.440233	-2.607508	-2.495027	H	-0.669390	-2.572163	2.528934	C	1.760168	-2.100420	0.060634
C	3.053693	-2.240742	-0.349865	C	-4.540207	-0.267117	0.348516	C	2.314810	-2.206459	-1.233564
C	3.726777	-2.001378	-1.566929	C	-4.933163	0.354400	1.552596	C	1.448481	-2.141682	-2.468113
C	3.060896	-2.254666	-2.896067	C	-4.345833	-0.067509	2.876586	H	2.056977	-2.265424	-3.374390
H	3.699892	-1.906951	-3.719943	H	-4.743266	0.553247	3.691423	H	0.924064	-1.175126	-2.536915
H	2.086936	-1.742141	-2.962617	H	-3.247756	0.020192	2.873229	H	0.675582	-2.926261	-2.474213
H	2.871340	-3.329331	-3.058338	H	-4.580877	-1.118424	3.112101	C	3.708018	-2.316614	-1.349374
C	5.038753	-1.507358	-1.509564	C	-5.858747	1.406601	1.482429	H	4.147235	-2.390828	-2.348822
H	5.565695	-1.310482	-2.448264	H	-6.161063	1.902304	2.409794	C	4.548232	-2.330259	-0.226419
C	5.691685	-1.268873	-0.293199	C	-6.400845	1.839069	0.264132	C	6.043012	-2.488395	-0.377585
C	7.095105	-0.712277	-0.256955	C	-7.425088	2.948758	0.218613	H	6.334418	-3.550539	-0.318043
H	7.715937	-1.233476	0.487800	H	-8.449195	2.539103	0.214697	H	6.586188	-1.955965	0.416815
H	7.085045	0.355260	0.018616	H	-7.315970	3.560239	-0.689220	H	6.392677	-2.107509	-1.348137
H	7.588664	-0.799967	-1.235505	H	-7.340536	3.611568	1.091902	C	3.961549	-2.218736	1.042317
C	4.999646	-1.540750	0.895797	C	-5.987163	1.196121	-0.912280	H	4.600844	-2.214022	1.930163
H	5.493521	-1.366198	1.856282	H	-6.389010	1.527824	-1.874374	C	2.574106	-2.107949	1.212811
C	3.688488	-2.032377	0.895999	C	-5.065754	0.140463	-0.897848	C	1.975890	-1.961144	2.589310
C	2.977079	-2.318402	2.193441	C	-4.610589	-0.497181	-2.187171	H	1.264680	-2.772293	2.814721
H	2.682699	-3.378049	2.271908	H	-4.800467	-1.582243	-2.200835	H	1.420530	-1.014533	2.681661
H	2.054663	-1.722326	2.288137	H	-3.528280	-0.358638	-2.338641	H	2.761125	-1.980463	3.357479
H	3.627014	-2.089648	3.049161	H	-5.136728	-0.054887	-3.044137	C	1.596970	1.023110	-0.171581
C	1.711351	0.454341	-0.309815	C	-1.948939	1.364938	-0.251946	C	3.676251	2.297365	-0.572299
C	3.649881	1.955361	-0.207661	C	-2.321771	3.793187	-0.406478	C	2.331833	2.278220	-0.123036
C	2.612813	1.286095	0.490556	C	-1.481481	2.678943	-0.667773	C	4.417970	3.477974	-0.569266
C	4.558421	2.777324	0.459241	C	-1.942357	5.081033	-0.778481	C	1.769184	3.491643	0.346336
C	2.541259	1.455238	1.892996	C	-0.253549	2.911410	-1.334007	C	3.839686	4.667831	-0.109074
C	4.473474	2.927244	1.848572	C	-0.720413	5.288784	-1.432889	H	5.451598	3.472599	-0.922907
H	5.336682	3.298462	-0.103258	H	-2.600359	5.926662	-0.564881	C	2.514786	4.667860	0.350407
C	3.468430	2.256075	2.559468	H	0.116635	4.200488	-1.712268	H	0.746377	3.500635	0.732099
H	1.752222	0.935627	2.441098	H	0.389813	2.063841	-1.575218	H	4.420532	5.592825	-0.102737
H	5.188612	3.562625	3.376594	H	-0.423588	6.297085	-1.730474	H	2.065261	5.592555	0.718728
H	3.406057	2.363425	3.645195	H	1.066721	4.360539	-2.225787	H	4.125302	1.366796	-0.928985
C	-2.807451	1.607077	-1.044246	C	3.842279	-0.050287	1.538377	H	2.202499	0.147370	-0.440042
C	-3.249898	2.449524	-2.075160	C	4.661358	0.670755	2.423044				
C	-3.614338	0.528062	-0.643667	C	3.736263	-1.444393	1.695102				
C	-4.486331	2.222864	-2.689864	C	5.370323	0.009622	3.433486				
H	-2.626324	3.282254	-2.404079	H	4.743644	1.755047	2.324607				
C	-4.853600	0.311617	-1.252922	C	4.454556	-2.104139	2.696153				
H	-3.280168	-0.145401	0.150104	H	3.082044	-2.014092	1.029604				
C	-5.292767	1.157539	-2.277720	C	5.273030	-1.378802	3.570557				
H	-4.817690	2.883420	-3.494496	H	6.002502	0.584555	4.114753				
H	-5.470660	-0.528897	-0.929555	H	4.367333	-3.188226	2.802453				
H	-6.258547	0.982675	-2.757467	H	5.827112	-1.893412	4.358985				
C	-0.402082	3.266532	-1.124988	C	3.033636	2.537530	0.539891				
C	-0.581448	4.603128	-0.728677	C	3.884229	3.414597	-0.152828				
C	0.354296	2.986158	-2.275174	C	2.205781	3.052233	1.557648				
C	-0.004886	5.642087	-1.468437	C	3.920820	4.775509	0.177830				
H	-1.168056	4.835939	0.161154	H	4.522746	3.033731	-0.952368				
C	0.920397	4.029475	-3.015273	C	2.257131	4.406875	1.895874				
C	0.476019	1.948329	-2.598583	H	1.514980	2.385170	2.081567				
C	0.747036	5.358655	-2.612983	C	3.114002	5.273675	1.205815				
H	-0.146019	6.676166	-1.145232	H	4.588521	5.446209	-0.368916				
H	1.501519	3.798789	-3.911372	H	1.613910	4.789913	2.691563				
H	1.196131	6.170875	-3.189474	H	3.147082	6.334519	1.464853				
C	-1.684052	2.685856	1.410337	C	4.008859	0.485490	-1.289491				
C	-3.022760	2.949811	1.737008	C	5.409011	0.416903	-1.176139				
C	-0.673074	3.058419	2.313253	C	3.419690	0.346295	-2.559091				
C	-3.344505	3.581604	2.944846	C	6.203638	0.232721	-2.312601				
H	-3.820285	2.666778	1.048578	H	5.878852	0.499418	-0.193407				
C	-0.996335	3.697772	3.512124	C	4.217257	0.168925	-3.695875				
H	0.371961	2.852366	2.075632	H	2.329708	0.350302	-2.651381				
C	-2.335759	3.958822	3.833284	C	5.609778	0.113016	-3.575351				
H	-4.391193	3.781126	3.186386	H	7.290550	0.180101	-2.211262				
H	-0.200071	3.983303	4.203249	H	3.745770	0.060020	-4.675468				
H											

Ru-II-III			Ru-III			Ru-III-IV			Ru-IV						
Ru	-0.241349	0.767658	-0.013148	Ru	-0.390561	0.932571	-0.372006	Ru	0.370019	-0.957875	-0.357235	Ru	0.248322	-0.866689	-0.327999
Cl	-0.261803	1.135649	2.311311	Cl	-0.337565	1.649069	1.936157	Cl	0.285461	-1.654111	1.959083	Cl	-0.015862	-1.529167	1.975409
Cl	-0.985024	1.018203	-2.232197	Cl	-0.845835	0.328745	-2.665154	Cl	0.828358	-0.438201	-2.685322	Cl	0.700549	-0.316033	-2.645397
N	-1.191510	-1.722104	0.306142	N	-1.827636	-1.480401	0.602498	N	1.932180	1.466164	0.546883	N	2.023279	1.419329	0.544806
N	0.470260	-2.166830	0.357604	N	0.314737	-1.966533	0.571046	N	-0.215124	1.944258	0.473238	N	-0.100879	2.015170	0.488476
C	-0.441487	-1.156626	0.173987	C	-0.591999	-0.996365	0.275108	C	0.701477	0.971402	0.246945	C	0.765400	1.002947	0.255839
C	-1.640811	-3.124636	0.763352	C	-1.772081	-2.795055	1.282988	C	1.871419	2.831590	1.123363	C	2.032902	2.786157	1.127795
H	-2.339576	-3.744541	0.183196	H	-2.502637	-3.486817	0.839562	H	2.590149	3.491681	0.617064	H	2.786512	3.406697	0.623160
H	-1.921372	-3.188644	1.828765	H	-2.008350	-2.676161	2.353294	H	2.123070	2.798749	2.195889	H	2.283271	2.733681	2.199643
C	-0.172191	-3.491424	0.527401	C	-0.318249	-3.222283	1.049688	C	0.408949	3.230638	0.876460	C	0.593918	3.266548	0.884243
H	0.279189	-4.026325	1.375241	H	0.180231	-3.573026	1.964403	H	-0.085295	3.627798	1.774408	H	0.126019	3.691971	1.782851
H	-0.029869	-4.103223	-0.380491	H	-0.224603	-4.008163	2.812176	H	0.301111	3.970892	0.066165	H	0.524407	4.008070	0.071223
C	-2.969060	-1.083198	0.118136	C	-3.100449	-0.837546	0.385800	C	3.201244	0.801726	0.376133	C	3.263160	0.703434	0.375851
C	-3.678949	-0.559648	1.221900	C	-3.724132	-0.118306	1.436288	C	3.795496	0.120299	1.462644	C	3.813342	-0.042816	1.423531
C	-3.187595	-0.698423	2.644488	C	-3.149828	-0.055147	2.823340	C	3.171774	0.098905	2.835079	C	3.149654	-0.122799	2.774678
H	-3.580759	0.112123	3.270971	H	-3.524544	0.828728	3.358004	H	3.651866	-0.663296	3.464306	H	3.707556	-0.801398	3.434768
H	-2.093669	-0.671039	2.712191	H	-2.054200	0.000751	2.819732	H	2.096724	-0.125064	2.795883	H	2.112990	-0.487591	2.704053
H	-3.544330	-1.649500	3.074773	H	-3.460506	-0.942735	3.402414	H	3.307531	1.071029	3.340437	H	3.274275	0.864311	3.266319
C	-4.928413	0.035939	0.982609	C	-4.964344	0.485194	1.169247	C	5.036195	-0.500744	1.251489	C	5.036890	-0.694682	1.205819
H	-5.470988	0.466374	1.829769	H	-5.438436	1.066036	1.966043	H	5.492028	-1.049290	2.081129	H	5.463546	-1.287020	2.020704
C	-5.504636	0.073920	-0.291637	C	-5.617116	0.346370	-0.061138	C	5.711112	-0.422249	0.027193	C	5.731820	-0.593524	-0.005906
C	-6.829171	0.758993	-0.529424	C	-6.928005	1.045719	-0.331263	C	7.023282	-1.139146	-0.185376	C	7.026608	-1.339749	-0.224912
H	-7.424214	0.231643	-1.289916	H	-7.583836	0.438860	-0.973121	H	7.689753	-0.571045	-0.851215	H	7.711145	-0.776212	-0.876042
H	-6.677256	1.789570	-0.891471	H	-6.760780	2.004318	-0.601543	H	6.859861	-2.125222	-0.651686	H	6.841263	-2.312582	-0.710459
H	-7.424300	0.819005	0.393322	H	-7.466839	1.266910	0.854458	H	7.549090	-1.309051	0.765454	H	7.542360	-1.540593	0.725406
C	-8.155669	-0.543041	-1.346466	C	-8.021167	-0.466365	-1.036183	C	8.134420	0.340795	-0.997729	C	8.190312	0.217318	-1.012603
H	-5.269356	-0.567907	-2.341527	H	-5.541631	-0.638492	-1.982895	H	5.668331	0.457926	-1.945396	H	5.753859	0.344250	-1.951781
C	-3.562311	-1.138800	-1.166747	C	-3.781488	-1.085568	-0.832624	C	3.894893	0.975928	-0.845128	C	3.969467	0.886828	-0.852510
C	-2.889350	-1.843473	-2.317041	C	-3.225701	-2.020575	-1.875011	C	3.348051	1.843486	-1.948902	C	3.452158	1.785611	-1.946355
H	-3.552009	-1.864703	-3.193322	H	-3.967633	-2.194782	-2.666725	H	4.081111	1.936395	-2.762170	H	4.197649	2.882798	-2.747716
H	-2.634574	-2.884892	-2.061422	H	-2.960132	-2.997407	-1.439438	H	3.116302	2.858790	-1.587816	H	3.229373	2.798126	-1.572139
H	-1.961310	-1.326943	-2.602254	H	-2.318973	-1.600318	-2.337211	H	2.422966	1.415195	-2.365905	H	2.525347	1.380567	-2.382781
C	1.893219	-2.155787	-0.164210	C	1.731520	-1.984405	0.334208	C	-1.636218	1.901567	0.250486	C	-1.529197	2.012232	0.291275
C	2.416653	-2.366463	-1.131152	C	2.216255	-2.461281	-0.902672	C	-2.152026	2.247584	-1.016668	C	-2.057502	2.377378	-0.967216
C	1.514639	-2.446116	-2.339236	C	1.279798	-2.815850	-0.830148	C	-1.249623	2.563500	-2.182797	C	-1.172047	2.713362	-2.140352
H	2.105767	-2.596592	-3.252982	H	1.846270	-3.143614	-2.913879	H	-1.843783	2.856237	-3.059645	H	-1.778474	3.052962	-2.991447
H	0.922676	-1.524292	-2.461411	H	0.651252	-1.957428	-2.324056	H	-0.626823	1.696571	-2.460879	H	-0.527805	1.842333	-2.464666
H	0.797027	-3.278906	-2.266538	H	0.594329	-3.633316	-1.754652	H	-0.562249	3.394392	-1.955268	H	-0.460694	3.519157	-1.897560
C	3.809184	-2.434112	-1.278973	C	3.605419	-2.563391	-1.071173	C	-3.546350	2.287809	-1.168786	C	-3.452799	2.436071	-1.101535
H	4.224147	-2.585205	-2.280233	H	3.991906	-2.925255	-2.028970	H	-3.957895	2.554230	-2.147050	H	-3.872013	2.714205	-2.073111
C	4.679047	-2.309294	-0.185727	C	4.504960	-2.220893	-0.052155	C	-4.420108	2.014220	-0.108374	C	-4.316788	2.170295	-0.031881
C	6.174566	-2.420916	-0.367663	C	5.995731	-2.369653	-0.246813	C	-5.916920	2.041439	-0.308357	C	-5.815042	2.210086	-0.214100
H	6.483874	-2.094947	-1.371410	H	6.540126	-1.496064	0.142569	H	-6.433623	2.454000	0.571175	H	-6.317995	2.628125	0.670742
H	6.509740	-3.464505	-0.244099	H	6.252719	-2.488436	-1.309071	H	-6.308377	1.022965	-0.468512	H	-6.214741	1.193646	-0.366012
H	6.715507	-1.813627	0.372559	H	6.377721	-3.255211	0.287861	H	-6.195161	2.645044	-1.184388	H	-6.099264	2.812964	-1.088671
C	4.122539	-2.103354	1.083808	C	3.984826	-1.753170	1.163399	C	-3.869027	1.694293	1.140232	C	-3.754414	1.835308	1.212032
C	4.784930	-1.993044	1.947570	H	4.670660	-1.471184	1.967796	H	-4.533990	1.484092	1.983048	H	-4.411554	1.664253	2.065718
C	2.736638	-2.030689	1.287128	C	2.606190	-1.632441	1.384828	C	-2.484374	1.637567	1.346987	C	-2.386667	1.781180	1.405115
C	2.173665	-1.799141	2.666589	C	2.078743	-1.126202	2.702998	C	-1.923967	1.297953	2.705134	C	-1.807153	1.480837	2.771243
H	1.514632	-2.625082	2.905203	H	1.451687	-1.881363	3.205393	H	-1.316845	2.122806	3.114373	H	-1.178392	2.307209	3.143134
H	1.570609	-0.878218	2.704021	H	1.451575	-0.229994	2.568066	H	-1.272028	0.410668	2.658546	H	-1.184664	0.572012	2.757326
H	2.982792	-1.717541	3.405459	H	2.906800	-0.876210	3.380398	H	-2.735408	1.098832	3.418736	H	-2.620236	1.332555	3.495152
C	1.572028	0.877382	-0.348694	C	1.456040	0.911315	-0.650796	C	-1.392399	-1.335862	-0.935601	C	-1.332884	-1.865083	-1.094050
C	3.573936	2.147086	-0.102829	C	3.798460	1.555466	-0.977705	C	-3.793634	-1.724011	-1.192012	C	-3.787181	-1.666197	-1.217126
C	2.400957	2.070548	-0.226199	C	2.570741	1.777076	-0.299558	C	-2.671736	-1.717533	-0.325072	C	-2.661361	-2.080783	-0.471502
C	4.407575	3.262074	-0.964410	C	4.921486	2.335872	-0.708272	C	-5.059471	-2.089828	-0.733884	C	-5.085017	-1.884988	-0.750050
C	2.117662	3.143509	0.653400	C	2.524482	2.802279	0.677549	C	-2.870936	-2.090709	1.023057	C	-2.883610	-2.715796	0.768042
C	4.108447	4.316279	-0.090458	C	4.854866	3.342737	0.263508	C	-5.233913	-2.466438	0.602848	C	-5.287984	-2.526652	0.476125
H	5.299146	3.308584	-1.594056	H	5.852335	2.158147	-1.251580	H	-5.908124	-2.091020	-1.421745	H	-5.939131	-1.566136	-1.352199
C	2.969419	4.245803	0.722456	C	3.657644	3.563510	0.958986	C	-4.135757	-2.466823	1.473924	C	-4.180805	-2.937510	1.230983
H	1.245337	3.075841	-1.305547	H	1.595469	2.956369	1.228822	H	-2.014183	-2.088395	1.699338	H	-2.029311	-2.999179	1.383786
H	4.767495	5.185838	-0.036103	H	5.735198	3.952090	0.481365	H	-6.221445	-2.762871	0.964452	H	-6.301166	-2.706616	0.842904
H	2.746941	5.057647	1.418950	H	3.608753	4.340855	1.725053	H	-4.268682	-2.762591	2.517183	H	-4.330548	-3.432777	2.193231
C	-1.119595	4.152145	-0.476301	C	-1.416633	2.948026	-0.683345	C	-0.092149	-3.161781	-1.027343	C	-0.100440	-2.999273	-0.961984
C	-1.988099	3.431186	0.244766	C	-0.215049	3.163648	-1.314642	C	1.270442	-2.872741	-0.794820	C	1.259399	-2.539996	-0.626315
H	-2.659352	2.712378	-0.231827	H	-2.277861	2.586096	-1.256684	H	-0.670237	-3.673456	-0.257196	H	-0.541292	-3.718841	-0.206576
H	-2.077264	3.546178	1.326851	H	-1.611925	3.345960	0.313445	H	-0.438159	-3.258503	-2.058789	H	-1.060855	-3.417166	-1.976691
H	-1.028887	4.017578	-1.556032	H	-0.088749	2.941301	-2.374755	H	1.712190	-3.190631	0.153280	H			

Ru-IV-V				Ru-V				Ru-V-VI				Ru-VI			
Ru	0.192325	-0.816956	-0.496227	Ru	-0.253980	-1.092364	-0.025175	Ru	-0.364192	-0.466649	0.577433	Ru	-0.097077	0.353440	-1.433386
Cl	0.079965	-1.788616	1.720058	Cl	-0.166961	-0.957558	-2.454733	Cl	0.574670	-1.448577	-1.363634	Cl	-1.028641	-1.597178	-2.278175
Cl	0.252509	0.043023	-2.765283	Cl	-0.306546	-1.135264	2.415130	Cl	-0.613460	0.059632	2.858862	Cl	-0.429092	2.640190	-1.197293
N	1.965846	1.393845	0.621230	N	-1.955599	1.465444	0.020842	N	-2.770561	0.920810	-0.578479	N	1.212061	-0.228614	1.219935
N	-0.154764	1.989118	0.584821	N	0.194015	1.929524	0.044082	N	-0.917696	2.131331	-0.565945	N	-0.995970	-0.278076	1.271982
C	0.710963	0.986751	0.283118	C	-0.707935	0.915409	0.014754	C	-1.446169	0.912547	-0.246768	C	0.088414	-0.094496	0.442332
C	1.994830	2.791005	1.122213	C	-1.932316	2.949059	-0.010887	C	-3.173347	2.180790	-1.243297	C	0.895780	-0.634970	2.608708
H	2.517774	3.438849	0.399819	H	-2.549789	3.355989	0.803094	H	-4.083146	2.585994	-0.776886	H	1.479396	-0.037504	3.322808
H	2.531594	2.841465	2.080521	H	-2.342278	3.311287	-0.967366	H	-3.84963	2.000107	-2.310671	H	1.146297	-1.699217	2.760224
C	0.504488	3.137160	1.253291	C	-0.441298	3.267132	0.151035	C	-1.944522	3.085068	-1.036353	C	-0.611086	-0.373536	2.694885
H	0.176439	3.198765	2.303553	H	-0.054223	3.932582	-0.633948	H	-1.614411	3.575038	-1.963774	H	-1.162304	-1.186158	3.189212
H	0.234670	4.077678	0.751120	H	-0.205529	3.714149	1.129939	H	-2.123460	3.864100	-0.276370	H	-0.842229	0.571663	3.216053
C	3.216272	0.709842	0.422130	C	-3.237930	0.814658	0.009036	C	-3.710950	-0.151058	-0.437783	C	2.590797	-0.206202	0.823954
C	3.785512	-0.003322	1.501297	C	-3.890871	0.581058	-1.225601	C	-3.917106	-1.045797	-1.516143	C	3.216462	-1.403008	0.413179
C	3.078307	-0.126120	2.825886	C	-3.240510	0.912378	-2.543466	C	-3.061798	-0.988253	-2.756296	C	2.435225	-2.668374	0.266102
H	3.691049	-0.696230	3.537975	H	-3.902685	0.640648	-3.377147	H	-3.362093	-1.768784	-3.468490	H	3.068030	-3.477313	-0.158912
H	2.108056	-0.637102	2.710794	H	-2.283226	0.380285	-2.670996	H	-1.995362	-1.133156	-2.515518	H	1.564265	-2.530309	-0.393587
H	2.877089	0.860899	3.273925	H	-3.026780	1.990635	-2.629315	H	-3.146732	-0.017544	-3.270685	H	2.056161	-3.051229	1.234693
C	5.037855	-0.605301	1.308963	C	-5.176044	0.020831	-1.196534	C	-4.915192	-2.019133	-1.383273	C	4.580061	-1.358156	0.088635
H	5.480357	-1.167049	2.137010	H	-5.677643	-0.183509	-2.147102	H	-5.072536	-2.723915	-2.205202	C	5.070357	-2.276911	-0.26933
C	5.738120	-0.498126	0.099991	C	-5.835352	-0.272658	0.004633	C	-5.711720	-2.116627	-0.231818	C	5.325115	-0.172866	0.171675
C	7.068667	-1.187375	-0.090970	C	-7.232388	-0.847129	0.002483	C	-6.801878	-3.156850	-0.134355	C	6.799876	-0.159250	-0.154775
H	7.724582	-0.617297	-0.765303	H	-7.988187	-0.044614	0.042138	H	-7.721120	-2.810403	-0.635843	H	7.405081	-0.337511	0.749967
H	6.937116	-2.187872	-0.535335	H	-7.401265	-1.497016	0.873863	H	-7.059039	-3.728888	0.912304	H	7.110970	0.103460	-0.569923
H	7.593251	-1.322948	0.866059	H	-7.425050	-1.434028	-0.906823	H	-6.503125	-0.098981	-0.617043	H	7.058485	-0.942828	-0.881564
C	5.163306	0.254932	-0.932979	C	-5.181647	0.023161	1.208881	C	-5.486311	-1.209584	0.813098	C	4.669535	0.995120	0.586262
H	5.705768	0.374903	-1.875658	H	-5.687390	-0.179016	2.157722	H	-6.094462	-1.274299	1.720017	H	5.231248	1.932051	0.646891
C	3.914459	0.878741	-0.795898	C	-3.897159	0.582522	1.241404	C	-4.502694	-0.214138	0.733376	C	3.308195	1.003997	0.922906
C	3.352579	1.703018	-1.925456	C	-3.246180	0.911129	2.559199	C	-4.278036	0.740486	1.877049	C	2.627816	2.283698	1.340503
H	4.040535	1.699525	-2.782220	H	-3.938088	0.713819	3.389651	H	-5.018257	0.575246	2.671759	H	3.352316	3.107843	1.394730
C	3.203019	2.753804	-1.627067	H	-2.951002	1.971711	2.613471	H	-4.357189	1.790802	1.553896	H	2.10329	2.188847	2.328891
H	2.377809	1.315831	-2.264640	H	-2.331984	0.313544	2.714284	H	-3.271109	0.612703	2.309167	H	1.836421	2.564783	0.627710
C	-1.585038	2.004113	0.401458	C	1.636665	1.875675	0.039058	C	0.449892	2.533323	-0.352607	C	-2.391676	-0.200922	0.922506
C	-2.111223	2.599998	0.768507	C	2.334364	1.886207	1.269017	C	0.815221	3.171231	0.855942	C	-3.079678	1.029317	1.007804
C	-1.217253	3.147864	-1.851135	C	1.619714	1.841107	2.595043	C	-0.188669	3.462551	1.942765	C	-2.432258	2.290479	1.525310
H	-1.814742	3.662003	-2.616944	H	2.345405	1.846811	3.420151	H	0.311261	3.903808	2.815704	H	-2.866593	3.176957	1.042926
H	-0.645578	2.341088	-2.338108	H	0.991985	0.940639	2.697126	H	-0.701395	2.548534	2.277621	H	-1.352868	2.316440	1.339442
H	-0.488113	3.871353	-1.452449	H	0.960766	2.714984	2.731207	H	-0.952601	4.181194	1.602309	H	-2.607074	2.388405	2.611293
C	-3.504170	2.682223	-0.898386	C	3.732841	1.974076	1.231299	C	2.152431	3.562094	1.014941	C	-4.442481	1.049167	0.671064
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H	-6.407634	1.684532	0.624241	H	6.329316	2.603011	-0.906446	H	5.025865	4.097978	-0.700905	H	-7.140852	-0.942279	0.248108
H	-6.191166	2.152951	-1.082034	H	6.390725	1.150387	0.113437	H	5.135393	2.889792	0.592427	H	-6.689203	-0.011269	-1.191979
H	-6.195274	3.391334	0.185494	H	6.325679	2.753143	0.869882	H	6.448025	4.552065	0.981629	H	-7.088932	0.838613	0.314373
C	-3.815266	1.675046	1.262711	C	3.714944	2.109190	-1.167719	C	2.696300	2.796414	-1.199275	H	-4.444597	-1.329363	0.329263
H	-4.476209	1.324659	2.060591	H	4.247182	2.220015	-1.217066	H	3.421096	2.670321	-2.008654	H	-4.980598	-2.254222	0.096620
C	-2.428446	1.568776	1.448575	C	2.315228	2.026213	-1.191290	C	1.374688	2.383168	-1.412697	C	-3.082899	-1.404518	0.646037
C	-1.881703	1.027818	2.744896	C	1.576263	2.127988	-2.500430	C	0.967388	1.803902	-2.742781	C	-2.393922	-2.744694	0.700302
H	-1.295774	1.790614	3.284333	H	0.896849	2.996629	-2.517193	H	0.066201	2.293193	-3.145258	H	-1.840044	-2.878396	1.643385
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C	-1.267479	-2.311592	-1.432869	C	1.142265	2.929217	0.407727	C	4.167152	-2.759375	1.720882	C	1.595750	0.263965	-2.071696
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C	-4.847362	-1.810231	-0.373824	C	4.721735	-1.974089	1.085958	C	3.355041	-2.140282	-0.210567				
C	-2.635311	-3.300659	0.480370	C	3.026916	-2.197927	-1.134378	C	4.598924	-2.162675	-0.702191				
C	-4.969594	-2.677846	0.715929	C	5.227701	-1.775102	-0.203795	C	6.876213	-1.874444	-1.497563				
H	-5.707254	-1.229289	-0.713873	C	5.379608	-1.886782	1.953548	H	8.429355	-2.130775	-0.011577				
C	-3.857732	-3.419558	1.139302	C	4.371889	-1.871108	-1.308714	C	5.494303	-1.884541	-1.734842				
H	-1.777423	-3.873321	0.831896	H	2.366851	-2.260280	-2.001721	H	3.525106	-2.144862	-0.903759				
H	-5.926724	-2.781721	1.232194	H	6.285148	-1.542204	-0.349073	H	7.572729	-1.655983	-2.310269				
H	-3.946593	-4.097982	1.990758	H	4.758154	-1.698435	-2.315675	H	5.110711	-1.667917	-2.734714				
C	-0.085760	-3.055025	-1.287020	C	0.250647	-3.365418	-0.555896	C	2.848698	-3.016260	1.658799				
C	1.769308	-1.710021	-0.800404	C	-1.974970	-1.694612	-0.022446	C	-1.703616	-1.703331	0.649806				
H	0.054249	-3.730825	-0.442319	H	0.476076	-3.343943	-1.621532	H	2.293050	-3.018884	0.717496				
H	0.509298	-3.244655	-2.181784	H	-0.599012	-3.977373	-0.253739	H	2.281853	-3.238207	2.564471				
H	2.239328	-2.327571	-0.016984	H	-2.504424	-1.908731	-0.966299	H	-1.916468	-2.386071	-0.188681				
H	-3.527972	-1.012760	-1.888978	H	2.975370	-2.453527	2.269692	H	6.837119	-2.625567	1.829770				
H	-1.420654	-1.846677	-2.411598	H	0.928008	-3.158865	1.453683	H	4.656268	-2.797242	2.701817				
H	2.283635	-													

Fe-I (with Py)	Fe-I (with PMe ₃)	Fe-I (with PCy ₃)
Fe 0.292390 0.536184 0.220784	Fe 0.265508 0.694275 0.307480	Fe -0.202710 0.365956 -0.098700
Cl 0.627367 0.791968 -2.028242	Cl 0.632616 1.178545 -1.913014	Cl 0.030709 0.647863 2.157516
Cl 0.458399 0.224896 2.503715	Cl 0.701335 0.326328 2.564739	Cl 0.074334 0.519898 -2.411623
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C 1.221807 -3.595371 -0.032160	C 0.566992 -1.236378 -0.005267	C -1.086978 4.480692 -0.806487
H 1.612735 -3.984152 0.922745	C 1.695807 -3.320530 -0.164100	H -0.704581 4.759834 -1.801865
H 1.751431 -4.095893 -0.855211	H 2.119595 -3.708759 0.776762	H -0.983965 5.347392 -0.137772
C -0.301601 -3.717740 -0.133424	H 2.265272 -3.744742 -1.003347	C -2.509885 3.924472 -0.864376
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H -0.733912 -4.371272 0.637593	H -0.116167 -3.901994 -1.277041	H -3.008114 4.116952 -1.824872
C 2.775646 -1.627101 -0.224269	H -0.184107 -4.294071 0.462981	C 1.038566 3.581989 0.154571
C 3.323717 -1.469470 -1.520323	C 3.082142 -1.228024 -0.296075	C 1.255052 3.98530 1.507682
C 2.565716 -1.873368 -2.759794	C 3.584315 -0.947469 -1.589512	C 0.117640 4.40867 2.491057
H 3.051249 -1.467979 -3.658225	C 2.807657 -1.293600 -2.834138	H 0.481162 4.408141 3.460922
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H 2.548706 -2.972793 -2.863342	H 1.850896 -0.752859 -2.864922	H -0.659387 4.738491 2.137207
C 4.636267 -0.992585 -1.634493	H 2.589295 -2.373537 -2.882704	C 2.559246 4.246053 1.914665
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H 2.632449 5.833434 1.395414	C 2.436713 3.221296 0.862507	H 1.179918 -5.084792 -3.325115
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		H 2.33265 -3.294039 1.237145
		C 0.422580 -2.944054 2.168598
		H -0.178393 -2.080424 2.487668
		H -0.179144 -3.482536 1.418854
		C 0.694247 -3.855317 3.378159
		H 1.235163 -4.761843 3.046235
		H -0.262638 -4.199510 3.803768
		C 1.528363 -3.130635 4.445150
		H 1.749508 -3.807068 5.287841
		H 0.938637 -2.291945 4.856565
		C 2.829709 -2.583585 3.841941
		H 3.470948 -3.431374 3.534346
		C 3.399260 -2.021062 4.60659
		C 2.563827 1.675276 2.625887
		H 3.529828 -1.343516 2.216115
		H 2.019167 -0.772738 2.941068

