

The Group 9 Cyclopentadienylmetal *cis*-Ethylenedithiolates as Metallodithiolene Ligands in Metal Carbonyl Chemistry: Analogies to Benzene Metal Carbonyl Complexes

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Supporting Information

Table S1. Initial structures.

Table S2A. Energy ranking for CpCoS₂C₂H₂·Cr(CO)_n structures.

Table S2B. Distance table for the lowest energy CpCoS₂C₂H₂·Cr(CO)_n structures.

Table S3A. Energy ranking for CpCoS₂C₂H₂·Fe(CO)_n structures.

Table S3B. Distance table for the lowest energy CpCoS₂C₂H₂·Fe(CO)_n structures.

Table S4A. Energy ranking for CpIrS₂C₂H₂·Cr(CO)_n structures.

Table S4B. Distance table for the lowest energy CpIrS₂C₂H₂·Cr(CO)_n structures.

Table S5A. Energy ranking for CpIrS₂C₂H₂·Fe(CO)_n structures.

Table S5B. Distance table for the lowest energy CpIrS₂C₂H₂·Fe(CO)_n structures.

Table S6A. Energy ranking for CpRhS₂C₂H₂·Cr(CO)_n structures.

Table S6B. Distance table for the lowest energy CpRhS₂C₂H₂·Cr(CO)_n structures.

Table S7A. Energy ranking for CpRhS₂C₂H₂·Fe(CO)_n structures.

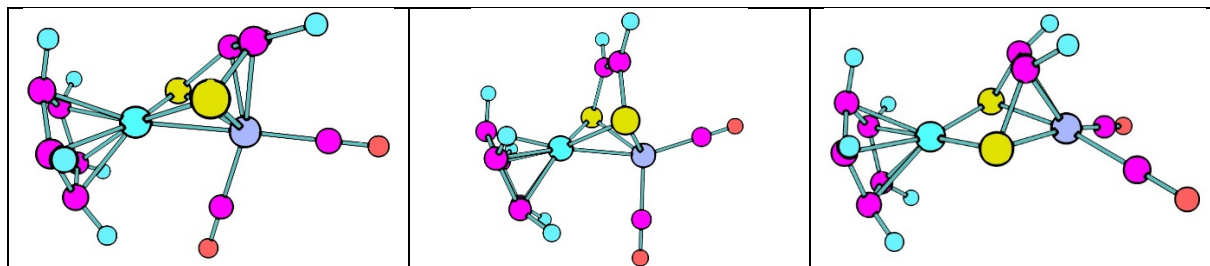
Table S7B. Distance table for the lowest energy CpRhS₂C₂H₂·Fe(CO)_n structures.

Table S8. Harmonic $\nu(\text{CO})$ vibrational frequencies and infrared intensities (in parentheses, in km/mol) for the CpMS₂C₂H₂·M'(CO)_n systems (M = Co, Rh, Ir; M' = Cr, Fe).

Table S9. Thermochemistry table for the CpH₂CpMS₂C₂H₂·M'(CO)_n systems (M = Co, Rh, Ir; M' = Cr, Fe).

Complete Gaussian09 Reference (reference 19)

Table S1. Initial structures.



Metal 1 – Co, Rh, Ir

Metal 2 – Fe (n CO = 2 – 4), Cr (n CO = 2 – 5)

Table S2A. Energy rank for all of the CpCoS₂C₂H₂·Cr(CO)_n optimized structures. PBE0/6-311G(d,p).

Co-Cr

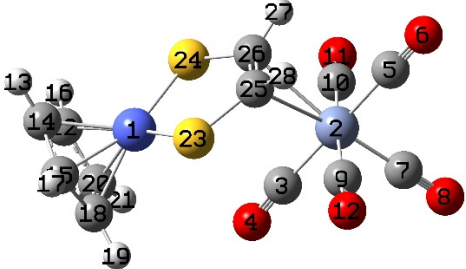
	name	E (a.u.)	ΔE (kcal/mol)
5-1	11-Co-Cr-CO-5-md2-freq	-4059.649109	0.0
5-2	10-ir-Cr-CO-5-md1-new-Cr-Co-f-r-ok	-4059.643976	3.2
5-3	12-rh-Cr-CO-5-md3-freq-fneg2-fneg1-new-Co-Cr-c-freq-ok	-4059.621753	17.2
4-1	8-Co-Cr-CO-4-md2-r1-freq	-3946.410367	0.0
4-2	7-Co-Cr-CO-4-md1-freq	-3946.397991	7.8
4-3	9-Co-Cr-CO-4-md3-r1-freq	-3946.389313	13.2
3-1	6-Co-Cr-CO-3-md3-r1-freq	-3833.185023	0.0
2-1	3-Co-Cr-CO-2-md3-r1-freq-fneg2-freq	-3719.897911	0.0

Table S2B. Distance table for the lowest-lying CpCoS₂C₂H₂·Cr(CO)_n structures after PBE0/6-311G(d,p) optimization.

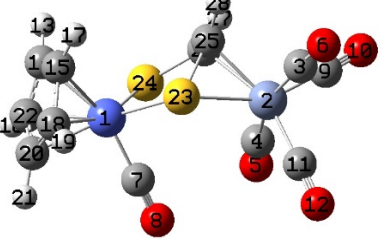
CpCoS₂C₂H₂·Cr(CO)₅

<p>1. -4059.649109 0.0</p>		1	2	3	4	5	
	1 Co	0.000000					
	2 Cr	2.746065	0.000000				
	3 C	3.571205	1.901191	0.000000			
	4 C	3.148811	1.874175	3.774500	0.000000		
	5 O	3.887152	3.017586	4.916598	1.144305	0.000000	
	6 O	4.453047	3.039299	1.140793	4.910295	6.050357	
	7 C	2.364520	1.889628	2.594577	2.773953	3.703171	
	8 O	3.068556	3.017264	3.433551	3.708014	4.481094	
	9 C	4.274001	1.896009	2.645695	2.665594	3.550695	
	10 O	5.320085	3.034844	3.529056	3.570742	4.267618	
	11 C	4.290073	1.835688	2.662724	2.560245	3.428323	
	12 O	5.343143	2.982573	3.567997	3.439503	4.093249	
	13 H	2.752994	5.069221	5.955879	4.884822	5.172162	
	14 C	2.012948	4.508551	5.498319	4.278830	4.583772	
	15 C	2.025783	4.748883	5.439303	4.841737	5.284983	
	16 H	2.802861	4.007716	5.606289	2.896070	2.732279	
	17 H	2.778900	5.477225	5.856491	5.806547	6.325742	
	18 C	2.049692	4.322402	5.172021	4.293239	4.700905	
	19 H	2.816913	4.763695	5.390480	4.912892	5.367583	
	20 C	2.075303	3.784217	5.104655	3.209061	3.402619	
	21 H	2.831995	3.764873	5.234413	2.926192	2.960912	
	22 C	2.050935	3.904091	5.301408	3.183521	3.289566	
	23 S	2.210413	3.709245	3.294945	4.921064	5.864602	
	24 S	2.172606	2.424747	3.178181	3.008134	3.830598	
	25 C	3.075280	3.869073	3.176042	5.224322	6.213352	
	26 C	3.089260	3.430697	3.142518	4.586321	5.516916	
	27 H	4.120545	4.137913	3.753008	5.240163	6.124902	
28 H	4.113667	4.802588	3.785834	6.262934	7.274002		
		6	7	8	9	10	
6 O	0.000000						
7 C	3.486742	0.000000					
8 O	4.112234	1.157608	0.000000				
9 C	3.515536	3.766571	4.858483	0.000000			
10 O	4.198600	4.898333	5.975535	1.139163	0.000000		
11 C	3.526062	2.453514	3.135723	2.580868	3.460060		
12 O	4.234233	3.304418	3.691925	3.471852	4.148373		
13 H	6.762264	5.086180	5.714109	6.031128	6.824148		
14 C	6.358122	4.242997	4.772292	5.737058	6.647679		
15 C	6.170881	3.946924	4.176233	6.274424	7.290219		
16 H	6.677065	4.227053	4.930932	4.912127	5.713189		
17 H	6.427391	4.621141	4.756701	6.978715	7.977644		
18 C	5.969405	3.120598	3.105472	6.056598	7.147439		
19 H	6.072370	3.211059	2.805605	6.606243	7.731107		

	20	C	6.081428	2.959068	3.216678	5.375511	6.421173
	21	H	6.247008	2.873484	3.005424	5.344260	6.381458
	22	C	6.311215	3.711149	4.284932	5.143625	6.070397
	23	S	3.631382	3.173338	3.598699	5.077887	6.048955
	24	S	4.063421	3.464048	4.534015	2.928002	3.716357
	25	C	3.354110	4.147249	4.873668	4.608413	5.349869
	26	C	3.570827	4.271399	5.221426	3.741811	4.356362
	27	H	4.035869	5.228666	6.219638	3.965475	4.306575
	28	H	3.642137	5.038757	5.668854	5.398890	6.035607
			11	12	13	14	15
	11	C	0.000000				
	12	O	1.146986	0.000000			
	13	H	6.750651	7.830579	0.000000		
	14	C	6.065042	7.097928	1.078263	0.000000	
	15	C	6.155308	7.125207	2.226201	1.414099	0.000000
	16	H	5.281390	6.212643	2.696665	2.234519	3.331628
	17	H	6.912771	7.886815	2.684713	2.233465	1.090359
	18	C	5.392956	6.234148	3.338258	2.297843	1.414989
	19	H	5.576453	6.294267	4.351091	3.344415	2.235933
	20	C	4.779148	5.607850	3.332948	2.289980	2.281843
	21	H	4.355711	5.024498	4.343101	3.333844	3.326803
	22	C	5.238402	6.194066	2.241363	1.426808	2.291903
	23	S	5.129163	6.127719	3.949269	3.547929	2.965939
	24	S	4.246126	5.389454	3.247020	3.161610	3.844845
	25	C	5.460975	6.523739	4.227764	4.209675	4.131762
	26	C	5.149157	6.260570	3.977387	4.094540	4.449669
	27	H	5.773153	6.852721	4.660977	4.947340	5.434710
	28	H	6.278402	7.288322	5.080476	5.147744	4.965353
			16	17	18	19	20
	16	H	0.000000				
	17	H	4.351989	0.000000			
	18	C	3.337443	2.232837	0.000000		
	19	H	4.346739	2.694750	1.081834	0.000000	
	20	C	2.223903	3.335395	1.417060	2.231776	0.000000
	21	H	2.674957	4.346125	2.228618	2.684581	1.081370
	22	C	1.076520	3.346147	2.296873	3.340399	1.409175
	23	S	4.949333	2.899136	3.303993	3.546590	4.033735
	24	S	3.221790	4.433693	4.183129	4.985684	3.817974
	25	C	5.388955	4.076647	4.716869	5.160417	5.141519
	26	C	4.818001	4.644068	5.029324	5.668869	5.095591
	27	H	5.520906	5.594787	6.078891	6.748233	6.069280
	28	H	6.451121	4.718534	5.609229	5.952417	6.158704
			21	22	23	24	25
	21	H	0.000000				
	22	C	2.218391	0.000000			
	23	S	4.746343	4.159571	0.000000		
	24	S	4.372767	3.150924	3.137532	0.000000	
	25	C	5.856334	4.862502	1.733442	2.681023	0.000000
	26	C	5.756691	4.549406	2.702157	1.750269	1.342269
	27	H	6.708760	5.397602	3.723634	2.439700	2.144735

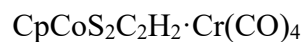
	<table border="0"> <tr> <td>28 H</td> <td>6.882977</td> <td>5.905649</td> <td>2.416754</td> <td>3.700853</td> <td>1.086884</td> </tr> <tr> <td></td> <td>26</td> <td>27</td> <td>28</td> <td></td> <td></td> </tr> <tr> <td>26 C</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>27 H</td> <td>1.086503</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>28 H</td> <td>2.123332</td> <td>2.513399</td> <td>0.000000</td> <td></td> <td></td> </tr> </table>	28 H	6.882977	5.905649	2.416754	3.700853	1.086884		26	27	28			26 C	0.000000					27 H	1.086503	0.000000				28 H	2.123332	2.513399	0.000000																																																																																																																																																																																																																																												
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 <p>2. -4059.643976 +3.2</p>	<table border="0"> <tr> <td></td> <td>1</td> <td>2</td> <td>3</td> <td>4</td> <td>5</td> </tr> <tr> <td>1 Co</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>2 Cr</td> <td>4.395459</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 C</td> <td>3.558280</td> <td>1.885863</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 O</td> <td>3.538034</td> <td>3.028919</td> <td>1.144090</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 C</td> <td>5.741112</td> <td>1.889197</td> <td>3.774988</td> <td>4.918079</td> <td>0.000000</td> </tr> <tr> <td>6 O</td> <td>6.693439</td> <td>3.031727</td> <td>4.917567</td> <td>6.060495</td> <td>1.142622</td> </tr> <tr> <td>7 C</td> <td>5.958998</td> <td>1.836722</td> <td>2.645629</td> <td>3.526027</td> <td>2.637937</td> </tr> <tr> <td>8 O</td> <td>7.002589</td> <td>2.983540</td> <td>3.545157</td> <td>4.229073</td> <td>3.535419</td> </tr> <tr> <td>9 C</td> <td>4.835783</td> <td>1.890396</td> <td>2.656200</td> <td>3.551803</td> <td>2.686486</td> </tr> <tr> <td>10 C</td> <td>4.831702</td> <td>1.890505</td> <td>2.657230</td> <td>3.553708</td> <td>2.687156</td> </tr> <tr> <td>11 O</td> <td>5.434502</td> <td>3.031686</td> <td>3.550485</td> <td>4.256702</td> <td>3.594050</td> </tr> <tr> <td>12 O</td> <td>5.440140</td> <td>3.031605</td> <td>3.549112</td> <td>4.253958</td> <td>3.593431</td> </tr> <tr> <td>13 H</td> <td>2.752387</td> <td>7.001414</td> <td>6.299795</td> <td>6.184648</td> <td>8.075646</td> </tr> <tr> <td>14 C</td> <td>2.008260</td> <td>6.395855</td> <td>5.477440</td> <td>5.243154</td> <td>7.663139</td> </tr> <tr> <td>15 C</td> <td>2.023601</td> <td>6.156259</td> <td>5.110304</td> <td>4.795008</td> <td>7.524875</td> </tr> <tr> <td>16 H</td> <td>2.779992</td> <td>6.370973</td> <td>5.368992</td> <td>5.069830</td> <td>7.701047</td> </tr> <tr> <td>17 H</td> <td>2.775902</td> <td>6.586463</td> <td>5.689370</td> <td>5.455760</td> <td>7.830095</td> </tr> <tr> <td>18 C</td> <td>2.015348</td> <td>5.584137</td> <td>4.207253</td> <td>3.658907</td> <td>7.188106</td> </tr> <tr> <td>19 H</td> <td>2.759716</td> <td>5.524962</td> <td>4.038923</td> <td>3.385616</td> <td>7.195633</td> </tr> <tr> <td>20 C</td> <td>2.009799</td> <td>5.494443</td> <td>4.060605</td> <td>3.467170</td> <td>7.134858</td> </tr> <tr> <td>21 H</td> <td>2.748646</td> <td>5.346899</td> <td>3.739722</td> <td>2.976139</td> <td>7.089135</td> </tr> <tr> <td>22 C</td> <td>2.028042</td> <td>6.037423</td> <td>4.925949</td> <td>4.567820</td> <td>7.456238</td> </tr> <tr> <td>23 S</td> <td>2.118586</td> <td>3.610239</td> <td>3.399554</td> <td>3.806752</td> <td>4.637073</td> </tr> <tr> <td>24 S</td> <td>2.119151</td> <td>3.610669</td> <td>3.402403</td> <td>3.811091</td> <td>4.636387</td> </tr> <tr> <td>25 C</td> <td>3.054627</td> <td>2.459832</td> <td>3.133060</td> <td>3.981272</td> <td>3.049459</td> </tr> <tr> <td>26 C</td> <td>3.054493</td> <td>2.460479</td> <td>3.134690</td> <td>3.983311</td> <td>3.049325</td> </tr> <tr> <td>27 H</td> <td>4.057372</td> <td>2.822796</td> <td>3.902514</td> <td>4.835359</td> <td>2.778534</td> </tr> <tr> <td>28 H</td> <td>4.057247</td> <td>2.822435</td> <td>3.900493</td> <td>4.832543</td> <td>2.779644</td> </tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr> <td>6 O</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>7 C</td> <td>3.538781</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8 O</td> <td>4.246021</td> <td>1.146818</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>9 C</td> <td>3.588900</td> <td>2.577661</td> <td>3.461780</td> <td>0.000000</td> <td></td> </tr> <tr> <td>10 C</td> <td>3.590040</td> <td>2.577179</td> <td>3.460954</td> <td>3.777060</td> <td>0.000000</td> </tr> <tr> <td>11 O</td> <td>4.316232</td> <td>3.448662</td> <td>4.123207</td> <td>4.915461</td> <td>1.141866</td> </tr> <tr> <td>12 O</td> <td>4.314946</td> <td>3.449299</td> <td>4.124385</td> <td>1.141894</td> <td>4.915489</td> </tr> <tr> <td>13 H</td> <td>8.871384</td> <td>8.656408</td> <td>9.722678</td> <td>7.396191</td> <td>7.228309</td> </tr> <tr> <td>14 C</td> <td>8.552939</td> <td>7.950750</td> <td>8.975488</td> <td>6.771064</td> <td>6.672318</td> </tr> <tr> <td>15 C</td> <td>8.460367</td> <td>7.610930</td> <td>8.593448</td> <td>6.161897</td> <td>6.794020</td> </tr> <tr> <td>16 H</td> <td>8.617018</td> <td>7.752844</td> <td>8.701055</td> <td>7.299170</td> <td>6.015242</td> </tr> <tr> <td>17 H</td> <td>8.706244</td> <td>8.061552</td> <td>9.049703</td> <td>6.314473</td> <td>7.441668</td> </tr> <tr> <td>18 C</td> <td>8.224372</td> <td>6.810656</td> <td>7.700210</td> <td>5.652651</td> <td>6.186212</td> </tr> <tr> <td>19 H</td> <td>8.257309</td> <td>6.553555</td> <td>7.356793</td> <td>5.324542</td> <td>6.347412</td> </tr> </table>		1	2	3	4	5	1 Co	0.000000					2 Cr	4.395459	0.000000				3 C	3.558280	1.885863	0.000000			4 O	3.538034	3.028919	1.144090	0.000000		5 C	5.741112	1.889197	3.774988	4.918079	0.000000	6 O	6.693439	3.031727	4.917567	6.060495	1.142622	7 C	5.958998	1.836722	2.645629	3.526027	2.637937	8 O	7.002589	2.983540	3.545157	4.229073	3.535419	9 C	4.835783	1.890396	2.656200	3.551803	2.686486	10 C	4.831702	1.890505	2.657230	3.553708	2.687156	11 O	5.434502	3.031686	3.550485	4.256702	3.594050	12 O	5.440140	3.031605	3.549112	4.253958	3.593431	13 H	2.752387	7.001414	6.299795	6.184648	8.075646	14 C	2.008260	6.395855	5.477440	5.243154	7.663139	15 C	2.023601	6.156259	5.110304	4.795008	7.524875	16 H	2.779992	6.370973	5.368992	5.069830	7.701047	17 H	2.775902	6.586463	5.689370	5.455760	7.830095	18 C	2.015348	5.584137	4.207253	3.658907	7.188106	19 H	2.759716	5.524962	4.038923	3.385616	7.195633	20 C	2.009799	5.494443	4.060605	3.467170	7.134858	21 H	2.748646	5.346899	3.739722	2.976139	7.089135	22 C	2.028042	6.037423	4.925949	4.567820	7.456238	23 S	2.118586	3.610239	3.399554	3.806752	4.637073	24 S	2.119151	3.610669	3.402403	3.811091	4.636387	25 C	3.054627	2.459832	3.133060	3.981272	3.049459	26 C	3.054493	2.460479	3.134690	3.983311	3.049325	27 H	4.057372	2.822796	3.902514	4.835359	2.778534	28 H	4.057247	2.822435	3.900493	4.832543	2.779644		6	7	8	9	10	6 O	0.000000					7 C	3.538781	0.000000				8 O	4.246021	1.146818	0.000000			9 C	3.588900	2.577661	3.461780	0.000000		10 C	3.590040	2.577179	3.460954	3.777060	0.000000	11 O	4.316232	3.448662	4.123207	4.915461	1.141866	12 O	4.314946	3.449299	4.124385	1.141894	4.915489	13 H	8.871384	8.656408	9.722678	7.396191	7.228309	14 C	8.552939	7.950750	8.975488	6.771064	6.672318	15 C	8.460367	7.610930	8.593448	6.161897	6.794020	16 H	8.617018	7.752844	8.701055	7.299170	6.015242	17 H	8.706244	8.061552	9.049703	6.314473	7.441668	18 C	8.224372	6.810656	7.700210	5.652651	6.186212	19 H	8.257309	6.553555	7.356793	5.324542	6.347412
	1	2	3	4	5																																																																																																																																																																																																																																																																				
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3 C	3.558280	1.885863	0.000000																																																																																																																																																																																																																																																																						
4 O	3.538034	3.028919	1.144090	0.000000																																																																																																																																																																																																																																																																					
5 C	5.741112	1.889197	3.774988	4.918079	0.000000																																																																																																																																																																																																																																																																				
6 O	6.693439	3.031727	4.917567	6.060495	1.142622																																																																																																																																																																																																																																																																				
7 C	5.958998	1.836722	2.645629	3.526027	2.637937																																																																																																																																																																																																																																																																				
8 O	7.002589	2.983540	3.545157	4.229073	3.535419																																																																																																																																																																																																																																																																				
9 C	4.835783	1.890396	2.656200	3.551803	2.686486																																																																																																																																																																																																																																																																				
10 C	4.831702	1.890505	2.657230	3.553708	2.687156																																																																																																																																																																																																																																																																				
11 O	5.434502	3.031686	3.550485	4.256702	3.594050																																																																																																																																																																																																																																																																				
12 O	5.440140	3.031605	3.549112	4.253958	3.593431																																																																																																																																																																																																																																																																				
13 H	2.752387	7.001414	6.299795	6.184648	8.075646																																																																																																																																																																																																																																																																				
14 C	2.008260	6.395855	5.477440	5.243154	7.663139																																																																																																																																																																																																																																																																				
15 C	2.023601	6.156259	5.110304	4.795008	7.524875																																																																																																																																																																																																																																																																				
16 H	2.779992	6.370973	5.368992	5.069830	7.701047																																																																																																																																																																																																																																																																				
17 H	2.775902	6.586463	5.689370	5.455760	7.830095																																																																																																																																																																																																																																																																				
18 C	2.015348	5.584137	4.207253	3.658907	7.188106																																																																																																																																																																																																																																																																				
19 H	2.759716	5.524962	4.038923	3.385616	7.195633																																																																																																																																																																																																																																																																				
20 C	2.009799	5.494443	4.060605	3.467170	7.134858																																																																																																																																																																																																																																																																				
21 H	2.748646	5.346899	3.739722	2.976139	7.089135																																																																																																																																																																																																																																																																				
22 C	2.028042	6.037423	4.925949	4.567820	7.456238																																																																																																																																																																																																																																																																				
23 S	2.118586	3.610239	3.399554	3.806752	4.637073																																																																																																																																																																																																																																																																				
24 S	2.119151	3.610669	3.402403	3.811091	4.636387																																																																																																																																																																																																																																																																				
25 C	3.054627	2.459832	3.133060	3.981272	3.049459																																																																																																																																																																																																																																																																				
26 C	3.054493	2.460479	3.134690	3.983311	3.049325																																																																																																																																																																																																																																																																				
27 H	4.057372	2.822796	3.902514	4.835359	2.778534																																																																																																																																																																																																																																																																				
28 H	4.057247	2.822435	3.900493	4.832543	2.779644																																																																																																																																																																																																																																																																				
	6	7	8	9	10																																																																																																																																																																																																																																																																				
6 O	0.000000																																																																																																																																																																																																																																																																								
7 C	3.538781	0.000000																																																																																																																																																																																																																																																																							
8 O	4.246021	1.146818	0.000000																																																																																																																																																																																																																																																																						
9 C	3.588900	2.577661	3.461780	0.000000																																																																																																																																																																																																																																																																					
10 C	3.590040	2.577179	3.460954	3.777060	0.000000																																																																																																																																																																																																																																																																				
11 O	4.316232	3.448662	4.123207	4.915461	1.141866																																																																																																																																																																																																																																																																				
12 O	4.314946	3.449299	4.124385	1.141894	4.915489																																																																																																																																																																																																																																																																				
13 H	8.871384	8.656408	9.722678	7.396191	7.228309																																																																																																																																																																																																																																																																				
14 C	8.552939	7.950750	8.975488	6.771064	6.672318																																																																																																																																																																																																																																																																				
15 C	8.460367	7.610930	8.593448	6.161897	6.794020																																																																																																																																																																																																																																																																				
16 H	8.617018	7.752844	8.701055	7.299170	6.015242																																																																																																																																																																																																																																																																				
17 H	8.706244	8.061552	9.049703	6.314473	7.441668																																																																																																																																																																																																																																																																				
18 C	8.224372	6.810656	7.700210	5.652651	6.186212																																																																																																																																																																																																																																																																				
19 H	8.257309	6.553555	7.356793	5.324542	6.347412																																																																																																																																																																																																																																																																				

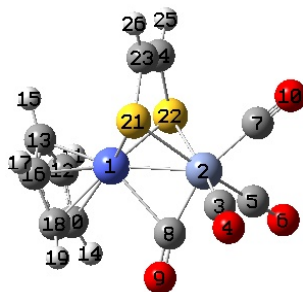
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	21	H	8.179323	6.301147	7.075271	6.032438	5.315190
	22	C	8.413956	7.441795	8.403303	6.715366	6.002115
	23	S	5.495207	5.236042	6.310045	3.355101	4.779910
	24	S	5.494297	5.235378	6.308903	4.783219	3.351145
	25	C	3.848923	4.253953	5.388781	2.724448	3.551768
	26	C	3.848626	4.254004	5.388614	3.554122	2.722485
	27	H	3.334766	4.456752	5.541819	4.087538	2.687850
	28	H	3.336179	4.457380	5.542838	2.688524	4.086700
			11	12	13	14	15
	11	O	0.000000				
	12	O	6.051797	0.000000			
	13	H	7.629372	7.882794	0.000000		
	14	C	7.113774	7.261538	1.080765	0.000000	
	15	C	7.414670	6.469347	2.235598	1.424854	0.000000
	16	H	6.112346	8.046613	2.687975	2.233497	3.349954
	17	H	8.154390	6.453449	2.690166	2.236744	1.080137
	18	C	6.800295	6.009992	3.335615	2.293241	1.414448
	19	H	7.056832	5.537758	4.346001	3.337840	2.229715
	20	C	6.051742	6.603511	3.333307	2.290335	2.299286
	21	H	5.624898	6.684105	4.343073	3.334433	3.339520
	22	C	6.291484	7.356187	2.232156	1.420447	2.306909
	23	S	5.700571	3.731495	4.186253	3.704662	3.154378
	24	S	3.725699	5.704774	3.946513	3.562568	4.082677
	25	C	4.501967	3.456591	5.203920	4.844073	4.657900
	26	C	3.453863	4.504731	5.118859	4.795702	4.970205
	27	H	3.238495	5.067855	5.869324	5.667755	5.970074
	28	H	5.066833	3.239633	6.003412	5.741684	5.492069
			16	17	18	19	20
	16	H	0.000000				
	17	H	4.357707	0.000000			
	18	C	3.347160	2.229562	0.000000		
	19	H	4.353050	2.689820	1.080137	0.000000	
	20	C	2.230861	3.343848	1.427043	2.235791	0.000000
	21	H	2.690699	4.349190	2.234913	2.683766	1.080381
	22	C	1.080152	3.349162	2.303118	3.343801	1.416475
	23	S	4.872962	3.229360	3.264369	3.424122	3.868653
	24	S	3.141481	4.806915	3.980723	4.635952	3.385237
	25	C	5.444057	4.876819	4.646846	4.849363	4.841249
	26	C	4.839161	5.427704	4.890464	5.281223	4.675990
	27	H	5.528237	6.414022	5.943616	6.360211	5.637019
	28	H	6.471586	5.549759	5.576157	5.699582	5.885289
			21	22	23	24	25
	21	H	0.000000				
	22	C	2.231540	0.000000			
	23	S	4.449066	4.124560	0.000000		
	24	S	3.634165	3.109790	3.076450	0.000000	
	25	C	5.189466	4.981246	1.742219	2.697554	0.000000
	26	C	4.896783	4.639061	2.697137	1.742153	1.378361
	27	H	5.806106	5.482722	3.684136	2.419630	2.152498

	28 H 6.251701 6.004095 2.419484 3.684538 1.083892 26 27 28
	26 C 0.000000
	27 H 1.083927 0.000000
	28 H 2.152725 2.509412 0.000000
	
3. -4059.621753 +17.2	1 2 3 4 5 1 Co 0.000000 2 Cr 3.968902 0.000000 3 C 5.102950 1.873714 0.000000 4 C 4.092734 1.878775 3.706495 0.000000 5 O 4.660623 3.018483 4.821544 1.143581 0.000000 6 O 6.034714 3.016256 1.145033 4.827533 5.926599 7 C 1.759041 3.740634 5.199441 3.285859 3.616062 8 O 2.890906 4.034438 5.576189 3.224334 3.310079 9 C 5.562859 1.821774 2.465510 2.468558 3.289283 10 O 6.616843 2.971352 3.330965 3.345087 3.926437 11 C 4.892295 1.854679 2.507054 2.528842 3.397179 12 O 5.658787 2.999255 3.389625 3.404051 4.058537 13 H 2.826319 5.824703 6.716329 6.028365 6.511923 14 C 2.089989 5.611635 6.516665 5.829016 6.337167 15 C 2.088810 5.345855 5.928342 5.936682 6.628992 16 H 2.808248 6.456215 7.789998 6.011716 6.131339 17 H 2.832327 5.339777 5.595292 6.236228 7.053614 18 C 2.054937 5.529478 6.203051 5.971414 6.594965 19 H 2.812136 5.723541 6.172517 6.338211 7.030719 20 C 2.058243 5.923348 6.948081 5.916341 6.307968 21 H 2.802206 6.407869 7.512071 6.216523 6.488203 22 C 2.050968 5.938777 7.098062 5.788914 6.101302 23 S 2.245383 2.463496 3.009546 3.568875 4.557466 24 S 2.238732 3.496348 5.002905 3.092813 3.459772 25 C 3.111706 2.078070 2.615496 3.315616 4.333962 26 C 3.117564 2.251372 3.485087 2.637975 3.435517 27 H 4.099428 2.885136 3.939148 3.127694 3.769774 28 H 3.979457 2.782291 2.621652 4.233810 5.270371 6 7 8 9 10 6 O 0.000000 7 C 6.239687 0.000000 8 O 6.631669 1.132052 0.000000 9 C 3.298319 5.314548 5.478784 0.000000 10 O 3.923047 6.376278 6.497386 1.150292 0.000000 11 C 3.379871 4.125428 3.993707 2.822976 3.798302 12 O 4.049250 4.686464 4.341170 3.802543 4.649688 13 H 7.495747 4.413056 5.492762 6.997232 7.836504 14 C 7.314044 3.717713 4.812920 7.000192 7.943503 15 C 6.599396 3.764956 4.870041 6.895183 7.912068 16 H 8.751837 3.513174 4.295358 7.791753 8.709308 17 H 6.115531 4.496670 5.595844 6.807740 7.787355 18 C 6.911726 3.236660 4.204284 7.246439 8.340399 19 H 6.774267 3.672842 4.497242 7.504628 8.628726 20 C 7.795937 2.834047 3.694380 7.580696 8.650203

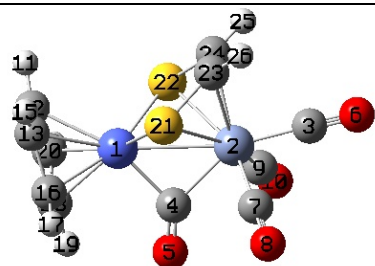
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	23	S	3.846482	2.841321	3.651562	4.184343	5.294979
	24	S	6.049213	2.705280	3.490844	4.492501	5.330326
	25	C	3.475519	3.848345	4.637454	3.209396	4.158033
	26	C	4.477026	3.604274	4.304266	3.019868	3.858956
	27	H	4.831737	4.590299	5.224989	2.994975	3.541174
	28	H	3.168463	4.885134	5.696175	3.543168	4.328923
			11	12	13	14	15
	11	C	0.000000				
	12	O	1.145339	0.000000			
	13	H	7.241992	8.177009	0.000000		
	14	C	6.819189	7.661614	1.079386	0.000000	
	15	C	6.386168	7.158503	2.218652	1.405416	0.000000
	16	H	7.418538	8.132355	2.691887	2.240168	3.337350
	17	H	6.458700	7.268905	2.674139	2.219281	1.079847
	18	C	6.181740	6.766650	3.339871	2.297129	1.428937
	19	H	6.117464	6.568253	4.348301	3.339509	2.242350
	20	C	6.544450	7.101345	3.338005	2.296349	2.294600
	21	H	6.772054	7.182659	4.349406	3.341723	3.340467
	22	C	6.891851	7.610179	2.233920	1.426329	2.294682
	23	S	3.375696	4.228115	4.255495	3.762264	3.097945
	24	S	4.897399	5.869990	3.078726	3.106266	3.741759
	25	C	3.749710	4.837746	4.160837	4.118378	3.839394
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	27	H	4.695866	5.827888	4.458861	4.794687	5.113774
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	19	H	4.355921	2.694583	1.080033	0.000000	
	20	C	2.237084	3.336536	1.415981	2.232569	0.000000
	21	H	2.692844	4.348479	2.228043	2.688290	1.081341
	22	C	1.080019	3.338131	2.300427	3.344991	1.421029
	23	S	5.035464	3.083767	3.224320	3.360420	3.959311
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	26	C	5.054143	4.347633	4.919174	5.498791	5.148017
	27	H	5.704287	5.099009	5.887115	6.513876	6.077575
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	22	C	2.232481	0.000000			
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	27	H	6.824765	5.423373	3.669328	2.405198	2.142231
	28	H	6.686358	5.595947	2.495341	3.684406	1.082971

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26 C	0.000000		
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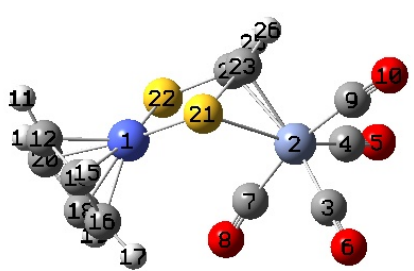
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	9 O	3.110628	2.971014	3.119545	3.699678	3.133029
	10 O	5.176565	3.037913	3.405851	4.071879	3.421842
	11 H	2.782525	4.752339	6.309248	7.339652	5.254471
	12 C	2.047231	4.333151	5.704894	6.664945	5.103897
	13 C	2.021046	4.470424	5.687820	6.579601	5.673201
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	16 C	2.047919	4.339351	5.127792	5.843693	5.701437
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	18 C	2.072474	4.086820	4.746955	5.423465	5.136816
	19 H	2.831197	4.339398	4.587277	5.065701	5.331757
	20 C	2.072575	4.083348	5.140932	5.984316	4.730285
	21 S	2.225128	2.429805	3.116170	3.921242	4.243774
	22 S	2.224699	2.428335	4.242830	5.381270	3.109886
	23 C	3.056033	3.278180	4.414277	5.314626	4.813546
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	25 H	4.034176	4.228919	5.786024	6.824929	5.136594
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12 C	5.811514	5.891847	3.777251	4.164371	6.924412	
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14 H	5.038592	6.155053	2.964513	2.732363	7.269828	
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16 C	6.656969	5.897221	3.778376	4.161457	6.926791	
17 H	7.339683	6.160544	4.369729	4.779941	7.124193	
18 C	5.976672	5.885895	2.963810	3.023783	6.995981	
19 H	6.144429	6.160858	2.965546	2.726276	7.272292	
20 C	5.400763	5.883142	2.963541	3.026802	6.995103	

	21	S	5.381754	3.215682	3.300759	4.303615	4.072673
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	23	C	5.854108	3.381020	4.550413	5.645381	3.943035
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	18	C	3.336564	2.293384	2.302343	2.236566	3.345531
	19	H	4.344044	3.335441	3.346275	2.689717	4.356050
	20	C	2.221929	1.411327	2.302541	1.079871	3.345873
	21	S	4.761496	4.092114	3.424859	4.974439	3.663817
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	25	H	4.582666	4.733686	4.436850	6.308634	4.025262
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	24	C	4.426911	4.768247	5.043847	5.828297	4.856025
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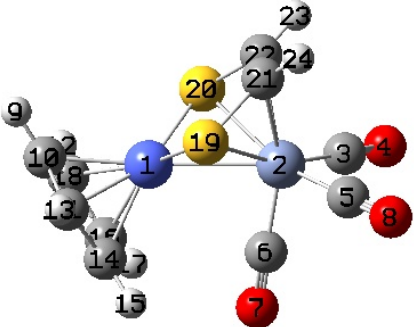
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7 C	3.674584	1.834442	2.405933	2.468626	3.004733
8 O	4.535687	2.977294	3.283052	3.265507	3.508490
9 C	3.689021	1.835330	2.405889	2.474736	2.964224
10 O	4.556949	2.977902	3.282304	3.269027	3.443695
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14 H	2.807478	4.891523	6.577653	3.713436	4.021346
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16 C	2.053380	4.502522	6.293879	3.152014	3.529134
17 H	2.812669	4.856367	6.560647	3.489855	3.710566
18 C	2.048537	4.455612	6.289373	2.784825	2.928755
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23 C	3.141721	2.193666	2.812579	3.686290	4.833152
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25 H	4.179307	2.929278	2.947342	4.593407	5.678270
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21 S	4.736644	2.950252	3.676314	4.226160	5.342053
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	13	C	2.038020	5.214995	5.736159	6.821644	7.870194			
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	12	C	1.080926	0.000000						
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	14	H	2.693001	2.239013	3.348031	0.000000				
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	19	H	4.348054	3.339389	3.342655	2.691702	4.351941			
	20	C	2.236577	1.426010	2.305454	1.080103	3.348409			
	21	S	4.095767	3.672567	3.164232	4.897297	3.194496			
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	23	C	5.100999	4.803395	4.661431	5.454541	4.846602			

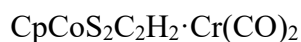
	24	C	5.242005	4.863686	4.968013	4.915009	5.425070
	25	H	6.108784	5.802834	6.015729	5.607131	6.487981
	26	H	5.760245	5.608576	5.471476	6.371241	5.506533
			16	17	18	19	20
	16	C	0.000000				
	17	H	1.080654	0.000000			
	18	C	1.426837	2.235973	0.000000		
	19	H	2.233977	2.682608	1.080415	0.000000	
	20	C	2.300322	3.341605	1.415251	2.231617	0.000000
	21	S	3.372605	3.580516	3.992842	4.614699	4.156435
	22	S	3.863491	4.456654	3.273272	3.439362	3.152170
	23	C	4.738795	4.990801	4.958718	5.361950	5.000143
	24	C	4.812321	5.154932	4.638198	4.828355	4.674189
	25	H	5.845492	6.188532	5.547754	5.632238	5.522760
	26	H	5.694813	5.924761	5.990814	6.435035	5.943429
			21	22	23	24	25
	21	S	0.000000				
	22	S	3.084758	0.000000			
	23	C	1.746007	2.714848	0.000000		
	24	C	2.662115	1.756013	1.384329	0.000000	
	25	H	3.685872	2.417828	2.154323	1.085068	0.000000
	26	H	2.453818	3.666836	1.082410	2.186642	2.560949
			26				
	26	H	0.000000				

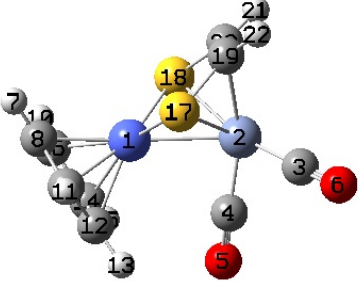
CpCoS₂C₂H₂·Cr(CO)₃

 <p>1. -3833.185023 0.0</p>			1	2	3	4	5	
	1	Co	0.000000					
	2	Cr	2.562463	0.000000				
	3	C	4.053391	1.835264	0.000000			
	4	O	5.105767	2.983222	1.148032	0.000000		
	5	C	4.061029	1.835154	2.603084	3.507127	0.000000	
	6	C	2.913631	1.823279	2.563593	3.475448	2.561326	
	7	O	3.631511	2.977481	3.465293	4.181082	3.464229	
	8	O	5.116185	2.982981	3.505622	4.216860	1.147899	
	9	H	2.781834	5.242872	6.637045	7.609114	6.691512	
	10	C	2.019854	4.579430	5.986184	6.973729	6.023054	
	11	C	2.022371	4.339723	5.952089	7.021644	5.449171	
	12	H	2.775782	4.761464	5.544708	6.271159	6.507954	
	13	H	2.772848	4.826302	6.566049	7.680381	5.667728	
	14	C	2.032047	3.879297	5.316365	6.328273	4.942727	
	15	H	2.787995	4.019035	5.436848	6.439183	4.712701	
	16	C	2.035636	3.856132	4.923993	5.800551	5.273640	
	17	H	2.788437	3.969342	4.680433	5.413546	5.339593	
	18	C	2.023147	4.300198	5.374816	6.238442	5.921928	
	19	S	2.149640	2.392459	4.178527	5.310969	3.049610	
	20	S	2.150014	2.393417	3.044610	3.863773	4.176595	
	21	C	3.050451	2.162944	3.428172	4.421343	2.849679	
22	C	3.051196	2.164560	2.857271	3.705132	3.420596		

23	H	4.090726	2.934435	3.024373	3.584644	3.954861
24	H	4.089676	2.931693	3.965745	4.850241	3.011030
		6	7	8	9	10
6	C	0.000000				
7	O	1.154224	0.000000			
8	O	3.471343	4.177813	0.000000		
9	H	5.639209	6.169224	7.687217	0.000000	
10	C	4.718019	5.156729	7.025837	1.079918	0.000000
11	C	4.235626	4.570350	6.326326	2.238196	1.422196
12	H	4.733124	5.072595	7.625158	2.695534	2.234409
13	H	4.852353	5.217847	6.418341	2.692709	2.232399
14	C	3.228697	3.315426	5.816945	3.349793	2.306206
15	H	3.054233	2.914767	5.436103	4.360105	3.349963
16	C	3.173375	3.243451	6.278643	3.349903	2.306328
17	H	2.935159	2.751178	6.324516	4.360613	3.350254
18	C	4.162570	4.482274	6.995514	2.240395	1.424197
19	S	3.440258	4.379099	3.872508	4.011911	3.596816
20	S	3.453722	4.394465	5.308423	3.915360	3.540008
21	C	3.878536	5.005585	3.698127	4.919950	4.664084
22	C	3.884821	5.012490	4.412251	4.885782	4.645264
23	H	4.649802	5.769662	4.835524	5.777119	5.614335
24	H	4.639625	5.758119	3.570307	5.830435	5.643099
		11	12	13	14	15
11	C	0.000000				
12	H	3.335971	0.000000			
13	H	1.080769	4.346723	0.000000		
14	C	1.418636	3.338968	2.229083	0.000000	
15	H	2.234825	4.346911	2.688677	1.080147	0.000000
16	C	2.296200	2.227607	3.339607	1.422988	2.233774
17	H	3.337997	2.688136	4.346524	2.231948	2.683960
18	C	2.291627	1.080741	3.336089	2.295568	3.338153
19	S	3.108196	4.848694	3.121645	3.402191	3.662613
20	S	4.088188	3.106843	4.808751	4.044506	4.737925
21	C	4.577881	5.359502	4.742261	4.782788	5.115116
22	C	4.904689	4.758868	5.325777	4.998056	5.489668
23	H	5.966752	5.498397	6.392807	6.041995	6.526773
24	H	5.469547	6.433262	5.485267	5.713191	5.941951
		16	17	18	19	20
16	C	0.000000				
17	H	1.079893	0.000000			
18	C	1.416950	2.233782	0.000000		
19	S	4.012285	4.679921	4.111929	0.000000	
20	S	3.459010	3.757238	3.098559	3.137567	0.000000
21	C	4.994150	5.476913	4.922359	1.741448	2.711082
22	C	4.809790	5.156392	4.585555	2.712063	1.741365
23	H	5.749255	6.000868	5.475176	3.726152	2.440125
24	H	6.030727	6.500949	5.987921	2.439470	3.725252
		21	22	23	24	
21	C	0.000000				
22	C	1.376904	0.000000			

	23 H	2.157132	1.083340	0.000000	
	24 H	1.083261	2.156941	2.526877	0.000000



 <p>1. -3719.897911 0.0</p>		1	2	3	4	5	
	1 Co	0.000000					
	2 Cr	2.462855	0.000000				
	3 C	3.966064	1.834330	0.000000			
	4 C	2.833798	1.816106	2.538704	0.000000		
	5 O	3.581148	2.971783	3.439584	1.155909	0.000000	
	6 O	5.030428	2.984049	1.149916	3.450722	4.151770	
	7 H	2.806044	5.156207	6.540201	5.580242	6.140877	
	8 C	2.039906	4.494735	5.890606	4.658648	5.128293	
	9 C	2.019020	4.172224	5.225893	4.068864	4.434862	
	10 H	2.776405	4.806326	6.537110	4.835518	5.206770	
	11 H	2.772963	4.610128	5.360183	4.625512	5.018385	
	12 C	2.039312	3.777437	4.821063	3.105150	3.208688	
	13 H	2.790094	3.897489	4.572465	2.869094	2.719316	
	14 C	2.032246	3.844717	5.263561	3.196384	3.295566	
	15 H	2.793947	4.041361	5.437082	3.072252	2.924116	
	16 C	2.028519	4.295104	5.896297	4.201725	4.552554	
	17 S	2.153549	2.331046	3.045167	3.505614	4.495670	
	18 S	2.202582	2.355441	4.161251	3.313957	4.227774	
	19 C	3.049464	2.169682	2.967797	3.925464	5.069213	
	20 C	3.047735	2.134234	3.462598	3.811409	4.928998	
	21 H	4.093886	2.904794	3.984412	4.542183	5.635625	
22 H	4.091358	2.957715	3.190088	4.718833	5.860061		
		6	7	8	9	10	
6 O	0.000000						
7 H	7.517072	0.000000					
8 C	6.883019	1.079888	0.000000				
9 C	6.094333	2.242918	1.426533	0.000000			
10 H	7.653048	2.685673	2.224615	3.329492	0.000000		
11 H	6.088371	2.698816	2.236926	1.080989	4.340241		
12 C	5.699514	3.355347	2.311808	1.418981	3.338266		
13 H	5.303406	4.365317	3.355242	2.234111	4.347669		
14 C	6.275568	3.354553	2.310222	2.293688	2.233622		
15 H	6.435456	4.364283	3.353261	3.337156	2.694748		
16 C	6.968211	2.233138	1.415209	2.284798	1.080955		
17 S	3.894829	3.830762	3.496430	3.100299	4.757257		
18 S	5.300655	4.166661	3.705861	4.173783	3.154651		
19 C	3.843669	4.839217	4.619390	4.588490	5.262453		
20 C	4.473157	4.965211	4.688145	4.931887	4.712740		
21 H	4.882445	5.918657	5.694951	6.007065	5.486857		
22 H	3.799910	5.715536	5.583058	5.483941	6.321204		
		11	12	13	14	15	
11 H	0.000000						
12 C	2.228818	0.000000					
13 H	2.686397	1.080110	0.000000				

	14	C	3.336749	1.419466	2.230671	0.000000		
	15	H	4.345770	2.231624	2.685291	1.079963	0.000000	
	16	C	3.329338	2.295431	3.339249	1.424987	2.241734	
	17	S	3.107903	3.539487	3.884835	4.087379	4.810304	
	18	S	4.929834	4.016749	4.661744	3.372399	3.587015	
	19	C	4.773840	4.856737	5.237676	5.009570	5.522172	
	20	C	5.386687	4.994282	5.478633	4.755952	5.082109	
	21	H	6.469669	6.023347	6.481785	5.684994	5.896580	
	22	H	5.520625	5.811007	6.106944	6.062471	6.572156	
			16	17	18	19	20	
	16	C	0.000000					
	17	S	4.060995	0.000000				
	18	S	3.149351	3.195586	0.000000			
	19	C	4.869375	1.741166	2.745024	0.000000		
	20	C	4.562507	2.712591	1.749997	1.377387	0.000000	
	21	H	5.476348	3.719518	2.442032	2.145434	1.085344	
	22	H	5.929065	2.443753	3.750379	1.083723	2.152828	
			21	22				
	21	H	0.000000					
	22	H	2.499388	0.000000				

Table S3A. Energy rank for all of the $\text{CpCoS}_2\text{C}_2\text{H}_2\cdot\text{Fe}(\text{CO})_n$ optimized structures. PBE0/6-311G(d,p).

Co-Fe

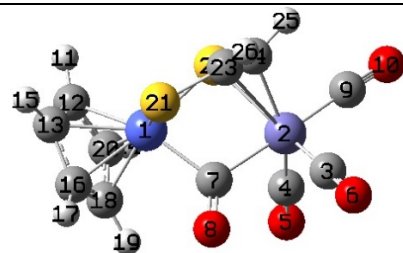
	name	E (a.u.)	ΔE (kcal/mol)
4-1	8-Co-fe-CO-4-md2-r1-freq	-4165.599957	0.0
4-2	7-ir-fe-CO-4-md1-new-Fe-Co-h-r-ok	-4165.597863	1.3
4-3	7-Co-fe-CO-4-md1-r1-freq	-4165.596538	2.1
4-4	9-Co-fe-CO-4-md3-r1	-4165.595131	3.0
4-5	7-rh-fe-CO-4-md1-r1-freq-new-Co-Fe-g-freq-ok	-4165.550276	31.2
	name		
3-1	5-Co-fe-CO-3-md2-r1	-4052.376675	0.0
3-2	4-Co-fe-CO-3-md1-r1	-4052.369928	4.2
3-3	6-Co-fe-CO-3-md3-r1-freq	-4052.353831	14.3
	name		
2-1	2-Co-fe-CO-2-md2-r1	-3939.121968	0.0
2-2	3-Co-fe-CO-2-md3-r1-freq	-3939.111699	6.4

Table S3B. Distance table for the lowest-lying CpCoS₂C₂H₂·Fe(CO)_n structures after PBE0/6-311G(d,p) optimization.

CpCoS₂C₂H₂·Fe(CO)₄

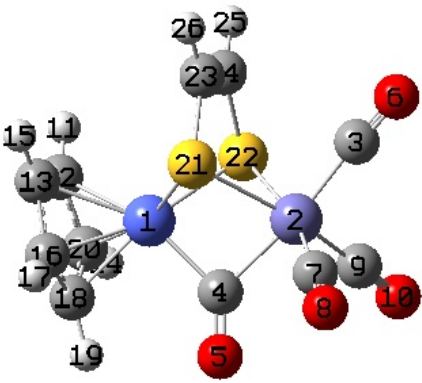
<p>1. -4165.599957 0.0</p>		1	2	3	4	5		
	1 Co	0.000000						
	2 Fe	2.558980	0.000000					
	3 C	3.219222	1.807621	0.000000				
	4 C	3.090459	1.789142	3.595674	0.000000			
	5 O	3.863848	2.928474	4.734141	1.139564	0.000000		
	6 O	4.103693	2.935427	1.134309	4.719628	5.855960		
	7 C	2.908157	1.756588	2.511299	2.561640	3.489373		
	8 O	3.655405	2.901422	3.408700	3.472173	4.220270		
	9 C	4.272033	1.757562	2.480797	2.491301	3.380526		
	10 O	5.409316	2.897747	3.367598	3.384797	4.071561		
	11 H	2.761444	5.063918	5.761900	5.008798	5.317416		
	12 C	2.009555	4.400319	5.200499	4.326548	4.674478		
	13 C	2.026705	4.508666	4.996422	4.780531	5.295791		
	14 H	2.807136	4.011526	5.451302	3.056125	2.915871		
	15 H	2.764901	5.221342	5.382526	5.725532	6.317828		
	16 C	2.044818	3.960353	4.636035	4.127880	4.633497		
	17 H	2.816422	4.328893	4.774248	4.682245	5.247823		
	18 C	2.068968	3.484030	4.678343	3.072314	3.352145		
	19 H	2.849453	3.467205	4.849660	2.747036	2.861788		
	20 C	2.047709	3.789696	5.025961	3.230314	3.381587		
	21 S	2.216432	3.627672	3.030124	4.888999	5.849703		
	22 S	2.172253	2.315520	3.030114	2.827474	3.608935		
	23 C	3.075116	3.815794	3.069442	5.117523	6.082096		
	24 C	3.093650	3.368593	3.075143	4.426092	5.308778		
	25 H	4.121343	4.094590	3.772845	5.047452	5.858179		
26 H	4.113181	4.778035	3.758494	6.161621	7.141271			
		6	7	8	9	10		
6 O	0.000000							
7 C	3.414560	0.000000						
8 O	4.118217	1.146022	0.000000					
9 C	3.297070	2.951192	3.934339	0.000000				
10 O	3.955204	3.923775	4.787485	1.141998	0.000000			
11 H	6.534912	5.587914	6.231287	6.592309	7.664250			
12 C	6.036973	4.681343	5.240139	6.029177	7.136042			
13 C	5.702172	4.342406	4.668495	6.253864	7.394872			
14 H	6.508319	4.520447	5.190629	5.286282	6.257569			
15 H	5.909426	5.029699	5.292794	6.956656	8.094626			
16 C	5.427618	3.338186	3.455142	5.687757	6.807801			
17 H	5.441919	3.300956	3.084110	5.996508	7.082207			
18 C	5.663342	3.108706	3.421041	5.081459	6.157663			
19 H	5.876542	2.839702	3.003095	4.857763	5.848320			

	20	C	6.026988	4.030088	4.603886	5.312258	6.376111
	21	S	3.310702	3.950592	4.575993	5.092745	6.141046
	22	S	3.917456	3.769583	4.848999	3.363948	4.340234
	23	C	3.214170	4.774780	5.643882	4.867436	5.773263
	24	C	3.490518	4.732453	5.761538	4.182686	5.027229
	25	H	4.058153	5.609263	6.678927	4.539250	5.198821
	26	H	3.591022	5.686686	6.500938	5.672268	6.483083
			11	12	13	14	15
	11	H	0.000000				
	12	C	1.079604	0.000000			
	13	C	2.233111	1.418991	0.000000		
	14	H	2.701365	2.238888	3.338887	0.000000	
	15	H	2.682460	2.226298	1.079566	4.347557	0.000000
	16	C	3.347046	2.304756	1.418208	3.344602	2.227820
	17	H	4.357828	3.349125	2.236130	4.353090	2.690924
	18	C	3.340034	2.296089	2.288641	2.225462	3.332186
	19	H	4.351172	3.340235	3.331727	2.679805	4.341713
	20	C	2.242107	1.426533	2.294328	1.080294	3.336698
	21	S	3.790818	3.443285	2.933169	4.900476	2.830645
	22	S	3.531732	3.334832	3.978768	3.224241	4.600972
	23	C	4.235815	4.219284	4.222326	5.317400	4.206840
	24	C	4.169413	4.214892	4.604876	4.770296	4.857112
	25	H	4.914891	5.101539	5.619070	5.464235	5.856438
	26	H	5.042585	5.132223	5.050105	6.360366	4.847745
			16	17	18	19	20
	16	C	0.000000				
	17	H	1.080015	0.000000			
	18	C	1.423235	2.237627	0.000000		
	19	H	2.231405	2.688796	1.079888	0.000000	
	20	C	2.301400	3.344134	1.411848	2.224231	0.000000
	21	S	3.377905	3.689453	4.086742	4.859407	4.120902
	22	S	4.175520	4.946285	3.736192	4.232232	3.173484
	23	C	4.787395	5.265267	5.143230	5.866741	4.828358
	24	C	5.080504	5.717648	5.060540	5.686120	4.545635
	25	H	6.131372	6.792305	6.018517	6.601278	5.395455
	26	H	5.696574	6.092059	6.171234	6.912416	5.859814
			21	22	23	24	25
	21	S	0.000000				
	22	S	3.138444	0.000000			
	23	C	1.724628	2.679885	0.000000		
	24	C	2.698757	1.750639	1.342806	0.000000	
	25	H	3.717797	2.434555	2.146224	1.083302	0.000000
	26	H	2.408400	3.697638	1.086132	2.119605	2.512078
			26				
	26	H	0.000000				

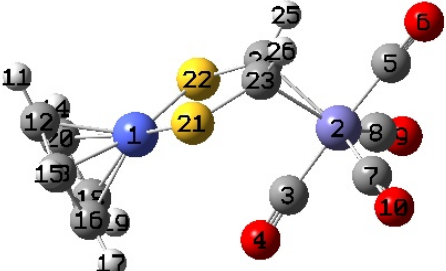


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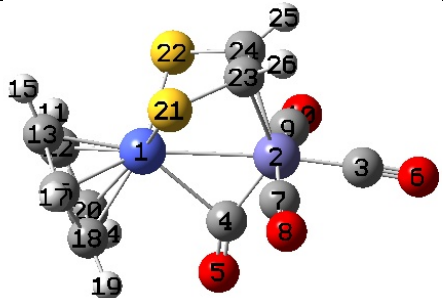
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12 C	2.133610	4.930990	6.327069	5.190858	5.642075
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14 H	2.807101	4.325536	5.852107	3.857817	3.951309
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16 C	2.045480	4.911071	5.769018	5.089243	5.508027
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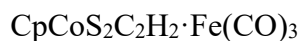
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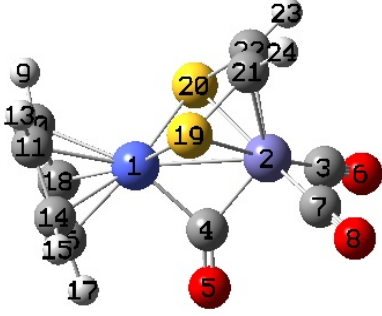
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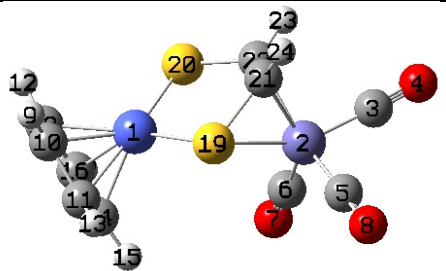
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	19	H	6.665887	4.090329	4.387985	5.255766	6.073023
	20	C	6.831790	4.822733	5.548443	4.401481	4.956652
	21	S	5.575793	2.906154	3.438246	4.452350	5.488040
	22	S	5.628885	4.422582	5.455677	2.932060	3.471794
	23	C	4.292014	2.611168	3.432171	3.399266	4.400434
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	20	C	2.219754	1.407389	2.294223	1.079150	3.335337
	21	S	4.681844	4.005707	3.209566	5.054690	3.327135
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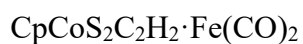
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	16 C	2.050069	3.513812	5.276687	6.411288	3.442384
	17 H	2.821240	3.625408	5.288598	6.384841	3.207069
	18 C	2.018483	3.787174	5.498119	6.616216	4.311103
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	21 C	3.110601	3.166468	3.542343	4.192529	4.338592
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23 H	4.087752	4.133183	4.272998	4.739164	5.736636	
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19 S	3.640542	3.962044	5.067014	4.525213	3.968912	
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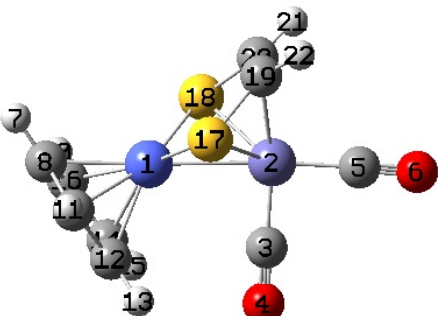
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	23	H	5.733130	5.840748	5.907637	6.135232	6.713206		
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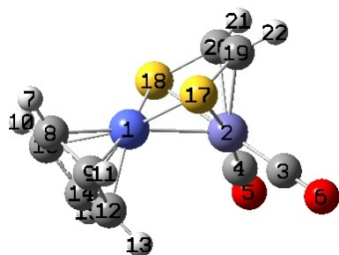
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	16 C	2.021297	5.118329	6.574356	7.590807	6.293995
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	15 H	3.750519	3.582467	5.829567	4.345222	3.336591
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	19 S	3.313195	4.199560	3.777925	3.966336	3.593198
	20 S	3.494113	4.015390	6.050706	4.352609	3.805386
	21 C	3.461540	4.524622	3.942333	5.061783	4.811809
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	21 C	4.684883	5.540211	4.816964	4.840652	5.116663
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	8 C	2.037933	4.477939	4.730098	5.229828	6.212320	
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	11 H	2.774271	4.690800	4.801165	5.212437	6.269378	
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	13 H	2.795637	3.888808	3.016798	2.917766	5.188377	
	14 C	2.035014	3.734606	3.199598	3.346451	5.263595	
15 H	2.795794	3.881241	3.005244	2.906288	5.179867		

	16	C	2.020544	4.193055	4.196113	4.588971	5.852285		
	17	S	2.149317	2.252265	3.317742	4.275252	3.586422		
	18	S	2.149802	2.252486	3.321808	4.281815	3.588993		
	19	C	3.017556	2.090272	3.760397	4.890731	2.957532		
	20	C	3.017844	2.090322	3.761886	4.893153	2.958726		
	21	H	4.062669	2.862604	4.487522	5.598066	3.192873		
	22	H	4.062288	2.862352	4.485074	5.594049	3.190579		
			6	7	8	9	10		
	6	O	0.000000						
	7	H	8.038668	0.000000					
	8	C	7.358275	1.079804	0.000000				
	9	C	6.972958	2.237288	1.420398	0.000000			
	10	H	7.337281	2.691412	2.230235	3.329178	0.000000		
	11	H	7.350126	2.691358	2.230241	1.080756	4.339823		
	12	C	6.329115	3.355163	2.311246	1.422915	3.338113		
	13	H	6.155349	4.364352	3.354037	2.237474	4.348794		
	14	C	6.324577	3.355111	2.311193	2.295273	2.231962		
	15	H	6.145894	4.364223	3.353924	3.339890	2.689213		
	16	C	6.965867	2.237391	1.420447	2.284764	1.080763		
	17	S	4.622857	4.083723	3.640353	3.119724	4.858247		
	18	S	4.625069	4.071680	3.632200	4.114286	3.137258		
	19	C	3.880436	4.969874	4.678521	4.561369	5.336099		
	20	C	3.881392	4.965774	4.675934	4.894196	4.739101		
	21	H	3.868043	5.896118	5.669421	5.965689	5.502784		
	22	H	3.865992	5.902488	5.673359	5.469180	6.413537		
			11	12	13	14	15		
	11	H	0.000000						
	12	C	2.232121	0.000000					
	13	H	2.689562	1.080100	0.000000				
	14	C	3.338190	1.419700	2.233239	0.000000			
	15	H	4.348898	2.233260	2.691275	1.080086	0.000000		
	16	C	3.329204	2.295191	3.339794	1.422720	2.237173		
	17	S	3.145829	3.390038	3.641723	3.997255	4.664899		
	18	S	4.855538	4.000135	4.671448	3.392664	3.647594		
	19	C	4.743055	4.745617	5.076879	4.947629	5.429595		
	20	C	5.336606	4.949038	5.433033	4.746187	5.077744		
	21	H	6.413601	5.986304	6.451111	5.682302	5.906349		
	22	H	5.508239	5.681321	5.904447	5.984262	6.446263		
			16	17	18	19	20		
	16	C	0.000000						
	17	S	4.116925	0.000000					
	18	S	3.114073	3.161497	0.000000				
	19	C	4.894255	1.729895	2.713271	0.000000			
	20	C	4.558997	2.713528	1.729819	1.382299	0.000000		
	21	H	5.465922	3.715938	2.433685	2.149874	1.083712		
	22	H	5.966142	2.433601	3.715696	1.083710	2.149819		
			21	22					
	21	H	0.000000						
	22	H	2.493969	0.000000					



2. -3939.111699 +6.4

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1 Co	0.000000				
2 Fe	2.465287	0.000000			
3 C	3.758479	1.736159	0.000000		
4 C	3.617970	1.734794	2.402802	0.000000	
5 O	4.599716	2.882751	3.292406	1.148153	0.000000
6 O	4.784612	2.883208	1.147526	3.282016	3.948845
7 H	2.820880	5.226687	6.386499	6.415234	7.338210
8 C	2.042370	4.497993	5.627182	5.555498	6.435786
9 C	2.014318	4.088645	4.825126	5.187397	6.093273
10 H	2.783867	4.839122	6.326112	5.351758	5.972239
11 H	2.771980	4.533611	4.980053	5.794860	6.756511
12 C	2.011509	3.576334	4.244981	4.264978	5.022686
13 H	2.768316	3.626186	3.859769	4.136088	4.812156
14 C	2.005370	3.693899	4.787306	4.061102	4.677574
15 H	2.762211	3.845205	4.918339	3.728827	4.101793
16 C	2.026035	4.273559	5.598914	4.934997	5.649991
17 S	2.152654	2.297177	2.990155	4.018229	5.163808
18 S	2.165549	2.283946	4.020017	2.938302	3.780689
19 C	3.097724	2.077946	2.992400	3.603240	4.689966
20 C	3.110283	2.060945	3.474290	3.088210	4.043141
21 H	4.144829	2.876444	4.111874	3.482294	4.237773
22 H	4.129173	2.879734	3.304896	4.280437	5.308723
	6	7	8	9	10
6 O	0.000000				
7 H	7.302723	0.000000			
8 C	6.541903	1.080073	0.000000		
9 C	5.585752	2.240172	1.424831	0.000000	
10 H	7.377464	2.689100	2.228846	3.334740	0.000000
11 H	5.590880	2.695461	2.235458	1.080802	4.344983
12 C	4.995219	3.354621	2.311167	1.420615	3.344306
13 H	4.416620	4.363435	3.353655	2.234418	4.354164
14 C	5.696693	3.350379	2.306042	2.294973	2.232757
15 H	5.807269	4.358740	3.348221	3.339171	2.688030
16 C	6.592598	2.232636	1.416498	2.289628	1.080742
17 S	3.854570	3.958333	3.575969	3.150578	4.796026
18 S	5.167006	4.332353	3.795546	4.160302	3.294074
19 C	3.925339	5.158736	4.821708	4.675829	5.423906
20 C	4.532575	5.307520	4.909142	5.023552	4.912268
21 H	5.084287	6.263261	5.906198	6.090066	5.671732
22 H	4.006870	6.043685	5.780765	5.555734	6.488039
	11	12	13	14	15
11 H	0.000000				
12 C	2.230126	0.000000			
13 H	2.686575	1.079262	0.000000		
14 C	3.338413	1.423605	2.237149	0.000000	
15 H	4.348775	2.236579	2.695973	1.079962	0.000000
16 C	3.333525	2.301851	3.345682	1.424255	2.237387
17 S	3.182198	3.503673	3.820648	4.051367	4.738886
18 S	4.915129	3.898926	4.490248	3.280752	3.431875

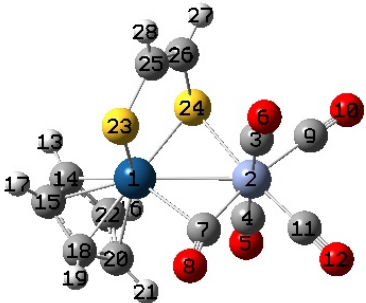
	19 C	4.880009	4.779232	5.068267	4.956227	5.383492
	20 C	5.491362	4.916725	5.305949	4.699809	4.922682
	21 H	6.573298	5.929366	6.289545	5.604361	5.700383
	22 H	5.611068	5.712533	5.904358	5.998013	6.421046
		16	17	18	19	20
	16 C	0.000000				
	17 S	4.090454	0.000000			
	18 S	3.212651	3.090530	0.000000		
	19 C	4.984999	1.743877	2.697757	0.000000	
	20 C	4.700772	2.707847	1.747713	1.377742	0.000000
	21 H	5.595981	3.728939	2.448498	2.168509	1.082523
	22 H	6.041279	2.439035	3.720396	1.082844	2.164703
		21	22			
	21 H	0.000000				
	22 H	2.556591	0.000000			

Table S4A. Energy rank for all of the CpIrS₂C₂H₂·Cr(CO)_n optimized structures. PBE0/6-311G(d,p).

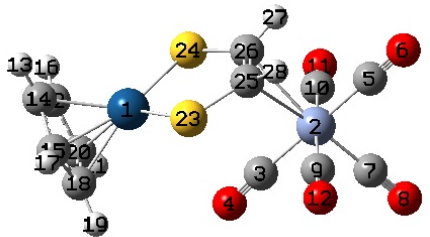
	name	E (a.u.)	ΔE (kcal/mol)
5-1	11-ir-Cr-CO-5-md2	-2781.572821	0.0
5-2	12-ir-Cr-CO-5-md3	-2781.563343	5.9
5-3	12-rh-Cr-CO-5-md3-freq-fneg2-fneg1-new-Cr-Ir-d-freq-ok	-2781.550056	14.3
	name		
4-1	7-ir-Cr-CO-4-md1-r1	-2668.327218	0.0
4-2	8-ir-Cr-CO-4-md2	-2668.325741	0.9
4-3	9-ir-Cr-CO-4-md3-fneg1	-2668.307465	12.4
	name		
3-1	6-ir-Cr-CO-3-md3	-2555.102274	0.0
	name		
2-1	2-ir-Cr-CO-2-md2	-2441.816596	0.0

Table S4B. Distance table for the lowest-lying CpIrS₂C₂H₂·Cr(CO)_n structures after PBE0/6-311G(d,p) optimization.

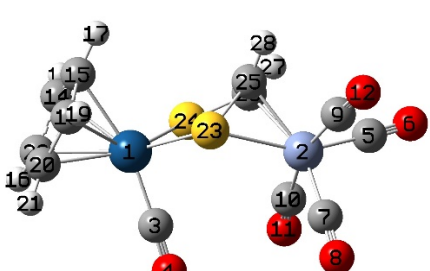
CpIrS₂C₂H₂·Cr(CO)₅

 <p>1. -2781.572821 0.0</p>							
	1	2	3	4	5		
	1 Ir	0.000000					
	2 Cr	2.824202	0.000000				
	3 C	3.638159	1.908331	0.000000			
	4 C	3.177204	1.878141	3.786322	0.000000		
	5 O	3.864274	3.023203	4.931231	1.145239	0.000000	
	6 O	4.526411	3.042356	1.138323	4.918561	6.062480	
	7 C	2.402144	1.914619	2.633097	2.766241	3.675716	
	8 O	3.135949	3.026422	3.460882	3.690497	4.441821	
	9 C	4.374136	1.892176	2.656574	2.676549	3.581109	
	10 O	5.422593	3.032234	3.541796	3.583095	4.306172	
	11 C	4.350893	1.840153	2.656654	2.609786	3.502641	
	12 O	5.390699	2.984831	3.555306	3.497351	4.191515	
	13 H	2.901409	5.381727	6.256518	5.133592	5.332719	
	14 C	2.167959	4.772725	5.751144	4.476510	4.689314	
	15 C	2.170910	4.949257	5.647504	4.964780	5.322497	
	16 H	2.961181	4.354953	5.923353	3.222484	2.955243	
	17 H	2.878051	5.645450	6.038963	5.902005	6.344225	
	18 C	2.211784	4.502038	5.381090	4.371863	4.682339	
19 H	2.952788	4.905156	5.584727	4.945319	5.307829		
20 C	2.238410	4.002087	5.336627	3.328589	3.402370		
21 H	2.979410	3.987181	5.484639	3.037001	2.934806		
22 C	2.221077	4.193564	5.573390	3.413241	3.406235		
23 S	2.336141	3.783992	3.298131	5.003131	5.926717		
24 S	2.312572	2.450946	3.153003	3.053350	3.864126		
25 C	3.209553	3.899141	3.140601	5.265294	6.242072		
26 C	3.230024	3.450860	3.097343	4.625284	5.549232		
27 H	4.258031	4.145166	3.698536	5.272448	6.157690		
28 H	4.245374	4.826982	3.747946	6.299286	7.300207		
	6	7	8	9	10		
6 O	0.000000						
7 C	3.534770	0.000000					
8 O	4.156450	1.156811	0.000000				
9 C	3.510126	3.784561	4.848467	0.000000			
10 O	4.192308	4.917443	5.963286	1.140208	0.000000		
11 C	3.505664	2.449267	3.075271	2.568937	3.451181		
12 O	4.202546	3.282872	3.594909	3.462211	4.143147		
13 H	7.064234	5.261181	5.871950	6.446912	7.268898		
14 C	6.613587	4.397005	4.918115	6.064705	6.989612		
15 C	6.393566	4.048093	4.276073	6.525814	7.555748		
16 H	6.986816	4.471062	5.154896	5.301464	6.101529		
17 H	6.632033	4.680256	4.814481	7.215226	8.236484		
18 C	6.199742	3.242584	3.237905	6.248574	7.341943		
19 H	6.300985	3.307554	2.924417	6.752518	7.879230		

	20	C	6.324389	3.146653	3.411699	5.580732	6.618629
	21	H	6.511230	3.106972	3.255477	5.525058	6.546031
	22	C	6.581918	3.915545	4.478543	5.458164	6.383445
	23	S	3.619093	3.290530	3.774452	5.142251	6.105861
	24	S	4.026194	3.532173	4.627717	2.945943	3.722227
	25	C	3.300055	4.221061	4.988288	4.639388	5.374791
	26	C	3.504393	4.331832	5.309864	3.769685	4.378161
	27	H	3.952527	5.278304	6.291468	3.982523	4.318478
	28	H	3.581104	5.112064	5.785007	5.420875	6.050619
			11	12	13	14	15
	11	C	0.000000				
	12	O	1.144868	0.000000			
	13	H	7.030630	8.089356	0.000000		
	14	C	6.292101	7.300950	1.079781	0.000000	
	15	C	6.294818	7.228657	2.244246	1.432404	0.000000
	16	H	5.640749	6.564893	2.717400	2.252166	3.361667
	17	H	7.010355	7.943358	2.695186	2.239843	1.080491
	18	C	5.510706	6.312602	3.363371	2.321056	1.427779
	19	H	5.642363	6.312142	4.374888	3.365689	2.244459
	20	C	4.970976	5.774370	3.354719	2.310425	2.306589
	21	H	4.580977	5.231632	4.366148	3.354739	3.350345
	22	C	5.511389	6.449071	2.254376	1.439338	2.316850
	23	S	5.183069	6.165888	4.176294	3.802556	3.279861
	24	S	4.278339	5.420874	3.708337	3.561716	4.192898
	25	C	5.462580	6.510021	4.615811	4.559944	4.511302
	26	C	5.149452	6.251049	4.458888	4.497486	4.839122
	27	H	5.756944	6.826101	5.187022	5.368264	5.835758
	28	H	6.265634	7.255730	5.464231	5.491872	5.349628
			16	17	18	19	20
	16	H	0.000000				
	17	H	4.372021	0.000000			
	18	C	3.362775	2.240089	0.000000		
	19	H	4.370121	2.704495	1.079673	0.000000	
	20	C	2.232181	3.352260	1.434792	2.247576	0.000000
	21	H	2.683660	4.362982	2.243398	2.701119	1.080680
	22	C	1.079976	3.360269	2.319669	3.361280	1.419336
	23	S	5.206931	3.190956	3.672852	3.943050	4.357847
	24	S	3.588885	4.760564	4.482907	5.252681	4.099417
	25	C	5.678105	4.480292	5.072501	5.522917	5.443558
	26	C	5.148860	5.047504	5.364752	5.988961	5.386745
	27	H	5.863130	6.023841	6.411451	7.064357	6.352494
	28	H	6.734280	5.146430	5.973804	6.337130	6.463224
			21	22	23	24	25
	21	H	0.000000				
	22	C	2.229247	0.000000			
	23	S	5.078536	4.434186	0.000000		
	24	S	4.613691	3.509629	3.194424	0.000000	
	25	C	6.140577	5.167175	1.727700	2.696724	0.000000
	26	C	6.014333	4.884582	2.711485	1.753657	1.340855
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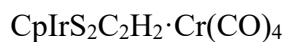
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	3 C 3.691894 1.891615 0.000000
	4 O 3.645783 3.033053 1.142768 0.000000
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	8 O 7.152907 2.981836 3.552004 4.232097 3.530324
	9 C 4.979932 1.889439 2.659157 3.554451 2.685475
	10 C 4.982026 1.889475 2.659186 3.554508 2.685581
	11 O 5.572091 3.031224 3.551149 4.255864 3.593694
	12 O 5.569083 3.031195 3.551055 4.255703 3.593639
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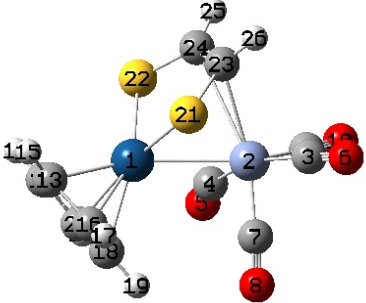
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	22	C	8.792316	7.850935	8.813926	7.070649	6.421495
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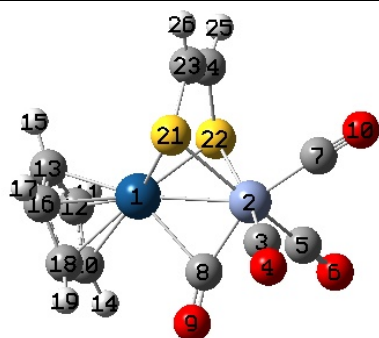
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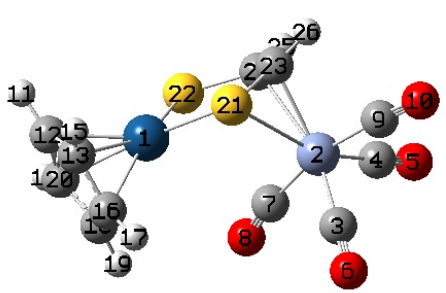
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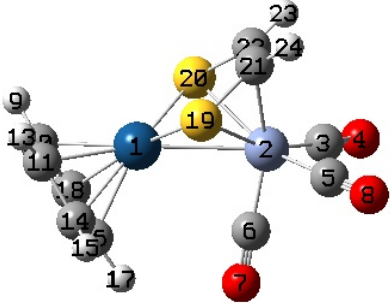
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16 C	6.799287	6.279323	3.888731	4.239991	7.345462
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22 S	3.957354	3.335919	3.346462	4.374877	4.213790
23 C	5.896201	3.529262	4.579588	5.700487	4.138175
24 C	5.361145	3.529545	4.579453	5.700296	4.138564
25 H	5.959624	4.187080	5.566275	6.675344	4.586936
26 H	6.866047	4.186627	5.566477	6.675644	4.586273
	11	12	13	14	15

	11 H 0.000000 12 C 1.080606 0.000000 13 C 2.241389 1.433206 0.000000 14 H 2.691126 2.238554 3.366725 0.000000 15 H 2.704706 2.249491 1.079093 4.376310 0.000000 16 C 3.347490 2.302888 1.433184 3.353190 2.249479 17 H 4.358875 3.347497 2.241370 4.363420 2.704696 18 C 3.353726 2.309893 2.323129 2.248543 3.365837 19 H 4.363400 3.353164 3.366661 2.706525 4.376245 20 C 2.232094 1.423231 2.323155 1.079726 3.365853 21 S 5.029562 4.383491 3.776637 5.260824 4.027249 22 S 3.473053 3.496166 3.776875 4.410965 4.027608 23 C 5.135886 4.802216 4.193707 6.140852 4.049253 24 C 4.538754 4.473166 4.193800 5.841401 4.049412 25 H 5.025611 5.148225 4.908410 6.638158 4.595907 26 H 6.033805 5.691642 4.908238 7.140744 4.595620 16 17 18 19 20 16 C 0.000000 17 H 1.080608 0.000000 18 C 1.423256 2.232142 0.000000 19 H 2.238486 2.691046 1.079723 0.000000 20 C 2.309948 3.353787 1.437373 2.248608 0.000000 21 S 3.496236 3.473403 4.005039 4.411341 4.517062 22 S 4.383738 5.030044 4.517091 5.260879 4.004815 23 C 4.473396 4.539342 5.202409 5.841725 5.382240 24 C 4.802501 5.136505 5.382365 6.141049 5.202203 25 H 5.691983 6.034494 6.326306 7.140936 6.028497 26 H 5.148434 5.026203 6.028719 6.638521 6.326175 21 22 23 24 25 21 S 0.000000 22 S 3.036472 0.000000 23 C 1.779611 2.681776 0.000000 24 C 2.681730 1.779629 1.325469 0.000000 25 H 3.720021 2.463866 2.136903 1.084194 0.000000 26 H 2.463851 3.720071 1.084194 2.136923 2.558279 26 26 H 0.000000
 <p>3. -2668.307465 +12.4</p>	1 2 3 4 5 1 Ir 0.000000 2 Cr 3.792542 0.000000 3 C 4.633817 1.834976 0.000000 4 C 5.335838 1.818304 2.704447 0.000000 5 O 6.379727 2.968910 3.656767 1.151022 0.000000 6 O 5.385750 2.983671 1.149272 3.661813 4.462168 7 C 3.423575 1.878978 2.520362 2.524766 3.406832 8 O 3.805418 3.020108 3.357909 3.364773 4.020539 9 C 5.160441 1.874954 2.508801 2.499883 3.377268 10 O 6.175616 3.018570 3.368747 3.345991 3.993978 11 H 2.889095 6.628500 7.494205 8.106657 9.093377 12 C 2.156343 5.945644 6.635316 7.465121 8.478884

	13	C	2.189798	5.617996	6.019128	7.306623	8.399282		
	14	H	2.928219	6.120165	6.836038	7.248871	8.084910		
	15	H	2.932318	6.063902	6.440724	7.825892	8.948381		
	16	C	2.194811	5.041776	5.112488	6.670837	7.747063		
	17	H	2.931281	4.994747	4.707034	6.645495	7.735590		
	18	C	2.163164	5.035475	5.255674	6.425322	7.401549		
	19	H	2.886139	4.981403	4.992945	6.173635	7.071168		
	20	C	2.193074	5.660639	6.257628	6.993760	7.930954		
	21	S	2.290545	2.642372	3.576306	4.390460	5.513467		
	22	S	2.245604	3.540098	5.010621	4.476726	5.291872		
	23	C	3.223020	2.174443	3.800808	3.430213	4.414661		
	24	C	3.174525	2.445111	4.225600	3.245992	4.080531		
	25	H	4.197194	3.047964	4.870388	3.262105	3.831200		
	26	H	4.219034	2.760109	4.289886	3.732789	4.601723		
			6	7	8	9	10		
	6	O	0.000000						
	7	C	3.391364	0.000000					
	8	O	3.998771	1.146734	0.000000				
	9	C	3.396037	3.727851	4.848723	0.000000			
	10	O	4.037272	4.855799	5.963340	1.146445	0.000000		
	11	H	8.165732	6.173262	6.303881	7.850068	8.772381		
	12	C	7.236314	5.391525	5.490067	7.251903	8.213839		
	13	C	6.485337	5.327451	5.582843	6.724876	7.608379		
	14	H	7.450980	4.942635	4.602795	7.784777	8.876713		
	15	H	6.877508	6.063338	6.450537	6.909554	7.675726		
	16	C	5.436972	4.519182	4.661994	6.299489	7.241939		
	17	H	4.837690	4.638460	4.854949	6.085163	6.954811		
	18	C	5.661564	4.019144	3.853358	6.598933	7.652932		
	19	H	5.298039	3.673980	3.263257	6.652410	7.734941		
	20	C	6.824811	4.682901	4.517957	7.224873	8.283028		
	21	S	4.431261	3.505329	4.429863	3.277999	4.124759		
	22	S	6.018048	3.080284	3.453870	5.002661	6.044639		
	23	C	4.885416	3.339913	4.365945	2.679808	3.539582		
	24	C	5.352604	2.897080	3.724827	3.520570	4.480650		
	25	H	6.015795	3.499693	4.242900	3.883060	4.723000		
	26	H	5.342143	4.233581	5.306759	2.506061	3.056698		
			11	12	13	14	15		
	11	H	0.000000						
	12	C	1.080187	0.000000					
	13	C	2.250041	1.442509	0.000000				
	14	H	2.702488	2.243706	3.373535	0.000000			
	15	H	2.704089	2.251959	1.079756	4.381188	0.000000		
	16	C	3.352120	2.310488	1.419026	3.369443	2.236076		
	17	H	4.366526	3.357624	2.235855	4.375676	2.701434		
	18	C	3.345232	2.300423	2.310882	2.241334	3.357329		
	19	H	4.356795	3.344956	3.352686	2.697759	4.366068		
	20	C	2.239345	1.427703	2.328558	1.079632	3.369594		
	21	S	4.684079	4.134578	3.584632	5.208214	3.734551		
	22	S	4.069099	3.760342	4.324854	3.524321	5.007336		
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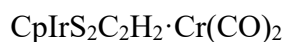
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	25 H	6.245878	6.000821	6.294728	5.927325	6.761603
	26 H	6.373133	6.078884	5.844361	6.837164	5.942717
		16	17	18	19	20
	16 C	0.000000				
	17 H	1.080044	0.000000			
	18 C	1.438404	2.246153	0.000000		
	19 H	2.247219	2.697754	1.080639	0.000000	
	20 C	2.325824	3.366444	1.427952	2.239273	0.000000
	21 S	3.561287	3.679015	4.097241	4.606912	4.462746
	22 S	4.358455	5.053625	3.822788	4.160505	3.466990
	23 C	5.016121	5.252179	5.179290	5.539860	5.331464
	24 C	5.212930	5.632557	4.994533	5.246845	4.966368
	25 H	6.268167	6.702940	5.953868	6.140537	5.837731
	26 H	5.932071	6.092969	6.211075	6.592405	6.349786
		21	22	23	24	25
	21 S	0.000000				
	22 S	3.158275	0.000000			
	23 C	1.748342	2.734131	0.000000		
	24 C	2.686295	1.761233	1.375772	0.000000	
	25 H	3.701827	2.418559	2.142715	1.085204	0.000000
	26 H	2.442215	3.692893	1.082151	2.170883	2.532270
		26				
	26 H	0.000000				

CpIrS₂C₂H₂·Cr(CO)₃

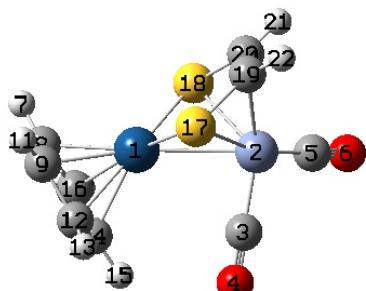
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	2 Cr	2.758374	0.000000				
	3 C	4.250900	1.834606	0.000000			
	4 O	5.300880	2.983764	1.149232	0.000000		
	5 C	4.251061	1.834635	2.579961	3.480298	0.000000	
	6 C	3.074663	1.826648	2.571575	3.484851	2.571869	
	7 O	3.753920	2.981032	3.477281	4.196373	3.477627	
	8 O	5.300932	2.983784	3.480514	4.183204	1.149221	
	9 H	2.914872	5.481321	6.615735	7.475792	7.121840	
	10 C	2.176821	4.862428	6.119358	7.044023	6.413812	
	11 C	2.176842	4.862111	6.413493	7.456336	6.118870	
	12 H	2.936859	4.734274	5.424198	6.113645	6.378959	
	13 H	2.914920	5.480821	7.121634	8.195035	6.614587	
	14 C	2.193554	4.428125	5.985312	7.035505	5.464739	
	15 H	2.936923	4.733309	6.377072	7.457500	5.423656	
	16 C	2.204569	4.141037	5.376156	6.309375	5.377276	
	17 H	2.926885	4.174213	5.214641	6.071649	5.216389	
	18 C	2.193429	4.428583	5.464728	6.311225	5.986488	
	19 S	2.288991	2.435948	4.212490	5.343272	3.085630	
	20 S	2.288687	2.436060	3.086418	3.901847	4.212325	
	21 C	3.209142	2.169714	3.416107	4.405209	2.849141	
22 C	3.209022	2.169758	2.850327	3.695603	3.415337		

	23	H	4.244742	2.923256	2.987645	3.540907	3.928012		
	24	H	4.244878	2.923204	3.928875	4.805527	2.986109		
			6	7	8	9	10		
	6	C	0.000000						
	7	O	1.154393	0.000000					
	8	O	3.485221	4.196867	0.000000				
	9	H	5.700278	6.127178	8.194960	0.000000			
	10	C	4.868683	5.218984	7.456485	1.079814	0.000000		
	11	C	4.867840	5.217887	7.043244	2.241703	1.430790		
	12	H	4.221739	4.290052	7.459675	2.708866	2.247434		
	13	H	5.698949	6.125443	7.474108	2.697244	2.241685		
	14	C	3.991298	4.134140	6.311222	3.360252	2.316683		
	15	H	4.218844	4.286075	6.113075	4.371491	3.360893		
	16	C	3.344003	3.300113	6.310782	3.359199	2.315240		
	17	H	2.933132	2.549292	6.073980	4.369609	3.358723		
	18	C	3.992852	4.136278	7.036833	2.247735	1.434381		
	19	S	3.506358	4.446838	3.900629	4.817187	4.217448		
	20	S	3.507231	4.447923	5.342999	3.823095	3.637268		
	21	C	3.893922	5.021816	3.693999	5.525628	5.155357		
	22	C	3.894238	5.022203	4.404193	5.179501	4.961012		
	23	H	4.638473	5.757942	4.804393	5.992731	5.883335		
	24	H	4.637977	5.757307	3.538691	6.535731	6.182481		
			11	12	13	14	15		
	11	C	0.000000						
	12	H	3.360871	0.000000					
	13	H	1.079816	4.371471	0.000000				
	14	C	1.434355	3.355825	2.247703	0.000000			
	15	H	2.247416	4.364447	2.708833	1.079902	0.000000		
	16	C	2.315208	2.238590	3.359166	1.427691	2.238588		
	17	H	3.358682	2.693671	4.369562	2.238802	2.693634		
	18	C	2.316658	1.079903	3.360229	2.313093	3.355825		
	19	S	3.637013	5.201933	3.822449	3.530752	3.626762		
	20	S	4.217690	3.626105	4.817777	4.453478	5.201523		
	21	C	4.961029	5.815779	5.179465	5.015480	5.275078		
	22	C	5.155483	5.274661	5.525964	5.322845	5.815765		
	23	H	6.182689	6.042739	6.536231	6.386565	6.894381		
	24	H	5.883291	6.894438	5.992563	5.912119	6.043287		
			16	17	18	19	20		
	16	C	0.000000						
	17	H	1.080217	0.000000					
	18	C	1.427694	2.238826	0.000000				
	19	S	4.068703	4.536761	4.453751	0.000000			
	20	S	4.067915	4.535617	3.530182	3.186419	0.000000		
	21	C	5.240313	5.636510	5.322813	1.744966	2.724788		
	22	C	5.240015	5.636079	5.015104	2.724816	1.744901		
	23	H	6.226665	6.576084	5.911670	3.736014	2.432268		
	24	H	6.227086	6.576728	6.386566	2.432283	3.736005		
			21	22	23	24			
	21	C	0.000000						
	22	C	1.374506	0.000000					

	23 H	2.154594	1.083263	0.000000
	24 H	1.083260	2.154652	2.523774 0.000000



	1	2	3	4	5
1 Ir	0.000000				
2 Cr	2.656645	0.000000			
3 C	3.002875	1.825228	0.000000		
4 O	3.696813	2.981235	1.156024	0.000000	
5 C	4.127613	1.833365	2.556052	3.466486	0.000000
6 O	5.173321	2.984698	3.468086	4.182655	1.151380
7 H	2.933853	5.399511	5.716025	6.187074	6.521342
8 C	2.196913	4.787203	4.867433	5.250320	6.012843
9 C	2.202582	4.790664	4.793822	5.135541	6.311424
10 H	2.925028	4.668352	4.319722	4.481750	5.273193
11 H	2.942770	5.406285	5.597503	6.002116	7.035860
12 C	2.194459	4.360097	3.880141	3.991953	5.851968
13 H	2.939212	4.681169	4.060401	4.053591	6.253911
14 C	2.205258	4.092564	3.324118	3.292609	5.230793
15 H	2.928526	4.160254	2.947395	2.576773	5.070218
16 C	2.180925	4.349092	4.023069	4.225736	5.312736
17 S	2.331645	2.394493	3.364514	4.274382	4.196668
18 S	2.293578	2.378150	3.593201	4.576010	3.049341
19 C	3.207506	2.135087	3.818688	4.935885	3.456022
20 C	3.212825	2.175302	3.948434	5.089976	2.947991
21 H	4.251222	2.949706	4.724816	5.865575	3.148727
22 H	4.249745	2.891151	4.524246	5.619257	3.970593
	6	7	8	9	10
6 O	0.000000				
7 H	7.375098	0.000000			
8 C	6.924405	1.079847	0.000000		
9 C	7.342806	2.234419	1.422178	0.000000	
10 H	5.923848	2.710210	2.250619	3.356992	0.000000
11 H	8.105629	2.691327	2.234796	1.079714	4.368563
12 C	6.878635	3.358050	2.313317	1.439466	3.350846
13 H	7.308872	4.367798	3.356219	2.250439	4.360862
14 C	6.127221	3.364448	2.321244	2.320413	2.240281
15 H	5.875098	4.376253	3.365898	3.364089	2.699659
16 C	6.129868	2.250719	1.438808	2.314004	1.079935
17 S	5.337822	4.856611	4.259009	3.676587	5.237181
18 S	3.874047	3.829223	3.651163	4.231133	3.625984
19 C	4.468774	5.523406	5.158618	4.970116	5.807780
20 C	3.816318	5.165505	4.960740	5.158521	5.276351
21 H	3.747483	5.984339	5.888365	6.188109	6.051873
22 H	4.876918	6.549111	6.198560	5.910373	6.885759



1. -2441.816596 0.0

		11	12	13	14	15
	11 H	0.000000				
	12 C	2.251559	0.000000			
	13 H	2.709935	1.080082	0.000000		
	14 C	3.363026	1.425030	2.235869	0.000000	
	15 H	4.373204	2.236533	2.690849	1.080016	0.000000
	16 C	3.358591	2.307672	3.351345	1.429517	2.242979
	17 S	3.853700	3.554828	3.643324	4.108607	4.582705
	18 S	4.829569	4.461318	5.213756	4.088716	4.569191
	19 C	5.187535	5.016590	5.282387	5.251673	5.661535
	20 C	5.521375	5.330446	5.831355	5.266579	5.684703
	21 H	6.533090	6.396166	6.910780	6.257145	6.629450
	22 H	6.025427	5.923909	6.061956	6.240072	6.597312
		16	17	18	19	20
	16 C	0.000000				
	17 S	4.482992	0.000000			
	18 S	3.527974	3.232219	0.000000		
	19 C	5.311032	1.753089	2.722385	0.000000	
	20 C	5.010877	2.755559	1.744265	1.375647	0.000000
	21 H	5.913436	3.759538	2.437249	2.152809	1.083744
	22 H	6.378599	2.435639	3.728049	1.085607	2.144755
		21	22			
	21 H	0.000000				
	22 H	2.501233	0.000000			

Table S5A. Energy rank for all of the $\text{CpIrS}_2\text{C}_2\text{H}_2\cdot\text{Fe}(\text{CO})_n$ optimized structures. PBE0/6-311G(d,p).

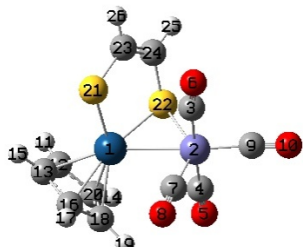
$\text{CpIrS}_2\text{C}_2\text{H}_2\cdot\text{Fe}(\text{CO})_n$

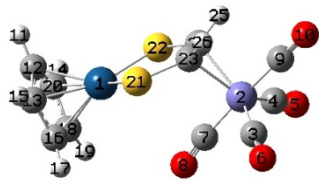
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4-1	8-ir-fe-CO-4-md2	-2887.529409	0.0
4-2	9-ir-fe-CO-4-md3	-2887.514336	9.5
4-3	7-ir-fe-CO-4-md1-new-Fe-Co-h-r-ok-new-Fe-Ir-o	-2887.51292	10.4
4-4	7-Co-fe-CO-4-md1-r1-freq-new-Fe-Ir-m-ok	-2887.505712	14.9
4-5	7-ir-fe-CO-4-md1	-2887.479272	31.5
	name		
3-1	5-ir-fe-CO-3-md2	-2774.29394	0.0
3-2	4-ir-fe-CO-3-md1	-2774.281945	7.5
3-3	6-ir-fe-CO-3-md3	-2774.270437	14.7
	name		
2-1	3-ir-fe-CO-2-md3-fneg1	-2661.045558	0.0

2-2	3-Co-fe-CO-2-md3-r1-freq-new-ir-fe-j- freq-ok	-2661.031538	8.8
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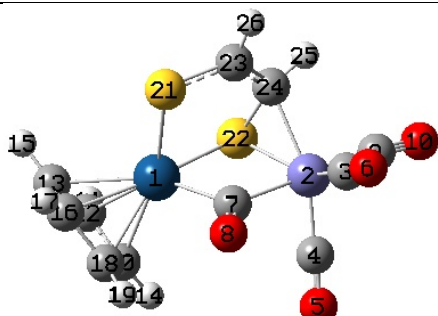
Table S5B. Distance table for the lowest-lying $\text{CpIrS}_2\text{C}_2\text{H}_2\cdot\text{Fe}(\text{CO})_n$ structures after PBE0/6-311G(d,p) optimization.

$\text{CpIrS}_2\text{C}_2\text{H}_2\cdot\text{Fe}(\text{CO})_4$

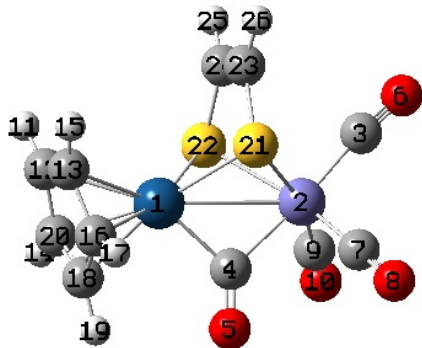
 <p>1. -2887.529409 0.0</p>							
	1	2	3	4	5		
	1 Ir	0.000000					
	2 Fe	2.697478	0.000000				
	3 C	3.431079	1.816025	0.000000			
	4 C	3.094581	1.794669	3.609415	0.000000		
	5 O	3.806721	2.934561	4.748556	1.140036	0.000000	
	6 O	4.311540	2.945461	1.134218	4.736521	5.874289	
	7 C	2.932658	1.767119	2.535126	2.579716	3.506567	
	8 O	3.639366	2.910709	3.436799	3.488444	4.236251	
	9 C	4.435909	1.764302	2.495075	2.508019	3.402309	
	10 O	5.575853	2.904687	3.384662	3.402043	4.096913	
	11 H	2.921698	5.409051	6.181593	5.214427	5.422332	
	12 C	2.175313	4.717384	5.590138	4.498209	4.740429	
	13 C	2.170659	4.767723	5.361198	4.885240	5.304589	
	14 H	2.950415	4.379495	5.834799	3.340070	3.084504	
	15 H	2.882682	5.459554	5.744362	5.814900	6.319868	
	16 C	2.201105	4.221411	5.006646	4.219065	4.617748	
	17 H	2.956509	4.568499	5.152375	4.748930	5.212739	
	18 C	2.219010	3.781272	5.037184	3.214083	3.362074	
	19 H	2.973930	3.757412	5.193219	2.897995	2.870138	
	20 C	2.206204	4.124146	5.400203	3.436486	3.462837	
	21 S	2.332825	3.686366	3.131436	4.905772	5.846603	
	22 S	2.316240	2.351131	3.040891	2.855660	3.630621	
	23 C	3.215389	3.827934	3.068267	5.123356	6.083824	
	24 C	3.238667	3.375655	3.039770	4.444697	5.331059	
25 H	4.266416	4.084806	3.691839	5.072999	5.899048		
26 H	4.250465	4.773866	3.726343	6.161578	7.141477		
	6	7	8	9	10		
6 O	0.000000						
7 C	3.436292	0.000000					
8 O	4.146210	1.145669	0.000000				
9 C	3.325137	2.934717	3.900275	0.000000			
10 O	3.992612	3.895851	4.731600	1.142557	0.000000		
11 H	6.961993	5.760859	6.320118	7.006681	8.098606		
12 C	6.428966	4.844570	5.323379	6.375707	7.485567		
13 C	6.079891	4.450349	4.691052	6.521171	7.656841		
14 H	6.884267	4.771700	5.375381	5.677001	6.644673		
15 H	6.297599	5.103442	5.276750	7.222606	8.363259		
16 C	5.809460	3.487023	3.518912	5.910535	7.006609		
17 H	5.846304	3.445162	3.144733	6.186219	7.241520		
18 C	6.020877	3.330793	3.573153	5.325163	6.371590		
19 H	6.221667	3.121996	3.239994	5.071471	6.020691		
20 C	6.395286	4.243677	4.745644	5.642991	6.695305		
21 S	3.407923	3.923407	4.524492	5.209129	6.274903		
22 S	3.916619	3.785772	4.863507	3.474318	4.471441		
23 C	3.197514	4.717062	5.569265	4.977357	5.920798		

	24 C 3.436148 4.692236 5.711362 4.304599 5.193566
	25 H 3.946745 5.562947 6.623033 4.653876 5.372656
	26 H 3.534359 5.609339 6.402406 5.766923 6.621626
	11 12 13 14 15
	11 H 0.000000
	12 C 1.079439 0.000000
	13 C 2.245555 1.432240 0.000000
	14 H 2.715407 2.249573 3.356154 0.000000
	15 H 2.695569 2.238350 1.080584 4.366525 0.000000
	16 C 3.368921 2.326997 1.428592 3.363741 2.238742
	17 H 4.379318 3.370768 2.245532 4.371963 2.702966
	18 C 3.359910 2.315905 2.305481 2.233810 3.350744
	19 H 4.370987 3.359885 3.349337 2.687188 4.361646
	20 C 2.254477 1.438326 2.311062 1.080342 3.354581
	21 S 4.116476 3.758056 3.270676 5.160679 3.183977
	22 S 3.996277 3.745567 4.309016 3.640584 4.913802
	23 C 4.716714 4.626233 4.597894 5.654956 4.610026
	24 C 4.695580 4.648119 4.971297 5.159413 5.233625
	25 H 5.479506 5.551390 5.993301 5.881942 6.247296
	26 H 5.537447 5.541398 5.432775 6.699246 5.275258
	16 17 18 19 20
	16 C 0.000000
	17 H 1.079460 0.000000
	18 C 1.436030 2.249615 0.000000
	19 H 2.244311 2.703770 1.080376 0.000000
	20 C 2.320383 3.362530 1.421714 2.232763 0.000000
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	22 S 4.473087 5.214572 4.042256 4.495069 3.562766
	23 C 5.109376 5.577080 5.433782 6.119368 5.164924
	24 C 5.391628 6.006755 5.357468 5.940646 4.915077
	25 H 6.442494 7.079273 6.317715 6.856139 5.779161
	26 H 6.020208 6.410575 6.459662 7.163232 6.194774
	21 22 23 24 25
	21 S 0.000000
	22 S 3.184736 0.000000
	23 C 1.725548 2.695863 0.000000
	24 C 2.707903 1.753643 1.342305 0.000000
	25 H 3.722941 2.429620 2.142364 1.083611 0.000000
	26 H 2.402470 3.709505 1.086291 2.117831 2.503654
	26
	26 H 0.000000
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	1 Ir 0.000000
	2 Fe 4.361511 0.000000
	3 C 5.325148 1.772322 0.000000
	4 C 5.323761 1.772393 3.022816 0.000000
	5 O 6.154956 2.915216 4.027591 1.143167 0.000000
	6 O 6.157654 2.915144 1.143200 4.026895 4.933089
	7 C 3.553817 1.803766 2.502545 2.504471 3.397597
	8 O 3.561383 2.938085 3.370434 3.373484 4.057874
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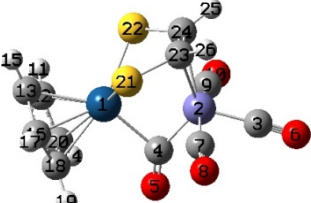
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	11	H	2.898731	7.089240	8.116602	7.970790	8.706790		
	12	C	2.165019	6.511506	7.461972	7.375571	8.110703		
	13	C	2.190152	6.336930	6.962083	7.415097	8.252683		
	14	H	2.937632	6.564746	7.823418	6.883747	7.336908		
	15	H	2.930584	6.780557	7.229353	8.034416	8.949004		
	16	C	2.177258	5.859754	6.394000	6.790176	7.562150		
	17	H	2.912300	5.908202	6.150694	6.904379	7.701830		
	18	C	2.168413	5.766486	6.609921	6.348850	6.956160		
	19	H	2.900795	5.734849	6.564850	6.068619	6.546886		
	20	C	2.203178	6.225104	7.305148	6.782144	7.368710		
	21	S	2.257124	3.416896	3.891704	4.963967	6.036460		
	22	S	2.259024	3.415715	4.964215	3.884276	4.566140		
	23	C	3.224474	2.142450	3.062285	3.685795	4.776395		
	24	C	3.225406	2.142574	3.689688	3.055363	3.984532		
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	7	C	3.395172	0.000000					
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	13	C	7.582222	5.350270	5.071547	7.677578	8.614119		
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	16	C	6.976410	4.553595	4.032250	7.412533	8.447516		
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	20	C	8.144499	5.161424	4.827296	7.620228	8.582755		
	21	S	4.577146	3.258122	3.725000	4.437892	5.302933		
	22	S	6.037552	3.254472	3.720897	4.440679	5.307599		
	23	C	3.994191	2.884989	3.798803	2.776401	3.609217		
	24	C	4.781728	2.884222	3.798011	2.778787	3.612413		
	25	H	5.326532	3.764229	4.733730	2.620198	3.174524		
	26	H	4.011515	3.765344	4.734854	2.616189	3.168565		
			11	12	13	14	15		
	11	H	0.000000						
	12	C	1.080136	0.000000					
	13	C	2.247108	1.438604	0.000000				
	14	H	2.697703	2.241867	3.370040	0.000000			
	15	H	2.702041	2.248840	1.079708	4.377639	0.000000		
	16	C	3.350447	2.308222	1.420785	3.367501	2.237331		
	17	H	4.364382	3.354838	2.236971	4.374353	2.701974		
	18	C	3.346423	2.302808	2.316605	2.238756	3.362949		
	19	H	4.359075	3.348251	3.357396	2.700396	4.370547		

	20 C 2.240436 1.429599 2.326770 1.079747 3.368348
	21 S 4.511594 4.024336 3.516922 5.174147 3.624231
	22 S 4.240334 3.860587 4.380435 3.519809 5.097789
	23 C 5.572091 5.191472 5.028467 5.807256 5.279120
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	22 S 3.151298 0.000000
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	26
	26 H 0.000000
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	1 Ir 0.000000
	2 Fe 3.296974 0.000000
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	10 O 5.930446 2.957931 3.555415 3.563008 4.306300
	11 H 3.050460 5.520179 7.078913 5.583698 5.889328
	12 C 2.323951 5.165516 6.572141 5.211812 5.529655
	13 C 2.354113 5.615532 6.790295 5.927171 6.370196
	14 H 2.963596 4.604299 5.953960 3.895077 3.800429
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	16 C 2.221451 5.363610 6.246638 5.563815 5.964120
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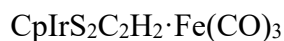
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	24	C	3.167909	2.103681	3.071068	3.770646	4.878889		
	25	H	4.205060	2.695239	3.498187	4.350766	5.451433		
	26	H	4.179071	3.768770	3.837035	5.478045	6.597822		
			6	7	8	9	10		
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	7	C	3.453238	0.000000					
	8	O	3.406776	1.189260	0.000000				
	9	C	3.572904	3.831736	4.682861	0.000000			
	10	O	4.329827	4.966950	5.794439	1.138127	0.000000		
	11	H	8.106999	4.852385	5.655767	6.555536	7.372404		
	12	C	7.532865	4.148492	4.816924	6.450973	7.379754		
	13	C	7.633247	4.295392	4.813358	7.066757	8.066274		
	14	H	6.909156	3.713123	4.185421	5.840594	6.736869		
	15	H	8.282772	5.088998	5.647571	7.672402	8.637109		
	16	C	6.955891	3.658510	3.848335	7.027418	8.110097		
	17	H	7.136885	4.102090	4.073162	7.660816	8.769977		
	18	C	6.490249	3.117668	3.222579	6.467305	7.538220		
	19	H	6.186230	3.080323	2.803476	6.603890	7.687829		
	20	C	6.815391	3.414193	3.895467	6.015917	6.991590		
	21	S	4.926032	2.884613	3.496036	5.228937	6.254383		
	22	S	4.993263	2.817339	4.005415	3.073033	3.959925		
	23	C	4.132259	3.074923	3.902188	4.023625	4.935239		
	24	C	3.978342	2.954786	4.005004	2.771604	3.657789		
	25	H	4.322675	3.956183	4.978821	2.624750	3.221685		
	26	H	4.250223	3.965814	4.643542	4.515838	5.301739		
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	12	C	1.080861	0.000000					
	13	C	2.213572	1.399593	0.000000				
	14	H	2.708277	2.257148	3.351900	0.000000			
	15	H	2.671815	2.216692	1.080033	4.364142	0.000000		
	16	C	3.343927	2.297134	1.446072	3.348342	2.256676		
	17	H	4.353345	3.339243	2.257353	4.358099	2.716910		
	18	C	3.356858	2.314858	2.322660	2.242170	3.364698		
	19	H	4.371639	3.362415	3.366491	2.707536	4.374504		
	20	C	2.251101	1.446391	2.314000	1.079727	3.359736		
	21	S	4.894372	4.289398	3.716058	5.273656	3.898457		
	22	S	3.706113	3.642278	4.193487	3.899912	4.689538		
	23	C	5.572263	5.184125	4.964629	5.865269	5.177594		
	24	C	5.259536	5.043615	5.208646	5.396670	5.559109		
	25	H	5.995414	5.919450	6.146740	6.265436	6.418590		
	26	H	6.598390	6.223291	5.903771	6.946135	6.012830		
			16	17	18	19	20		
	16	C	0.000000						
	17	H	1.080317	0.000000					
	18	C	1.422738	2.231879	0.000000				
	19	H	2.232556	2.682896	1.080298	0.000000			
	20	C	2.303947	3.347021	1.427282	2.242492	0.000000		

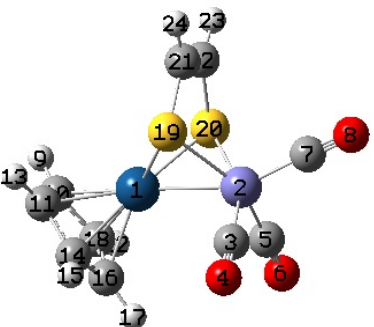
	21 S 3.493983 3.565028 4.078525 4.535986 4.481305 22 S 4.519381 5.278440 4.305124 4.877875 3.691897 23 C 4.900972 5.134588 5.189363 5.582523 5.302129 24 C 5.290585 5.768325 5.277649 5.684108 5.063371 25 H 6.335209 6.819894 6.326164 6.742283 6.009639 26 H 5.806893 5.907263 6.178435 6.517646 6.371312 21 22 23 24 25 21 S 0.000000 22 S 3.239432 0.000000 23 C 1.662139 2.751496 0.000000 24 C 2.720483 1.779867 1.406852 0.000000 25 H 3.640219 2.446519 2.114641 1.086251 0.000000 26 H 2.360277 3.739589 1.088150 2.152105 2.421635 26 26 H 0.000000																																																																																																																																																																																																																		
 <p>4. -2887.505712 +14.9</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Fe</td><td>3.006792</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>4.476373</td><td>1.846560</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>1.990258</td><td>2.002047</td><td>3.843495</td><td>0.000000</td><td></td></tr> <tr><td>5 O</td><td>2.899999</td><td>2.935007</td><td>4.758710</td><td>1.187279</td><td>0.000000</td></tr> <tr><td>6 O</td><td>5.541232</td><td>2.977324</td><td>1.135516</td><td>4.977294</td><td>5.867961</td></tr> <tr><td>7 C</td><td>4.063755</td><td>1.762946</td><td>2.693992</td><td>2.608837</td><td>3.030895</td></tr> <tr><td>8 O</td><td>4.942050</td><td>2.900201</td><td>3.623583</td><td>3.435051</td><td>3.569081</td></tr> <tr><td>9 C</td><td>4.063799</td><td>1.762959</td><td>2.694136</td><td>2.608551</td><td>3.030452</td></tr> <tr><td>10 O</td><td>4.942451</td><td>2.900230</td><td>3.623906</td><td>3.434613</td><td>3.568098</td></tr> <tr><td>11 H</td><td>3.103815</td><td>5.721029</td><td>6.740596</td><td>4.966502</td><td>5.716732</td></tr> <tr><td>12 C</td><td>2.365225</td><td>5.250933</td><td>6.489563</td><td>4.221932</td><td>4.880502</td></tr> <tr><td>13 C</td><td>2.364781</td><td>5.249790</td><td>6.489342</td><td>4.219619</td><td>4.877333</td></tr> <tr><td>14 H</td><td>2.933353</td><td>5.289641</td><td>6.772203</td><td>3.901712</td><td>4.163929</td></tr> <tr><td>15 H</td><td>3.103105</td><td>5.718928</td><td>6.740063</td><td>4.962703</td><td>5.711553</td></tr> <tr><td>16 C</td><td>2.194331</td><td>4.943246</td><td>6.447323</td><td>3.519576</td><td>3.905335</td></tr> <tr><td>17 H</td><td>2.933601</td><td>5.287754</td><td>6.773098</td><td>3.895586</td><td>4.153951</td></tr> <tr><td>18 C</td><td>2.173431</td><td>4.845520</td><td>6.517167</td><td>3.114180</td><td>3.257404</td></tr> <tr><td>19 H</td><td>2.848146</td><td>5.032084</td><td>6.818890</td><td>3.092229</td><td>2.827886</td></tr> <tr><td>20 C</td><td>2.194387</td><td>4.944591</td><td>6.447096</td><td>3.523428</td><td>3.911187</td></tr> <tr><td>21 S</td><td>2.411410</td><td>2.417563</td><td>3.163554</td><td>2.875303</td><td>3.934732</td></tr> <tr><td>22 S</td><td>2.411300</td><td>2.417643</td><td>3.163667</td><td>2.875126</td><td>3.934542</td></tr> <tr><td>23 C</td><td>3.214965</td><td>3.132939</td><td>3.079014</td><td>4.082978</td><td>5.258045</td></tr> <tr><td>24 C</td><td>3.214953</td><td>3.132940</td><td>3.079015</td><td>4.082926</td><td>5.257987</td></tr> <tr><td>25 H</td><td>4.165253</td><td>4.060965</td><td>3.688951</td><td>5.085231</td><td>6.241570</td></tr> <tr><td>26 H</td><td>4.165262</td><td>4.060948</td><td>3.688941</td><td>5.085297</td><td>6.241648</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 O</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 C</td><td>3.585076</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 O</td><td>4.344991</td><td>1.137667</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>3.585254</td><td>2.585545</td><td>3.519197</td><td>0.000000</td><td></td></tr> <tr><td>10 O</td><td>4.345393</td><td>3.518530</td><td>4.288502</td><td>1.137665</td><td>0.000000</td></tr> <tr><td>11 H</td><td>7.607614</td><td>7.070174</td><td>8.006155</td><td>6.567752</td><td>7.262376</td></tr> <tr><td>12 C</td><td>7.448935</td><td>6.425671</td><td>7.287248</td><td>6.141230</td><td>6.868917</td></tr> </tbody> </table>		1	2	3	4	5	1 Ir	0.000000					2 Fe	3.006792	0.000000				3 C	4.476373	1.846560	0.000000			4 C	1.990258	2.002047	3.843495	0.000000		5 O	2.899999	2.935007	4.758710	1.187279	0.000000	6 O	5.541232	2.977324	1.135516	4.977294	5.867961	7 C	4.063755	1.762946	2.693992	2.608837	3.030895	8 O	4.942050	2.900201	3.623583	3.435051	3.569081	9 C	4.063799	1.762959	2.694136	2.608551	3.030452	10 O	4.942451	2.900230	3.623906	3.434613	3.568098	11 H	3.103815	5.721029	6.740596	4.966502	5.716732	12 C	2.365225	5.250933	6.489563	4.221932	4.880502	13 C	2.364781	5.249790	6.489342	4.219619	4.877333	14 H	2.933353	5.289641	6.772203	3.901712	4.163929	15 H	3.103105	5.718928	6.740063	4.962703	5.711553	16 C	2.194331	4.943246	6.447323	3.519576	3.905335	17 H	2.933601	5.287754	6.773098	3.895586	4.153951	18 C	2.173431	4.845520	6.517167	3.114180	3.257404	19 H	2.848146	5.032084	6.818890	3.092229	2.827886	20 C	2.194387	4.944591	6.447096	3.523428	3.911187	21 S	2.411410	2.417563	3.163554	2.875303	3.934732	22 S	2.411300	2.417643	3.163667	2.875126	3.934542	23 C	3.214965	3.132939	3.079014	4.082978	5.258045	24 C	3.214953	3.132940	3.079015	4.082926	5.257987	25 H	4.165253	4.060965	3.688951	5.085231	6.241570	26 H	4.165262	4.060948	3.688941	5.085297	6.241648		6	7	8	9	10	6 O	0.000000					7 C	3.585076	0.000000				8 O	4.344991	1.137667	0.000000			9 C	3.585254	2.585545	3.519197	0.000000		10 O	4.345393	3.518530	4.288502	1.137665	0.000000	11 H	7.607614	7.070174	8.006155	6.567752	7.262376	12 C	7.448935	6.425671	7.287248	6.141230	6.868917
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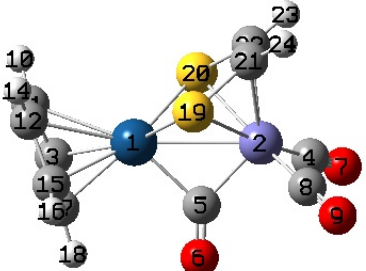
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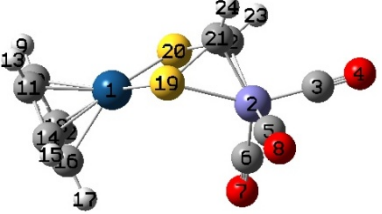
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	18 C	3.353800	2.309327	2.319091	2.250375	3.361479
	19 H	4.362348	3.351628	3.363055	2.706599	4.372452
	20 C	2.228792	1.419844	2.319095	1.079451	3.361529
	21 S	4.969224	4.308113	3.599981	5.324302	3.756085
	22 S	3.291362	3.352193	3.598950	4.443674	3.754911
	23 C	5.521456	5.113393	4.793008	5.894542	4.948545
	24 C	4.949774	4.794159	4.792682	5.570411	4.948208
	25 H	5.734239	5.710551	5.802288	6.401987	5.907153
	26 H	6.606477	6.188501	5.802748	6.904192	5.907625
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	17 H	1.080834	0.000000			
	18 C	1.419824	2.228775	0.000000		
	19 H	2.236297	2.688822	1.079455	0.000000	
	20 C	2.309319	3.353793	1.440502	2.250327	0.000000
	21 S	3.352868	3.292034	3.983602	4.443684	4.521850
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	23 C	4.794551	4.950323	5.131746	5.570656	5.320815
	24 C	5.113231	5.521432	5.320681	5.894479	5.131485
	25 H	6.188289	6.606455	6.349896	6.904109	6.063428
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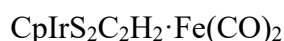
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	14 C	2.180475	4.139767	3.902833	4.123471	4.528729
	15 H	2.935093	4.443773	3.782199	3.713267	4.940272
	16 C	2.196297	3.944296	3.926376	4.288065	3.778926
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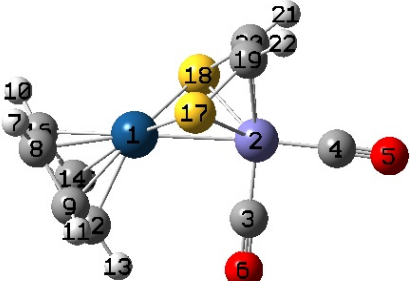
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 <p>3. -2774.270437 +14.7</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Fe</td><td>3.779215</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>5.313545</td><td>1.745225</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 O</td><td>6.360550</td><td>2.888602</td><td>1.144157</td><td>0.000000</td><td></td></tr> <tr><td>5 C</td><td>4.957910</td><td>1.783929</td><td>2.534839</td><td>3.467042</td><td>0.000000</td></tr> <tr><td>6 C</td><td>3.859109</td><td>1.787914</td><td>2.685150</td><td>3.631437</td><td>2.851373</td></tr> <tr><td>7 O</td><td>4.275373</td><td>2.929938</td><td>3.648335</td><td>4.447306</td><td>3.844122</td></tr> <tr><td>8 O</td><td>5.866552</td><td>2.926428</td><td>3.461751</td><td>4.219112</td><td>1.142614</td></tr> <tr><td>9 H</td><td>2.904638</td><td>6.559161</td><td>7.916223</td><td>8.852209</td><td>7.827855</td></tr> <tr><td>10 C</td><td>2.174057</td><td>5.946135</td><td>7.425898</td><td>8.429119</td><td>7.098432</td></tr> <tr><td>11 C</td><td>2.188868</td><td>5.740758</td><td>7.363008</td><td>8.436766</td><td>6.580728</td></tr> <tr><td>12 H</td><td>2.921498</td><td>6.002531</td><td>7.301995</td><td>8.224085</td><td>7.316679</td></tr> <tr><td>13 H</td><td>2.929963</td><td>6.212477</td><td>7.811228</td><td>8.871811</td><td>6.934118</td></tr> <tr><td>14 C</td><td>2.221670</td><td>5.290713</td><td>6.997412</td><td>8.117064</td><td>5.925761</td></tr> <tr><td>15 H</td><td>2.949402</td><td>5.359480</td><td>7.103625</td><td>8.245181</td><td>5.661532</td></tr> <tr><td>16 C</td><td>2.170347</td><td>5.157370</td><td>6.762608</td><td>7.838854</td><td>6.023920</td></tr> <tr><td>17 H</td><td>2.903874</td><td>5.151491</td><td>6.704289</td><td>7.764052</td><td>5.894089</td></tr> <tr><td>18 C</td><td>2.184181</td><td>5.627221</td><td>7.085595</td><td>8.085836</td><td>6.805166</td></tr> <tr><td>19 S</td><td>2.334536</td><td>2.358861</td><td>3.980543</td><td>5.079919</td><td>3.007828</td></tr> <tr><td>20 S</td><td>2.205855</td><td>3.308083</td><td>4.241649</td><td>5.059153</td><td>4.990893</td></tr> <tr><td>21 C</td><td>3.321914</td><td>1.926126</td><td>2.907739</td><td>3.835499</td><td>3.012876</td></tr> <tr><td>22 C</td><td>3.201101</td><td>2.038794</td><td>2.691182</td><td>3.513578</td><td>3.688885</td></tr> <tr><td>23 H</td><td>4.174394</td><td>2.737515</td><td>2.696995</td><td>3.186475</td><td>4.316813</td></tr> <tr><td>24 H</td><td>4.204185</td><td>2.739210</td><td>3.335115</td><td>4.077252</td><td>3.405291</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 O</td><td>1.142727</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 O</td><td>3.830834</td><td>4.706798</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 H</td><td>6.557542</td><td>6.759213</td><td>8.725432</td><td>0.000000</td><td></td></tr> <tr><td>10 C</td><td>5.848624</td><td>6.021726</td><td>7.949830</td><td>1.080115</td><td>0.000000</td></tr> <tr><td>11 C</td><td>5.871663</td><td>6.188919</td><td>7.286627</td><td>2.252691</td><td>1.445780</td></tr> <tr><td>12 H</td><td>5.272447</td><td>5.038084</td><td>8.246747</td><td>2.698017</td><td>2.235990</td></tr> <tr><td>13 H</td><td>6.599373</td><td>7.038484</td><td>7.568317</td><td>2.707139</td><td>2.255110</td></tr> <tr><td>14 C</td><td>5.174331</td><td>5.381916</td><td>6.547732</td><td>3.357138</td><td>2.316150</td></tr> <tr><td>15 H</td><td>5.344638</td><td>5.612925</td><td>6.113503</td><td>4.368954</td><td>3.361591</td></tr> <tr><td>16 C</td><td>4.600299</td><td>4.546381</td><td>6.762919</td><td>3.353816</td><td>2.306932</td></tr> <tr><td>17 H</td><td>4.283454</td><td>4.021629</td><td>6.578216</td><td>4.364149</td><td>3.349748</td></tr> <tr><td>18 C</td><td>5.118777</td><td>5.057288</td><td>7.676317</td><td>2.232505</td><td>1.417954</td></tr> <tr><td>19 S</td><td>3.353103</td><td>4.249149</td><td>3.811533</td><td>5.006211</td><td>4.338093</td></tr> <tr><td>20 S</td><td>3.490796</td><td>3.999965</td><td>6.094664</td><td>3.888825</td><td>3.673230</td></tr> <tr><td>21 C</td><td>3.457361</td><td>4.519859</td><td>3.973856</td><td>5.716167</td><td>5.308616</td></tr> <tr><td>22 C</td><td>3.014262</td><td>3.924737</td><td>4.792846</td><td>5.419242</td><td>5.108480</td></tr> <tr><td>23 H</td><td>3.676222</td><td>4.531570</td><td>5.394308</td><td>6.095971</td><td>5.926312</td></tr> <tr><td>24 H</td><td>4.423837</td><td>5.522957</td><td>4.180275</td><td>6.370706</td><td>6.049992</td></tr> <tr> <th></th> <th>11</th> <th>12</th> <th>13</th> <th>14</th> <th>15</th> </tr> <tr><td>11 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 H</td><td>3.367339</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 Ir	0.000000					2 Fe	3.779215	0.000000				3 C	5.313545	1.745225	0.000000			4 O	6.360550	2.888602	1.144157	0.000000		5 C	4.957910	1.783929	2.534839	3.467042	0.000000	6 C	3.859109	1.787914	2.685150	3.631437	2.851373	7 O	4.275373	2.929938	3.648335	4.447306	3.844122	8 O	5.866552	2.926428	3.461751	4.219112	1.142614	9 H	2.904638	6.559161	7.916223	8.852209	7.827855	10 C	2.174057	5.946135	7.425898	8.429119	7.098432	11 C	2.188868	5.740758	7.363008	8.436766	6.580728	12 H	2.921498	6.002531	7.301995	8.224085	7.316679	13 H	2.929963	6.212477	7.811228	8.871811	6.934118	14 C	2.221670	5.290713	6.997412	8.117064	5.925761	15 H	2.949402	5.359480	7.103625	8.245181	5.661532	16 C	2.170347	5.157370	6.762608	7.838854	6.023920	17 H	2.903874	5.151491	6.704289	7.764052	5.894089	18 C	2.184181	5.627221	7.085595	8.085836	6.805166	19 S	2.334536	2.358861	3.980543	5.079919	3.007828	20 S	2.205855	3.308083	4.241649	5.059153	4.990893	21 C	3.321914	1.926126	2.907739	3.835499	3.012876	22 C	3.201101	2.038794	2.691182	3.513578	3.688885	23 H	4.174394	2.737515	2.696995	3.186475	4.316813	24 H	4.204185	2.739210	3.335115	4.077252	3.405291		6	7	8	9	10	6 C	0.000000					7 O	1.142727	0.000000				8 O	3.830834	4.706798	0.000000			9 H	6.557542	6.759213	8.725432	0.000000		10 C	5.848624	6.021726	7.949830	1.080115	0.000000	11 C	5.871663	6.188919	7.286627	2.252691	1.445780	12 H	5.272447	5.038084	8.246747	2.698017	2.235990	13 H	6.599373	7.038484	7.568317	2.707139	2.255110	14 C	5.174331	5.381916	6.547732	3.357138	2.316150	15 H	5.344638	5.612925	6.113503	4.368954	3.361591	16 C	4.600299	4.546381	6.762919	3.353816	2.306932	17 H	4.283454	4.021629	6.578216	4.364149	3.349748	18 C	5.118777	5.057288	7.676317	2.232505	1.417954	19 S	3.353103	4.249149	3.811533	5.006211	4.338093	20 S	3.490796	3.999965	6.094664	3.888825	3.673230	21 C	3.457361	4.519859	3.973856	5.716167	5.308616	22 C	3.014262	3.924737	4.792846	5.419242	5.108480	23 H	3.676222	4.531570	5.394308	6.095971	5.926312	24 H	4.423837	5.522957	4.180275	6.370706	6.049992		11	12	13	14	15	11 C	0.000000					12 H	3.367339	0.000000			
	1	2	3	4	5																																																																																																																																																																																																																																																																																												
1 Ir	0.000000																																																																																																																																																																																																																																																																																																
2 Fe	3.779215	0.000000																																																																																																																																																																																																																																																																																															
3 C	5.313545	1.745225	0.000000																																																																																																																																																																																																																																																																																														
4 O	6.360550	2.888602	1.144157	0.000000																																																																																																																																																																																																																																																																																													
5 C	4.957910	1.783929	2.534839	3.467042	0.000000																																																																																																																																																																																																																																																																																												
6 C	3.859109	1.787914	2.685150	3.631437	2.851373																																																																																																																																																																																																																																																																																												
7 O	4.275373	2.929938	3.648335	4.447306	3.844122																																																																																																																																																																																																																																																																																												
8 O	5.866552	2.926428	3.461751	4.219112	1.142614																																																																																																																																																																																																																																																																																												
9 H	2.904638	6.559161	7.916223	8.852209	7.827855																																																																																																																																																																																																																																																																																												
10 C	2.174057	5.946135	7.425898	8.429119	7.098432																																																																																																																																																																																																																																																																																												
11 C	2.188868	5.740758	7.363008	8.436766	6.580728																																																																																																																																																																																																																																																																																												
12 H	2.921498	6.002531	7.301995	8.224085	7.316679																																																																																																																																																																																																																																																																																												
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14 C	2.221670	5.290713	6.997412	8.117064	5.925761																																																																																																																																																																																																																																																																																												
15 H	2.949402	5.359480	7.103625	8.245181	5.661532																																																																																																																																																																																																																																																																																												
16 C	2.170347	5.157370	6.762608	7.838854	6.023920																																																																																																																																																																																																																																																																																												
17 H	2.903874	5.151491	6.704289	7.764052	5.894089																																																																																																																																																																																																																																																																																												
18 C	2.184181	5.627221	7.085595	8.085836	6.805166																																																																																																																																																																																																																																																																																												
19 S	2.334536	2.358861	3.980543	5.079919	3.007828																																																																																																																																																																																																																																																																																												
20 S	2.205855	3.308083	4.241649	5.059153	4.990893																																																																																																																																																																																																																																																																																												
21 C	3.321914	1.926126	2.907739	3.835499	3.012876																																																																																																																																																																																																																																																																																												
22 C	3.201101	2.038794	2.691182	3.513578	3.688885																																																																																																																																																																																																																																																																																												
23 H	4.174394	2.737515	2.696995	3.186475	4.316813																																																																																																																																																																																																																																																																																												
24 H	4.204185	2.739210	3.335115	4.077252	3.405291																																																																																																																																																																																																																																																																																												
	6	7	8	9	10																																																																																																																																																																																																																																																																																												
6 C	0.000000																																																																																																																																																																																																																																																																																																
7 O	1.142727	0.000000																																																																																																																																																																																																																																																																																															
8 O	3.830834	4.706798	0.000000																																																																																																																																																																																																																																																																																														
9 H	6.557542	6.759213	8.725432	0.000000																																																																																																																																																																																																																																																																																													
10 C	5.848624	6.021726	7.949830	1.080115	0.000000																																																																																																																																																																																																																																																																																												
11 C	5.871663	6.188919	7.286627	2.252691	1.445780																																																																																																																																																																																																																																																																																												
12 H	5.272447	5.038084	8.246747	2.698017	2.235990																																																																																																																																																																																																																																																																																												
13 H	6.599373	7.038484	7.568317	2.707139	2.255110																																																																																																																																																																																																																																																																																												
14 C	5.174331	5.381916	6.547732	3.357138	2.316150																																																																																																																																																																																																																																																																																												
15 H	5.344638	5.612925	6.113503	4.368954	3.361591																																																																																																																																																																																																																																																																																												
16 C	4.600299	4.546381	6.762919	3.353816	2.306932																																																																																																																																																																																																																																																																																												
17 H	4.283454	4.021629	6.578216	4.364149	3.349748																																																																																																																																																																																																																																																																																												
18 C	5.118777	5.057288	7.676317	2.232505	1.417954																																																																																																																																																																																																																																																																																												
19 S	3.353103	4.249149	3.811533	5.006211	4.338093																																																																																																																																																																																																																																																																																												
20 S	3.490796	3.999965	6.094664	3.888825	3.673230																																																																																																																																																																																																																																																																																												
21 C	3.457361	4.519859	3.973856	5.716167	5.308616																																																																																																																																																																																																																																																																																												
22 C	3.014262	3.924737	4.792846	5.419242	5.108480																																																																																																																																																																																																																																																																																												
23 H	3.676222	4.531570	5.394308	6.095971	5.926312																																																																																																																																																																																																																																																																																												
24 H	4.423837	5.522957	4.180275	6.370706	6.049992																																																																																																																																																																																																																																																																																												
	11	12	13	14	15																																																																																																																																																																																																																																																																																												
11 C	0.000000																																																																																																																																																																																																																																																																																																
12 H	3.367339	0.000000																																																																																																																																																																																																																																																																																															

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	14 C	1.420071	3.366852	2.235348	0.000000	
	15 H	2.232931	4.376061	2.694044	1.080112	0.000000
	16 C	2.304035	2.254139	3.348622	1.426099	2.235939
	17 H	3.346977	2.710211	4.358229	2.237808	2.690789
	18 C	2.320675	1.079711	3.361401	2.325111	3.368307
	19 S	3.742365	5.171518	4.012321	3.476082	3.484518
	20 S	4.194392	3.710627	4.780699	4.414614	5.113697
	21 C	5.034060	5.980028	5.237886	5.041731	5.209371
	22 C	5.222906	5.345662	5.626534	5.268322	5.667806
	23 H	6.162164	6.070218	6.526192	6.304662	6.741613
	24 H	5.671205	6.935458	5.689043	5.798892	5.885492
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	16 C	0.000000				
	17 H	1.080223	0.000000			
	18 C	1.443512	2.252988	0.000000		
	19 S	3.894843	4.273895	4.438102	0.000000	
	20 S	4.019393	4.490165	3.571922	3.112860	0.000000
	21 C	5.253394	5.628669	5.457614	1.775227	2.808831
	22 C	5.120683	5.446156	5.065202	2.615842	1.803393
	23 H	6.104394	6.423773	5.909758	3.647975	2.395622
	24 H	6.177165	6.608775	6.366521	2.496442	3.698445
		21	22	23	24	
	21 C	0.000000				
	22 C	1.423067	0.000000			
	23 H	2.163524	1.087635	0.000000		
	24 H	1.083873	2.263229	2.629985	0.000000	

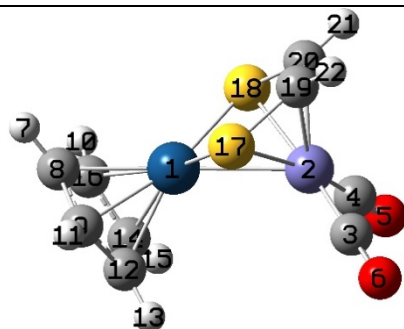


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	6 O	3.813512	2.898283	1.149441	3.369820	4.048892
	7 H	2.938417	5.395819	5.738645	7.096920	8.227457
	8 C	2.199744	4.767469	4.911852	6.489393	7.625778
	9 C	2.198469	4.319855	4.031722	5.926584	7.011289
	10 H	2.938670	5.397845	5.742785	7.098297	8.228355
	11 H	2.941281	4.637771	4.259628	6.105542	7.129817
	12 C	2.219053	4.044191	3.403018	5.574852	6.626692
	13 H	2.948163	4.107667	3.019319	5.409392	6.363340
	14 C	2.198579	4.321835	4.036618	5.927816	7.012017
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	16 C	2.199988	4.768750	4.914467	6.490256	7.626358
	17 S	2.287450	2.293690	3.382899	3.623858	4.658852



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	19 C	3.177615	2.093181	3.774279	2.945417	3.869762
	20 C	3.177563	2.093120	3.774678	2.943905	3.867635
	21 H	4.218586	2.847189	4.474727	3.144306	3.817738
	22 H	4.218641	2.847587	4.474460	3.147369	3.822170
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	6 O	0.000000				
	7 H	6.229072	0.000000			
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	10 H	6.234194	2.695169	2.237571	3.357699	0.000000
	11 H	4.391482	2.706675	2.247641	1.080047	4.367923
	12 C	3.433963	3.362320	2.319515	1.427456	3.362289
	13 H	2.713757	4.373330	3.363739	2.240382	4.373315
	14 C	4.252036	3.357667	2.313279	2.307315	2.248429
	15 H	4.402777	4.367866	3.356531	3.350813	2.706586
	16 C	5.332584	2.237559	1.425190	2.313324	1.079608
	17 S	4.341328	3.909953	3.693130	3.521340	4.891255
	18 S	4.342129	4.894329	4.268639	4.447962	3.914008
	19 C	4.905268	5.214439	4.974127	4.987422	5.559208
	20 C	4.905763	5.560455	5.168452	5.296424	5.215396
	21 H	5.584312	6.590164	6.209720	6.361002	6.058666
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	12 C	2.238115	0.000000			
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	19 C	5.244813	5.209633	5.606809	5.296443	5.788593
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	21 H	0.000000				
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	2 Fe	2.621746	0.000000			



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4	C	3.715173	1.738494	2.400855	0.000000				
5	O	4.663422	2.889688	3.291926	1.151290	0.000000			
6	O	4.810074	2.896023	1.155594	3.291935	3.959586			
7	H	2.980768	5.538645	6.688692	6.631397	7.495872			
8	C	2.223510	4.844740	5.919510	5.819503	6.643086			
9	C	2.184401	4.528839	5.211696	5.581341	6.443899			
10	H	2.923519	5.075001	6.457398	5.474111	6.015507			
11	H	2.921097	5.004217	5.460514	6.232112	7.160952			
12	C	2.172901	4.063489	4.597530	4.747037	5.461547			
13	H	2.910663	4.194499	4.310781	4.761748	5.413397			
14	C	2.173504	4.091555	5.004431	4.427441	4.984534			
15	H	2.914092	4.249315	5.097661	4.143849	4.464491			
16	C	2.187932	4.572276	5.784100	5.146427	5.794376			
17	S	2.298055	2.321313	2.985264	4.040919	5.186242			
18	S	2.306964	2.307999	4.046240	2.960700	3.801766			
19	C	3.264368	2.092336	3.069322	3.641927	4.743707			
20	C	3.273952	2.084616	3.557378	3.151517	4.126054			
21	H	4.303697	2.893767	4.217014	3.555433	4.345221			
22	H	4.291602	2.891434	3.410646	4.325520	5.376488			
		6	7	8	9	10			
6	O	0.000000							
7	H	7.586132	0.000000						
8	C	6.793614	1.079263	0.000000					
9	C	5.917500	2.247421	1.431544	0.000000				
10	H	7.457574	2.699532	2.237897	3.345365	0.000000			
11	H	6.039598	2.703219	2.240727	1.080505	4.356896			
12	C	5.251389	3.369878	2.326821	1.429591	3.356347			
13	H	4.753565	4.378856	3.369188	2.243267	4.367637			
14	C	5.820190	3.369348	2.326247	2.312419	2.238410			
15	H	5.874549	4.378400	3.368662	3.356461	2.697480			
16	C	6.718973	2.244643	1.428838	2.300585	1.080534			
17	S	3.836178	4.381471	3.969469	3.521519	5.122174			
18	S	5.200858	4.496095	4.036557	4.446971	3.591104			
19	C	4.026106	5.491780	5.163330	5.029562	5.756735			
20	C	4.643167	5.541507	5.194413	5.347268	5.233419			
21	H	5.234633	6.464390	6.169396	6.405575	5.985656			
22	H	4.156273	6.395459	6.127640	5.910961	6.826440			
		11	12	13	14	15			
11	H	0.000000							
12	C	2.237202	0.000000						
13	H	2.694775	1.079386	0.000000					
14	C	3.355771	1.435737	2.248466	0.000000				
15	H	4.366548	2.247915	2.708901	1.079406	0.000000			
16	C	3.345204	2.312998	3.357391	1.430890	2.245340			
17	S	3.575178	3.794701	4.079580	4.339373	5.003139			
18	S	5.172083	4.295658	4.929388	3.726062	3.963187			
19	C	5.243008	5.149514	5.468195	5.326795	5.783347			
20	C	5.802814	5.323706	5.769472	5.125041	5.423269			
21	H	6.878113	6.348732	6.785201	6.042957	6.240109			

	22 H	5.987979	6.074080	6.299209	6.358410	6.811679
		16	17	18	19	20
	16 C	0.000000				
	17 S	4.418235	0.000000			
	18 S	3.532027	3.142134	0.000000		
	19 C	5.319970	1.752032	2.714605	0.000000	
	20 C	5.029607	2.722454	1.754540	1.373753	0.000000
	21 H	5.915671	3.742286	2.442284	2.165799	1.082754
	22 H	6.374833	2.434867	3.735543	1.082866	2.162873
		21	22			
	21 H	0.000000				
	22 H	2.556513	0.000000			

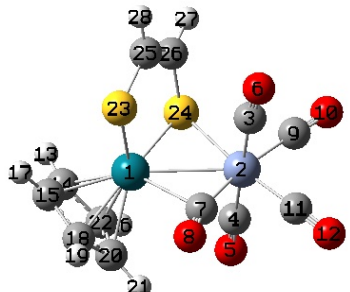
Table S6A. Energy rank for all of the $\text{CpRhS}_2\text{C}_2\text{H}_2 \cdot \text{Cr}(\text{CO})_n$ optimized structures. PBE0/6-311G(d,p).

Rh-Cr

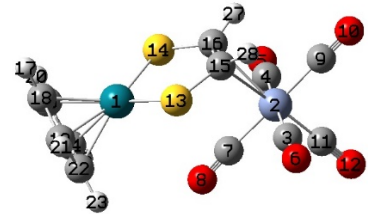
	name	E(a.u.)	ΔE (kcal/mol)
5-1	11-rh-Cr-CO-5-md2	-2787.754554	0.0
5-2	12-ir-Cr-CO-5-md3-new-Rh-Cr-k-ok	-2787.740342	8.92
5-3	12-rh-Cr-CO-5-md3-freq-fneg2-fneg1	-2787.72102	21.0
5-4	10-rh-Cr-CO-5-md1	-2787.696236	36.6
	name		
4-1	8-rh-Cr-CO-4-md2	-2674.508827	0.0
4-2	7-rh-Cr-CO-4-md1	-2674.497551	7.1
4-3	9-rh-Cr-CO-4-md3	-2674.485493	14.6
	name		
3-1	6-rh-Cr-CO-3-md3	-2561.285037	0.0
	name		
2-1	3-rh-Cr-CO-2-md3	-2448.001988	0.0
2-2	2-rh-Cr-CO-2-md2	-2447.996221	3.6

Table S6B. Distance table for the lowest-lying CpRhS₂C₂H₂·Cr(CO)_n structures after PBE0/6-311G(d,p) optimization.

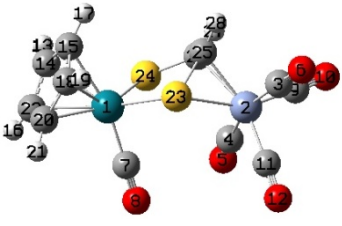
CpRhS₂C₂H₂·Cr(CO)₅

 <p>1. -2787.754554 0.0</p>							
		1	2	3	4	5	
	1 Rh	0.000000					
	2 Cr	2.822617	0.000000				
	3 C	3.632976	1.906854	0.000000			
	4 C	3.164044	1.879136	3.785906	0.000000		
	5 O	3.851967	3.023768	4.930477	1.144860	0.000000	
	6 O	4.509734	3.041889	1.138078	4.919998	6.063829	
	7 C	2.433958	1.907077	2.626572	2.762577	3.675412	
	8 O	3.139738	3.026416	3.459924	3.694698	4.449744	
	9 C	4.357967	1.894263	2.655156	2.682763	3.584976	
	10 O	5.403359	3.033941	3.540265	3.590035	4.310946	
	11 C	4.369261	1.841576	2.670309	2.612840	3.503426	
	12 O	5.417176	2.986337	3.571564	3.501584	4.193493	
	13 H	2.886886	5.348489	6.222778	5.082608	5.279675	
	14 C	2.161977	4.757322	5.735422	4.443118	4.653515	
	15 C	2.165222	4.946373	5.642454	4.948134	5.305131	
	16 H	2.955425	4.334623	5.903556	3.182086	2.908619	
	17 H	2.869472	5.639957	6.030828	5.883714	6.325587	
	18 C	2.211945	4.516677	5.392012	4.376499	4.686765	
	19 H	2.948246	4.923728	5.598212	4.959001	5.323506	
	20 C	2.244004	4.019559	5.347938	3.339073	3.412859	
	21 H	2.983926	4.011769	5.500781	3.064644	2.966678	
	22 C	2.218988	4.185927	5.563875	3.389699	3.380430	
	23 S	2.318168	3.792623	3.317616	4.992469	5.911934	
	24 S	2.291680	2.447048	3.146002	3.036719	3.846115	
	25 C	3.183730	3.915459	3.168733	5.260855	6.231816	
	26 C	3.203570	3.462131	3.113218	4.618002	5.536520	
27 H	4.231323	4.167483	3.727165	5.274700	6.152321		
28 H	4.220472	4.852960	3.792611	6.301875	7.295153		
		6	7	8	9	10	
6 O	0.000000						
7 C	3.526674	0.000000					
8 O	4.154157	1.153689	0.000000				
9 C	3.514027	3.779199	4.856976	0.000000			
10 O	4.197499	4.911349	5.972772	1.139896	0.000000		
11 C	3.531496	2.455737	3.118004	2.563540	3.441377		
12 O	4.236501	3.296652	3.658464	3.452146	4.125244		
13 H	7.017744	5.278960	5.872676	6.378165	7.188618		
14 C	6.586264	4.425572	4.926295	6.023802	6.941012		
15 C	6.375304	4.092847	4.300091	6.501513	7.524600		
16 H	6.960781	4.474478	5.144150	5.265907	6.062307		
17 H	6.608455	4.726562	4.841883	7.184748	8.197489		
18 C	6.199972	3.295874	3.271695	6.252383	7.342170		
19 H	6.304025	3.360732	2.965190	6.765694	7.890272		


	20	C	6.327204	3.184831	3.428126	5.592775	6.628881
	21	H	6.521470	3.133109	3.263806	5.554909	6.577006
	22	C	6.563831	3.936109	4.479926	5.435785	6.357142
	23	S	3.624900	3.313776	3.765662	5.143219	6.105274
	24	S	4.009489	3.536313	4.615409	2.926175	3.701753
	25	C	3.313312	4.242443	4.984480	4.646408	5.379909
	26	C	3.505946	4.346502	5.304737	3.767629	4.373417
	27	H	3.969489	5.298517	6.294851	3.995015	4.328439
	28	H	3.616718	5.141825	5.791434	5.439533	6.067608
			11	12	13	14	15
	11	C	0.000000				
	12	O	1.144879	0.000000			
	13	H	7.012973	8.079907	0.000000		
	14	C	6.295584	7.314239	1.080006	0.000000	
	15	C	6.324805	7.275070	2.241407	1.428900	0.000000
	16	H	5.620225	6.546451	2.710672	2.246765	3.354996
	17	H	7.042612	7.994744	2.693067	2.237285	1.080433
	18	C	5.563444	6.384307	3.356908	2.314014	1.424514
	19	H	5.710023	6.405308	4.368501	3.358745	2.240860
	20	C	5.011986	5.827346	3.348451	2.303940	2.300432
	21	H	4.628162	5.290623	4.359660	3.348281	3.344587
	22	C	5.515459	6.460096	2.248849	1.433638	2.310036
	23	S	5.216693	6.209623	4.148332	3.777154	3.242371
	24	S	4.272575	5.414068	3.649391	3.522046	4.154511
	25	C	5.496255	6.549444	4.551018	4.510954	4.453384
	26	C	5.167148	6.269782	4.382148	4.443745	4.782846
	27	H	5.784474	6.853493	5.090054	5.302247	5.769605
	28	H	6.315390	7.314056	5.388662	5.435367	5.284347
			16	17	18	19	20
	16	H	0.000000				
	17	H	4.365284	0.000000			
	18	C	3.355110	2.237366	0.000000		
	19	H	4.362913	2.700547	1.079911	0.000000	
	20	C	2.230012	3.345873	1.428703	2.242058	0.000000
	21	H	2.681378	4.356872	2.238417	2.695743	1.080954
	22	C	1.080197	3.353497	2.311837	3.353943	1.416649
	23	S	5.186538	3.146852	3.637736	3.898311	4.332899
	24	S	3.569033	4.715259	4.460973	5.230262	4.092380
	25	C	5.651967	4.407212	5.032836	5.478880	5.420448
	26	C	5.121492	4.978086	5.330357	5.953503	5.369397
	27	H	5.831262	5.940556	6.374146	7.028226	6.335351
	28	H	6.704157	5.061472	5.930896	6.290470	6.438032
			21	22	23	24	25
	21	H	0.000000				
	22	C	2.226968	0.000000			
	23	S	5.054996	4.410840	0.000000		
	24	S	4.616454	3.488895	3.188853	0.000000	
	25	C	6.126949	5.136115	1.725377	2.694122	0.000000
	26	C	6.009136	4.853688	2.709834	1.750730	1.342451
	27	H	6.951831	5.701497	3.722887	2.430471	2.139821

	28 H 7.159920 6.169267 2.402163 3.707411 1.086894 26 27 28 26 C 0.000000 27 H 1.084157 0.000000 28 H 2.117459 2.497925 0.000000																																																																																																																																																																																																																																																																														
 <p>2. -2787.740342 +8.92</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 Rh</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Cr</td><td>4.539282</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 C</td><td>4.967644</td><td>1.889796</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 C</td><td>4.967416</td><td>1.889796</td><td>3.775528</td><td>0.000000</td><td></td></tr> <tr><td>5 O</td><td>5.561888</td><td>3.031367</td><td>4.914039</td><td>1.142379</td><td>0.000000</td></tr> <tr><td>6 O</td><td>5.562196</td><td>3.031367</td><td>1.142379</td><td>4.914038</td><td>6.050212</td></tr> <tr><td>7 C</td><td>3.672025</td><td>1.890995</td><td>2.659972</td><td>2.659959</td><td>3.552719</td></tr> <tr><td>8 O</td><td>3.620168</td><td>3.032822</td><td>3.555821</td><td>3.555660</td><td>4.258194</td></tr> <tr><td>9 C</td><td>5.883253</td><td>1.887373</td><td>2.685282</td><td>2.685254</td><td>3.592559</td></tr> <tr><td>10 O</td><td>6.833575</td><td>3.030402</td><td>3.588265</td><td>3.588162</td><td>4.314379</td></tr> <tr><td>11 C</td><td>6.094647</td><td>1.833711</td><td>2.573154</td><td>2.573207</td><td>3.442903</td></tr> <tr><td>12 O</td><td>7.136044</td><td>2.981187</td><td>3.456923</td><td>3.457032</td><td>4.116075</td></tr> <tr><td>13 S</td><td>2.243681</td><td>3.648398</td><td>3.382979</td><td>4.822386</td><td>5.746305</td></tr> <tr><td>14 S</td><td>2.243678</td><td>3.648446</td><td>4.822524</td><td>3.382898</td><td>3.753965</td></tr> <tr><td>15 C</td><td>3.181467</td><td>2.501210</td><td>2.764426</td><td>3.583230</td><td>4.531273</td></tr> <tr><td>16 C</td><td>3.181463</td><td>2.501232</td><td>3.583218</td><td>2.764486</td><td>3.493427</td></tr> <tr><td>17 H</td><td>2.893061</td><td>7.324911</td><td>7.626453</td><td>7.626075</td><td>8.059732</td></tr> <tr><td>18 C</td><td>2.164199</td><td>6.702863</td><td>7.017743</td><td>7.017423</td><td>7.471218</td></tr> <tr><td>19 C</td><td>2.189390</td><td>6.416155</td><td>6.400238</td><td>7.051040</td><td>7.665134</td></tr> <tr><td>20 H</td><td>2.923491</td><td>6.816317</td><td>7.677736</td><td>6.514569</td><td>6.628548</td></tr> <tr><td>21 H</td><td>2.923428</td><td>6.816424</td><td>6.514989</td><td>7.677585</td><td>8.389691</td></tr> <tr><td>22 C</td><td>2.169471</td><td>5.864449</td><td>5.967902</td><td>6.406547</td><td>6.985202</td></tr> <tr><td>23 H</td><td>2.896270</td><td>5.796022</td><td>5.682723</td><td>6.516411</td><td>7.173176</td></tr> <tr><td>24 C</td><td>2.169472</td><td>5.864379</td><td>6.406631</td><td>5.967668</td><td>6.331728</td></tr> <tr><td>25 H</td><td>2.896283</td><td>5.795908</td><td>6.516375</td><td>5.682519</td><td>5.929066</td></tr> <tr><td>26 C</td><td>2.189414</td><td>6.416074</td><td>7.051210</td><td>6.399877</td><td>6.687238</td></tr> <tr><td>27 H</td><td>4.189546</td><td>2.833165</td><td>4.093199</td><td>2.705330</td><td>3.259768</td></tr> <tr><td>28 H</td><td>4.189545</td><td>2.833159</td><td>2.705130</td><td>4.093319</td><td>5.074232</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 O</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 C</td><td>3.552719</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 O</td><td>4.258388</td><td>1.142949</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 C</td><td>3.592609</td><td>3.778229</td><td>4.920186</td><td>0.000000</td><td></td></tr> <tr><td>10 O</td><td>4.314537</td><td>4.921329</td><td>6.063143</td><td>1.143129</td><td>0.000000</td></tr> <tr><td>11 C</td><td>3.442843</td><td>2.654058</td><td>3.534816</td><td>2.633982</td><td>3.535040</td></tr> <tr><td>12 O</td><td>4.115932</td><td>3.555320</td><td>4.241128</td><td>3.530710</td><td>4.240556</td></tr> <tr><td>13 S</td><td>3.754096</td><td>3.455278</td><td>3.868272</td><td>4.649177</td><td>5.497724</td></tr> <tr><td>14 S</td><td>5.746464</td><td>3.455534</td><td>3.868502</td><td>4.649043</td><td>5.497485</td></tr> <tr><td>15 C</td><td>3.493356</td><td>3.170548</td><td>4.014460</td><td>3.072901</td><td>3.863797</td></tr> <tr><td>16 C</td><td>4.531249</td><td>3.170661</td><td>4.014548</td><td>3.072807</td><td>3.863646</td></tr> <tr><td>17 H</td><td>8.060288</td><td>6.561633</td><td>6.397628</td><td>8.423493</td><td>9.227175</td></tr> <tr><td>18 C</td><td>7.471679</td><td>5.735415</td><td>5.456598</td><td>7.982850</td><td>8.875759</td></tr> <tr><td>19 C</td><td>6.687725</td><td>5.292360</td><td>4.910192</td><td>7.819047</td><td>8.767628</td></tr> <tr><td>20 H</td><td>8.389943</td><td>5.810885</td><td>5.494140</td><td>8.121014</td><td>9.022444</td></tr> </tbody> </table>		1	2	3	4	5	1 Rh	0.000000					2 Cr	4.539282	0.000000				3 C	4.967644	1.889796	0.000000			4 C	4.967416	1.889796	3.775528	0.000000		5 O	5.561888	3.031367	4.914039	1.142379	0.000000	6 O	5.562196	3.031367	1.142379	4.914038	6.050212	7 C	3.672025	1.890995	2.659972	2.659959	3.552719	8 O	3.620168	3.032822	3.555821	3.555660	4.258194	9 C	5.883253	1.887373	2.685282	2.685254	3.592559	10 O	6.833575	3.030402	3.588265	3.588162	4.314379	11 C	6.094647	1.833711	2.573154	2.573207	3.442903	12 O	7.136044	2.981187	3.456923	3.457032	4.116075	13 S	2.243681	3.648398	3.382979	4.822386	5.746305	14 S	2.243678	3.648446	4.822524	3.382898	3.753965	15 C	3.181467	2.501210	2.764426	3.583230	4.531273	16 C	3.181463	2.501232	3.583218	2.764486	3.493427	17 H	2.893061	7.324911	7.626453	7.626075	8.059732	18 C	2.164199	6.702863	7.017743	7.017423	7.471218	19 C	2.189390	6.416155	6.400238	7.051040	7.665134	20 H	2.923491	6.816317	7.677736	6.514569	6.628548	21 H	2.923428	6.816424	6.514989	7.677585	8.389691	22 C	2.169471	5.864449	5.967902	6.406547	6.985202	23 H	2.896270	5.796022	5.682723	6.516411	7.173176	24 C	2.169472	5.864379	6.406631	5.967668	6.331728	25 H	2.896283	5.795908	6.516375	5.682519	5.929066	26 C	2.189414	6.416074	7.051210	6.399877	6.687238	27 H	4.189546	2.833165	4.093199	2.705330	3.259768	28 H	4.189545	2.833159	2.705130	4.093319	5.074232		6	7	8	9	10	6 O	0.000000					7 C	3.552719	0.000000				8 O	4.258388	1.142949	0.000000			9 C	3.592609	3.778229	4.920186	0.000000		10 O	4.314537	4.921329	6.063143	1.143129	0.000000	11 C	3.442843	2.654058	3.534816	2.633982	3.535040	12 O	4.115932	3.555320	4.241128	3.530710	4.240556	13 S	3.754096	3.455278	3.868272	4.649177	5.497724	14 S	5.746464	3.455534	3.868502	4.649043	5.497485	15 C	3.493356	3.170548	4.014460	3.072901	3.863797	16 C	4.531249	3.170661	4.014548	3.072807	3.863646	17 H	8.060288	6.561633	6.397628	8.423493	9.227175	18 C	7.471679	5.735415	5.456598	7.982850	8.875759	19 C	6.687725	5.292360	4.910192	7.819047	8.767628	20 H	8.389943	5.810885	5.494140	8.121014	9.022444
	1	2	3	4	5																																																																																																																																																																																																																																																																										
1 Rh	0.000000																																																																																																																																																																																																																																																																														
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3 C	4.967644	1.889796	0.000000																																																																																																																																																																																																																																																																												
4 C	4.967416	1.889796	3.775528	0.000000																																																																																																																																																																																																																																																																											
5 O	5.561888	3.031367	4.914039	1.142379	0.000000																																																																																																																																																																																																																																																																										
6 O	5.562196	3.031367	1.142379	4.914038	6.050212																																																																																																																																																																																																																																																																										
7 C	3.672025	1.890995	2.659972	2.659959	3.552719																																																																																																																																																																																																																																																																										
8 O	3.620168	3.032822	3.555821	3.555660	4.258194																																																																																																																																																																																																																																																																										
9 C	5.883253	1.887373	2.685282	2.685254	3.592559																																																																																																																																																																																																																																																																										
10 O	6.833575	3.030402	3.588265	3.588162	4.314379																																																																																																																																																																																																																																																																										
11 C	6.094647	1.833711	2.573154	2.573207	3.442903																																																																																																																																																																																																																																																																										
12 O	7.136044	2.981187	3.456923	3.457032	4.116075																																																																																																																																																																																																																																																																										
13 S	2.243681	3.648398	3.382979	4.822386	5.746305																																																																																																																																																																																																																																																																										
14 S	2.243678	3.648446	4.822524	3.382898	3.753965																																																																																																																																																																																																																																																																										
15 C	3.181467	2.501210	2.764426	3.583230	4.531273																																																																																																																																																																																																																																																																										
16 C	3.181463	2.501232	3.583218	2.764486	3.493427																																																																																																																																																																																																																																																																										
17 H	2.893061	7.324911	7.626453	7.626075	8.059732																																																																																																																																																																																																																																																																										
18 C	2.164199	6.702863	7.017743	7.017423	7.471218																																																																																																																																																																																																																																																																										
19 C	2.189390	6.416155	6.400238	7.051040	7.665134																																																																																																																																																																																																																																																																										
20 H	2.923491	6.816317	7.677736	6.514569	6.628548																																																																																																																																																																																																																																																																										
21 H	2.923428	6.816424	6.514989	7.677585	8.389691																																																																																																																																																																																																																																																																										
22 C	2.169471	5.864449	5.967902	6.406547	6.985202																																																																																																																																																																																																																																																																										
23 H	2.896270	5.796022	5.682723	6.516411	7.173176																																																																																																																																																																																																																																																																										
24 C	2.169472	5.864379	6.406631	5.967668	6.331728																																																																																																																																																																																																																																																																										
25 H	2.896283	5.795908	6.516375	5.682519	5.929066																																																																																																																																																																																																																																																																										
26 C	2.189414	6.416074	7.051210	6.399877	6.687238																																																																																																																																																																																																																																																																										
27 H	4.189546	2.833165	4.093199	2.705330	3.259768																																																																																																																																																																																																																																																																										
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	6	7	8	9	10																																																																																																																																																																																																																																																																										
6 O	0.000000																																																																																																																																																																																																																																																																														
7 C	3.552719	0.000000																																																																																																																																																																																																																																																																													
8 O	4.258388	1.142949	0.000000																																																																																																																																																																																																																																																																												
9 C	3.592609	3.778229	4.920186	0.000000																																																																																																																																																																																																																																																																											
10 O	4.314537	4.921329	6.063143	1.143129	0.000000																																																																																																																																																																																																																																																																										
11 C	3.442843	2.654058	3.534816	2.633982	3.535040																																																																																																																																																																																																																																																																										
12 O	4.115932	3.555320	4.241128	3.530710	4.240556																																																																																																																																																																																																																																																																										
13 S	3.754096	3.455278	3.868272	4.649177	5.497724																																																																																																																																																																																																																																																																										
14 S	5.746464	3.455534	3.868502	4.649043	5.497485																																																																																																																																																																																																																																																																										
15 C	3.493356	3.170548	4.014460	3.072901	3.863797																																																																																																																																																																																																																																																																										
16 C	4.531249	3.170661	4.014548	3.072807	3.863646																																																																																																																																																																																																																																																																										
17 H	8.060288	6.561633	6.397628	8.423493	9.227175																																																																																																																																																																																																																																																																										
18 C	7.471679	5.735415	5.456598	7.982850	8.875759																																																																																																																																																																																																																																																																										
19 C	6.687725	5.292360	4.910192	7.819047	8.767628																																																																																																																																																																																																																																																																										
20 H	8.389943	5.810885	5.494140	8.121014	9.022444																																																																																																																																																																																																																																																																										

	21	H	6.629126	5.811039	5.494438	8.121096	9.022547
	22	C	6.332020	4.430685	3.821060	7.486287	8.529250
	23	H	5.929289	4.224192	3.479789	7.502545	8.578493
	24	C	6.985336	4.430593	3.820898	7.486228	8.529184
	25	H	7.173154	4.224027	3.479469	7.502453	8.578389
	26	C	7.665404	5.292252	4.910002	7.818978	8.767548
	27	H	5.074080	3.914777	4.847100	2.778869	3.330292
	28	H	3.259511	3.914636	4.846989	2.779083	3.330630
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	11	C	0.000000				
	12	O	1.147476	0.000000			
	13	S	5.276388	6.352676	0.000000		
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	15	C	4.293069	5.428563	1.737999	2.706894	0.000000
	16	C	4.293108	5.428616	2.706890	1.738000	1.376570
	17	H	8.961248	10.020542	4.368233	4.367919	5.485509
	18	C	8.239459	9.256804	3.935144	3.934993	5.125793
	19	C	7.827928	8.791640	3.471147	4.393827	4.970901
	20	H	8.229048	9.189698	5.121348	3.542868	5.752004
	21	H	8.229269	9.189950	3.542738	5.121166	5.202501
	22	C	7.059218	7.932768	3.644892	4.217409	4.974189
	23	H	6.780253	7.559905	3.862144	4.831917	5.210128
	24	C	7.059107	7.932648	4.217213	3.645185	5.169400
	25	H	6.780054	7.559685	4.831656	3.862621	5.554708
	26	C	7.827786	8.791482	4.393890	3.471230	5.282402
	27	H	4.464473	5.549706	3.692759	2.411863	2.148597
	28	H	4.464440	5.549645	2.411863	3.692755	1.084384
			16	17	18	19	20
	16	C	0.000000				
	17	H	5.485401	0.000000			
	18	C	5.125741	1.080584	0.000000		
	19	C	5.282320	2.240833	1.430137	0.000000	
	20	H	5.202679	2.696775	2.241935	3.362458	0.000000
	21	H	5.751805	2.696790	2.241940	1.080021	4.371343
	22	C	5.169440	3.342845	2.299505	1.418111	3.358215
	23	H	5.554745	4.356584	3.346041	2.234805	4.365136
	24	C	4.974306	3.342837	2.299499	2.312362	2.234003
	25	H	5.210339	4.356574	3.346034	3.353092	2.697791
	26	C	4.970985	2.240821	1.430130	2.319578	1.080021
	27	H	1.084383	6.288807	6.026163	6.301114	5.909686
	28	H	2.148595	6.288960	6.026229	5.822923	6.771287
			21	22	23	24	25
	21	H	0.000000				
	22	C	2.234001	0.000000			
	23	H	2.697792	1.080338	0.000000		
	24	C	3.358208	1.438190	2.245347	0.000000	
	25	H	4.365131	2.245348	2.693980	1.080338	0.000000
	26	C	3.362456	2.312369	3.353098	1.418113	2.234803
	27	H	6.771042	6.217898	6.624490	5.921850	6.095245
	28	H	5.909450	5.921673	6.094937	6.217834	6.624424

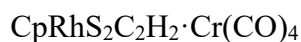
	26	27	28				
	26 C	0.000000					
	27 H	5.823044	0.000000				
	28 H	6.301213	2.499385	0.000000			
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	1 Rh	0.000000					
	2 Cr	4.074845	0.000000				
	3 C	5.253124	1.875095	0.000000			
	4 C	4.083884	1.878063	3.711599	0.000000		
	5 O	4.581726	3.019100	4.830771	1.143970	0.000000	
	6 O	6.199649	3.018178	1.145721	4.834237	5.938842	
	7 C	1.874476	3.932936	5.417917	3.341078	3.552854	
	8 O	3.007742	4.290746	5.840159	3.379269	3.337016	
	9 C	5.657513	1.824864	2.474593	2.491232	3.330553	
	10 O	6.706022	2.974453	3.342338	3.371698	3.981422	
	11 C	4.987766	1.850525	2.502545	2.523094	3.381517	
	12 O	5.751757	2.996179	3.383005	3.398175	4.037124	
	13 H	2.951817	6.365437	7.525961	6.157215	6.403156	
	14 C	2.248870	6.024659	7.088163	5.975981	6.326416	
	15 C	2.225723	5.576709	6.301682	5.973791	6.562314	
	16 H	2.977685	6.911187	8.218507	6.421686	6.484052	
	17 H	2.947889	5.587851	6.106663	6.197771	6.879030	
	18 C	2.246604	5.656759	6.265720	6.141918	6.767747	
	19 H	2.953516	5.698782	5.996545	6.465508	7.212615	
	20 C	2.244559	6.095753	6.989452	6.198825	6.623224	
	21 H	2.978771	6.538692	7.393695	6.607320	6.992827	
	22 C	2.243145	6.309327	7.461589	6.093687	6.341889	
	23 S	2.362468	2.446336	3.038510	3.494927	4.462402	
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	26 C	3.237143	2.295460	3.509025	2.680594	3.479144	
	27 H	4.228070	2.914355	3.931147	3.197458	3.864593	
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	6 O	0.000000					
	7 C	6.463137	0.000000				
	8 O	6.893573	1.133490	0.000000			
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	10 O	3.937474	6.527556	6.705115	1.150248	0.000000	
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	12 O	4.035583	4.788370	4.518815	3.783218	4.623883	
	13 H	8.415681	4.354978	5.339072	7.544425	8.382167	
	14 C	7.947858	3.798341	4.840134	7.401872	8.337068	
	15 C	7.029058	4.067189	5.188861	7.028738	7.999622	
	16 H	9.170407	3.479416	4.160937	8.383066	9.362990	
	17 H	6.737643	4.820284	5.953713	6.885469	7.784338	
	18 C	6.944376	3.785455	4.826291	7.315727	8.380641	
	19 H	6.531044	4.338905	5.320422	7.391052	8.471063	
	20 C	7.781140	3.255218	4.153809	7.790378	8.873814	
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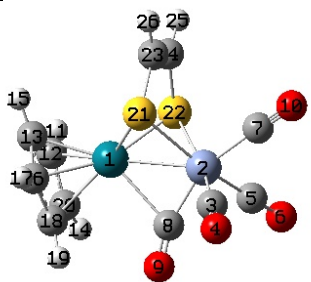
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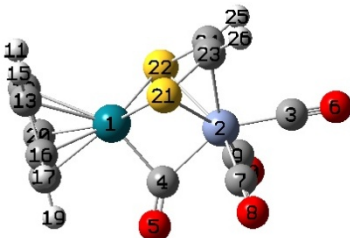
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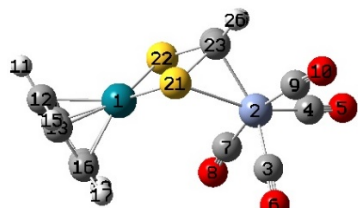
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8 O	4.615269	2.978017	3.266798	3.248695	3.496150
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13 C	7.973594	5.857926	6.516143	6.186957	6.995931
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16 C	7.684573	5.125144	5.629478	5.729427	6.513118
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19 H	7.726366	5.097211	5.559426	5.097825	5.560363
20 C	7.685079	5.728929	6.512302	5.126375	5.631217
21 S	4.768216	3.008749	3.735312	4.290721	5.409239
22 S	4.768060	4.289780	5.408247	3.008994	3.735962
23 C	3.662066	3.314715	4.248502	3.864468	4.950335
24 C	3.662225	3.863950	4.949709	3.315453	4.249467
25 H	3.470329	4.537987	5.605838	3.669709	4.446088
26 H	3.469956	3.669010	4.445112	4.538323	5.606237
	11	12	13	14	15
11 H	0.000000				
12 C	1.080937	0.000000			
13 C	2.199474	1.379286	0.000000		
14 H	2.712900	2.262213	3.332926	0.000000	
15 H	2.660260	2.199474	1.080939	4.349069	0.000000
16 C	3.343961	2.295364	1.454402	3.331383	2.258325
17 H	4.349068	3.332924	2.262220	4.343382	2.712918
18 C	3.360045	2.319956	2.319965	2.230311	3.360059

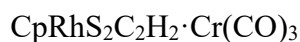
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	22 S	3.734980	3.648135	4.220282	3.696955	4.757407
	23 C	5.280854	5.033513	4.841122	5.866468	4.921701
	24 C	4.922219	4.841469	5.033485	5.332943	5.280652
	25 H	5.701045	5.749998	6.040950	6.124276	6.254475
	26 H	6.254665	6.040945	5.749585	6.950870	5.700438
		16	17	18	19	20
	16 C	0.000000				
	17 H	1.080711	0.000000			
	18 C	1.418285	2.230322	0.000000		
	19 H	2.232433	2.689793	1.079908	0.000000	
	20 C	2.286277	3.331383	1.418274	2.232415	0.000000
	21 S	3.554878	3.696009	4.219247	4.769398	4.483570
	22 S	4.483825	5.276678	4.219579	4.769544	3.555606
	23 C	4.998113	5.332175	5.399968	5.946331	5.303776
	24 C	5.303649	5.866036	5.400115	5.946466	4.998552
	25 H	6.370869	6.950445	6.407622	6.928635	5.907732
	26 H	5.907212	6.123382	6.407421	6.928443	6.370969
		21	22	23	24	25
	21 S	0.000000				
	22 S	3.264609	0.000000			
	23 C	1.744624	2.745179	0.000000		
	24 C	2.745190	1.744648	1.376055	0.000000	
	25 H	3.745274	2.429316	2.145231	1.084906	0.000000
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		26				
	26 H	0.000000				
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	1 Rh	0.000000				
	2 Cr	3.848266	0.000000			
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	5 O	6.369248	2.971555	3.665261	1.150570	0.000000
	6 O	5.517833	2.984573	1.148793	3.667856	4.470501
	7 C	3.399435	1.879293	2.523002	2.541670	3.426305
	8 O	3.717905	3.021317	3.358902	3.398875	4.065681
	9 C	5.249570	1.872193	2.503165	2.500350	3.379227
	10 O	6.272959	3.016266	3.363178	3.348607	3.999500
	11 H	2.891981	6.658002	7.540776	8.154081	9.145851
	12 C	2.164609	5.996693	6.726918	7.504562	8.509742
	13 C	2.193370	5.583379	5.983892	7.244092	8.323073
	14 H	2.917157	6.325631	7.200354	7.425358	8.239065
	15 H	2.930182	5.939268	6.247863	7.694091	8.812743
	16 C	2.178331	5.044687	5.186198	6.595834	7.637496
	17 H	2.909619	4.938418	4.699457	6.491216	7.540093
	18 C	2.162288	5.187217	5.569683	6.484516	7.414963
	19 H	2.879432	5.196002	5.450546	6.264827	7.098816
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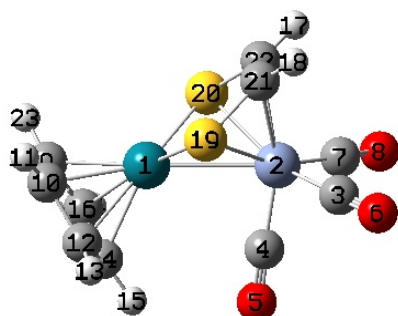


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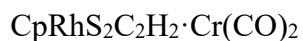
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	23	C	3.217376	2.162773	3.764649	3.458129	4.452654		
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	25	H	4.188014	3.032436	4.863053	3.250464	3.821345		
	26	H	4.204130	2.753365	4.235747	3.800792	4.693870		
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	9	C	3.387549	3.726652	4.850618	0.000000			
	10	O	4.027285	4.856192	5.968284	1.146583	0.000000		
	11	H	8.222522	6.249556	6.386183	7.832570	8.732627		
	12	C	7.349436	5.430208	5.497543	7.299104	8.257207		
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	14	H	7.891377	5.226106	4.921158	7.945732	9.021105		
	15	H	6.656136	5.825675	6.131918	6.858809	7.654493		
	16	C	5.552374	4.306793	4.297595	6.430930	7.420305		
	17	H	4.867684	4.273171	4.291080	6.227479	7.172201		
	18	C	6.054658	4.037058	3.743484	6.820513	7.899864		
	19	H	5.875785	3.734446	3.159469	6.950148	8.064636		
	20	C	7.157433	4.826207	4.633907	7.366046	8.422259		
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	23	C	4.841924	3.330584	4.353704	2.665139	3.523817		
	24	C	5.360138	2.947679	3.789129	3.470460	4.418079		
	25	H	6.010701	3.585803	4.368091	3.783345	4.597181		
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	16	C	3.343169	2.300306	1.417459	3.360833	2.233882		
	17	H	4.356884	3.347012	2.234144	4.368025	2.697757		
	18	C	3.341526	2.297485	2.309731	2.236326	3.355857		
	19	H	4.354868	3.343782	3.351236	2.697850	4.363710		
	20	C	2.239443	1.428491	2.320709	1.079908	3.362975		
	21	S	4.559370	4.063047	3.532260	5.195137	3.629925		
	22	S	4.240372	3.859630	4.356696	3.523045	5.064087		
	23	C	5.496634	5.147952	4.988112	5.790769	5.208841		
	24	C	5.470479	5.114553	5.263197	5.209277	5.726847		
	25	H	6.321940	6.047393	6.304341	5.932244	6.775169		
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			16	17	18	19	20		
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	17	H	1.080399	0.000000					
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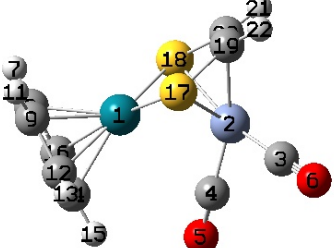
	20 C	2.315607	3.356678	1.420794	2.235991	0.000000
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	22 S	4.264481	4.913352	3.709546	3.969531	3.457815
	23 C	5.012536	5.254237	5.208050	5.588433	5.317877
	24 C	5.164434	5.554076	4.970604	5.200039	4.969770
	25 H	6.211824	6.611521	5.911384	6.060969	5.836124
	26 H	5.945401	6.135755	6.243230	6.656571	6.308349
		21	22	23	24	25
	21 S	0.000000				
	22 S	3.142709	0.000000			
	23 C	1.745750	2.726456	0.000000		
	24 C	2.681580	1.752571	1.379673	0.000000	
	25 H	3.699761	2.414810	2.148463	1.085727	0.000000
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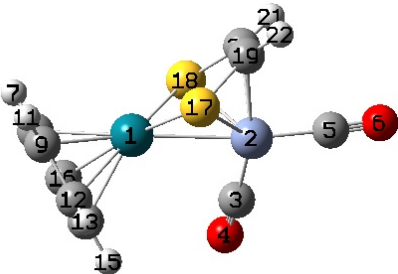


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	7 C	4.211216	1.840808	2.571722	3.470451	2.591429	
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	18 C	2.187595	4.400849	3.967995	4.126510	5.438417	
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23 H	4.228117	2.929813	4.648468	5.767499	3.003618		
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	14	C	7.009550	5.437919	6.282694	3.352718	2.307843
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	21	C	4.925679	5.795067	5.121665	4.993839	5.252811
	22	C	5.120366	5.252806	5.471271	5.301359	5.795038
	23	H	6.149447	6.026765	6.481844	6.367190	6.874797
	24	H	5.851804	6.874836	5.937219	5.895663	6.026780
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	17	H	1.080364	0.000000			
	18	C	1.422864	2.235283	0.000000		
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	21	C	5.248606	5.663725	5.301371	1.742949	2.725189
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	24	H	6.239162	6.608588	6.367205	2.434493	3.733929
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	21	C	0.000000				
	22	C	1.375317	0.000000			
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	5 O	3.684117	2.984129	3.460143	1.154386	0.000000
	6 O	5.126219	2.988535	1.150026	3.464217	4.172159
	7 H	2.939386	5.357795	6.989399	5.535527	5.942748
	8 C	2.207117	4.756014	6.269699	4.751423	5.100127
	9 C	2.206536	4.767932	5.988557	4.863709	5.265455
	10 H	2.933293	4.637319	6.185025	3.975941	3.955927
	11 H	2.937462	5.376398	6.502096	5.716694	6.209794
	12 C	2.176312	4.328960	5.271912	4.033756	4.266955
	13 H	2.913759	4.651235	5.232134	4.354315	4.558919
	14 C	2.218614	4.088237	5.190614	3.324669	3.309828
	15 H	2.941668	4.170789	5.029737	2.967408	2.618643
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	17 S	2.282033	2.347133	3.007574	3.578419	4.570273
	18 S	2.323299	2.382003	4.194598	3.336830	4.242929
	19 C	3.191986	2.177439	2.971540	3.958745	5.101176
	20 C	3.183475	2.136640	3.481394	3.816230	4.929706
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11 H	7.354091	2.686546	2.227881	1.080119	4.361159	
12 C	6.077863	3.348651	2.302596	1.437230	3.340279	
13 H	5.869639	4.358167	3.345203	2.247526	4.351119	
14 C	6.070179	3.358061	2.316028	2.318963	2.232002	
15 H	5.811039	4.368658	3.360386	3.363836	2.688518	
16 C	6.807240	2.249692	1.438748	2.306237	1.080533	
17 S	3.829945	4.840143	4.235244	3.659177	5.192468	
18 S	5.336085	3.813219	3.658316	4.240831	3.644853	
19 C	3.843236	5.497153	5.141033	4.940647	5.817605	
20 C	4.498291	5.145046	4.943348	5.128837	5.272878	
21 H	4.912755	5.984808	5.887278	6.170034	6.060579	
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16 C	3.352342	2.295291	3.339417	1.419497	2.232435	

	17 S 3.842806 3.496450 3.573981 4.067112 4.539068 18 S 4.824896 4.471317 5.222520 4.130850 4.622072 19 C 5.134297 4.979354 5.231906 5.262945 5.689799 20 C 5.478005 5.282079 5.771284 5.257475 5.684121 21 H 6.502499 6.352483 6.851085 6.251641 6.627571 22 H 5.959571 5.885965 6.010557 6.254654 6.634237 16 17 18 19 20 16 C 0.000000 17 S 4.441682 0.000000 18 S 3.554191 3.240426 0.000000 19 C 5.313723 1.743448 2.758977 0.000000 20 C 5.002447 2.721089 1.750250 1.376255 0.000000 21 H 5.916331 3.723289 2.434788 2.140228 1.086348 22 H 6.380674 2.441272 3.759464 1.084253 2.150080 21 22 21 H 0.000000 22 H 2.487892 0.000000
 <p>2. -2447.996221 +3.6</p>	1 2 3 4 5 1 Rh 0.000000 2 Cr 2.710005 0.000000 3 C 3.155170 1.867779 0.000000 4 O 3.840074 3.013856 1.148841 0.000000 5 C 4.528099 1.835804 2.734305 3.683569 0.000000 6 O 5.670818 2.985893 3.684970 4.481389 1.150774 7 H 2.954799 5.468063 5.589101 5.893840 7.162294 8 C 2.217634 4.860585 4.886539 5.188731 6.632881 9 C 2.206393 4.851350 5.138623 5.591535 6.683817 10 H 2.919853 4.717993 3.933787 3.770271 6.243409 11 H 2.943590 5.458561 6.008292 6.560737 7.258153 12 C 2.187919 4.419126 4.438883 4.812473 6.220517 13 H 2.929798 4.735775 4.861005 5.283150 6.455292 14 C 2.214430 4.171180 3.637574 3.737203 5.888255 15 H 2.946721 4.256911 3.339117 3.210610 5.802385 16 C 2.182359 4.412274 3.929014 3.996676 6.108751 17 S 2.278035 2.308238 3.805193 4.852320 3.770443 18 S 2.303527 2.307339 2.919832 3.671663 3.517746 19 C 3.234013 2.163407 3.988058 5.110729 2.963999 20 C 3.225970 2.097260 3.584635 4.601036 2.756063 21 H 4.262849 2.879481 4.215806 5.162712 2.896145 22 H 4.268541 2.967389 4.830728 5.972276 3.254811 6 7 8 9 10 6 O 0.000000 7 H 8.248800 0.000000 8 C 7.756735 1.079873 0.000000 9 C 7.830181 2.230464 1.415035 0.000000 10 H 7.282363 2.703943 2.245509 3.343732 0.000000 11 H 8.386206 2.689919 2.229536 1.080300 4.357184 12 C 7.363160 3.354885 2.309210 1.437500 3.340279 13 H 7.567030 4.363222 3.350934 2.247221 4.352425 14 C 7.006808 3.362998 2.320519 2.315704 2.234837

15	H	6.863481	4.372318	3.363790	3.361917	2.689411
16	C	7.213566	2.247228	1.434702	2.300311	1.080647
17	S	4.805187	4.861141	4.257449	3.695385	5.169454
18	S	4.487084	3.924019	3.717961	4.275136	3.607882
19	C	3.818049	5.551239	5.192315	4.993447	5.826902
20	C	3.583475	5.227532	5.009079	5.194881	5.266979
21	H	3.412419	6.037336	5.929329	6.218737	6.038114
22	H	3.856368	6.538394	6.204291	5.902238	6.909023
		11	12	13	14	15
11	H	0.000000				
12	C	2.247276	0.000000			
13	H	2.701260	1.080407	0.000000		
14	C	3.357631	1.421839	2.234984	0.000000	
15	H	4.370765	2.238996	2.698941	1.080108	0.000000
16	C	3.346611	2.296549	3.341958	1.425371	2.237478
17	S	3.896772	3.549175	3.650996	4.079587	4.559460
18	S	4.890364	4.459096	5.203017	4.075571	4.540470
19	C	5.199708	5.045020	5.310610	5.300690	5.735588
20	C	5.568019	5.339276	5.835614	5.275676	5.695427
21	H	6.573965	6.403708	6.916156	6.265608	6.641728
22	H	5.990212	5.944172	6.086351	6.297137	6.697910
		16	17	18	19	20
16	C	0.000000				
17	S	4.435646	0.000000			
18	S	3.532609	3.153620	0.000000		
19	C	5.338573	1.734214	2.739432	0.000000	
20	C	5.019107	2.700600	1.744235	1.388323	0.000000
21	H	5.918020	3.714064	2.434147	2.163131	1.084000
22	H	6.402344	2.437998	3.751640	1.083253	2.172541
		21	22			
21	H	0.000000				
22	H	2.539266	0.000000			

Table S7A. Energy rank for all of the $\text{CpRhS}_2\text{C}_2\text{H}_2 \cdot \text{Fe}(\text{CO})_n$ optimized structures. PBE0/6-311G(d,p).

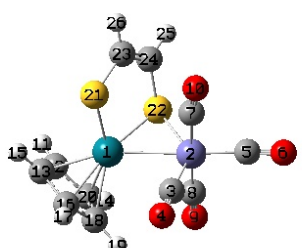
Rh-Fe

	name	E (a.u.)	ΔE (kcal/mol)
4-1	8-rh-fe-CO-4-md2	-2893.711607	0.0
4-2	7-ir-fe-CO-4-md1-new-Fe-Co-h-r-ok-new-Fe-Rh-n	-2893.695783	9.9
4-3	7-Co-fe-CO-4-md1-r1-freq-new-Fe-Rh-l	-2893.691537	12.6
4-4	9-rh-fe-CO-4-md3	-2893.691238	12.8
4-5	7-rh-fe-CO-4-md1-r1-freq	-2893.660889	31.8

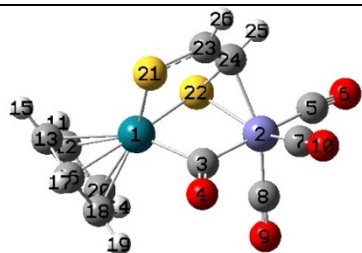
	name		
3-1	5-rh-fe-CO-3-md2	-2780.479877	0.0
3-2	4-rh-fe-CO-3-md1	-2780.469128	6.7
3-3	6-rh-fe-CO-3-md3	-2780.449273	19.2
	name		
2-1	1-rh-fe-CO-2-md1	-2667.231223	0.0
2-2	3-rh-fe-CO-2-md3-fneg1	-2667.216735	9.1

Table S7B. Distance table for the lowest-lying CpRhS₂C₂H₂·Fe(CO)_n structures after PBE0/6-311G(d,p) optimization.

CpRhS₂C₂H₂·Fe(CO)₄

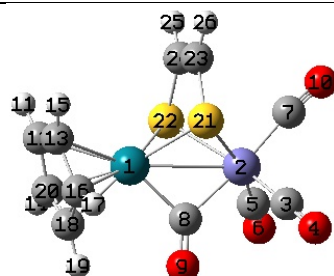
 <p>1. -2893.711607 0.0</p>							
	1 Rh	0.000000					
	2 Fe	2.667396	0.000000				
	3 C	2.898236	1.767646	0.000000			
	4 O	3.608716	2.910893	1.145350	0.000000		
	5 C	4.408796	1.764182	2.925694	3.888110	0.000000	
	6 O	5.548422	2.904509	3.886951	4.718427	1.142219	
	7 C	3.405936	1.815544	2.539974	3.437521	2.496776	
	8 C	3.068138	1.796269	2.583223	3.496888	2.508049	
	9 O	3.789740	2.935728	3.510961	4.248045	3.398436	
	10 O	4.288693	2.945005	3.447072	4.154181	3.326950	
	11 H	2.913865	5.340502	5.717991	6.295353	6.931297	
	12 C	2.178393	4.675548	4.816459	5.307830	6.330273	
	13 C	2.170429	4.755393	4.457157	4.712211	6.507652	
	14 H	2.951469	4.322688	4.708030	5.316806	5.611143	
	15 H	2.877884	5.447641	5.120879	5.313610	7.210568	
	16 C	2.201688	4.238995	3.511560	3.550049	5.926775	
	17 H	2.948646	4.602794	3.493383	3.204564	6.222019	
	18 C	2.225828	3.789642	3.320894	3.558594	5.330275	
	19 H	2.976547	3.778495	3.105986	3.207045	5.089459	
	20 C	2.210136	4.087195	4.201741	4.709128	5.601690	
	21 S	2.321473	3.677861	3.896579	4.486826	5.210466	
	22 S	2.300412	2.332723	3.766232	4.844197	3.471810	
	23 C	3.192182	3.831906	4.708015	5.551457	5.005158	
	24 C	3.216666	3.377943	4.685184	5.698786	4.333422	
	25 H	4.244577	4.101158	5.570020	6.624391	4.707407	
26 H	4.228424	4.789389	5.613454	6.396835	5.812011		
		6	7	8	9	10	
6 O	0.000000						
7 C	3.387789	0.000000					
8 C	3.400698	3.610316	0.000000				
9 O	4.089940	4.748865	1.139694	0.000000			
10 O	3.996895	1.133991	4.737400	5.874346	0.000000		
11 H	8.018812	6.131697	5.124230	5.330290	6.918380		
12 C	7.437373	5.563731	4.438489	4.680838	6.407995		
13 C	7.642764	5.356564	4.864562	5.286533	6.079325		
14 H	6.573287	5.794329	3.255668	2.993919	6.847715		
15 H	8.351538	5.740736	5.794236	6.300982	6.298853		
16 C	7.022891	5.021362	4.238892	4.642972	5.824948		
17 H	7.279528	5.176488	4.793160	5.264571	5.869494		
18 C	6.374830	5.040975	3.229812	3.387444	6.024237		
19 H	6.036705	5.200279	2.945417	2.937175	6.226011		
20 C	6.650794	5.374495	3.384449	3.413764	6.372927		
21 S	6.278698	3.128703	4.894535	5.837664	3.406666		

	22 S	4.470946	3.018458	2.841946	3.622920	3.889255
	23 C	5.955358	3.077907	5.120714	6.080788	3.203331
	24 C	5.228690	3.038409	4.443938	5.330834	3.425122
	25 H	5.437284	3.704404	5.084042	5.908482	3.947313
	26 H	6.677064	3.754220	6.166181	7.143305	3.563272
		11	12	13	14	15
	11 H	0.000000				
	12 C	1.079771	0.000000			
	13 C	2.239998	1.426401	0.000000		
	14 H	2.708323	2.244405	3.349204	0.000000	
	15 H	2.690478	2.233921	1.080533	4.359343	0.000000
	16 C	3.360471	2.317756	1.426114	3.355707	2.237101
	17 H	4.371109	3.361767	2.242692	4.364802	2.700233
	18 C	3.352459	2.308109	2.299696	2.232060	3.344744
	19 H	4.363685	3.352400	3.344215	2.685583	4.356243
	20 C	2.248244	1.432380	2.304204	1.080491	3.347698
	21 S	4.117200	3.755555	3.240726	5.161430	3.144578
	22 S	3.914624	3.698196	4.266458	3.630176	4.856514
	23 C	4.655221	4.583044	4.534489	5.646123	4.523391
	24 C	4.608472	4.593718	4.908251	5.150063	5.147332
	25 H	5.368555	5.483252	5.919950	5.869557	6.145539
	26 H	5.469596	5.493118	5.362756	6.688084	5.177581
		16	17	18	19	20
	16 C	0.000000				
	17 H	1.079833	0.000000			
	18 C	1.429320	2.243696	0.000000		
	19 H	2.239003	2.698266	1.080735	0.000000	
	20 C	2.312127	3.355078	1.419195	2.230712	0.000000
	21 S	3.657241	3.951863	4.338571	5.083460	4.389098
	22 S	4.463113	5.206623	4.055706	4.527365	3.549038
	23 C	5.065336	5.521910	5.415853	6.111725	5.144159
	24 C	5.360722	5.972425	5.354516	5.955673	4.895415
	25 H	6.411150	7.047783	6.318553	6.882097	5.755552
	26 H	5.971525	6.349654	6.438574	7.153837	6.170657
		21	22	23	24	25
	21 S	0.000000				
	22 S	3.187466	0.000000			
	23 C	1.725286	2.695175	0.000000		
	24 C	2.710150	1.753389	1.342823	0.000000	
	25 H	3.724321	2.431600	2.142119	1.083940	0.000000
	26 H	2.403948	3.708167	1.086938	2.116161	2.498922
		26				
	26 H	0.000000				
		1	2	3	4	5
	1 Rh	0.000000				
	2 Fe	3.251523	0.000000			
	3 C	2.047157	1.996512	0.000000		
	4 O	2.851824	2.915194	1.182919	0.000000	
	5 C	4.812072	1.822457	3.817784	4.690952	0.000000
	6 O	5.873506	2.958732	4.953159	5.806141	1.137179



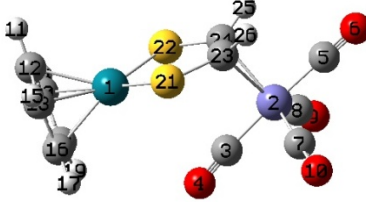
2. -2893.695783 +9.9	7 C	4.421060	1.769338	2.624824	2.932737	2.633719	
	8 C	3.811360	1.770632	2.500401	3.063942	2.652949	
	9 O	4.505150	2.910669	3.321604	3.650799	3.569649	
	10 O	5.322907	2.906473	3.448073	3.429778	3.567063	
	11 H	3.064803	5.655769	4.965912	5.745703	6.705514	
	12 C	2.336875	5.219944	4.212508	4.858590	6.504679	
	13 C	2.340832	5.579547	4.213926	4.654164	7.063980	
	14 H	2.955140	4.599072	3.885084	4.464310	5.739191	
	15 H	3.071992	6.281292	4.969956	5.413295	7.716110	
	16 C	2.218462	5.228980	3.510311	3.623243	6.907575	
	17 H	2.947305	5.746173	3.868414	3.703125	7.502945	
	18 C	2.229557	4.689157	3.102457	3.237304	6.309486	
	19 H	2.910423	4.708255	3.060949	2.872795	6.357589	
	20 C	2.220075	4.587302	3.514982	4.045489	5.945836	
	21 S	2.305315	3.791816	2.854334	3.429040	5.216032	
	22 S	2.342063	2.276530	2.841279	4.022021	3.048150	
	23 C	3.098549	3.014995	3.047084	3.856871	4.016493	
	24 C	3.134065	2.101007	2.940463	3.985680	2.759707	
	25 H	4.175918	2.696333	3.940724	4.959095	2.616902	
	26 H	4.153388	3.764951	3.940034	4.601547	4.510720	
			6	7	8	9	10
		6 O	0.000000				
		7 C	3.553976	0.000000			
		8 C	3.556030	2.726838	0.000000		
		9 O	4.296356	3.690205	1.140223	0.000000	
		10 O	4.323051	1.137877	3.686341	4.513127	0.000000
		11 H	7.525417	7.192698	5.843235	6.212600	8.210268
		12 C	7.430940	6.623718	5.342501	5.700027	7.584114
		13 C	8.073369	6.719209	5.909714	6.364978	7.549318
		14 H	6.600432	6.057092	3.994367	3.969927	7.059302
		15 H	8.703741	7.362490	6.811739	7.348228	8.150585
		16 C	7.992240	6.109275	5.379732	5.760600	6.825809
		17 H	8.618378	6.352819	5.972922	6.374658	6.917427
		18 C	7.364983	5.689080	4.416429	4.596294	6.482398
		19 H	7.416934	5.485656	4.154683	4.167350	6.181834
		20 C	6.901673	5.943823	4.302054	4.476238	6.896884
		21 S	6.235598	4.309747	5.069554	6.022092	4.917958
		22 S	3.922035	3.910238	3.256998	4.160077	4.999410
		23 C	4.919918	3.473110	4.657315	5.752842	4.125871
		24 C	3.635468	3.063701	3.774172	4.883049	3.970749
		25 H	3.199378	3.479530	4.354653	5.455249	4.296939
		26 H	5.286738	3.830028	5.481680	6.602238	4.244696
			11	12	13	14	15
	11 H	0.000000					
	12 C	1.080629	0.000000				
	13 C	2.211669	1.393348	0.000000			
	14 H	2.708643	2.255453	3.337923	0.000000		
	15 H	2.671074	2.210859	1.080812	4.352762	0.000000	
	16 C	3.346283	2.298555	1.445597	3.335624	2.253356	
	17 H	4.354165	3.339168	2.256563	4.346684	2.710818	

	18 C	3.357800	2.316570	2.315760	2.231699	3.357344
	19 H	4.371787	3.363688	3.360314	2.695223	4.367609
	20 C	2.254648	1.447021	2.298291	1.080740	3.346279
	21 S	4.752290	4.202706	3.632963	5.257503	3.746870
	22 S	3.799619	3.686160	4.266056	3.710197	4.826030
	23 C	5.481157	5.123406	4.921018	5.792458	5.115111
	24 C	5.259753	5.031463	5.212279	5.275616	5.588823
	25 H	6.008736	5.917066	6.176930	6.114049	6.492410
	26 H	6.480787	6.151074	5.853542	6.880830	5.930838
		16	17	18	19	20
	16 C	0.000000				
	17 H	1.080424	0.000000			
	18 C	1.418970	2.230688	0.000000		
	19 H	2.229305	2.683325	1.080177	0.000000	
	20 C	2.290150	3.334367	1.417664	2.234263	0.000000
	21 S	3.553637	3.677285	4.188061	4.717893	4.476584
	22 S	4.516951	5.287431	4.215644	4.734603	3.591336
	23 C	4.921366	5.190166	5.223584	5.652787	5.259786
	24 C	5.279775	5.773404	5.237696	5.629880	4.993674
	25 H	6.338538	6.845098	6.277141	6.666665	5.927746
	26 H	5.843811	5.989801	6.236518	6.627255	6.336068
		21	22	23	24	25
	21 S	0.000000				
	22 S	3.257445	0.000000			
	23 C	1.659935	2.754624	0.000000		
	24 C	2.725282	1.775288	1.410498	0.000000	
	25 H	3.645049	2.444135	2.115553	1.086845	0.000000
	26 H	2.361160	3.736714	1.089068	2.150882	2.410741
		26				
	26 H	0.000000				
		1	2	3	4	5
	1 Rh	0.000000				
	2 Fe	2.934241	0.000000			
	3 C	4.021161	1.765379	0.000000		
	4 O	4.913513	2.901914	1.136920	0.000000	
	5 C	4.021113	1.765383	2.598167	3.533837	0.000000
	6 O	4.913748	2.901935	3.533283	4.308214	1.136920
	7 C	4.388510	1.848723	2.686625	3.611396	2.686682
	8 C	1.976250	1.977272	2.607445	3.444106	2.607069
	9 O	2.875523	2.931647	3.063242	3.618263	3.062759
	10 O	5.444914	2.979324	3.579824	4.333935	3.579873
	11 H	3.106645	5.665601	7.035633	7.981438	6.527751
	12 C	2.369397	5.188694	6.387456	7.261075	6.100966
	13 C	2.368928	5.187440	6.097030	6.835113	6.387281
	14 H	2.922084	5.207600	6.413136	7.295585	5.461205
	15 H	3.105936	5.663355	6.520951	7.221428	7.035029
	16 C	2.194883	4.872536	5.458212	6.052678	5.977798
	17 H	2.922151	5.205203	5.456568	5.866199	6.407640
	18 C	2.188274	4.785266	5.495097	6.155905	5.493272
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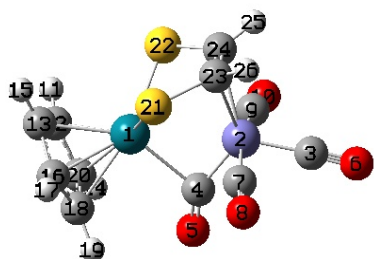


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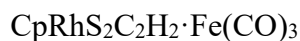
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	14	H	5.872441	6.678338	3.857924	4.098104	7.701010			
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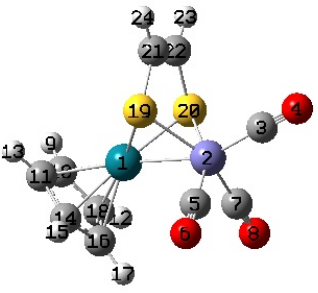
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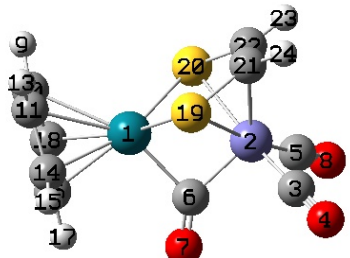
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	23 C	3.615290	3.062442	3.691425	4.783442	3.994363
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17 H 7.766904 4.722632 4.905672 6.258134 7.153678	
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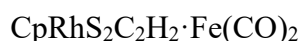
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	22 C	3.252120	3.166420	3.555856	4.217324	4.715383
	23 H	4.220979	4.127846	4.267389	4.739482	5.740867
24 H	4.220454	4.127818	4.270833	4.744791	5.144116	
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7 C	3.439892	0.000000				
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17 H	3.921002	3.536778	3.642953	4.373264	3.365205	
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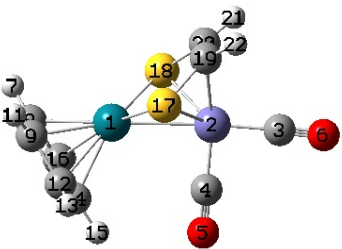
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23	H	4.310747	2.868325	4.043832	4.994526	3.180905
24	H	4.310626	2.868418	3.183449	3.829532	4.041677
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10	C	4.277697	4.888372	7.021461	1.080958	0.000000
11	C	4.276747	4.887337	7.413786	2.199473	1.378874
12	H	3.854865	4.091923	6.145646	2.712798	2.262405
13	H	5.045789	5.743258	8.093592	2.660949	2.199432
14	C	3.490982	3.849446	6.987966	3.344241	2.295320
15	H	3.852099	4.088540	7.457242	4.349013	3.332581
16	C	3.054313	3.170676	6.397820	3.362798	2.322938
17	H	2.969640	2.676219	6.276619	4.375778	3.369715
18	C	3.492784	3.851495	6.280819	2.259501	1.455511
19	S	3.012532	4.042943	5.297544	4.809862	4.264892
20	S	3.011608	4.041450	3.824468	3.805467	3.702561
21	C	3.632061	4.764724	4.525581	5.388744	5.122181
22	C	3.631676	4.764131	3.851291	5.040002	4.934934
23	H	4.504508	5.579441	3.825831	5.834815	5.851286
24	H	4.505134	5.580433	4.991397	6.376528	6.136968
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11	C	0.000000				
12	H	3.332484	0.000000			
13	H	1.080963	4.348914	0.000000		
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15	H	2.262422	4.342136	2.712800	1.080731	0.000000
16	C	2.322882	2.230426	3.362749	1.418786	2.230464
17	H	3.369644	2.691206	4.375707	2.233963	2.691167
18	C	2.295193	1.080737	3.344119	2.284239	3.329629
19	S	3.700232	5.286547	3.802078	3.580973	3.713307
20	S	4.267039	3.712387	4.812854	4.503064	5.287013
21	C	4.934289	5.895825	5.039122	5.046971	5.368058
22	C	5.123012	5.367170	5.390063	5.348344	5.896525
23	H	6.138251	6.154939	6.378507	6.415310	6.980266
24	H	5.850142	6.979593	5.833158	5.954516	6.155807
		16	17	18	19	20
16	C	0.000000				
17	H	1.080191	0.000000			
18	C	1.418743	2.233987	0.000000		
19	S	4.232349	4.768754	4.502602	0.000000	
20	S	4.231568	4.766840	3.581127	3.262180	0.000000
21	C	5.428535	5.949793	5.348029	1.760364	2.751735
22	C	5.428252	5.949112	5.046816	2.751648	1.760405
23	H	6.429937	6.919722	5.954481	3.755433	2.442723
24	H	6.430343	6.920783	6.414926	2.442648	3.755555
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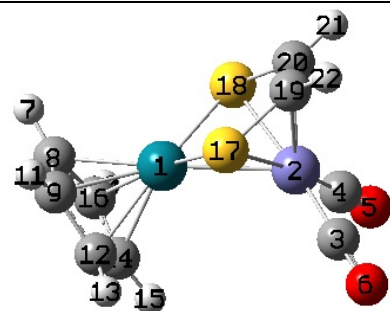
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	1 Rh	0.000000					
	2 Fe	3.759090	0.000000				
	3 C	4.952064	1.780544	0.000000			
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	5 O	4.245948	2.930955	3.821601	1.142779	0.000000	
	6 O	5.867467	2.922883	1.142457	3.813406	4.676661	
	7 C	5.287466	1.747541	2.532368	2.697856	3.668611	
	8 O	6.331638	2.890755	3.464541	3.646332	4.474113	
	9 H	2.917469	6.570074	7.849286	6.530617	6.710149	
	10 C	2.188885	5.938265	7.103856	5.799941	5.947756	
	11 C	2.195041	5.740324	6.597855	5.820461	6.104416	
	12 H	2.912754	5.912388	7.245762	5.154862	4.907476	
	13 H	2.931691	6.237511	6.976812	6.569253	6.972419	
	14 C	2.208545	5.233257	5.889573	5.068265	5.243176	
	15 H	2.933150	5.296861	5.619165	5.232397	5.465566	
	16 C	2.166108	5.069197	5.957488	4.465510	4.381270	
	17 H	2.894399	5.020772	5.785525	4.098610	3.798957	
	18 C	2.182619	5.560568	6.756709	5.016947	4.934968	
	19 S	2.327561	2.342935	2.999382	3.317921	4.204572	
	20 S	2.188001	3.285821	4.969476	3.495842	4.026059	
	21 C	3.309501	1.928283	3.001606	3.466953	4.532460	
22 C	3.185965	2.058486	3.695272	3.066380	3.989972		
23 H	4.165904	2.748092	4.309283	3.729502	4.607532		
24 H	4.201041	2.734761	3.377689	4.427342	5.530083		
		6	7	8	9	10	
6 O	0.000000						
7 C	3.457922	0.000000					
8 O	4.214735	1.143958	0.000000				
9 H	8.752865	7.925300	8.860072	0.000000			
10 C	7.962627	7.413641	8.414439	1.080426	0.000000		
11 C	7.312963	7.364022	8.437760	2.247591	1.439039		
12 H	8.187011	7.187164	8.098073	2.691452	2.231088		
13 H	7.619851	7.844933	8.908808	2.702348	2.249389		
14 C	6.524432	6.937754	8.055600	3.351101	2.309338		
15 H	6.084666	7.042269	8.183310	4.362761	3.354775		
16 C	6.709954	6.662514	7.733152	3.349412	2.302885		
17 H	6.485317	6.555248	7.607007	4.359508	3.345883		
18 C	7.638396	7.004165	7.997617	2.228270	1.413560		
19 S	3.806833	3.972425	5.073807	5.047238	4.365135		
20 S	6.074574	4.209600	5.024434	3.920913	3.688443		
21 C	3.959088	2.915999	3.845604	5.771639	5.343409		
22 C	4.795956	2.700625	3.518366	5.451555	5.124788		
23 H	5.381497	2.695852	3.180255	6.146443	5.955932		
24 H	4.144891	3.340182	4.087110	6.455719	6.109584		
		11	12	13	14	15	
11 C	0.000000						
12 H	3.357430	0.000000					

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	14	C	1.417107	3.358961	2.232232	0.000000			
	15	H	2.230435	4.369005	2.690094	1.080393	0.000000		
	16	C	2.300051	2.249180	3.344734	1.423845	2.234530		
	17	H	3.343910	2.705396	4.355312	2.237498	2.691767		
	18	C	2.310888	1.080091	3.352340	2.316552	3.360489		
	19	S	3.777169	5.133851	4.067471	3.453756	3.450189		
	20	S	4.198725	3.664148	4.795366	4.378894	5.072860		
	21	C	5.071882	5.935021	5.300220	5.018024	5.174115		
	22	C	5.240202	5.287204	5.661777	5.237420	5.631819		
	23	H	6.191075	6.015573	6.576474	6.279807	6.709586		
	24	H	5.734505	6.907437	5.782816	5.792737	5.863756		
			16	17	18	19	20		
	16	C	0.000000						
	17	H	1.080537	0.000000					
	18	C	1.438846	2.249581	0.000000				
	19	S	3.853366	4.202730	4.415814	0.000000			
	20	S	3.973939	4.424113	3.542714	3.096654	0.000000		
	21	C	5.207686	5.547946	5.433552	1.773128	2.797377		
	22	C	5.070990	5.367575	5.029770	2.614941	1.786719		
	23	H	6.057673	6.342864	5.881336	3.649151	2.395036		
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	21	C	0.000000						
	22	C	1.422431	0.000000					
	23	H	2.167206	1.087820	0.000000				
	24	H	1.083839	2.257601	2.628581	0.000000			



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	5	O	3.787401	2.899414	3.371756	1.148047	0.000000			
	6	O	5.493942	2.893983	1.146947	3.358540	4.051094			
	7	H	2.936198	5.356787	7.060613	5.704176	6.210083			
	8	C	2.204296	4.739779	6.465708	4.884010	5.315470			
	9	C	2.204440	4.740370	6.466533	4.884784	5.316268			
	10	H	2.932969	4.615300	6.085395	4.236132	4.381859			
	11	H	2.936304	5.357680	7.061949	5.705381	6.211357			
	12	C	2.194172	4.297585	5.908287	4.006758	4.234718			
	13	H	2.932937	4.616734	6.087662	4.238524	4.384574			
	14	C	2.231955	4.048918	5.582616	3.398074	3.437394			
15	H	2.961911	4.132180	5.436925	3.034796	2.734592				

16	C	2.194184	4.296759	5.907040	4.005410	4.233224
17	S	2.280650	2.274335	3.600703	3.359171	4.320263
18	S	2.280662	2.274384	3.600285	3.359812	4.321174
19	C	3.155204	2.097629	2.953156	3.780489	4.910824
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21	H	4.199893	2.854148	3.154931	4.486970	5.595116
22	H	4.199924	2.854193	3.155382	4.486673	5.594647
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6	O	0.000000				
7	H	8.189360	0.000000			
8	C	7.600909	1.080012	0.000000		
9	C	7.601838	2.230773	1.415945	0.000000	
10	H	7.108501	2.701932	2.245515	3.347263	0.000000
11	H	8.190901	2.690644	2.230719	1.080009	4.359988
12	C	6.992229	3.350455	2.304551	1.435505	3.340237
13	H	7.111136	4.359920	3.347160	2.245424	4.351643
14	C	6.633488	3.358836	2.316601	2.316636	2.234241
15	H	6.390045	4.370119	3.361406	3.361404	2.693121
16	C	6.990801	2.247019	1.435560	2.304651	1.080553
17	S	4.632612	4.878652	4.258937	3.685845	5.179550
18	S	4.632043	3.890306	3.684799	4.258276	3.582721
19	C	3.875776	5.513600	5.136954	4.943152	5.767212
20	C	3.875472	5.165320	4.942771	5.136726	5.220762
21	H	3.827577	6.012542	5.889896	6.180438	6.003878
22	H	3.828185	6.543919	6.180796	5.890431	6.842414
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11	H	0.000000				
12	C	2.247053	0.000000			
13	H	2.701946	1.080556	0.000000		
14	C	3.358901	1.422349	2.234270	0.000000	
15	H	4.370145	2.236702	2.693058	1.080309	0.000000
16	C	3.350526	2.295590	3.340238	1.422324	2.236738
17	S	3.892064	3.506446	3.582045	4.049739	4.509937
18	S	4.877431	4.436291	5.179937	4.050696	4.511646
19	C	5.165848	4.964626	5.220338	5.215394	5.630486
20	C	5.513065	5.274140	5.767119	5.215690	5.631051
21	H	6.543152	6.341576	6.842418	6.204157	6.564172
22	H	6.013364	5.876246	6.003392	6.203718	6.563319
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16	C	0.000000				
17	S	4.436062	0.000000			
18	S	3.506774	3.216320	0.000000		
19	C	5.274198	1.731910	2.727418	0.000000	
20	C	4.964831	2.727360	1.731930	1.380180	0.000000
21	H	5.876470	3.722611	2.427781	2.143264	1.084505
22	H	6.341585	2.427798	3.722664	1.084504	2.143268
		21	22			
21	H	0.000000				
22	H	2.476081	0.000000			



3. -2667.216735 +9.1

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2 Fe	2.603442	0.000000			
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4 C	3.760327	1.743429	2.408551	0.000000	
5 O	4.728935	2.890702	3.293542	1.147435	0.000000
6 O	4.781510	2.891039	1.147270	3.292263	3.955404
7 H	2.957769	5.415983	6.750943	6.279293	7.040670
8 C	2.213389	4.765763	5.943033	5.638947	6.420490
9 C	2.203963	4.716414	5.577581	5.862948	6.763666
10 H	2.910169	4.638125	5.844368	4.774090	5.204471
11 H	2.943618	5.332819	6.130296	6.657332	7.626472
12 C	2.171294	4.225781	4.741818	5.217211	6.059112
13 H	2.908175	4.506358	4.634384	5.565359	6.424542
14 C	2.184274	3.978140	4.648519	4.518677	5.176231
15 H	2.911800	4.036279	4.433013	4.234835	4.725966
16 C	2.174064	4.302588	5.404191	4.787656	5.407935
17 S	2.291599	2.306895	2.966284	4.042105	5.187014
18 S	2.295142	2.302561	4.043311	2.959231	3.802698
19 C	3.251038	2.092264	3.079544	3.608173	4.695496
20 C	3.254889	2.089133	3.573863	3.112433	4.072034
21 H	4.286749	2.893118	4.229815	3.484760	4.246826
22 H	4.281951	2.893097	3.428889	4.274258	5.301029
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6 O	0.000000				
7 H	7.726017	0.000000			
8 C	6.858027	1.080071	0.000000		
9 C	6.357018	2.231865	1.416946	0.000000	
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11 H	6.864601	2.689974	2.230607	1.080363	4.358578
12 C	5.381558	3.353931	2.308685	1.434036	3.344270
13 H	5.069847	4.363449	3.351427	2.246052	4.355135
14 C	5.363772	3.361140	2.318321	2.314995	2.234912
15 H	5.017535	4.371496	3.362140	3.359524	2.692565
16 C	6.291926	2.246250	1.433734	2.302411	1.080479
17 S	3.811539	4.820625	4.230717	3.666529	5.182748
18 S	5.189549	3.994327	3.751086	4.298812	3.582564
19 C	4.029642	5.637974	5.246875	5.056106	5.807113
20 C	4.652318	5.351820	5.088238	5.272814	5.254456
21 H	5.240744	6.184446	6.017528	6.306409	6.008506
22 H	4.171073	6.641720	6.266926	5.970890	6.886698
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11 H	0.000000				
12 C	2.244332	0.000000			
13 H	2.701410	1.080235	0.000000		
14 C	3.357704	1.425772	2.237264	0.000000	
15 H	4.368864	2.239830	2.696744	1.079667	0.000000
16 C	3.348102	2.300416	3.344762	1.425076	2.238813
17 S	3.843039	3.552943	3.653680	4.097298	4.590287
18 S	4.931052	4.429406	5.155121	4.009457	4.438722

	19 C	5.295246	5.041218	5.284865	5.250114	5.636252
	20 C	5.679549	5.338498	5.808464	5.222189	5.583889
	21 H	6.707303	6.396272	6.880055	6.192516	6.496447
	22 H	6.100463	5.933201	6.047920	6.235576	6.577930
		16	17	18	19	20
	16 C	0.000000				
	17 S	4.446470	0.000000			
	18 S	3.517620	3.143069	0.000000		
	19 C	5.337591	1.748760	2.715825	0.000000	
	20 C	5.027813	2.718608	1.750119	1.375328	0.000000
	21 H	5.915987	3.736887	2.441054	2.163106	1.083352
	22 H	6.399426	2.437805	3.734508	1.083423	2.161862
		21	22			
	21 H	0.000000				
	22 H	2.546754	0.000000			

Table S8. Harmonic $\nu(\text{CO})$ vibrational frequencies and infrared intensities (in parantheses, in km/mol) for the $\text{CpH}_2\text{C}_2\text{S}_2\text{M}_1\text{M}_2(\text{CO})_n$ systems.

Co-Cr	
2-1-co-cr	1885(629) 1935(1414)
3-1-co-cr	1908(626) 1934(692) 1977(1542)
4-1-co-cr	1872(511) 1939(882) 1970(551) 2018(1199)
4-2-co-cr	1816(363) 1951(558) 1957(825) 2012(1232)
4-3-co-cr	1931(1247) 1933(883) 1947(279) 2012(1081)
5-1-co-cr	1887(498) 1943(1004) 1971(767) 1988(511) 2039(943)
5-2-co-cr	1948(1345) 1957(797) 1963(1322) 1983(37) 2052(417)
5-3-co-cr	1934(926) 1951(1068) 1963(324) 2011(1219) 2046(663)
Co-Fe	
2-1-co-fe	1941(538) 1987(1284)
2-2-co-fe	1946(602) 1996(1220)
3-1-co-fe	1973(573) 1983(672) 2037(821)
3-2-co-fe	1825(405) 1977(592) 2026(1065)
3-3-co-fe	1968(710) 1971(709) 2028(1000)
4-1-co-fe	1975(667) 1988(713) 2003(652) 2055(663)
4-2-co-fe	1761(275) 1981(642) 1988(708) 2041(1022)
4-3-co-fe	1780(402) 1996(583) 1999(620) 2054(935)
4-4-co-fe	1984(933) 1989(1060) 1998(306) 2061(620)
4-5-co-fe	1761(275) 1981(642) 1988(709) 2042(1022)
Ir-Cr	
2-1-ir-cr	1880(634) 1927(1448)
3-1-ir-cr	1903(645) 1926(685) 1970(1615)
4-1-ir-cr	1859(472) 1914(740) 1957(642) 2004(1264)
4-2-ir-cr	1847(496) 1932(905) 1963(537) 2013(1202)
4-3-ir-cr	1926(939) 1927(1283) 1941(355) 2011(886)
5-1-ir-cr	1881(533) 1940(1031) 1968(741) 1982(543) 2035(983)
5-2-ir-cr	1950(1430) 1954(810) 1959(1334) 1982(5) 2052(375)
5-3-ir-cr	1929(914) 1941(1122) 1955(333) 2006(1053) 2040(737)
Ir-Fe	
2-1-ir-fe	1936(537) 1982(1314)
2-2-ir-fe	1939(590) 1988(1205)
3-1-ir-fe	1971(574) 1980(679) 2035(861)
3-2-ir-fe	1807(417) 1974(595) 2022(1083)
3-3-ir-fe	1966(682) 1967(776) 2026(935)
4-1-ir-fe	1974(676) 1981(685) 1999(668)
4-2-ir-fe	1980(928) 1988(1019) 1996(425) 2060(562)
4-3-ir-fe	1738(300) 1977(651) 1984(719) 2039(1051)
4-4-ir-fe	1755(416) 1989(590) 1994(624) 2050(974)
4-5-ir-fe	1817(378) 1977(489) 1998(878) 2054(658)

Rh-Cr	
2-1-rh-cr	1884(614) 1932(1443)
2-2-rh-cr	1899(742) 1936(1525)
3-1-rh-cr	1906(620) 1931(668) 1973(1644)
4-1-rh-cr	1868(510) 1935(893) 1967(533) 2016(1247)
4-2-rh-cr	1817(375) 1952(538) 1956(828) 2013(1230)
4-3-rh-cr	1928(1224) 1930(940) 1943(329) 2010(1078)
5-1-rh-cr	1894(545) 1943(1006) 1969(766) 1985(518) 2037(981)
5-2-rh-cr	1950(1406) 1954(802) 1960(1329) 1982(9) 2052(397)
5-3-rh-cr	1932(959) 1943(1111) 1954(261) 2005(1334) 2043(655)
5-4-rh-cr	1836(350) 1965(725) 1969(1022) 1979(523) 2036(964)
Rh-Fe	
2-1-rh-fe	1940(526) 1985(1316)
2-2-rh-fe	1943(584) 1992(1233)
3-1-rh-fe	1973(571) 1982(660) 2036(877)
3-2-rh-fe	1828(411) 1978(587) 2026(1081)
3-3-rh-fe	1968(706) 1969(693) 2026(1075)
4-1-rh-fe	1974(646) 1984(657) 2001(689) 2053(708)
4-2-rh-fe	1762(291) 1981(634) 1988(702) 2042(1068)
4-3-rh-fe	1777(416) 1995(560) 1998(615) 2054(985)
4-4-rh-fe	1980(936) 1988(1020) 1995(400) 2059(616)
4-5-rh-fe	1844(367) 1981(492) 2000(863) 2056(685)

Table S9. CO dissociation energies for the CpH₂C₂S₂M₁M₂(CO)_n systems.

Reaction	ΔE, kcal/mol	ΔG, kcal/mol
CoCr5-1 → CoCr4-1 + CO	18.3	7.3
CoCr4-1 → CoCr3-1 + CO	9.8	-0.2
CoCr3-1 → CoCr2-1 + CO	48.6	38.8
CoFe4-1 → CoFe3-1 + CO	8.6	-1.8
CoFe3-1 → CoFe2-1 + CO	28.3	18.6
IrCr5-1 → IrCr4-1 + CO	22.6	11.8
IrCr4-1 → IrCr3-1 + CO	9.6	0
IrCr3-1 → IrCr2-1 + CO	47.7	37.2
IrFe4-1 → IrFe3-1 + CO	16.2	5.6
IrFe3-1 → IrFe2-1 + CO	24.3	15.1
RhCr5-1 → RhCr4-1 + CO	22.6	11.5
RhCr4-1 → RhCr3-1 + CO	8.9	-0.5
RhCr3-1 → RhCr2-1 + CO	46.1	35.7
RhFe4-1 → RhFe3-1 + CO	13.9	3.3
RhFe3-1 → RhFe2-1 + CO	24.5	15.3

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