

Supporting Information

Controlling the Spin-Crossover behavior of the [Cr(indenyl)₂] family via ligand functionalization

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Table S1: Calculated average Cr-C bond length in both spin states (low-spin S = 1 and high-spin S = 2) for both ligand configurations. Experimental data (when available) in parenthesis. All bond lengths in Angstroms.

System	Eclipsed		Staggered	
	high-spin	low-spin	high-spin	low-spin
[Cr(Indenyl) ₂]	2.325	2.162	2.313	2.168
[Cr(¹ -MeIndenyl) ₂]	2.313 (2.262)	2.165 (2.179)	2.304	2.165
[Cr(² -MeIndenyl) ₂]	2.329	2.164	2.305 (2.308)	2.169
[Cr(⁶ -MeIndenyl) ₂]	2.318	2.162	2.314	2.167
[Cr(⁷ -MeIndenyl) ₂]	2.318	2.160	2.311	2.165
[Cr(^{1,3} -MeIndenyl) ₂]	2.304	2.164	2.296 (2.317) ^a	2.164
[Cr(^{4,7} -MeIndenyl) ₂]	2.318	2.161 (2.174)	2.309	2.163
[Cr(^{5,6} -MeIndenyl) ₂]	2.321	2.161	2.298	2.167
[Cr(^{1,2,3} -MeIndenyl) ₂]	2.296	2.164	2.286 (2.239) ^b	2.166 (2.239) ^b
[Cr(^{2,4,7} -MeIndenyl) ₂]	2.311	2.161 (2.168, 2.187) ^c	2.299 (2.227)	2.163 (2.172)
[Cr(^{2,4,5,6,7} -MeIndenyl) ₂]	2.312	2.159	2.298	2.161 (2.168)
[Cr(^{1,2,3,4,5,6,7} -MeIndenyl) ₂]	2.300	2.160	2.286	2.161 (2.182)

^aExperimental data of [Cr(^{1,3}-iPrIndenyl)₂].

^bThe experimental data is in between the high spin and the low spin states, since its experimental T_{1/2} is 150 K and the crystal was obtained at 173 K.

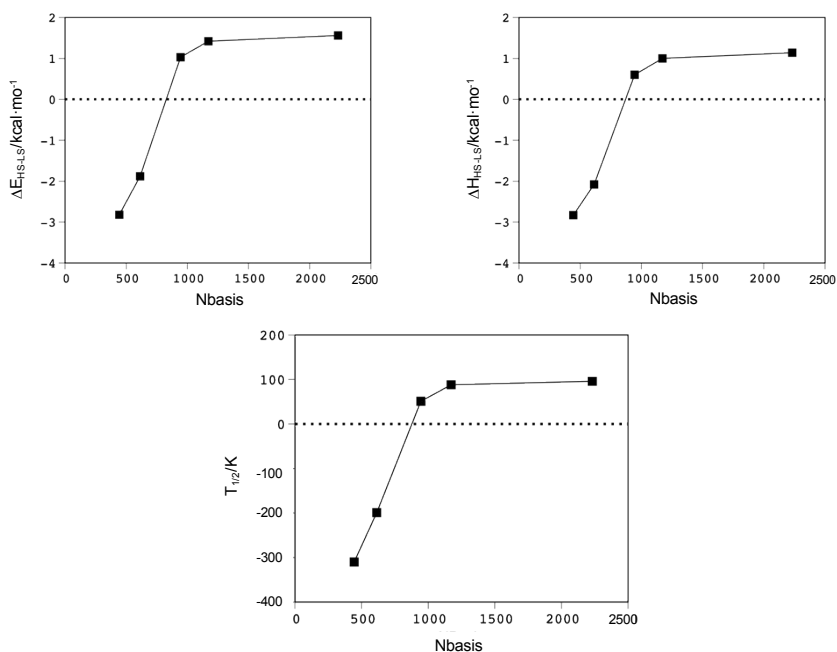
^cFirst crystal was obtained at 173 K and the second crystal at 293 K. Both are low spin complexes since the experimental T_{1/2} is above 350 K.

S2. DFT and Basis set benchmarking for the $\text{Cr}^{(1,2,3\text{-MeIndenyl)}_2}$ (staggered configuration) system, and basis set calibration

<i>DFT</i>	<i>E(HS)/a.u.</i>	<i>E(LS)/a.u.</i>	<i>ΔE/kcal·mol</i>
OLYP	-1974.8787	-1974.8679	-6.7373001
OPBE	-1974.8584	-1974.8491	-5.8746753
TPSSh	-1975.1847	-1975.1806	-2.5745963
B3LYP	-1975.0967	-1975.0816	-9.4892871
B3LYP*	-1966.0464	-1966.0382	-5.1609522
M06L	-1974.9494	-1974.9436	-3.6207677
TPSSTPSS	-1975.3002	-1975.3038	2.25250825
TPSSh-GD3BJ	-1975.2755	-1975.2772	1.03210259
TPSSTPSS_GD3BJ	-1975.3911	-1975.4001	5.61891496

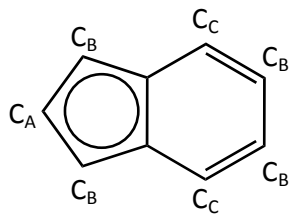
	Number of Basis functions	$\Delta E/\text{kcal}\cdot\text{mol}^{-1}$	$\Delta H/\text{kcal}\cdot\text{mol}^{-1}$	$\Delta S/\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$T_{1/2}/\text{K}$
Def2TZV	444	-2.82	-2.83	9.138	-310
Def2QZV	614	-1.88	-2.08	10.482	-199
Def2TZVP	945	1.03	0.60	11.757	51
Def2TZVPP	1172	1.42	1.00	11.336	88
Def2QZVP	2232	1.56	1.14	11.833	96

Convergence of ΔE , ΔH and $T_{1/2}$ with the size of the basis set



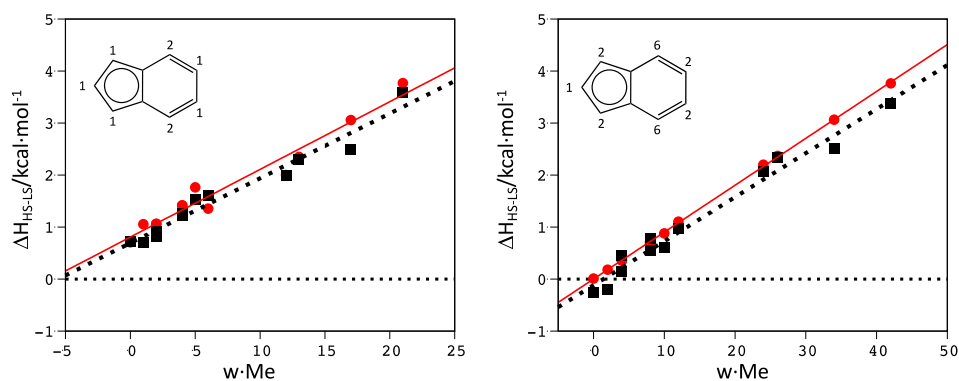
S3. Coefficients for the multilinear fitting model. Current model uses 3 types of carbon atoms (see below) and has the following functional form:

$$\Delta E_{\text{HS-LS}} = \omega_A \cdot C_A + \omega_B \cdot C_B + \omega_C \cdot C_C + b$$



	Eclipsed	Staggered
ω_A	0.348158982	0.169994076
ω_B	0.354777977	0.348849344
ω_C	0.647119268	1.092757488
b	0.706617529	0.011610141
R^2	0.976570954	0.986540932

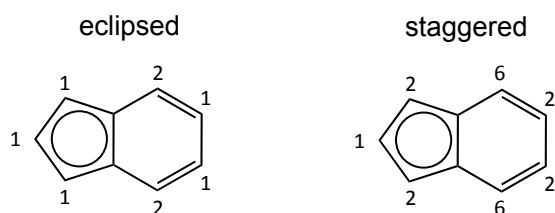
This model, which is based on the $\Delta E_{\text{HS-LS}}$, can also be used to predict the $\Delta H_{\text{HS-LS}}$ in the $[\text{Cr}^{(n-\text{Me})}\text{Indenyl}]_2$ family without further modification, as shown below.



$\Delta H_{\text{HS-LS}}$ vs the $w \cdot \text{Me}$ coefficient. Left, eclipsed ($R^2 = 0.95$), right, staggered ($R^2 = 0.97$)

S4. Computed ($\Delta E(\text{DFT})$) and calculated with our model ($\Delta E(\text{M})$) spin-state energy gaps for the different members of the $[\text{Cr}(\text{n-MeIndenyl})_2]$ ($n=0-7$) in both eclipsed and staggered configurations. All energies in kcal/mol

To compute the $w \cdot \text{Me}$ parameter, one must multiply the number of methyl groups by the weight the position has (see Scheme below). For instance, the $[\text{Cr}(\text{1,4,7-MeIndenyl})_2]$, which has 1 methyl group in the C2 position, and two methyl groups in the C4 and C7 position, will have a $w \cdot \text{Me} = 1 \cdot 1 + 0 \cdot 1 + 2 \cdot 2 = 5$, by two indenyl ligands will $w \cdot \text{Me} = 10$. For the staggered configuration, the same compound will give $w \cdot \text{Me} = 1 \cdot 1 + 2 \cdot 0 + 2 \cdot 6 = 13$, by two indenyl ligands will $w \cdot \text{Me} = 26$



				Eclipsed			Staggered		
n	# C1	# C2	# C3	w·Me	$\Delta E(\text{DFT})$	$\Delta E(\text{M})$	w·Me	$\Delta E(\text{DFT})$	$\Delta E(\text{M})$
-	0	0	0	0	0.728	0.707	0	-0.148	0.011
1	0	1	0	2	0.998	1.062	4	0.288	0.360
2	1	0	0	2	1.041	1.055	2	0.020	0.182
6	0	1	0	2	0.821	1.062	4	0.556	0.360
7	0	0	1	4	0.824	1.354	12	1.051	1.104
1,3	0	2	0	4	1.437	1.416	8	0.790	0.709
4,7	0	0	2	8	2.044	2.001	24	2.188	2.197
5,6	0	2	0	4	1.334	1.416	8	0.903	0.709
1,2,3	1	2	0	6	1.821	1.764	10	1.032	0.879
1,4,7	1	0	2	10	2.492	2.349	26	2.595	2.367
1,4,7,5,6	1	2	2	14	2.732	3.058	34	2.825	3.065
1,2,3,4,5,6,7	1	4	2	18	3.908	3.768	42	3.784	3.763

S5. Cartesian atomic coordinates for the [Cr(^RIndenyl)₂] optimized geometries

Low-spin eclipsed [Cr(Indenyl)₂] (S = 1), E = -1739.24184575 a.u., $\nu_1 = 22.7829 \text{ cm}^{-1}$

Cr	0.544756290000	0.556563380000	0.401462770000
C	-0.427714180000	0.246088380000	2.274262660000
C	0.956446090000	0.559848420000	2.469247280000
C	1.737280200000	-0.464994400000	1.842470240000
C	0.840373000000	-1.446695180000	1.307314450000
C	1.049378520000	-2.607406060000	0.520373520000
H	2.058407070000	-2.941223420000	0.306582880000
C	-0.035454090000	-3.297245100000	0.042339490000
H	0.115892120000	-4.186747310000	-0.557970260000
C	-1.359450520000	-2.862936180000	0.307976940000
H	-2.190022510000	-3.430651490000	-0.094995290000
C	-1.603594770000	-1.737040110000	1.052278180000
H	-2.618270140000	-1.407143070000	1.244465070000
C	-0.509855830000	-1.003250280000	1.577356390000
C	-0.358345970000	2.201453940000	-0.609202190000
C	1.019625890000	2.476359570000	-0.328934990000
C	1.816074330000	1.508152700000	-1.022226760000
C	0.938592610000	0.666618050000	-1.780666280000
C	1.164747090000	-0.490665070000	-2.568117500000
H	2.178162280000	-0.824583680000	-2.759999300000
C	0.090877990000	-1.171773560000	-3.081973250000
H	0.255380370000	-2.055990990000	-3.686652350000
C	-1.239123440000	-0.748900540000	-2.828284450000
H	-2.061013590000	-1.319636310000	-3.244521550000
C	-1.500148540000	0.357051640000	-2.060166120000
H	-2.519631430000	0.669424560000	-1.864306020000
C	-0.417749480000	1.098436390000	-1.522679510000
H	-1.265814640000	0.834781730000	2.615571560000
H	-1.205763650000	2.746821420000	-0.222027750000
H	1.342991900000	1.400131960000	3.024247880000
H	1.393592250000	3.293048970000	0.268296190000
H	2.815278220000	-0.506520830000	1.802909300000
H	2.893138810000	1.438951420000	-0.998992490000

Low-spin staggered [Cr(Indenyl)₂] (S = 1), E = -1739.23911700 a.u., $\nu_1 = 23.4908 \text{ cm}^{-1}$

Cr	-0.007781180000	-0.020438540000	-0.015649860000
C	-0.750174080000	-1.187803310000	-1.643431900000
C	-0.047634570000	-0.037938010000	-2.125311730000
C	-0.729604610000	1.132172290000	-1.663085370000
C	-1.897358160000	0.710922120000	-0.944228570000
C	-2.897965600000	1.424011880000	-0.236412620000
H	-2.894256860000	2.508225300000	-0.240653880000

C	-3.878546750000	0.726835950000	0.423834840000
H	-4.656384170000	1.264912170000	0.953278660000
C	-3.891146080000	-0.691283970000	0.435891110000
H	-4.678335760000	-1.206387320000	0.974280140000
C	-2.923207330000	-1.416882450000	-0.212273290000
H	-2.938741750000	-2.500906550000	-0.198057070000
C	-1.910188930000	-0.733813890000	-0.931960240000
C	0.733815760000	1.146740430000	1.612633290000
C	0.031455000000	-0.003375420000	2.094096210000
C	0.713751800000	-1.173235410000	1.631827380000
C	1.881679840000	-0.751597940000	0.913419480000
C	2.882777030000	-1.464304950000	0.205930860000
H	2.879299620000	-2.548520210000	0.209892630000
C	3.863572460000	-0.766747960000	-0.453604570000
H	4.641820140000	-1.304511320000	-0.982759280000
C	3.875869400000	0.651375730000	-0.465288690000
H	4.663252870000	1.166767730000	-1.003121790000
C	2.907422400000	1.376616480000	0.182521350000
H	2.922756210000	2.460646430000	0.168641340000
C	1.894210210000	0.693131840000	0.901540170000
H	0.418998610000	-2.195221110000	1.816473250000
H	-0.860247830000	0.009319490000	2.702152110000
H	0.843415150000	-0.051035940000	-2.734308140000
H	-0.435027150000	2.154048670000	-1.848592020000
H	-0.473504860000	-2.217721630000	-1.811215780000
H	0.457380210000	2.176593340000	1.781174100000

High-spin eclipsed [Cr(Indenyl)₂] (S = 2), E = -1739.24068506 a.u., $\nu_1 = 21.6979 \text{ cm}^{-1}$

Cr	0.662318057859	0.808315881673	0.576088536442
C	-0.209647367053	0.147870860285	2.559362933863
C	1.197341164743	0.222386527895	2.678762643654
C	1.782216372876	-0.716444674306	1.791065400658
C	0.722408905219	-1.518889475627	1.232494414683
C	0.715979206924	-2.608595119905	0.344823319424
H	1.647543054957	-3.012105405873	-0.034622688960
C	-0.495188976728	-3.157459629967	-0.028776360291
H	-0.512685863313	-4.003281439579	-0.705974883158
C	-1.712295973379	-2.626857112356	0.438830132921
H	-2.643346834192	-3.081672854006	0.120312312430
C	-1.740983298239	-1.538753124518	1.289661768851
H	-2.683097422393	-1.130195409770	1.637600183599
C	-0.523014733325	-0.972525395931	1.705933947356
C	-0.547518422051	2.137043508008	-0.776143400065
C	0.735297296957	2.717983817657	-0.607581734558
C	1.706625409977	1.843495757351	-1.147197740418
C	1.012978837925	0.770432692004	-1.817396017263
C	1.463971116836	-0.334550175122	-2.561084521942
H	2.524214365804	-0.486482426927	-2.729502348397
C	0.531950181337	-1.214099645523	-3.077206683147

H	0.864689994703	-2.063155518954	-3.663348008751
C	-0.846112105871	-1.033211648592	-2.853985483507
H	-1.546673186119	-1.751499466234	-3.263380801358
C	-1.317506162450	0.029996600579	-2.108871313111
H	-2.378953374877	0.150966401860	-1.926362550081
C	-0.397047517884	0.958845811805	-1.593638459649
H	-0.925316097811	0.745358451102	3.105044315828
H	-1.485138616497	2.571693887463	-0.461268889083
H	1.740020133703	0.930163995215	3.289622968804
H	0.941611827088	3.641815197530	-0.085516195356
H	2.840717380440	-0.887459196166	1.658694678562
H	2.773686644834	2.011197328928	-1.160998477981

High-spin staggered [Cr(Indenyl)₂] (S = 2), E = -1739.23935260 a.u., $\nu_1 = 13.9830 \text{ cm}^{-1}$

Cr	-0.007287020000	-0.020371830000	-0.016263810000
C	-0.931855490000	-1.180102800000	-1.713066440000
C	-0.286065070000	-0.038800170000	-2.246976920000
C	-0.912731690000	1.122760170000	-1.734429160000
C	-2.080696820000	0.708229530000	-0.995756590000
C	-3.080582730000	1.423584580000	-0.312270740000
H	-3.076198200000	2.507836530000	-0.313365630000
C	-4.070455830000	0.721069220000	0.349903120000
H	-4.856167160000	1.260843430000	0.865949140000
C	-4.082167720000	-0.687420340000	0.362964280000
H	-4.876676290000	-1.204425150000	0.888767850000
C	-3.104213800000	-1.418471530000	-0.285888340000
H	-3.117908350000	-2.502478420000	-0.266867870000
C	-2.092661660000	-0.732647640000	-0.982368120000
C	0.915488490000	1.139960970000	1.681076510000
C	0.269152930000	-0.001085520000	2.214870250000
C	0.896205760000	-1.162885030000	1.703337980000
C	2.064741180000	-0.748734870000	0.965375920000
C	3.065202730000	-1.464397460000	0.283009750000
H	3.060792850000	-2.548646550000	0.284502720000
C	4.055693960000	-0.762177960000	-0.378523060000
H	4.841846020000	-1.302198810000	-0.893642800000
C	4.067501040000	0.646324150000	-0.392113230000
H	4.862503840000	1.163052060000	-0.917437160000
C	3.089023450000	1.377662360000	0.255581680000
H	3.102766460000	2.461664030000	0.236190130000
C	2.076815780000	0.692158260000	0.951469810000
H	0.616454910000	-2.182738940000	1.923686080000
H	-0.614392760000	0.012330520000	2.837422900000
H	0.597005510000	-0.051955110000	-2.870216300000
H	-0.633216120000	2.142712500000	-1.954623370000
H	-0.669435840000	-2.208440350000	-1.914489740000
H	0.652888680000	2.168384130000	1.881823200000

Low-spin eclipsed $[\text{Cr}(\text{}^1\text{-MeIndenyl})_2]$ ($S = 1$), $E = -1817.91976425$ a.u., $\nu_1 = 16.9979$ cm^{-1}

Cr	0.552968333657	0.555891931210	0.396651948944
C	-0.452239517781	0.268293601876	2.273533676969
C	0.938021724503	0.563563978633	2.470167995544
C	1.719343546629	-0.465106139781	1.849195770440
C	0.818004209805	-1.440625193026	1.310504830217
C	1.018809906572	-2.603375856915	0.525450584726
H	2.025688656021	-2.945583237536	0.314397340401
C	-0.070267601101	-3.285184728263	0.044658313269
H	0.075290617118	-4.176422480646	-0.554423503232
C	-1.390904916151	-2.839427898174	0.307471341162
H	-2.225618458191	-3.401677090468	-0.094815241949
C	-1.627342989943	-1.711150240460	1.051091475467
H	-2.640992908809	-1.379293572463	1.245099693144
C	-0.528659319292	-0.983679837987	1.576222676651
C	-1.609531319443	1.053570248875	2.804622865549
H	-1.929245537040	0.668461685693	3.779387966961
H	-2.470205944302	1.005167098336	2.133539242078
H	-1.344089298040	2.104635542496	2.933614331719
C	-0.329458313669	2.207316056980	-0.651333995253
C	1.050892406771	2.462701072381	-0.352656982866
C	1.854304489862	1.475426973758	-1.011084176701
C	0.982819136148	0.632262733156	-1.774079009478
C	1.207877328308	-0.540438602795	-2.537670232555
H	2.220233182696	-0.891550817124	-2.703114323955
C	0.135225370031	-1.215581848247	-3.062722119531
H	0.299389623049	-2.111756428128	-3.649555897055
C	-1.193010440879	-0.769202492072	-2.843327562110
H	-2.014701006893	-1.333625214772	-3.268646496104
C	-1.453365463130	0.353825435204	-2.099674494978
H	-2.472741997092	0.685219716170	-1.937562299011
C	-0.371667038419	1.087831744420	-1.549360742595
C	-1.499364026395	3.030523260532	-0.213483609410
H	-1.740552185054	3.796067112986	-0.959475535256
H	-1.289767123490	3.539563969402	0.729218340034
H	-2.392092077334	2.416888180710	-0.071764876880
H	1.420245882566	3.286957203763	0.238643086454
H	1.325410340650	1.402579053997	3.028239627664
H	2.929920178359	1.396381051359	-0.963693628552
H	2.797339859704	-0.513491913080	1.817787520077

Low-spin staggered $[\text{Cr}(\text{}^1\text{-MeIndenyl})_2]$ ($S = 1$), $E = -1817.91756366$ a.u., $\nu_1 = 18.9450$ cm^{-1}

Cr	0.000030295496	0.000061258586	0.000056014413
C	-0.773873820554	-1.179345145104	-1.614144312163
C	-0.087203520545	-0.022037220386	-2.107174765524
C	-0.752068216708	1.151990865794	-1.627857833154

C	-1.901302694189	0.733040550444	-0.880930726207
C	-2.878071325195	1.444756776952	-0.139466144125
H	-2.872646783650	2.529090521162	-0.140597233758
C	-3.840327040046	0.747091031170	0.547770702666
H	-4.600395162372	1.284511172548	1.103062581244
C	-3.856182097789	-0.670734292384	0.551956703814
H	-4.629148414124	-1.187142470177	1.109462756920
C	-2.910713837144	-1.395580948000	-0.130477774574
H	-2.935307725446	-2.479493970585	-0.124294577151
C	-1.915281419295	-0.712787851429	-0.875244674555
C	-0.416978792843	-2.605888384982	-1.893824511825
H	-0.932494156466	-2.975413154468	-2.787441209666
H	-0.692217447909	-3.256499449098	-1.060428726910
H	0.657224321665	-2.709886947092	-2.060576105308
C	0.773900097704	1.179466969288	1.614280116797
C	0.087260942690	0.022131222104	2.107287027051
C	0.752158473305	-1.151870018610	1.627948578592
C	1.901382818176	-0.732872257787	0.881029887808
C	2.878173685898	-1.444546589814	0.139554679794
H	2.872779272979	-2.528880545266	0.140664692238
C	3.840411653424	-0.746840641261	-0.547666150093
H	4.600496386920	-1.284228214180	-1.102966716421
C	3.856225407032	0.670985302557	-0.551824878829
H	4.629178332854	1.187426380878	-1.109319114109
C	2.910735412426	1.395792309979	0.130621377510
H	2.935299150027	2.479706122053	0.124459295804
C	1.915320863943	0.712956740573	0.875373688395
C	0.416957069144	2.605994497835	1.893978329791
H	0.932446333027	2.975520124342	2.787609645507
H	0.692189868871	3.256627471572	1.060597729245
H	-0.657252118249	2.709957020847	2.060713287730
H	-0.791234022055	0.038247942282	2.735536957973
H	0.791289372619	-0.038189546749	-2.735426645941
H	0.456011940333	-2.172814096805	1.817055530918
H	-0.455889453956	2.172922883212	-1.816979553896

High-spin eclipsed $[\text{Cr}(\text{}^1\text{-MeIndenyl})_2]$ ($S = 2$), $E = -1817.91817442$ a.u., $\nu_1 = 19.0153$ cm^{-1}

Cr	0.717890287375	0.785862196206	0.545355351719
C	-0.256444266150	0.234861003508	2.526878849327
C	1.150969114067	0.210333654253	2.674063833379
C	1.701207500121	-0.775792876392	1.812531066059
C	0.606834406391	-1.509185667634	1.230810503158
C	0.545100448732	-2.600609127414	0.347348184104
H	1.454732457164	-3.072909211718	-0.004933818798
C	-0.692558727769	-3.062464972106	-0.058158749550
H	-0.751916702124	-3.908301230178	-0.732951323428
C	-1.881008488886	-2.443303223724	0.372057549134
H	-2.833065451009	-2.832879515755	0.029827993227

C	-1.854499673354	-1.351240307709	1.218967615254
H	-2.775028194157	-0.877916521471	1.541992157755
C	-0.609723713816	-0.870167449512	1.664070846491
C	-1.225362960261	1.104646901168	3.266856346433
H	-1.697879062568	0.553639290247	4.087742580727
H	-2.026621668970	1.462297392672	2.614692824072
H	-0.724159730776	1.975822187767	3.693088760139
C	-0.500868580087	2.106752360724	-0.819782183954
C	0.769897208149	2.705431341740	-0.607455603376
C	1.781904132788	1.862209671952	-1.126837560090
C	1.133764281004	0.779473331120	-1.822521622470
C	1.627350606373	-0.314140627343	-2.557594480293
H	2.694875902834	-0.447263144764	-2.692734435254
C	0.727287000215	-1.205264765257	-3.110156874052
H	1.094168343938	-2.044060106624	-3.690895281947
C	-0.660608624526	-1.048293245863	-2.935317662356
H	-1.334591039712	-1.774353596667	-3.374519049460
C	-1.174140295009	0.001523707993	-2.198335083514
H	-2.243235697292	0.103694417640	-2.053755462290
C	-0.286411442447	0.938843735139	-1.642689779320
C	-1.836060976748	2.673215857453	-0.445391119943
H	-2.303252567027	3.173241230114	-1.300937805286
H	-1.741508895604	3.405120087469	0.359199389080
H	-2.522263589171	1.889921424636	-0.112712937626
H	0.936282139012	3.629209472340	-0.069406502064
H	1.721272333598	0.888190980157	3.295125472117
H	2.844129361929	2.056862323077	-1.106250496045
H	2.749512133777	-1.017052917246	1.713782408942

High-spin staggered $[\text{Cr}(\text{}^1\text{-MeIndenyl})_2]$ ($S = 2$), $E = -1817.91710399$ a.u., $\nu_1 = 11.7386$ cm^{-1}

Cr	-0.054081336824	0.048795321883	0.086502430862
C	-0.840111703230	-1.143702298809	-1.670227636474
C	-0.231313092520	0.038701118572	-2.157756753034
C	-0.919504566639	1.170298504439	-1.650837944341
C	-2.088249004112	0.698571650145	-0.954610471831
C	-3.136171502750	1.357314640933	-0.284848020024
H	-3.180611491226	2.440681881066	-0.270109170520
C	-4.110733543474	0.601039964948	0.339744194689
H	-4.932651045752	1.097356321825	0.842905996302
C	-4.061485115865	-0.807268312299	0.330011768231
H	-4.846838159302	-1.366751069043	0.825198593024
C	-3.035910752832	-1.484014555518	-0.303476794462
H	-3.006132237382	-2.567838387075	-0.303933620225
C	-2.034528857171	-0.743021312028	-0.960092034471
C	-0.426376398282	-2.551564929680	-1.970023217039
H	-1.008133373415	-2.963083387116	-2.802233900105
H	-0.581811325449	-3.205920300835	-1.108676500698
H	0.629962319098	-2.597299975412	-2.241510158271

C	1.000209359622	1.244624383693	1.693826085775
C	0.355979814424	0.128457314571	2.285540834456
C	0.912242284321	-1.068931206841	1.768103314013
C	2.043648167550	-0.709483309565	0.951148518588
C	2.970117813639	-1.469020502562	0.214249364247
H	2.931168987319	-2.552442288014	0.236217489603
C	3.932970385520	-0.810496724970	-0.530115834933
H	4.662718309898	-1.385379499341	-1.088900370842
C	3.990345298876	0.595594153289	-0.570557591073
H	4.763267906800	1.076746728885	-1.158892255653
C	3.083578379542	1.369827995923	0.132315943031
H	3.133150851493	2.452197642441	0.091806250701
C	2.098982793621	0.730052959564	0.905538011765
C	0.731569344404	2.689987357526	1.981903351023
H	1.439538732128	3.079534258403	2.721903837731
H	0.830061301514	3.303324520039	1.082822694935
H	-0.276783132132	2.829270667460	2.376142908344
H	-0.485264917047	0.187020034947	2.963199716492
H	0.676297158128	0.069547206709	-2.745455794504
H	0.613676866600	-2.072939490386	2.032181458047
H	-0.671911519096	2.203439922235	-1.846625693359

Low-spin eclipsed $[\text{Cr}(\text{}^2\text{-MeIndenyl})_2]$ ($S = 1$), $E = -1817.91961784$ a.u., $\nu_1 = 16.5731$ cm^{-1}

Cr	0.553930622100	0.556571531331	0.396814569214
C	-0.446555986572	0.270581257906	2.257399351068
C	0.937973651853	0.577724613895	2.480291446924
C	1.706086273530	-0.468354484227	1.866058723375
C	0.808846676462	-1.443296937366	1.319889508070
C	1.015235854739	-2.609049158901	0.541177425338
H	2.023052027983	-2.956872502953	0.344332260845
C	-0.071241251092	-3.287811375405	0.049117263212
H	0.078271402621	-4.182049461356	-0.544611342181
C	-1.392666856691	-2.834698052566	0.290798610127
H	-2.224378127823	-3.392815159582	-0.123130336613
C	-1.633417699717	-1.700621448200	1.025110089206
H	-2.646614707767	-1.355608495021	1.197948137442
C	-0.539056811848	-0.980591166300	1.565581297740
C	-0.308172213682	2.202151223807	-0.644843589772
C	1.067468064472	2.476161128918	-0.337875591273
C	1.855616831520	1.484400107522	-1.013234537660
C	0.985543092858	0.641244133556	-1.777905841347
C	1.211986911581	-0.527943668722	-2.546097588496
H	2.224653750992	-0.875425306727	-2.717071033733
C	0.138910120905	-1.204216577520	-3.069903607489
H	0.303951129133	-2.097531007706	-3.660944924337
C	-1.189659619952	-0.765019588712	-2.842278744871
H	-2.011168851905	-1.332439767048	-3.263804588972
C	-1.450852357984	0.352971156836	-2.090490508862

H	-2.470125487798	0.677149954971	-1.913241367248
C	-0.369633449337	1.090069667424	-1.546810684209
C	1.472121800261	1.676783271904	3.342544350652
H	1.549334082446	1.347870307756	4.385009740872
H	2.467609080545	1.986317477253	3.018133892914
H	0.819501878182	2.551695782328	3.318514784174
C	1.588596037575	3.671966110254	0.393661162961
H	2.544330953947	3.456040861107	0.875187108857
H	1.745074664327	4.509304708950	-0.295732135256
H	0.887544149430	4.002426646275	1.162687660224
H	-1.154799168961	2.763582572725	-0.276645511672
H	2.932437849899	1.406042230721	-0.969811539760
H	2.785074047927	-0.522566369328	1.846223068017
H	-1.281177604157	0.874372592199	2.583608112520

Low-spin staggered [Cr(²-MeIndenyl)₂] (S = 2), E = -1817.91940910 a.u., ν₁ = 21.7748 cm⁻¹

Cr	0.000035263649	0.000040806086	0.000054331647
C	-0.785189250194	-1.159227871192	-1.612649779436
C	-0.083081634292	-0.014655871391	-2.117481823594
C	-0.761688162998	1.151223289846	-1.629524030877
C	-1.910107049656	0.735379001779	-0.878762914495
C	-2.886945272044	1.448599893461	-0.139938524860
H	-2.881451214941	2.532909242852	-0.142047367866
C	-3.847238543703	0.752006315086	0.551562635474
H	-4.606245202390	1.290522420845	1.107307580269
C	-3.861648855492	-0.665527671780	0.561956655014
H	-4.631383670372	-1.180308373722	1.125387310175
C	-2.915833028277	-1.391565141934	-0.119118851684
H	-2.932380065768	-2.475677572738	-0.105348719494
C	-1.924795751325	-0.709251577837	-0.868170975345
C	1.081928341742	-0.033301868127	-3.055558974552
H	0.742034801721	-0.034006327746	-4.097193213938
H	1.696353428494	-0.921762090294	-2.899566369964
H	1.718074544540	0.841190271760	-2.907844180622
C	0.785192118714	1.159310456244	1.612801319403
C	0.083147682100	0.014681779781	2.117590959837
C	0.761820329750	-1.151142612857	1.629592612148
C	1.910218281786	-0.735204529032	0.878846390135
C	2.887098588205	-1.448342725243	0.139998698585
H	2.881665579889	-2.532652501622	0.142067859808
C	3.847352861422	-0.751669852186	-0.551476687855
H	4.606390186548	-1.290121788781	-1.107241666791
C	3.861679719003	0.665865271944	-0.561819528592
H	4.631385793356	1.180711145904	-1.125230153605
C	2.915822105457	1.391824620087	0.119281440127
H	2.932307991083	2.475938449926	0.105550675844
C	1.924824224907	0.709427350144	0.868310334019
C	-1.081863849532	0.033231359118	3.055668016661

H	-0.741969105779	0.034042343491	4.097301779762
H	-1.696408482436	0.921600220916	2.899623676857
H	-1.717892655035	-0.841354552776	2.908005664902
H	0.467731617200	-2.172909719589	1.821595372234
H	0.511767500911	2.189473325261	1.789911044992
H	-0.467533891234	2.172966507651	-1.821553879446
H	-0.511830965009	-2.189412773335	-1.789733304879

High-spin eclipsed [Cr(^{2-Me}Indenyl)₂] (S = 2), E = -1817.91795874 a.u., $\nu_1 = 17.1313$ cm⁻¹

Cr	0.668542757461	0.803551289826	0.565886093486
C	-0.490393915727	0.010082612549	2.310666937700
C	0.794119503434	0.397500013394	2.780555649746
C	1.757791792541	-0.410290288657	2.127050256300
C	1.066808320010	-1.430295129904	1.374579781801
C	1.517866272102	-2.506737363465	0.592120053983
H	2.579128152270	-2.704160640104	0.489802892695
C	0.584404902878	-3.310672014378	-0.036439391986
H	0.918305293552	-4.152511592565	-0.632293265563
C	-0.793690324687	-3.054942824208	0.077360946793
H	-1.495934906675	-3.697410254306	-0.440772671560
C	-1.265428857243	-1.989313752212	0.821696589959
H	-2.328401680494	-1.788056578565	0.887839569039
C	-0.344069386852	-1.172564835277	1.497068606871
C	-0.226666566428	2.446424034749	-0.697050954767
C	1.180164216793	2.615157126239	-0.676895928432
C	1.765982444153	1.464384313394	-1.271334028036
C	0.714262596764	0.652557423951	-1.834067085244
C	0.717527264334	-0.552954691325	-2.554546628108
H	1.653355459142	-1.033686603539	-2.815148606458
C	-0.491006536339	-1.111200675215	-2.928330348567
H	-0.500589463705	-2.036647880018	-3.492067874384
C	-1.711908818203	-0.510055659310	-2.573864159372
H	-2.640273150907	-0.978498100271	-2.880306241165
C	-1.748690321289	0.661220911087	-1.839465568694
H	-2.694540199116	1.111961181811	-1.560346866568
C	-0.535713298977	1.263970419595	-1.465368276332
C	1.078281223362	1.486494289322	3.770294468871
H	1.074314706680	1.083501951889	4.788568213070
H	2.057905438294	1.937029084246	3.597381068344
H	0.323059721122	2.274025673411	3.724911851902
C	1.921828230892	3.785100160903	-0.104638847264
H	2.902490771082	3.489344023419	0.274077169807
H	2.081422967044	4.546513594605	-0.875390963737
H	1.363555922159	4.251737262810	0.709722140156
H	-0.947300130077	3.153848626103	-0.310841597425
H	2.827026008015	1.299628551820	-1.398390026718
H	2.827363248849	-0.350038797860	2.273082100579
H	-1.427778636213	0.447746556057	2.625101229278

High-spin staggered [Cr(^{2-Me}Indenyl)₂] (S = 2), E = -1817.91937755 a.u., ν_1 = 16.6548 cm⁻¹

Cr	-0.000092294979	-0.000394328326	-0.000384662656
C	-0.904446989503	-1.151744817801	-1.700045194992
C	-0.247607187241	-0.015603850030	-2.241032823546
C	-0.880819783342	1.142271647115	-1.718319380310
C	-2.051726634588	0.733525102710	-0.979990710890
C	-3.043749176998	1.449500158357	-0.287574310522
H	-3.036573760483	2.533826555727	-0.286248869632
C	-4.031661733250	0.747849099583	0.382056399380
H	-4.812042218389	1.289258522006	0.904548081077
C	-4.046185554390	-0.659061992381	0.393251313163
H	-4.837488595943	-1.175876445125	0.924151890733
C	-3.073074629902	-1.391515289988	-0.264962954340
H	-3.088288391661	-2.475601154366	-0.246402422649
C	-2.066605784741	-0.707281071798	-0.968543460102
C	0.945116680695	-0.035020367327	-3.148114135806
H	0.625376161421	-0.040094301619	-4.195378125316
H	1.556369910255	-0.923369210563	-2.979487059110
H	1.574362753201	0.843268502910	-2.993553414245
C	0.903518339768	1.150137251149	1.700297285482
C	0.247363375760	0.013145915531	2.240284850051
C	0.881293790666	-1.143907871481	1.716579014006
C	2.052000544175	-0.733822509525	0.978684802669
C	3.044483693033	-1.448602981061	0.285710800371
H	3.038004153322	-2.532933028993	0.283520402921
C	4.031966012061	-0.745785209186	-0.383336141213
H	4.812705462589	-1.286272607372	-0.906244802309
C	4.045580054127	0.661143706496	-0.393397773443
H	4.836565829212	1.178893302505	-0.923860999408
C	3.071987476238	1.392447848284	0.265374599805
H	3.086507777020	2.476557062456	0.247680458783
C	2.065926161703	0.707002241662	0.968376487840
C	-0.945386155277	0.031068873154	3.147362751122
H	-0.625667059527	0.035167785384	4.194637530699
H	-1.557023597560	0.919327303408	2.979659890050
H	-1.574247363250	-0.847330987508	2.991864624598
H	0.640335755690	2.178609888832	1.904617144320
H	0.598397623131	-2.164095611394	1.935572155248
H	-0.641972178101	-2.180556464651	-1.903566914513
H	-0.597230534943	2.162094553224	-1.938113687315

Low-spin eclipsed [Cr(^{6-Me}Indenyl)₂] (S = 1), E = -1817.91855069 a.u., ν_1 = 11.9680 cm⁻¹

Cr	0.541282635175	0.559059897948	0.404103627300
C	-0.429985307736	0.255686628773	2.272687899650
C	0.955635925956	0.564728626123	2.468123564409

C	1.733883277139	-0.465781266643	1.845951229817
C	0.834576855983	-1.447444376815	1.316750745306
C	1.043458983740	-2.619126489549	0.545592154256
H	2.055396655314	-2.952166545771	0.339004669448
C	-0.029378352319	-3.334212971588	0.071206041621
C	-1.353127234391	-2.877295278204	0.337331030948
C	-1.601040031408	-1.740895154380	1.060298846350
H	-2.617967285668	-1.410651994312	1.240249279564
C	-0.511761433889	-0.998065578296	1.581547091553
C	-0.357945375116	2.203040153662	-0.600045537233
C	1.020910191117	2.476567828274	-0.320368619679
C	1.817074570862	1.511119384969	-1.019018221198
C	0.939631055525	0.675541041151	-1.782493299045
C	1.169247588421	-0.470151655755	-2.586239644893
H	2.186450633400	-0.796178677046	-2.777706474006
C	0.110267989962	-1.157447800302	-3.127797461041
C	-1.221254098700	-0.726608506032	-2.856645170079
C	-1.489676109788	0.362790228607	-2.071286672086
H	-2.512468089167	0.663515384345	-1.873804601339
C	-0.414028432256	1.103991409249	-1.520302849842
H	-1.267173368297	0.844678000370	2.615375562673
H	-1.205469047081	2.749719473151	-0.215258117928
H	1.345217928852	1.406163678396	3.019396682986
H	1.396015918357	3.289775672256	0.281029697538
H	2.811833334346	-0.510953283100	1.807968217083
H	2.894204048569	1.441982547491	-0.996640274197
C	0.164921059499	-4.597495257950	-0.721999213074
H	-0.197761303618	-5.468909852463	-0.167232860665
H	-0.390806420347	-4.562216511042	-1.663221650699
H	1.218729130276	-4.759540629136	-0.954469061417
C	0.328358339136	-2.357953319556	-4.007542843285
H	-0.236039051373	-3.221477255485	-3.644483871258
H	-0.007709942696	-2.161141541670	-5.030682768714
H	1.383730895687	-2.632909852859	-4.045226949588
H	-2.043700949976	-1.291980095070	-3.282574357659
H	-2.185989783488	-3.449294091742	-0.058469501577

Low-spin staggered [Cr(^{6-Me}Indenyl)₂] (S = 1), E = -1817.91463278 a.u., ν₁ = 21.3561 cm⁻¹

Cr	1.781415113779	0.000186393719	1.088549578569
C	0.049198873370	-1.195096465604	1.218851294360
C	3.514385244779	1.194499774439	0.954775958840
C	0.121546188534	-0.358826188825	2.378151074158
C	-0.062022170043	-0.355214467563	0.064410401473
C	-0.124444960051	1.006087096862	0.509785036295
C	-0.189352022343	2.239952865337	-0.186968871690
H	-0.274531508404	2.240864027331	-1.268914205427
C	-0.169456539392	3.427146113270	0.505113724011
C	-0.055491208598	3.410658291659	1.925863178390

C	0.039352568462	2.242899639036	2.636228833502
H	0.127326149319	2.258639793070	3.716898985014
C	-0.007966837792	1.004261078125	1.947303539698
C	3.440603799294	0.355301228849	-0.202350967636
C	3.625982056811	0.357552227945	2.111240519116
C	3.687175669767	-1.004855809321	1.669490380765
C	3.750904615883	-2.237037248711	2.369415215917
H	3.836935104033	-2.235259338977	3.451293809044
C	3.729008870763	-3.426005410220	1.680479731470
C	3.614192997791	-3.413224085635	0.259741843264
C	3.520270813587	-2.247213510764	-0.453586890820
H	3.431539503896	-2.265631460116	-1.534154836255
C	3.569524112209	-1.006821858777	0.232042549140
H	0.221770451911	-0.693911854680	3.399421430790
H	3.340428359454	0.687786668239	-1.224469864982
H	0.072896901618	-2.274204809418	1.214831229595
H	3.491613484791	2.273631200108	0.956021821722
H	-0.119914719093	-0.689196155043	-0.960568890788
H	3.684398692135	0.694221392430	3.135316474544
C	3.812479799870	-4.745848189799	2.398621142935
H	2.919844970956	-5.351993697785	2.214162070205
H	4.673247091969	-5.327592672177	2.054729254973
H	3.908152481455	-4.602718794980	3.476205833542
C	-0.254214261088	4.748787505142	-0.209550094271
H	-1.116088806037	5.328375250606	0.135216843721
H	0.637406582641	5.355721376683	-0.022813291543
H	-0.348879610677	4.608384248515	-1.287584573611
H	3.591767395840	-4.362691106091	-0.265414379716
H	-0.034591801398	4.358751143121	2.453572081685

High-spin eclipsed [Cr(^{6-Me}Indenyl)₂] (S = 2), E = -1817.91724310 a.u., $\nu_1 = 28.7550$ cm⁻¹

Cr	0.662391737100	0.801567042457	0.568118519471
C	-0.061676592228	0.142935156460	2.610642324601
C	1.348479200512	0.233880563535	2.634039007625
C	1.882475549880	-0.702005898044	1.709940475850
C	0.796604949343	-1.515309171469	1.223663824498
C	0.743676651040	-2.607100753597	0.338938527135
H	1.657071360093	-3.001501222633	-0.093667492613
C	-0.475602443900	-3.181555734403	0.027438625385
C	-1.661771515577	-2.644516236211	0.579756002966
C	-1.651554780539	-1.559603725345	1.430946271818
H	-2.577215981354	-1.164234872988	1.834155151539
C	-0.417810513249	-0.978371921799	1.775685516281
C	-0.677868512676	2.045643333196	-0.742078144357
C	0.572645104331	2.703597058857	-0.619135560037
C	1.575064621280	1.887549567648	-1.194587642438
C	0.923152262701	0.772262971344	-1.835865259759
C	1.414989910669	-0.303835723907	-2.597028273965

H	2.478333385498	-0.387730154377	-2.797336790836
C	0.536862414788	-1.246229282576	-3.102516141334
C	-0.845703682437	-1.130544521713	-2.828440963375
C	-1.358792392704	-0.105009164285	-2.061012470435
H	-2.420779014312	-0.052426441771	-1.851015803833
C	-0.485137097278	0.877843840257	-1.565360347725
H	-0.746514167203	0.734404481914	3.200612948377
H	-1.627937537401	2.423300861888	-0.392792984535
H	1.923680384321	0.948680120297	3.205586565546
H	0.741181350790	3.639869319766	-0.105804509664
H	2.931474402564	-0.860698320896	1.505792409994
H	2.628928134481	2.118944425347	-1.247514380675
C	-0.561516458882	-4.356907209246	-0.907412419452
H	-1.082623977219	-5.198417651117	-0.441323564586
H	-1.115503011925	-4.095096182930	-1.814619078142
H	0.432042880282	-4.696817410458	-1.204890477047
C	1.036134042799	-2.389117481149	-3.946095852649
H	0.787672023856	-3.353140384930	-3.493234911404
H	0.581804375764	-2.373079426434	-4.941517516154
H	2.119677933916	-2.342384612486	-4.069062435178
H	-1.519593813911	-1.880460357713	-3.229567098509
H	-2.609195183216	-3.105923880491	0.319670947619

High-spin staggered [Cr(⁶-MeIndenyl)₂] (S = 2), E = -1817.91374742 a.u., $\nu_1 = 8.1547$ cm⁻¹

Cr	1.779802047517	-0.001061582171	1.091929794362
C	-0.200978937925	-1.053563809148	1.241593169267
C	3.759606269678	1.053956632807	0.943751408413
C	-0.054791390332	-0.228660420906	2.382799264451
C	-0.222891481175	-0.234269047140	0.086007597133
C	-0.258376644234	1.141679475905	0.517733425692
C	-0.320359029732	2.359089194363	-0.185478357296
H	-0.393110269510	2.358073092198	-1.268394887692
C	-0.297290277721	3.557918379385	0.507229281731
C	-0.193845410607	3.546232917987	1.918270612020
C	-0.115504726246	2.371404414951	2.639612851540
H	-0.030890115086	2.392574338961	3.720490099037
C	-0.154913700832	1.144863577672	1.952488429123
C	3.614294229769	0.230370159282	-0.198480495307
C	3.781988450762	0.233246519706	2.098334565430
C	3.818532754400	-1.142125538278	1.664952240008
C	3.881203208855	-2.360374083045	2.366687727088
H	3.953745291596	-2.360628632503	3.449618343250
C	3.859195439877	-3.558354472570	1.672507454626
C	3.756105741476	-3.544997886493	0.261436421720
C	3.676974213325	-2.369371750098	-0.458480687053
H	3.592628404066	-2.389287951098	-1.539402280779
C	3.715228522992	-1.143609551179	0.230158126460
H	0.003361218264	-0.568342284404	3.406634599623

H	3.555939169281	0.571225435084	-1.221912804246
H	-0.203742706322	-2.134466401464	1.244489475755
H	3.761432960594	2.134860751750	0.942211667169
H	-0.314912456293	-0.579768266012	-0.933396016030
H	3.873395512490	0.577595572131	3.118182063689
C	3.952830802206	-4.874294189372	2.399144537809
H	3.100227491856	-5.518478506550	2.163625155098
H	4.857848134284	-5.419808030669	2.113916987454
H	3.976479741407	-4.725642659635	3.480196647552
C	-0.390131401623	4.873025608449	-0.221013197220
H	-1.294809456138	5.419437783003	0.063568047229
H	0.462872230213	5.516976638084	0.013694708641
H	-0.413900320643	4.723062864227	-1.301881712189
H	3.742569332301	-4.492876732160	-0.267067349968
H	-0.179399392789	4.494752628951	2.445600056410

Low-spin eclipsed [Cr(^{7-Me}Indenyl)₂] (S = 1), E = -1817.92256721 a.u., ν_1 = 12.9605 cm⁻¹

Cr	8.871775008598	0.746862027377	8.143135202937
C	7.788527875637	-0.068403182801	9.793328279303
C	9.041080345091	0.476902218878	10.225722759253
H	9.171145209837	1.270122175194	10.945166627764
C	10.090649413874	-0.249717646918	9.575314605053
H	11.149462343577	-0.069542006858	9.683922396768
C	9.494325875273	-1.282911356705	8.780246647098
C	10.038225941554	-2.223413077603	7.870146491612
H	11.112269353969	-2.309143523782	7.753191155529
C	9.182669417498	-3.014608562581	7.148366870131
H	9.582170571820	-3.738187385973	6.447249332042
C	7.776393502502	-2.903727447229	7.289359937062
H	7.138901816473	-3.549013387130	6.694007597113
C	7.195305180923	-2.003030345761	8.150219226873
C	8.060051565449	-1.168911359924	8.915383003276
C	7.797490898019	2.344101411544	7.224445914680
C	9.035991302603	2.813863714744	7.772032961295
H	9.145058773672	3.572759376666	8.530877388164
C	10.104383374722	2.137364309638	7.099392913968
H	11.158403549947	2.262410989823	7.296379526543
C	9.536020905170	1.288036724445	6.095044629935
C	10.107280615407	0.339305213497	5.210319658037
H	11.183951390600	0.230510587756	5.150214141510
C	9.274350445697	-0.429740558275	4.439908601183
H	9.694678443250	-1.161117786646	3.759287630086
C	7.864932999388	-0.299207136642	4.517564876623
H	7.245864685467	-0.933340398168	3.891614616654
C	7.258057540257	0.599177732417	5.362906024583
C	8.098608864404	1.414374886017	6.174244420083
H	6.811964979354	0.273152810974	10.100320083841
H	6.811994898216	2.660789564298	7.529360860437

C	5.769066248496	0.755876670256	5.437196447415
H	5.461938274952	1.745226022616	5.082431805386
H	5.263388354916	0.002029383747	4.832222734170
H	5.416125573855	0.664047054045	6.468587262029
C	5.709850274865	-1.893665648753	8.320573576729
H	5.183677702602	-2.521845932223	7.600488669928
H	5.408750132977	-2.198517938595	9.328270049474
H	5.374142419088	-0.860870441365	8.187635295430

Low-spin staggered [Cr(⁷-MeIndenyl)₂] (S = 1), E = -1817.91959668 a.u., ν_1 = 22.0316 cm⁻¹

Cr	1.7810470818	0.0002021219	1.0888897987
C	0.0561089513	-1.203755443	1.2378258282
C	3.5064589674	1.2033694674	0.9371510226
C	0.1291344188	-0.3659766977	2.3957563372
C	-0.0639035646	-0.3659050062	0.0835680081
C	-0.1211813658	0.997336671	0.5302592644
C	-0.1743357009	2.2258691691	-0.1892965503
C	-0.1509943091	3.3928015873	0.5386181204
C	-0.0487204026	3.3971606952	1.9524971594
C	0.039941753	2.2296680205	2.6670304849
H	0.1238013343	2.240429231	3.7476825378
C	-0.0076595625	0.9967770728	1.9689568508
C	3.4324194881	0.363222273	-0.219025341
C	3.6267842211	0.3678645509	2.0930403004
C	3.6832764992	-0.9962608392	1.6492360642
C	3.7361155261	-2.2233297295	2.3713504824
C	3.7118233115	-3.3917595479	1.6458920742
C	3.6088995244	-3.3991065201	0.2320615066
C	3.5203996889	-2.2330746289	-0.4848587939
H	3.43595291	-2.2460439985	-1.5654409462
C	3.5688856986	-0.9987542431	0.2106109459
H	0.2324593552	-0.7005687725	3.4169855185
H	3.329009062	0.695697567	-1.240933106
H	0.0856903257	-2.2827552728	1.2349043573
H	3.4774444296	2.2823871623	0.9378809674
H	-0.1246621621	-0.7036441418	-0.9395155305
H	3.6879010486	0.7077298486	3.1154021562
H	3.5896362196	-4.3512736872	-0.2858746288
H	-0.0301608551	4.3482340562	2.4724704374
H	-0.2038642091	4.3415542621	0.0146663527
H	3.7644787364	-4.3394266938	2.1718317053
C	-0.2660309516	2.2081452263	-1.6854738253
H	0.5916129223	1.6826493466	-2.1192612298
H	-1.1653233763	1.6803110983	-2.0186224937
H	-0.2908733216	3.2204738551	-2.0910792848
C	3.8284948034	-2.2025111333	3.8674422462
H	4.7281601223	-1.6743647945	4.1990856052
H	2.9712687805	-1.6757302446	4.3005067031

H 3.8530763314 -3.2139964177 4.2751624749

High-spin eclipsed [$\text{Cr}^{(7\text{-Me})}\text{Indenyl}_2$] ($S = 2$), $E = -1817.92035530$ a.u., $\nu_1 = 26.8858$ cm^{-1}

Cr	8.906091174010	0.983686871995	8.352268349087
C	7.609350000555	-0.236677764190	9.727659498477
C	8.691349430620	0.288273322094	10.480318740063
H	8.610161913484	1.030683388920	11.261847109988
C	9.898161397307	-0.245816883027	9.974504402914
H	10.891265003471	-0.025914398659	10.338431504993
C	9.563767588706	-1.250225836170	8.993991877123
C	10.352338124691	-2.120996103834	8.220851053548
H	11.431818265971	-2.122213298452	8.319452463025
C	9.716303618852	-2.976679729378	7.344285634281
H	10.302758734572	-3.665847935854	6.747157442386
C	8.316051606364	-2.974973554091	7.203735667879
H	7.858230905335	-3.657394319632	6.495462729816
C	7.503509934121	-2.119053501982	7.926951761068
C	8.133274395858	-1.252074327652	8.846288554078
C	8.024965210638	2.627099871926	7.063399197218
C	9.367686302894	2.952626274964	7.363442958492
H	9.692057028978	3.779879642464	7.979048304136
C	10.214049755927	1.961576645895	6.804107517665
H	11.292046074271	1.938699772696	6.872591752720
C	9.403638870280	1.088781388115	5.992613532488
C	9.708415813311	-0.021194134025	5.186343399776
H	10.733339855760	-0.351384394017	5.066843428938
C	8.672597456915	-0.676954476787	4.552472158977
H	8.885895599789	-1.532551540345	3.922479505121
C	7.335436269496	-0.271138554916	4.721957463934
H	6.551790235620	-0.818632020067	4.208003456995
C	6.985472033645	0.800695784754	5.525121313313
C	8.034563981102	1.494887795085	6.167888922389
H	6.565226751368	-0.009317723271	9.884529150128
H	7.155627895141	3.194168647980	7.361219018730
C	5.560924804097	1.238495486677	5.706747787890
H	5.405361718135	2.249886305188	5.316581707319
H	4.874931513526	0.566008524140	5.189244617498
H	5.283390398835	1.260790696062	6.766250424873
C	6.011984273518	-2.107553959301	7.765686759151
H	5.696130578660	-2.825736614039	7.007664219796
H	5.510152142432	-2.357919524803	8.706160984162
H	5.658809411748	-1.117992074466	7.462475849562

High-spin staggered [$\text{Cr}^{(7\text{-Me})}\text{Indenyl}_2$] ($S = 2$), $E = -1817.91792166$ a.u., $\nu_1 = 16.6751$ cm^{-1}

Cr	1.7810786885	0.0004511681	1.089109754
C	-0.1863823794	-1.0822609882	1.2450824112

C	3.7489267506	1.0819359405	0.9305209236
C	-0.04986245	-0.254721434	2.3853912007
C	-0.2169362963	-0.2645832098	0.0895316659
C	-0.260755202	1.112502426	0.5210364815
C	-0.3210941863	2.3229952908	-0.2048081794
C	-0.3067007467	3.501451188	0.5235246777
C	-0.2177746384	3.5129509182	1.929158588
C	-0.134994493	2.3396332404	2.6538686734
H	-0.0567663201	2.3557685989	3.7349354746
C	-0.1627325126	1.1183814754	1.9567312493
C	3.611657464	0.2523118852	-0.2082169989
C	3.7795793143	0.266410067	2.0875651635
C	3.8226333348	-1.1115035057	1.65858162
C	3.8826929232	-2.3206813663	2.3866498092
C	3.867624618	-3.5004736971	1.6604971151
C	3.7783157112	-3.5145552279	0.2549169497
C	3.6958351509	-2.342530378	-0.4719373455
H	3.6173000557	-2.360626469	-1.5529513305
C	3.724272649	-1.1200263134	0.2229289199
H	0.009851692	-0.593064267	3.4096764953
H	3.5517697095	0.5887803177	-1.2331100019
H	-0.1775406691	-2.1631312888	1.2488854449
H	3.7405999796	2.1628018698	0.9246907951
H	-0.3026083577	-0.6148588323	-0.9283288795
H	3.8657620351	0.6185319032	3.1047446226
H	3.7756492396	-4.4675827406	-0.261792285
H	-0.2156414944	4.4650209222	2.4476337898
H	-0.3678603819	4.4463917544	-0.0066305319
H	3.9285374094	-4.4444543274	2.1923899794
C	-0.3902799981	2.3078089693	-1.704140971
H	0.4900637888	1.8162301095	-2.1333328001
H	-1.267745956	1.7558547564	-2.0559431687
H	-0.441825506	3.3214069701	-2.1045563737
C	3.9522425732	-2.3027547478	3.8859333657
H	4.8299767664	-1.7504489081	4.2365142439
H	3.0721656501	-1.8100864705	4.3144269877
H	4.003537814	-3.3156301291	4.2882060442

Low-spin eclipsed [$\text{Cr}^{(1,3\text{-MeIndenyl})_2}$] ($S = 1$), $E = -1896.59746972$ a.u., $\nu_1 = 9.1329$ cm^{-1}

Cr	0.557863000000	0.558803000000	0.398350000000
C	-0.435109000000	0.278591000000	2.277757000000
C	0.962954000000	0.540751000000	2.468626000000
C	1.732202000000	-0.495529000000	1.839128000000
C	0.798522000000	-1.444867000000	1.301348000000
C	0.975161000000	-2.608305000000	0.510671000000
H	1.973544000000	-2.972948000000	0.297151000000
C	-0.127555000000	-3.267721000000	0.029163000000
H	0.000303000000	-4.159117000000	-0.573794000000

C	-1.439230000000	-2.800742000000	0.299511000000
H	-2.285317000000	-3.346459000000	-0.101742000000
C	-1.652275000000	-1.672126000000	1.050115000000
H	-2.659210000000	-1.323708000000	1.250499000000
C	-0.539343000000	-0.966980000000	1.574470000000
C	-1.571378000000	1.083706000000	2.823914000000
H	-1.882306000000	0.706889000000	3.804866000000
H	-2.442760000000	1.047277000000	2.166160000000
H	-1.287433000000	2.130913000000	2.945625000000
C	-0.352973000000	2.186660000000	-0.644156000000
C	1.024159000000	2.472932000000	-0.355247000000
C	1.859085000000	1.509941000000	-1.015101000000
C	0.996063000000	0.651205000000	-1.773285000000
C	1.250508000000	-0.511293000000	-2.544559000000
H	2.270783000000	-0.831138000000	-2.724078000000
C	0.194875000000	-1.215444000000	-3.066409000000
H	0.382153000000	-2.103136000000	-3.659374000000
C	-1.144778000000	-0.808871000000	-2.839320000000
H	-1.952040000000	-1.395156000000	-3.262519000000
C	-1.432585000000	0.304466000000	-2.090815000000
H	-2.460205000000	0.605794000000	-1.921944000000
C	-0.370298000000	1.067246000000	-1.543446000000
C	-1.538823000000	2.987739000000	-0.208121000000
H	-1.791717000000	3.751110000000	-0.952673000000
H	-1.342256000000	3.498000000000	0.736761000000
H	-2.420794000000	2.357643000000	-0.071040000000
C	3.221349000000	-0.637379000000	1.862228000000
H	3.707670000000	0.336050000000	1.950267000000
H	3.543757000000	-1.248858000000	2.712639000000
H	3.593272000000	-1.116456000000	0.953508000000
C	3.354718000000	1.486832000000	-1.018254000000
H	3.753219000000	2.051976000000	-1.868397000000
H	3.755640000000	1.933094000000	-0.106046000000
H	3.741122000000	0.467627000000	-1.090515000000
H	1.378676000000	3.305954000000	0.234443000000
H	1.371293000000	1.367445000000	3.031826000000

Low-spin staggered [Cr(^{1,3}-MeIndenyl)₂] (S = 2), E = -1896.59674013 a.u., $\nu_1 = 16.8113$ cm⁻¹

Cr	0.000034155192	0.000050041075	0.000054614998
C	-0.766627416254	-1.175375890679	-1.615870259365
C	-0.082934671565	-0.014765605532	-2.107079966294
C	-0.742997305262	1.166607254655	-1.633395313738
C	-1.892257328727	0.736008968703	-0.887416124601
C	-2.867363046449	1.448061546841	-0.143518800950
H	-2.869962794290	2.532329474675	-0.151577178900
C	-3.823717232319	0.751669659763	0.554504427545
H	-4.581526818589	1.290865714142	1.111239676197
C	-3.837906193587	-0.665661948374	0.565301410619

H	-4.606233225382	-1.181052369773	1.130109512172
C	-2.895862307071	-1.391608446823	-0.121968305613
H	-2.920170673052	-2.475611073311	-0.113507156683
C	-1.906834021875	-0.710616549040	-0.876536743374
C	-0.406544208297	-2.600516641380	-1.896375596066
H	-0.892241540771	-2.959924391170	-2.810563030003
H	-0.715409923914	-3.257550689280	-1.080024271020
H	0.672518794600	-2.709329740647	-2.026475095523
C	-0.354223249863	2.579874799098	-1.934918341285
H	-0.833102261519	2.935635307010	-2.854117153554
H	0.726754354407	2.664762339704	-2.066947713525
H	-0.649108166693	3.254993440483	-1.128189306460
C	0.766644282358	1.175477430132	1.616012217442
C	0.082998574719	0.014826474111	2.107189129715
C	0.743111191927	-1.166507204364	1.633474110489
C	1.892355688598	-0.735839224591	0.887507530705
C	2.867493723378	-1.447830349419	0.143594378052
H	2.870138461384	-2.532098466329	0.151623045085
C	3.823820541517	-0.751379434575	-0.554407612499
H	4.581654361192	-1.290527768689	-1.111155938803
C	3.837947415299	0.665953030712	-0.565166497054
H	4.606253731600	1.181391865159	-1.129958752862
C	2.895871635107	1.391841414001	0.122120823172
H	2.920134942380	2.475845211505	0.113689264659
C	1.906871058020	0.710787245812	0.876669984652
C	0.406488610625	2.600595206026	1.896540773430
H	0.892149465858	2.960005978334	2.810746293671
H	0.715341450957	3.257660784483	1.080209899906
H	-0.672582425091	2.709354326826	2.026618445458
C	0.354407825475	-2.579799434507	1.934972944927
H	0.833318797024	-2.935557419975	2.854156190189
H	-0.726563483000	-2.664740739508	2.067019658249
H	0.649310361950	-3.254887515591	1.128224810049
H	-0.797197518724	0.028337489561	2.734461425733
H	0.797259188726	-0.028328949252	-2.734354258943

High-spin eclipsed $[\text{Cr}(\text{}^{1,3}\text{-MeIndenyl})_2]$ ($S = 2$), $E = -1896.59517995$ a.u., $\nu_1 = 17.5449$ cm^{-1}

Cr	0.665475508579	0.786415769882	0.557269851962
C	-0.239432717863	0.263583185208	2.565092468730
C	1.174008700720	0.219092293066	2.662032310982
C	1.693839724895	-0.779954351546	1.792445500656
C	0.562232886465	-1.495793338124	1.254807180726
C	0.462899552208	-2.595910608326	0.385779420049
H	1.355328470777	-3.086245111721	0.014955366950
C	-0.791511702873	-3.044390069419	0.016514121210
H	-0.880692334673	-3.895878635953	-0.647802239557
C	-1.958997078608	-2.402851880257	0.470717181413
H	-2.925217983381	-2.781711320325	0.156992720518

C	-1.896208368195	-1.304639354831	1.308239531973
H	-2.801846625140	-0.817061536810	1.651536588953
C	-0.633310516213	-0.837519426517	1.718863827446
C	-1.169690840131	1.153038709431	3.331137220307
H	-1.617852161082	0.618776519580	4.176669915324
H	-1.990594353412	1.513106194904	2.704893392382
H	-0.642788975957	2.023467577568	3.727157232555
C	-0.496545912499	2.073252095904	-0.869165926768
C	0.763396792091	2.686290542246	-0.621953586733
C	1.811836336975	1.849212209814	-1.079477449968
C	1.190648804649	0.742091504262	-1.766550555013
C	1.729952458612	-0.363838928723	-2.450608703632
H	2.803651848932	-0.484349876660	-2.542381064277
C	0.865102983533	-1.284495464449	-3.012628393060
H	1.266183854332	-2.134240109434	-3.553571864128
C	-0.530453468992	-1.141239503510	-2.899877558205
H	-1.176208740713	-1.889441157631	-3.344293142762
C	-1.089025168133	-0.077075619444	-2.216825852303
H	-2.164630198565	0.012994876881	-2.120322319009
C	-0.238805547591	0.889622307743	-1.653029290132
C	-1.848771873290	2.637660642848	-0.557138481954
H	-2.285706280952	3.122712608774	-1.437142207716
H	-1.789513559844	3.382127354813	0.239466552082
H	-2.542840415660	1.855476120894	-0.238396737037
C	3.132658403455	-1.157424985379	1.613524385535
H	3.792953321002	-0.339212796686	1.908287410926
H	3.389496779255	-2.031203306085	2.222730597601
H	3.351557368837	-1.410452112053	0.572712524325
C	3.281298513200	2.135524385303	-1.033995702634
H	3.642705810936	2.494019745766	-2.004619212554
H	3.508905984982	2.900740506276	-0.289175778007
H	3.858847710622	1.241125834144	-0.784625503431
H	0.902157725809	3.624096384958	-0.098764567687
H	1.776012112897	0.892910843621	3.258706273964

High-spin staggered [Cr(^{1,3}-MeIndenyl)₂] (S = 2), E = -1896.59548053 a.u., ν_1 = 11.8482 cm⁻¹

Cr	-0.058862562266	-0.000314966257	0.093095547792
C	-0.846421800760	-1.168204479528	-1.663282389852
C	-0.179390060495	-0.014962215522	-2.151721282307
C	-0.821348471424	1.159149213162	-1.679701604730
C	-2.017326902950	0.734918661992	-0.991624419386
C	-3.043421429610	1.450664035578	-0.344991643088
H	-3.041225689741	2.534976792540	-0.346446748811
C	-4.058580028426	0.748597849882	0.278826076504
H	-4.862908986165	1.288841913144	0.764961058449
C	-4.073790121186	-0.660553733657	0.288705749511
H	-4.889506167601	-1.176458234182	0.782245603491
C	-3.074093564451	-1.393012324453	-0.325052621666

H	-3.095262588225	-2.477037193158	-0.311264154900
C	-2.032900524361	-0.708687825801	-0.981469166804
C	-0.485188267546	-2.594840598022	-1.940238682732
H	-1.043193968539	-2.983709868632	-2.799237514177
H	-0.714478230311	-3.237804886360	-1.086593141855
H	0.580106590353	-2.691922483143	-2.159255194481
C	-0.428950238320	2.573648552978	-1.975806527776
H	-0.976239322812	2.962216850983	-2.841815798046
H	0.638756369769	2.644738014990	-2.193036119297
H	-0.646607834223	3.233378081322	-1.131978480229
C	0.944958596738	1.167400010864	1.731923382404
C	0.335845315214	0.013054186494	2.291154359029
C	0.923123648529	-1.161109569297	1.750155157971
C	2.041066854128	-0.734635892270	0.940660762222
C	2.986256053740	-1.449878966890	0.183695770937
H	2.983565956472	-2.534201270916	0.183700406452
C	3.922741134273	-0.746694061484	-0.555253135739
H	4.665704702820	-1.286909929409	-1.130938440317
C	3.935971046982	0.660693468349	-0.566243282650
H	4.688889718208	1.177800829134	-1.150161299117
C	3.013015144753	1.392847009030	0.161489154033
H	3.030759531517	2.476899940957	0.144580091092
C	2.054621089272	0.707435129044	0.929414011484
C	0.628137346522	2.595024162850	2.055976255424
H	1.304118884322	2.983350858010	2.826034032687
H	0.733873420160	3.237781796868	1.178214947691
H	-0.394359056080	2.695235999231	2.425425503524
C	0.580278579696	-2.577299939871	2.097127040910
H	1.251619794684	-2.966588912682	2.870742016020
H	-0.442546316475	-2.652288600596	2.471588085011
H	0.670444825585	-3.235437708250	1.229068295592
H	-0.507727055070	0.026238428193	2.969695030472
H	0.741988583299	-0.028912125213	-2.719850690744

Low-spin eclipsed $[\text{Cr}(\text{}^{4,7}\text{-MeIndenyl})_2]$ ($S = 1$), $E = -1896.60300885$ a.u., $\nu_1 = 22.3136$ cm^{-1}

Cr	0.540488000000	0.544083000000	0.394428000000
C	-0.545868000000	0.147550000000	2.169716000000
C	0.783206000000	0.580167000000	2.492132000000
C	1.703909000000	-0.372120000000	1.954665000000
C	0.956509000000	-1.425964000000	1.342303000000
C	1.374043000000	-2.570764000000	0.604637000000
C	0.391289000000	-3.331183000000	0.019896000000
H	0.674666000000	-4.208687000000	-0.552502000000
C	-0.985295000000	-3.012784000000	0.136139000000
H	-1.710161000000	-3.652876000000	-0.355699000000
C	-1.430263000000	-1.922960000000	0.844327000000
C	-0.445592000000	-1.103536000000	1.466409000000
C	-0.242737000000	2.286247000000	-0.595161000000

C	1.167426000000	2.401552000000	-0.391369000000
C	1.810396000000	1.336305000000	-1.105053000000
C	0.792460000000	0.584804000000	-1.789961000000
C	0.854103000000	-0.610307000000	-2.562063000000
C	-0.337455000000	-1.148320000000	-2.983889000000
H	-0.324847000000	-2.062255000000	-3.568367000000
C	-1.588097000000	-0.554260000000	-2.679269000000
H	-2.491970000000	-1.030179000000	-3.045980000000
C	-1.694447000000	0.597748000000	-1.939340000000
C	-0.482650000000	1.185298000000	-1.475251000000
H	-1.460180000000	0.650794000000	2.443762000000
H	-0.995735000000	2.927960000000	-0.163751000000
H	2.779912000000	-0.308326000000	2.010170000000
H	2.873298000000	1.156522000000	-1.152755000000
C	2.830672000000	-2.915931000000	0.518311000000
H	3.228965000000	-3.181234000000	1.503357000000
H	2.996135000000	-3.758079000000	-0.155303000000
H	3.418916000000	-2.065343000000	0.158455000000
C	2.179179000000	-1.227983000000	-2.890116000000
H	2.050493000000	-2.156128000000	-3.448723000000
H	2.793294000000	-0.547098000000	-3.488622000000
H	2.741309000000	-1.451839000000	-1.979283000000
C	-3.008716000000	1.253586000000	-1.637675000000
H	-3.079857000000	2.230954000000	-2.126554000000
H	-3.842678000000	0.638863000000	-1.979686000000
H	-3.127047000000	1.428493000000	-0.563164000000
C	-2.884281000000	-1.588191000000	0.980894000000
H	-3.500918000000	-2.280645000000	0.406174000000
H	-3.201094000000	-1.631402000000	2.028171000000
H	-3.085995000000	-0.573939000000	0.625575000000
H	1.662607000000	3.174867000000	0.174937000000
H	1.043207000000	1.454892000000	3.067608000000

Low-spin staggered [$\text{Cr}^{(4,7\text{-Me})}\text{Indenyl}_2$] ($S = 1$), $E = -1896.59983398$ a.u., $\nu_1 = 19.1909$ cm^{-1}

Cr	0.000019382685	-0.000074448398	-0.000057506396
C	1.049227372260	-1.737966236104	0.659370541004
H	2.056541248847	-1.979347436904	0.356579202609
C	-0.146871763167	-2.102782424736	-0.036933427075
C	-1.265322281598	-1.576763611051	0.684842469323
H	-2.302839450821	-1.676070371803	0.405005241372
C	-0.766646474765	-0.926470972786	1.863653360546
C	-1.428024098910	-0.185723959870	2.884477705185
C	-0.640824631759	0.387884165445	3.854396348032
H	-1.114204271623	0.948664046182	4.653964723334
C	0.772891188274	0.288466489557	3.839391504948
H	1.336835794010	0.775986416257	4.628163605087
C	1.451365234574	-0.387884599148	2.853682568528
C	0.671484490661	-1.026880522472	1.847984170616

C	-2.922352185014	-0.066331397178	2.874371274407
H	-3.274997312136	0.532790194020	3.715142613328
H	-3.398180521943	-1.050757319498	2.929011768780
H	-3.267700030656	0.404223541526	1.947191105315
C	2.947019743572	-0.479718605983	2.811768398533
H	3.398343579719	0.064459674314	3.642646347365
H	3.334995259096	-0.063341819937	1.875610255933
H	3.280577123063	-1.521314916147	2.860151742115
C	-1.049127333443	1.737888739376	-0.659441260374
H	-2.056411087208	1.979328117731	-0.356595616341
C	0.147027388737	2.102627042144	0.036806087475
C	1.265410163885	1.576530335454	-0.685019798306
H	2.302948143096	1.675778352166	-0.405239574445
C	0.766632598560	0.926265136926	-1.863806466415
C	1.427912217963	0.185473118962	-2.884661110091
C	0.640628089545	-0.388088783731	-3.854538368902
H	1.113930886773	-0.948902966343	-4.654128033925
C	-0.773080791014	-0.288580898931	-3.839460317411
H	-1.337096813308	-0.776069716247	-4.628200726862
C	-1.451462591574	0.387820758002	-2.853722832590
C	-0.671490566560	1.026774713253	-1.848067764871
C	2.922233291727	0.065985800620	-2.874629047494
H	3.274797735637	-0.533166202871	-3.715412528221
H	3.398120933945	1.050381159663	-2.929303476559
H	3.267598344750	-0.404581702119	-1.947461884976
C	-2.947108996947	0.479750230365	-2.811733434829
H	-3.398509931091	-0.064403588109	-3.642585518800
H	-3.335063149474	0.063402823571	-1.875553159619
H	-3.280602776433	1.521367472562	-2.860104867925
H	0.197008409519	2.676417515888	0.949773786596
H	-0.196773701454	-2.676572333617	-0.949905808004

High-spin eclipsed $[\text{Cr}^{(4,7\text{-Me})}\text{Indenyl}]_2$ ($S = 2$), $E = -1896.59975162$ a.u., $v_1 = 31.0949$ cm^{-1}

Cr	0.651095612244	0.785185604815	0.565285149321
C	-0.610203793012	-0.008328636697	2.255556586045
C	0.649888364629	0.376753249138	2.780950433031
C	1.651591972074	-0.429766206257	2.194894515332
C	0.997360939308	-1.442350695772	1.400741087485
C	1.515655437449	-2.519236287515	0.647784424052
C	0.598909070188	-3.311489573364	-0.018648897417
H	0.958214536485	-4.153521197464	-0.601855174873
C	-0.785806423143	-3.064232869893	0.030714528888
H	-1.452851505016	-3.717592815806	-0.521816530326
C	-1.323244614198	-2.008940291986	0.744801300214
C	-0.416284970713	-1.189971716848	1.451579533763
C	-0.143476592418	2.444727644464	-0.755686638768
C	1.266905927374	2.528929134514	-0.720917131581
C	1.807895671549	1.345551297849	-1.285770924772
C	0.719854319902	0.577184453366	-1.838900694879

C	0.692670511184	-0.641322392888	-2.550974630533
C	-0.551301268190	-1.126740131981	-2.910614047574
H	-0.611350714124	-2.059092096689	-3.462208029848
C	-1.744841159913	-0.462055214550	-2.572002866283
H	-2.690177409216	-0.897838753217	-2.879705580840
C	-1.754635276015	0.724311424692	-1.861488257150
C	-0.498662068319	1.255565352942	-1.493113895513
H	-1.561356638721	0.431920645258	2.516612990784
H	-0.830826626386	3.192868270295	-0.389644148375
H	2.711212352782	-0.365771000922	2.393103713378
H	2.859533307801	1.123945636681	-1.393587135553
C	2.993261017046	-2.779962033579	0.604020935145
H	3.383153354037	-3.020969471355	1.598698553948
H	3.224308227997	-3.613330679812	-0.061510540343
H	3.543032019165	-1.899951927326	0.252198308702
C	1.965343446251	-1.352260657433	-2.905015720866
H	1.756495361175	-2.287372820018	-3.426806740405
H	2.598265256244	-0.733782022289	-3.550199920226
H	2.546017138609	-1.587595690301	-2.008985001824
C	-3.023328046342	1.441944923157	-1.502734185410
H	-3.068633214241	2.428174073787	-1.976823573473
H	-3.898378465169	0.872699117363	-1.820636023913
H	-3.097307097439	1.605602917110	-0.421887283130
C	-2.798239492758	-1.739197244620	0.791384327313
H	-3.344264722387	-2.454419407225	0.174426373627
H	-3.181268620173	-1.807069019539	1.815092530428
H	-3.025509113489	-0.734369476269	0.424978165002
H	0.821393461434	1.198688919763	3.461775571237
H	1.839247976455	3.329128846419	-0.272994553818

High-spin staggered [Cr(^{4,7}-MeIndenyl)₂] (S = 2), E = -1896.59634712 a.u., $\nu_1 = 3.5755$ cm⁻¹

Cr	-0.005134910861	-0.018508901519	-0.000948639113
C	1.026332342705	-1.852238229629	0.808332283212
H	2.029650652240	-2.123835720564	0.515144558154
C	-0.163462963197	-2.262782479471	0.160552317527
C	-1.268479652617	-1.688533455963	0.833557898633
H	-2.306335390586	-1.814169252249	0.562489401261
C	-0.775775921600	-1.031532769145	2.020822164110
C	-1.440573852916	-0.324387158610	3.047124885935
C	-0.648688186262	0.237875068427	4.033169826222
H	-1.124846199912	0.775596894817	4.846891194625
C	0.756443205522	0.138500035739	4.017199111438
H	1.321810201022	0.602817748753	4.818939882548
C	1.438783260035	-0.528387689972	3.014633404985
C	0.658002609325	-1.133549816820	2.004940359051
C	-2.935939088779	-0.195307131540	3.042313910165
H	-3.282692203286	0.370587932989	3.908405893583
H	-3.420571071291	-1.176837114303	3.059263017435

H	-3.284725948187	0.318109072684	2.139038963407
C	2.936886601458	-0.610561904785	2.975198366481
H	3.379607895506	-0.099777141148	3.831745951963
H	3.332907890705	-0.150188814163	2.062855886807
H	3.279302320023	-1.650382973368	2.983081677093
C	-1.037514508914	1.804865798249	-0.831118450585
H	-2.040970965392	2.079479950094	-0.541256850303
C	0.151982358347	2.222463410619	-0.187137494725
C	1.257493894126	1.642103949294	-0.854221079187
H	2.295247242086	1.771508907440	-0.584530706336
C	0.765286940475	0.973772859154	-2.035478489322
C	1.430715217124	0.256406512194	-3.054041217939
C	0.639351446083	-0.316653636358	-4.034418150829
H	1.115978271093	-0.862706084738	-4.842299261173
C	-0.765715635696	-0.217724493192	-4.019870036109
H	-1.330690645268	-0.690668643924	-4.816831619204
C	-1.448610066577	0.459438636127	-3.024431653214
C	-0.668403406338	1.075273135844	-2.020985962799
C	2.926069320165	0.127388060194	-3.046974439689
H	3.273423671771	-0.446838465695	-3.907321528945
H	3.410808850574	1.108662617122	-3.072999051888
H	3.274142270958	-0.377339660009	-2.138525974782
C	-2.946797883283	0.540731540682	-2.985938846298
H	-3.388994567989	0.021620316696	-3.837745961278
H	-3.342558858224	0.088458457967	-2.069420614805
H	-3.290158986531	1.580115888497	-3.003505742288
H	0.202987958905	2.813540487033	0.716390203141
H	-0.214847506544	-2.843657743453	-0.749534386965

Low-spin eclipsed $[\text{Cr}(\text{}^5,6\text{-MeIndenyl})_2]$ ($S = 1$), $E = -1896.59486275$ a.u., $\nu_1 = 20.3760$ cm^{-1}

Cr	0.548941543682	0.555872207377	0.405196429693
C	-0.292368185687	0.229236989134	2.346404038825
C	1.110817591907	0.500406915019	2.434823842312
C	1.810388042827	-0.528519607583	1.720603288893
C	0.838359218816	-1.470176661076	1.238766811736
C	0.934206377639	-2.618714590503	0.415176687034
H	1.910376270123	-2.970884471822	0.097748381669
C	-0.195738623200	-3.294244788749	0.021938725866
C	-1.493273927874	-2.830469410287	0.425102495609
C	-1.615260471733	-1.703851289134	1.200832689938
H	-2.600043036872	-1.354787956075	1.494649289155
C	-0.465529477848	-1.000105987015	1.635146019641
C	-0.488035827454	2.127149110850	-0.571250582125
C	0.864944436547	2.517037126423	-0.295962399393
C	1.737177119917	1.635093817707	-1.011290085667
C	0.931461755104	0.738487550055	-1.782034553324
C	1.248357973727	-0.366625298031	-2.608958922442
H	2.287709390385	-0.598050821461	-2.819098235930

C	0.252591952812	-1.137030834136	-3.157518937828
C	-1.124984080523	-0.845997750536	-2.876643868871
C	-1.457820775266	0.209652856576	-2.062660267300
H	-2.501342844376	0.416477860530	-1.848252065492
C	-0.451627593887	1.036915119804	-1.506062102639
H	-1.082646766240	0.834377534211	2.764533570778
H	-1.377735386728	2.595428071764	-0.178431248284
H	1.563970500723	1.317337964829	2.974355666782
H	1.172100068428	3.350631733692	0.316045698287
H	2.880375537665	-0.605105378064	1.600530566122
H	2.816391290636	1.657041733709	-0.991463351332
C	-0.080814524582	-4.526059527274	-0.833070831271
H	-0.464416555237	-5.411229065344	-0.314980589596
H	-0.657864911355	-4.429833744562	-1.758145179267
H	0.959593410986	-4.715256012656	-1.100977029198
C	-2.721384900420	-3.582309318034	-0.009249587968
H	-2.703791679075	-4.617942245701	0.345137063105
H	-3.622529813573	-3.106550245590	0.380348910997
H	-2.804670426828	-3.622046022123	-1.099628205125
C	0.602253302846	-2.293732285205	-4.053001833589
H	0.231073551856	-3.241134370616	-3.650408367694
H	0.161403447749	-2.177960945799	-5.048326906431
H	1.683706434631	-2.377853577501	-4.169497740591
C	-2.202424055318	-1.704439896157	-3.479942461220
H	-3.187266625944	-1.392363863814	-3.129613643197
H	-2.196790959381	-1.646182026115	-4.573389184537
H	-2.068544429603	-2.759648710717	-3.221652926132

Low-spin staggered $[\text{Cr}^{(5,6\text{-MeIndenyl})_2}]$ ($S = 1$), $E = -1896.58958484$ a.u., $\nu_1 = 19.4435$ cm^{-1}

Cr	1.781094499124	0.000784114481	1.088421469473
C	0.047502149877	-1.191992065935	1.211088525883
C	3.515877380466	1.191972495163	0.962472395990
C	0.112279428367	-0.355531635137	2.371535216703
C	-0.053454488504	-0.352209914927	0.055581044636
C	-0.117661127556	1.009262254044	0.504334347854
C	-0.173906687389	2.247665847113	-0.181044254826
H	-0.249050145753	2.257595000686	-1.263824552785
C	-0.158049502876	3.433774618367	0.512979633883
C	-0.054975388456	3.431688256587	1.944623225879
C	0.028338223440	2.243586861673	2.630364206399
H	0.108894802816	2.250356319577	3.712776390400
C	-0.014764174599	1.007154198439	1.940469291959
C	3.449333050299	0.352916381296	-0.196030334016
C	3.616890138960	0.354745936136	2.119775332932
C	3.679386038202	-1.007743659745	1.674217155087
C	3.734506923677	-2.244657116592	2.362438256712
H	3.810251907325	-2.252190661775	3.445194706833
C	3.716892825643	-3.432327257793	1.671164591318

C	3.613123613663	-3.433520653853	0.239543819743
C	3.530659227480	-2.246930788597	-0.448870417433
H	3.449452801189	-2.256079836499	-1.531216328349
C	3.575338557778	-1.008965801232	0.238165125437
H	0.205979365569	-0.691416851333	3.393190494030
H	3.355787061149	0.686525700126	-1.218440022597
H	0.069531160252	-2.271153399849	1.207955039078
H	3.495161297948	2.271161645851	0.963132486100
H	-0.106876357849	-0.685138963310	-0.969931435045
H	3.670812889268	0.690011186754	3.144506429970
C	3.792863786904	-4.739112192500	2.413140071401
H	2.908569299175	-5.357968602189	2.228692050672
H	4.661308499400	-5.328251612315	2.101458685566
H	3.867987165061	-4.568848994776	3.488110398013
C	3.581284931966	-4.741508648136	-0.503527632088
H	4.484718457907	-5.331230734715	-0.317952850181
H	2.731728202429	-5.359039053760	-0.193831044030
H	3.502421450271	-4.572933467454	-1.578498920364
C	-0.024789214186	4.737966902592	2.690765332037
H	0.824276619043	5.357062478861	2.382851119365
H	-0.928735869412	5.327209242411	2.506167916612
H	0.053788849622	4.566974161733	3.765375049500
C	-0.235125199081	4.742196473141	-0.225989583871
H	-1.104383776125	5.329640250479	0.086623568833
H	0.648384812671	5.361624819149	-0.039698549625
H	-0.309541895155	4.574340477763	-1.301389483088

High-spin eclipsed [Cr(^{5,6}-MeIndenyl)₂] (S = 2), E = -1896.59273629 a.u., ν_1 = 31.4954 cm⁻¹

Cr	0.659979531563	0.800789468335	0.575214069380
C	-0.181353331296	0.094836270705	2.551232555941
C	1.222050361294	0.229922719461	2.671933002414
C	1.846391214351	-0.681409904638	1.782237937423
C	0.820344353113	-1.529480429596	1.226813596713
C	0.852768810858	-2.629641616068	0.355364118572
H	1.802093490037	-2.999351283199	-0.018418119825
C	-0.321841078199	-3.261665661872	-0.013115465983
C	-1.575313506887	-2.773579810450	0.452100045733
C	-1.628287564551	-1.669957875819	1.285055843315
H	-2.589297881102	-1.301452796040	1.629677842998
C	-0.443340880447	-1.039792714817	1.698999298421
C	-0.579027604515	2.169404095308	-0.711329861593
C	0.719263655024	2.724847778315	-0.578226476515
C	1.654849726353	1.841447540217	-1.167224192409
C	0.915568063614	0.797329517934	-1.834716539216
C	1.308348265362	-0.297079443983	-2.622439087078
H	2.359939182714	-0.468776883257	-2.829293777474
C	0.356543366856	-1.149587516864	-3.153484020762
C	-1.024999717477	-0.939828492994	-2.882998604368

C	-1.426178864631	0.111974403075	-2.078150682785
H	-2.480679548290	0.252986434661	-1.864203148454
C	-0.477089088838	1.006334650953	-1.558367169363
H	-0.922339828139	0.659501537827	3.098156896130
H	-1.497032597655	2.614914417675	-0.356307251380
H	1.733384424486	0.960007572662	3.283544405015
H	0.961376669406	3.634468784542	-0.046700427336
H	2.911264222659	-0.807342088083	1.650160254678
H	2.723720269350	1.990212419300	-1.216491260726
C	-0.271244126965	-4.480826833030	-0.893249142257
H	-0.643024062013	-5.367992511433	-0.369284854436
H	-0.890591368980	-4.362992217147	-1.787118620667
H	0.751650868149	-4.683959388775	-1.213912895696
C	-2.847854863209	-3.466824672961	0.046289698954
H	-2.856295544037	-4.513045417437	0.369296594999
H	-3.714677811774	-2.971349516183	0.486465463097
H	-2.975790407060	-3.469547252672	-1.040309452005
C	0.783870102719	-2.296129463889	-4.029549140803
H	0.466514522273	-3.258366374919	-3.616632778499
H	0.347142972855	-2.221237821804	-5.030879573615
H	1.869610095411	-2.316702520990	-4.136236478817
C	-2.055105371035	-1.853618371541	-3.489165940510
H	-3.055085268511	-1.597470061568	-3.135844417713
H	-2.055892740479	-1.786136797702	-4.582435352605
H	-1.865039112359	-2.901793871236	-3.240628890893

High-spin staggered $[\text{Cr}^{(5,6\text{-Me})}\text{Indenyl}]_2$ ($S = 2$), $E = -1896.58814651$ a.u., $\nu_1 = 6.9068$ cm^{-1}

Cr	1.778212128902	-0.001944312409	1.093177388157
C	-0.208944214903	-1.041437461132	1.237378440886
C	3.763850945815	1.041393459500	0.951453310168
C	-0.058903916357	-0.218720469987	2.380619094778
C	-0.224706468961	-0.220391592494	0.083268309943
C	-0.254096708433	1.154903759777	0.519067846731
C	-0.306799026449	2.377812166064	-0.171197873883
H	-0.378853071875	2.387552512412	-1.254242897728
C	-0.275024150000	3.574580478668	0.524993625442
C	-0.172747055897	3.575615477507	1.945307511853
C	-0.104368261057	2.379828635220	2.640559085906
H	-0.020434726048	2.391076448185	3.722732918693
C	-0.150880118020	1.155946441452	1.951589135973
C	3.615188472765	0.220862327857	-0.193490535995
C	3.780596424980	0.217978815319	2.103873322568
C	3.811941997414	-1.156352503442	1.665281262043
C	3.866324073651	-2.380623704047	2.353029728569
H	3.938405708130	-2.392477795860	3.436051601677
C	3.836254279864	-3.575984533130	1.654386772480
C	3.733978126531	-3.574221197903	0.234043075436
C	3.663914526092	-2.377140819054	-0.458749400059

H	3.580044500763	-2.386287809096	-1.540947215390
C	3.708757583743	-1.154557651222	0.232733635700
H	-0.004221218154	-0.560397893690	3.404000550514
H	3.559951135170	0.564577486665	-1.216158019619
H	-0.218032529591	-2.122317414530	1.238821805163
H	3.771180326651	2.122285030808	0.952282376608
H	-0.317234517270	-0.563572021972	-0.936881786882
H	3.872421858573	0.559182633207	3.124749276497
C	3.916994584276	-4.882037665091	2.398413497846
H	3.039697179004	-5.509231523096	2.208529131537
H	4.792966393781	-5.464867654357	2.095050561047
H	3.982771491885	-4.710763653633	3.474022045986
C	3.706874415589	-4.878430473999	-0.517092990270
H	4.616401536317	-5.462689684912	-0.342676871809
H	2.864767256668	-5.505469294859	-0.206009652222
H	3.619299458082	-4.704467622034	-1.590715407921
C	-0.143848306361	4.881321852816	2.693769962784
H	0.698970117329	5.506685254945	2.381248206692
H	-1.052687689952	5.466358767376	2.518352625953
H	-0.056281159390	4.709438682433	3.767728657167
C	-0.353909436045	4.879203144948	-0.221743628975
H	-1.228928643235	5.464003059156	0.080564421863
H	0.524383794398	5.505448830116	-0.033322457073
H	-0.420135508373	4.705793197521	-1.296982478836

Low-spin eclipsed [$\text{Cr}^{(1,2,3\text{-MeIndenyl})_2}$] ($S = 1$), $E = -1975.27537003$ a.u., $\nu_1 = 12.8700$ cm^{-1}

Cr	0.557590000000	0.558424000000	0.398339000000
C	-0.356803000000	0.314124000000	2.329234000000
C	1.061908000000	0.517531000000	2.459137000000
C	1.735337000000	-0.558358000000	1.775158000000
C	0.729511000000	-1.453512000000	1.272379000000
C	0.806650000000	-2.609514000000	0.456870000000
H	1.772966000000	-3.017933000000	0.183910000000
C	-0.351299000000	-3.205636000000	0.022815000000
H	-0.299539000000	-4.091013000000	-0.599871000000
C	-1.620804000000	-2.676992000000	0.366764000000
H	-2.513509000000	-3.172169000000	0.002338000000
C	-1.737546000000	-1.550369000000	1.142393000000
H	-2.714253000000	-1.155711000000	1.399319000000
C	-0.564566000000	-0.912853000000	1.620703000000
C	-1.429350000000	1.175203000000	2.917155000000
H	-1.674529000000	0.858258000000	3.937297000000
H	-2.346463000000	1.124936000000	2.326560000000
H	-1.121534000000	2.221897000000	2.963988000000
C	-0.413262000000	2.125052000000	-0.665847000000
C	0.934134000000	2.514761000000	-0.331163000000
C	1.839205000000	1.601857000000	-0.977919000000
C	1.061948000000	0.685906000000	-1.757375000000

C	1.415821000000	-0.459193000000	-2.515357000000
H	2.459883000000	-0.707670000000	-2.669964000000
C	0.424261000000	-1.236278000000	-3.060804000000
H	0.688034000000	-2.110195000000	-3.645296000000
C	-0.945108000000	-0.924396000000	-2.868475000000
H	-1.699319000000	-1.567558000000	-3.306458000000
C	-1.326869000000	0.168782000000	-2.130966000000
H	-2.376693000000	0.395787000000	-1.984491000000
C	-0.334002000000	1.004898000000	-1.562978000000
C	-1.670872000000	2.832678000000	-0.269309000000
H	-1.948867000000	3.591208000000	-1.010260000000
H	-1.561417000000	3.337561000000	0.692199000000
H	-2.507439000000	2.135001000000	-0.183434000000
C	1.720470000000	1.565776000000	3.298746000000
H	1.852991000000	1.217166000000	4.329988000000
H	2.707661000000	1.824673000000	2.911065000000
H	1.126320000000	2.480487000000	3.334165000000
C	3.212652000000	-0.787912000000	1.710185000000
H	3.767207000000	0.151545000000	1.745351000000
H	3.554982000000	-1.404523000000	2.549378000000
H	3.492332000000	-1.303054000000	0.788087000000
C	1.325060000000	3.750172000000	0.416015000000
H	2.282943000000	3.623438000000	0.923283000000
H	1.420650000000	4.606150000000	-0.262738000000
H	0.580780000000	4.011819000000	1.170721000000
C	3.333317000000	1.658650000000	-0.930710000000
H	3.728062000000	2.306237000000	-1.721973000000
H	3.689012000000	2.052929000000	0.023515000000
H	3.772959000000	0.668141000000	-1.065302000000

Low-spin staggered [Cr(^{1,2,3}-MeIndenyl)₂] (S = 1), E = -1975.27719081 a.u., $\nu_1 = 19.1092 \text{ cm}^{-1}$

Cr	0.000037840000	0.000035400000	0.000054080000
C	-0.764629720000	-1.170987960000	-1.620715560000
C	-0.068010620000	-0.014978200000	-2.120294340000
C	-0.740999480000	1.162203730000	-1.637992890000
C	-1.887803130000	0.735526380000	-0.888858820000
C	-2.858529650000	1.447306640000	-0.139920460000
H	-2.861943900000	2.531655260000	-0.148029430000
C	-3.810881290000	0.751230710000	0.565382360000
H	-4.564238540000	1.290851640000	1.127773020000
C	-3.825134040000	-0.665344250000	0.576015710000
H	-4.589136720000	-1.181193520000	1.146303300000
C	-2.887147450000	-1.390960900000	-0.118679110000
H	-2.912380350000	-2.475022370000	-0.110523880000
C	-1.902414040000	-0.710153020000	-0.878093770000
C	-0.406490680000	-2.599763980000	-1.885865550000
H	-0.830298930000	-2.949159540000	-2.834277840000
H	-0.783721180000	-3.252725440000	-1.095741350000

H	0.676670700000	-2.732513540000	-1.938945920000
C	1.095228430000	-0.033459650000	-3.059870600000
H	0.757831520000	-0.031626110000	-4.103058060000
H	1.711647650000	-0.920906110000	-2.908109870000
H	1.736053690000	0.837368060000	-2.912785120000
C	-0.354069730000	2.579272070000	-1.924603350000
H	-0.770852330000	2.922750880000	-2.878279750000
H	0.731547290000	2.689182140000	-1.979620030000
H	-0.717859360000	3.251661620000	-1.144509590000
C	0.764621430000	1.171058980000	1.620876180000
C	0.068076610000	0.014984320000	2.120402870000
C	0.741144470000	-1.162135010000	1.638054240000
C	1.887924560000	-0.735349120000	0.888940440000
C	2.858701730000	-1.447031160000	0.139975380000
H	2.862189240000	-2.531379680000	0.148036840000
C	3.811007180000	-0.750861260000	-0.565296850000
H	4.564400800000	-1.290406640000	-1.127710890000
C	3.825160500000	0.665714990000	-0.575871020000
H	4.589128790000	1.181641130000	-1.146135400000
C	2.887124180000	1.391239080000	0.118853450000
H	2.912282840000	2.475302650000	0.110743720000
C	1.902437400000	0.710332150000	0.878241010000
C	0.406377440000	2.599798990000	1.886075290000
H	0.830162020000	2.949192730000	2.834498780000
H	0.783557870000	3.252815910000	1.095972930000
H	-0.676794050000	2.732463390000	1.939162770000
C	-1.095169360000	0.033353030000	3.059972310000
H	-0.757776710000	0.031669310000	4.103161770000
H	-1.711742630000	0.920679410000	2.908130490000
H	-1.735841380000	-0.837599090000	2.912961640000
C	0.354302580000	-2.579238110000	1.924613750000
H	0.771007310000	-2.922687540000	2.878334560000
H	-0.731311480000	-2.689243700000	1.979510930000
H	0.718236340000	-3.251589100000	1.144555680000

High-spin eclipsed $[\text{Cr}(\text{}^{1,2,3\text{-Me}}\text{Indenyl})_2]$ ($S = 2$), $E = -1975.27246793$ a.u., $\nu_1 = 18.2054$ cm^{-1}

Cr	0.650633178592	0.766499493435	0.542146231469
C	-0.561739657932	-0.037612182074	2.240598215431
C	0.685616125454	0.422912421287	2.764034143202
C	1.740210335494	-0.334870133449	2.181912340617
C	1.135862968225	-1.385042891719	1.396821121853
C	1.690346740967	-2.432754969405	0.638155943434
H	2.764825145589	-2.571315230021	0.592563217719
C	0.838638579918	-3.287241428829	-0.039325244868
H	1.251597230855	-4.106289936338	-0.617441649152
C	-0.556522156137	-3.117134401268	0.008043167463
H	-1.192072474587	-3.799333660366	-0.544208171801
C	-1.128598887451	-2.085268933920	0.730967046620

H	-2.204059846536	-1.952591464379	0.744972366767
C	-0.292677037719	-1.213808279021	1.448695934513
C	-1.927827374638	0.465196422968	2.594808130043
H	-2.355931420400	-0.100923460788	3.430079563254
H	-2.611538491700	0.367064496003	1.748042616267
H	-1.907387868319	1.517424796432	2.886331232826
C	-0.154197575655	2.491455850496	-0.666977297186
C	1.267877701256	2.542231705947	-0.689479486619
C	1.765763533070	1.352836020688	-1.305249485308
C	0.632905439493	0.627243350539	-1.827785440196
C	0.526547867598	-0.575596283359	-2.545357610484
H	1.415326752256	-1.119438928257	-2.843193254359
C	-0.731485060398	-1.053074357459	-2.868121609869
H	-0.825473213529	-1.976520342504	-3.427342449916
C	-1.894215448506	-0.371144275144	-2.467358518331
H	-2.863328009874	-0.775854945671	-2.736848702353
C	-1.823831147126	0.804088052308	-1.740381113470
H	-2.726850103538	1.320498460535	-1.434343237651
C	-0.557249990075	1.323691117124	-1.414207828619
C	-1.088051511318	3.536125273987	-0.138304419814
H	-1.405912244322	4.223516152909	-0.931110100441
H	-0.621815779780	4.133757264944	0.647854994288
H	-1.991118720205	3.083604354404	0.279198507474
C	0.853278585504	1.542317717605	3.745781695240
H	0.816580404332	1.162854254141	4.773004043988
H	1.811924844503	2.049131099587	3.618431473392
H	0.061026948347	2.286904652595	3.644898606854
C	3.206217925712	-0.207752242395	2.460509024702
H	3.469299130761	0.800868076325	2.786222491792
H	3.523373322701	-0.902201083283	3.247415270765
H	3.798318969926	-0.434841173678	1.570241148500
C	2.111615289121	3.647347597304	-0.131165014471
H	3.072205972652	3.274750627414	0.230258943703
H	2.320589773219	4.399491999761	-0.899991832282
H	1.612885097866	4.155349718364	0.696657275862
C	3.200325355179	1.001286560815	-1.555842191919
H	3.529183829744	1.351447286662	-2.541082284465
H	3.861462856090	1.447943736806	-0.810256096039
H	3.348046115319	-0.081017958058	-1.526904708422

High-spin staggered [$\text{Cr}^{(1,2,3\text{-Me})}\text{Indenyl}_2$] ($S = 2$), $E = -1975.27554618$ a.u., $v_1 = 9.9449$ cm^{-1}

Cr	0.000006000000	0.025253000000	-0.000193000000
C	-0.848228000000	-1.149901000000	-1.707264000000
C	-0.216493000000	0.012511000000	-2.238273000000
C	-0.866124000000	1.171151000000	-1.719746000000
C	-2.021747000000	0.726466000000	-0.976646000000
C	-3.020793000000	1.422818000000	-0.272632000000
H	-3.038685000000	2.507048000000	-0.272331000000
C	-3.986965000000	0.701680000000	0.410030000000

H	-4.772070000000	1.227833000000	0.941063000000
C	-3.974690000000	-0.705101000000	0.419633000000
H	-4.750654000000	-1.237480000000	0.957919000000
C	-2.996568000000	-1.418891000000	-0.253476000000
H	-2.996192000000	-2.503148000000	-0.238819000000
C	-2.009629000000	-0.714924000000	-0.967591000000
C	-0.488348000000	-2.574855000000	-1.994715000000
H	-1.005931000000	-2.944526000000	-2.887316000000
H	-0.768240000000	-3.225101000000	-1.162549000000
H	0.584639000000	-2.691273000000	-2.161758000000
C	0.977598000000	0.015099000000	-3.142604000000
H	0.665484000000	-0.003932000000	-4.192656000000
H	1.612148000000	-0.855351000000	-2.968238000000
H	1.589602000000	0.906071000000	-2.993663000000
C	-0.535122000000	2.598781000000	-2.028338000000
H	-1.087510000000	2.954287000000	-2.905748000000
H	0.529587000000	2.728753000000	-2.232983000000
H	-0.795940000000	3.252113000000	-1.192239000000
C	0.889779000000	1.179563000000	1.701648000000
C	0.217244000000	0.042144000000	2.237659000000
C	0.825414000000	-1.140608000000	1.724291000000
C	1.995068000000	-0.740224000000	0.978111000000
C	2.967495000000	-1.474492000000	0.274721000000
H	2.945600000000	-2.558621000000	0.276686000000
C	3.959189000000	-0.790635000000	-0.409546000000
H	4.724140000000	-1.346469000000	-0.939823000000
C	3.999372000000	0.615612000000	-0.421575000000
H	4.794428000000	1.117861000000	-0.960883000000
C	3.048131000000	1.366164000000	0.250258000000
H	3.087469000000	2.449703000000	0.233355000000
C	2.035894000000	0.700595000000	0.965149000000
C	0.588176000000	2.618149000000	1.988824000000
H	1.152977000000	2.976951000000	2.856940000000
H	0.856142000000	3.252813000000	1.140653000000
H	-0.472462000000	2.771960000000	2.197932000000
C	-0.976580000000	0.081858000000	3.141488000000
H	-0.665157000000	0.068386000000	4.191826000000
H	-1.568742000000	0.984257000000	2.981663000000
H	-1.630148000000	-0.776414000000	2.977151000000
C	0.436881000000	-2.553495000000	2.033233000000
H	0.944297000000	-2.918899000000	2.933391000000
H	-0.638727000000	-2.646342000000	2.198313000000
H	0.706663000000	-3.222226000000	1.212485000000

Low-spin eclipsed [Cr(^{2,4,7-Me}Indenyl)₂] (S = 1), E = -1975.28091762 a.u., $\nu_1 = 24.7698$ cm⁻¹

Cr	0.538122590000	0.537676980000	0.390214310000
C	-0.567686530000	0.138502200000	2.150278470000
C	0.749451580000	0.596675080000	2.500322460000

C	1.681199670000	-0.356229570000	1.977099320000
C	0.959666680000	-1.420281170000	1.351647470000
C	1.402053150000	-2.556618900000	0.616624800000
C	0.437185240000	-3.329677900000	0.017273550000
H	0.740365240000	-4.202361400000	-0.552429780000
C	-0.944256810000	-3.028665220000	0.113463550000
H	-1.654171000000	-3.676628050000	-0.389731770000
C	-1.412234420000	-1.942635670000	0.813864960000
C	-0.447222470000	-1.113333810000	1.451405990000
C	-0.208733840000	2.294145690000	-0.599519870000
C	1.204763220000	2.392228610000	-0.393878400000
C	1.814556120000	1.306512000000	-1.112707030000
C	0.782601090000	0.569339420000	-1.792264850000
C	0.818219870000	-0.629495720000	-2.558558670000
C	-0.385699160000	-1.148133230000	-2.971571420000
H	-0.392914020000	-2.064673730000	-3.552045760000
C	-1.622981440000	-0.531746630000	-2.659599310000
H	-2.538101560000	-0.993715750000	-3.016247740000
C	-1.703533550000	0.624932280000	-1.922404530000
C	-0.478626840000	1.194955880000	-1.473023410000
C	1.073760410000	1.763464590000	3.378293440000
H	1.054146450000	1.472685060000	4.434725270000
H	2.068335680000	2.157278870000	3.160492050000
H	0.351152900000	2.571456540000	3.244018700000
C	1.923116420000	3.503235450000	0.304190210000
H	2.858550100000	3.153007450000	0.746218150000
H	2.168723370000	4.308632420000	-0.397246210000
H	1.310468990000	3.931118240000	1.100017610000
H	-1.491114960000	0.635233450000	2.408942860000
H	-0.946250980000	2.952235800000	-0.163525830000
H	2.756164940000	-0.278055000000	2.050816560000
H	2.874965010000	1.107825490000	-1.162527350000
C	2.864672820000	-2.879775910000	0.546139170000
H	3.258435270000	-3.133502700000	1.536059210000
H	3.049828960000	-3.722633140000	-0.121510170000
H	3.442405340000	-2.021508020000	0.186794170000
C	2.129942250000	-1.273446090000	-2.890230260000
H	1.981208080000	-2.199187220000	-3.447909850000
H	2.755979920000	-0.605290630000	-3.490805300000
H	2.689594860000	-1.508394360000	-1.980666050000
C	-3.004478380000	1.301188100000	-1.607861000000
H	-3.062722670000	2.283076750000	-2.089337370000
H	-3.851162810000	0.702966560000	-1.948011750000
H	-3.112303330000	1.470300590000	-0.531085350000
C	-2.871764890000	-1.622310570000	0.924779550000
H	-3.471624280000	-2.323969280000	0.343441210000
H	-3.205754710000	-1.663242970000	1.966838100000
H	-3.077488070000	-0.612180800000	0.560157710000

Low-spin staggered [Cr(^{2,4,7}-MeIndenyl)₂] (S = 1), E = -1975.28076608 a.u., $\nu_1 = 17.4411 \text{ cm}^{-1}$

Cr	0.000026020000	-0.000074680000	-0.000055860000
C	1.043981510000	-1.741816280000	0.653688290000
H	2.051221260000	-1.983791470000	0.348038820000
C	-0.147997350000	-2.110737990000	-0.054694900000
C	-1.261410980000	-1.581132610000	0.679161720000
H	-2.299100090000	-1.681296330000	0.396892480000
C	-0.767146410000	-0.931422330000	1.859094730000
C	-1.427955240000	-0.189253590000	2.878224180000
C	-0.640950900000	0.386154600000	3.848074270000
H	-1.114385340000	0.949608760000	4.645759060000
C	0.772283660000	0.286889120000	3.832923470000
H	1.336699470000	0.777196620000	4.619658980000
C	1.450239750000	-0.391217110000	2.847220760000
C	0.670731210000	-1.031845400000	1.843390140000
C	-0.220869740000	-2.964850030000	-1.280413820000
H	-0.294352080000	-4.025048180000	-1.013572600000
H	0.666045780000	-2.833128470000	-1.902975540000
H	-1.091275980000	-2.707216540000	-1.886714420000
C	-2.921857440000	-0.064772260000	2.865026650000
H	-3.274533710000	0.534897810000	3.705480610000
H	-3.401735020000	-1.047344870000	2.917352440000
H	-3.263217220000	0.407738770000	1.937159960000
C	2.946093310000	-0.477723780000	2.801940560000
H	3.397640340000	0.067877940000	3.631851270000
H	3.329874450000	-0.059638570000	1.864641500000
H	3.284084230000	-1.517948510000	2.848775070000
C	-1.043855360000	1.741749080000	-0.653749160000
H	-2.051060200000	1.983791350000	-0.348037090000
C	0.148191260000	2.110581030000	0.054566220000
C	1.261523000000	1.580885200000	-0.679349040000
H	2.299236440000	1.680982420000	-0.397146230000
C	0.767139950000	0.931205840000	-1.859253330000
C	1.427832200000	0.188982470000	-2.878417500000
C	0.640728490000	-0.386367250000	-3.848221200000
H	1.114072500000	-0.949865140000	-4.645928520000
C	-0.772497310000	-0.286990400000	-3.832987710000
H	-1.336997610000	-0.777253770000	-4.619690330000
C	-1.450345000000	0.391174800000	-2.847250120000
C	-0.670728670000	1.031747390000	-1.843467400000
C	0.221197740000	2.964693450000	1.280277000000
H	0.294368370000	4.024911840000	1.013430190000
H	-0.665513960000	2.832764280000	1.903086770000
H	1.091832320000	2.707246720000	1.886327320000
C	2.921725180000	0.064380980000	-2.865303100000
H	3.274305780000	-0.535323860000	-3.705772450000
H	3.401679070000	1.046914570000	-2.917663460000
H	3.263099180000	-0.408150130000	-1.937452130000

C	-2.946189140000	0.477800690000	-2.801886580000
H	-3.397826240000	-0.067765280000	-3.631771700000
H	-3.329951700000	0.059746480000	-1.864565730000
H	-3.284099740000	1.518052590000	-2.848702560000

High-spin eclipsed [Cr(^{2,4,7}-MeIndenyl)₂] (S = 2), E = -1975.27694669 a.u., $\nu_1 = 27.2113$ cm⁻¹

Cr	0.639255220000	0.757326730000	0.544996320000
C	-0.610688510000	-0.005891630000	2.245125360000
C	0.645102640000	0.396369750000	2.776515190000
C	1.643847990000	-0.418841150000	2.190378720000
C	0.996827700000	-1.444987200000	1.406124010000
C	1.520026210000	-2.521290130000	0.657812490000
C	0.606672540000	-3.321110100000	-0.007018600000
H	0.970530770000	-4.163876420000	-0.586409040000
C	-0.777630800000	-3.078237380000	0.038810660000
H	-1.442310570000	-3.735148140000	-0.512406390000
C	-1.319360910000	-2.020096660000	0.748297190000
C	-0.416977150000	-1.197695140000	1.454336400000
C	-0.133352630000	2.439539930000	-0.747302340000
C	1.279622120000	2.527709590000	-0.705695320000
C	1.806188250000	1.338907410000	-1.281131490000
C	0.717467830000	0.578908120000	-1.847196140000
C	0.685309500000	-0.637480550000	-2.560122570000
C	-0.561699960000	-1.117966790000	-2.921478100000
H	-0.624945770000	-2.049033190000	-3.474930980000
C	-1.751267330000	-0.449998570000	-2.580670620000
H	-2.698983550000	-0.880767750000	-2.888263940000
C	-1.755104490000	0.734749410000	-1.864797010000
C	-0.497555570000	1.259954480000	-1.497333920000
C	0.871286740000	1.502551270000	3.762192720000
H	0.809989950000	1.118253670000	4.785888080000
H	1.858523420000	1.952337050000	3.636936760000
H	0.119193570000	2.287818520000	3.659940180000
C	2.079503280000	3.658973110000	-0.134127990000
H	3.029484760000	3.308616260000	0.275196660000
H	2.306930820000	4.395391640000	-0.912169330000
H	1.531798330000	4.173821360000	0.658057650000
H	-1.563198960000	0.434752390000	2.504354130000
H	-0.816257250000	3.190795440000	-0.376569290000
H	2.703425870000	-0.349267000000	2.392046920000
H	2.858414090000	1.115679160000	-1.389016760000
C	2.999120860000	-2.773981490000	0.613717270000
H	3.392140240000	-3.008557260000	1.608806910000
H	3.234322020000	-3.608762780000	-0.048681250000
H	3.543370880000	-1.892277920000	0.257236180000
C	1.954979870000	-1.355203750000	-2.911854110000
H	1.742371010000	-2.287037990000	-3.438066170000
H	2.595171640000	-0.738701100000	-3.551839130000

H	2.529920540000	-1.598055070000	-2.013989100000
C	-3.020804810000	1.453975650000	-1.498313820000
H	-3.065399080000	2.443231450000	-1.966336600000
H	-3.898491100000	0.888907220000	-1.816619360000
H	-3.091050460000	1.611346060000	-0.416172760000
C	-2.794952710000	-1.751489720000	0.787010210000
H	-3.338043650000	-2.473024610000	0.174741480000
H	-3.182295930000	-1.809686260000	1.809746850000
H	-3.021618000000	-0.750469850000	0.409663610000

High-spin staggered [Cr(^{2,4,7}-MeIndenyl)₂] (S = 2), E = -1975.27663048 a.u., $\nu_1 = 12.6269 \text{ cm}^{-1}$

Cr	-0.005220000000	0.000665000000	-0.001103000000
C	1.022544000000	-1.828765000000	0.792741000000
H	2.026157000000	-2.101325000000	0.498249000000
C	-0.163261000000	-2.248862000000	0.135912000000
C	-1.263792000000	-1.666815000000	0.817137000000
H	-2.301774000000	-1.794417000000	0.544034000000
C	-0.775705000000	-1.007781000000	2.006176000000
C	-1.439835000000	-0.288745000000	3.022973000000
C	-0.648030000000	0.284782000000	4.004982000000
H	-1.125129000000	0.831427000000	4.812241000000
C	0.755592000000	0.186060000000	3.989630000000
H	1.321924000000	0.659514000000	4.785384000000
C	1.437798000000	-0.491380000000	2.991673000000
C	0.657623000000	-1.109093000000	1.990825000000
C	-0.236868000000	-3.099558000000	-1.095631000000
H	-0.310440000000	-4.157949000000	-0.824378000000
H	0.651179000000	-2.973330000000	-1.717545000000
H	-1.109948000000	-2.846343000000	-1.699757000000
C	-2.934828000000	-0.154560000000	3.012810000000
H	-3.281926000000	0.424684000000	3.870017000000
H	-3.423743000000	-1.133712000000	3.042034000000
H	-3.279609000000	0.347182000000	2.101252000000
C	2.936240000000	-0.567167000000	2.948322000000
H	3.379601000000	-0.045331000000	3.797975000000
H	3.327260000000	-0.114747000000	2.029622000000
H	3.284225000000	-1.605046000000	2.965762000000
C	-1.032723000000	1.830227000000	-0.794859000000
H	-2.036341000000	2.102832000000	-0.500422000000
C	0.153062000000	2.250109000000	-0.137870000000
C	1.253581000000	1.667998000000	-0.819077000000
H	2.291543000000	1.795370000000	-0.545781000000
C	0.765530000000	1.009189000000	-2.008245000000
C	1.429654000000	0.290178000000	-3.025061000000
C	0.637854000000	-0.283204000000	-4.007162000000
H	1.114966000000	-0.829784000000	-4.814458000000
C	-0.765758000000	-0.184369000000	-3.991889000000
H	-1.332079000000	-0.657694000000	-4.787726000000

C	-1.447963000000	0.493067000000	-2.993928000000
C	-0.667795000000	1.110642000000	-1.992990000000
C	0.226642000000	3.100687000000	1.093755000000
H	0.302294000000	4.158949000000	0.822572000000
H	-0.662365000000	2.975910000000	1.714577000000
H	1.098572000000	2.846051000000	1.698950000000
C	2.924629000000	0.155743000000	-3.014748000000
H	3.271857000000	-0.422029000000	-3.872894000000
H	3.413693000000	1.134866000000	-3.042057000000
H	3.269085000000	-0.347710000000	-2.104002000000
C	-2.946406000000	0.568973000000	-2.950646000000
H	-3.389755000000	0.047527000000	-3.800544000000
H	-3.337519000000	0.116197000000	-2.032160000000
H	-3.294286000000	1.606892000000	-2.967675000000

Low-spin eclipsed [Cr(^{2,4,5,6,7}-MeIndenyl)₂] (S = 1), E = -2132.61983015 a.u., ν_1 = 30.2827 cm⁻¹

Cr	0.537408506633	0.539471685960	0.389154817228
C	-0.264802485410	0.220847111236	2.350070352669
C	1.145458014377	0.463886366145	2.414934902241
C	1.790596217876	-0.582676447089	1.670815918861
C	0.782632590569	-1.494754667452	1.193865748317
C	0.849271439899	-2.637352238513	0.351294104126
C	-0.334581523408	-3.253753121522	-0.004285520757
C	-1.611289964046	-2.751989879250	0.430019424637
C	-1.702810851948	-1.620453415796	1.217373676023
C	-0.493123354041	-0.990986256260	1.622838126892
C	-0.528101449296	2.067755661289	-0.610296541580
C	0.803765403941	2.517457015115	-0.311409861968
C	1.707918791758	1.656694603958	-1.014228530328
C	0.949691356940	0.717747615811	-1.784344017378
C	1.365770984350	-0.384055978954	-2.582346708117
C	0.387916590556	-1.185895472666	-3.138853765078
C	-1.007067579568	-0.941313078993	-2.884671980793
C	-1.429626412270	0.103765749112	-2.086429345186
C	-0.443669270874	0.965845089329	-1.534466303324
H	-1.023024403161	0.846863334427	2.796739409986
H	-1.432854348821	2.521629348954	-0.234709488026
H	2.857860257372	-0.682127612464	1.541578600049
H	2.785014325587	1.724841893125	-0.975830322124
C	1.826655881386	1.514508804330	3.233277005332
H	2.777775054134	1.810247525451	2.784809283253
H	1.204528403441	2.406800344979	3.327348714299
H	2.036595281631	1.146440623714	4.244123062796
C	1.168262667701	3.747334621470	0.457837683419
H	1.191154267203	4.625354284812	-0.197832189499
H	0.444504329490	3.945811960323	1.251527778887
H	2.154547915441	3.648736154299	0.915561908163
C	-2.981700007077	-0.995814345077	1.701974787196

H	-3.105536543531	-1.144364067904	2.780250923580
H	-2.953197782032	0.084534318514	1.530206487958
H	-3.867796208860	-1.385237994142	1.205181851426
C	-2.882647525845	0.368783761322	-1.792680570325
H	-2.989356215079	1.194812517456	-1.090238876642
H	-3.438312217414	0.630270900496	-2.698435917864
H	-3.366381225767	-0.505498216345	-1.350055985820
C	-2.014870366291	-1.858459339329	-3.528197156569
H	-3.024116076807	-1.665833050184	-3.169539478838
H	-2.023730074875	-1.738391311148	-4.617331918573
H	-1.784803144000	-2.909571237265	-3.332551045376
C	-2.836152155399	-3.513500231316	-0.009276167453
H	-2.752310767937	-4.572472007446	0.251576383949
H	-3.745806031649	-3.136254370477	0.452144314156
H	-2.967400425763	-3.466771853929	-1.095198408862
C	0.730892398930	-2.349094521805	-4.034649007716
H	0.443564521809	-3.302156790586	-3.578885804057
H	0.194731594127	-2.281529697358	-4.985683349963
H	1.793071648339	-2.396793323873	-4.263018935830
C	-0.315505069910	-4.494019411199	-0.860053535866
H	-0.649150373272	-5.372006423162	-0.295622097591
H	-0.987342941491	-4.401478793279	-1.717992560649
H	0.681831653462	-4.708422407758	-1.239167790891
C	2.195586445408	-3.133838384752	-0.105500722371
H	2.415078964580	-4.130953677400	0.288334241168
H	2.251590974730	-3.190139573115	-1.195477152759
H	2.987117159374	-2.464780779843	0.230548782049
C	2.847864816055	-0.565037410051	-2.758874724784
H	3.116401928317	-1.520961554434	-3.203498477693
H	3.266496562605	0.229381193847	-3.386335821347
H	3.346496397822	-0.499552983338	-1.786948546668

Low-spin staggered [$\text{Cr}^{(2,4,5,6,7\text{-Me})\text{Indenyl}}_2$] ($S = 1$), $E = -2132.61589068$ a.u., $\nu_1 = 15.2855 \text{ cm}^{-1}$

Cr	-0.000089182226	0.000313551187	-0.000153183108
C	-0.691667808891	-1.234078125591	-1.594510953288
C	0.020881078497	-0.101378431479	-2.110746363904
C	-0.692976501547	1.073921221160	-1.703610147998
C	-1.870013539896	0.670332450162	-0.982743973560
C	-2.867728678516	1.413603335320	-0.295617826412
C	-3.839475993166	0.715903099159	0.396337831798
C	-3.840342922211	-0.720753103848	0.458342508900
C	-2.851563913280	-1.461442048695	-0.162295219221
C	-1.865575354296	-0.763789963922	-0.913855375747
C	0.691606238516	1.235208404250	1.593645877369
C	-0.021104721243	0.102839668545	2.110400490538
C	0.692604480540	-1.072746336691	1.703832815373
C	1.869700642588	-0.669667449090	0.982819776514
C	2.867301559484	-1.413414560933	0.296033893579

C	3.838926400926	-0.716199303745	-0.396592771193
C	3.840213738787	0.720430170786	-0.458975933443
C	2.851636684708	1.461565069966	0.161449765296
C	1.865465549860	0.764421812532	0.913225949437
H	-0.396741131992	2.086540931611	-1.932871477096
H	-0.400735403686	-2.265611181057	-1.725699916374
H	0.396111681537	-2.085231922878	1.933366022338
H	0.400808083014	2.266840988612	1.724346834026
C	2.823660685001	-2.918616761601	0.351360179007
H	3.746734692010	-3.338309854171	0.760821358262
H	2.000404080018	-3.256668306975	0.979851072629
H	2.679942120815	-3.353424917348	-0.642912886099
C	2.726718064710	2.958880666746	0.107743221091
H	1.687471048002	3.232220842813	-0.100466398375
H	2.988361669931	3.411548256174	1.070445110344
H	3.349514503755	3.414743569661	-0.659270598311
C	-2.824216271893	2.918847342684	-0.350008556545
H	-1.997295278918	3.257424917466	-0.973378616790
H	-3.744980392178	3.338399625433	-0.764899209863
H	-2.686699502758	3.353305463753	0.645245249053
C	-2.726280539321	-2.958748639456	-0.109229594343
H	-2.987747711535	-3.411035962781	-1.072157702624
H	-1.686988376341	-3.231936720097	0.098949841295
H	-3.349049196734	-3.415128262713	0.657500597271
C	1.237358753013	-0.140788951490	-2.981041420786
H	1.846790716633	0.754027575365	-2.840220998594
H	1.859409494666	-1.006222021077	-2.744020531296
H	0.961626806949	-0.200790182946	-4.039988770296
C	-1.237645357756	0.142804204540	2.980586633457
H	-1.859361096321	1.008425934177	2.743385259836
H	-1.847387746994	-0.751813405026	2.839831665231
H	-0.961989069296	0.202852860304	4.039551561219
C	4.922172801415	-1.458274277878	-1.137584853242
H	4.773804476414	-2.535732467317	-1.098720175912
H	4.956637999044	-1.164706585465	-2.191393741592
H	5.911947494894	-1.245011632137	-0.719774677037
C	4.947237625928	1.376572827713	-1.245173600358
H	5.926010174109	1.012368276680	-0.920711214295
H	4.867186892591	1.151466482319	-2.314602610133
H	4.949395532373	2.458226755830	-1.132366521697
C	-4.923352503013	1.457432397308	1.136920645907
H	-4.956212054889	1.166062275773	2.191424087626
H	-4.777210897638	2.535095939326	1.095531366449
H	-5.913091234458	1.241276246012	0.720581913254
C	-4.947217950483	-1.377325135489	1.244356827592
H	-4.868993960547	-1.149860954992	2.313401923849
H	-5.926235865905	-1.015526921494	0.917865526450
H	-4.947312472799	-2.459203244986	1.133766994542

High-spin eclipsed [Cr(^{2,4,5,6,7}-Me₅Indenyl)₂] (S = 2), E = -2132.61547579 a.u., $\nu_1 = 25.5289 \text{ cm}^{-1}$

Cr	0.644346000000	0.773160000000	0.548765000000
C	-0.196176000000	0.130652000000	2.536042000000
C	1.210559000000	0.231357000000	2.660795000000
C	1.793073000000	-0.709910000000	1.771156000000
C	0.741902000000	-1.539488000000	1.224736000000
C	0.767134000000	-2.645029000000	0.354690000000
C	-0.449576000000	-3.231098000000	0.013083000000
C	-1.684197000000	-2.700216000000	0.477572000000
C	-1.728296000000	-1.573567000000	1.295532000000
C	-0.502837000000	-1.004658000000	1.692747000000
C	-0.564488000000	2.127700000000	-0.761300000000
C	0.716784000000	2.715631000000	-0.590385000000
C	1.674274000000	1.835032000000	-1.149092000000
C	0.974760000000	0.769756000000	-1.834881000000
C	1.439143000000	-0.322613000000	-2.592740000000
C	0.488876000000	-1.179789000000	-3.142888000000
C	-0.901569000000	-0.990878000000	-2.914115000000
C	-1.371248000000	0.055858000000	-2.123967000000
C	-0.427032000000	0.959558000000	-1.602868000000
H	-0.908546000000	0.723992000000	3.090964000000
H	-1.493363000000	2.573455000000	-0.435236000000
H	2.855773000000	-0.863441000000	1.649085000000
H	2.739696000000	2.014024000000	-1.166973000000
C	1.954077000000	1.179399000000	3.552237000000
H	2.919907000000	1.455552000000	3.123487000000
H	1.381848000000	2.092874000000	3.728237000000
H	2.145571000000	0.716005000000	4.526037000000
C	1.004091000000	4.022356000000	0.084995000000
H	0.973712000000	4.841502000000	-0.641490000000
H	0.265822000000	4.241670000000	0.859445000000
H	1.995231000000	4.024721000000	0.543783000000
C	-3.017542000000	-0.969305000000	1.789294000000
H	-3.476197000000	-1.577234000000	2.576980000000
H	-2.840964000000	0.023909000000	2.203858000000
H	-3.753193000000	-0.862424000000	0.989523000000
C	-2.835575000000	0.263773000000	-1.841171000000
H	-2.976917000000	1.039040000000	-1.088090000000
H	-3.384244000000	0.568867000000	-2.738416000000
H	-3.304289000000	-0.648206000000	-1.464624000000
C	-1.869300000000	-1.940046000000	-3.573094000000
H	-2.889480000000	-1.787448000000	-3.225573000000
H	-1.871097000000	-1.809704000000	-4.661501000000
H	-1.602904000000	-2.983192000000	-3.384730000000
C	-2.957743000000	-3.398389000000	0.071871000000
H	-2.916388000000	-4.465679000000	0.309225000000
H	-3.828283000000	-2.983449000000	0.576872000000
H	-3.130133000000	-3.324021000000	-1.007461000000

C	0.917751000000	-2.334206000000	-4.012833000000
H	0.654808000000	-3.296177000000	-3.559819000000
H	0.421446000000	-2.301917000000	-4.987731000000
H	1.991789000000	-2.333270000000	-4.190418000000
C	-0.480934000000	-4.471571000000	-0.842758000000
H	-0.789633000000	-5.346861000000	-0.259183000000
H	-1.194997000000	-4.377074000000	-1.664547000000
H	0.494520000000	-4.694596000000	-1.271475000000
C	2.087032000000	-3.171634000000	-0.143284000000
H	2.316327000000	-4.156714000000	0.276269000000
H	2.094410000000	-3.269429000000	-1.231359000000
H	2.899679000000	-2.498806000000	0.130568000000
C	2.920475000000	-0.503566000000	-2.803312000000
H	3.245100000000	-1.521476000000	-2.575222000000
H	3.212500000000	-0.291872000000	-3.837527000000
H	3.485711000000	0.170642000000	-2.159318000000

High-spin staggered [Cr(^{2,4,5,6,7}-Me₅Indenyl)₂] (S = 2), E = -2132.61138908 a.u., $\nu_1 = 6.2967 \text{ cm}^{-1}$

Cr	-0.000142000000	0.000338000000	-0.000208000000
C	-0.872111000000	-1.157967000000	-1.709171000000
C	-0.212413000000	-0.024941000000	-2.248493000000
C	-0.852118000000	1.131993000000	-1.736596000000
C	-2.028073000000	0.723759000000	-0.998693000000
C	-2.999504000000	1.460380000000	-0.292478000000
C	-3.979803000000	0.750586000000	0.399354000000
C	-3.991089000000	-0.671370000000	0.418013000000
C	-3.024596000000	-1.414456000000	-0.258135000000
C	-2.040758000000	-0.711858000000	-0.981721000000
C	0.871972000000	1.158541000000	1.708773000000
C	0.212108000000	0.025608000000	2.248083000000
C	0.851649000000	-1.131416000000	1.736184000000
C	2.027665000000	-0.723344000000	0.998290000000
C	2.998992000000	-1.460102000000	0.292071000000
C	3.979399000000	-0.750444000000	-0.399747000000
C	3.990898000000	0.671511000000	-0.418388000000
C	3.024512000000	1.414731000000	0.257764000000
C	2.040563000000	0.712271000000	0.981332000000
H	-0.559662000000	2.147349000000	-1.962370000000
H	-0.596639000000	-2.183388000000	-1.909398000000
H	0.559038000000	-2.146733000000	1.961933000000
H	0.596646000000	2.184000000000	1.909010000000
C	2.937643000000	-2.965916000000	0.292996000000
H	3.835034000000	-3.410367000000	0.734211000000
H	2.081490000000	-3.317573000000	0.868514000000
H	2.841012000000	-3.368172000000	-0.720447000000
C	2.991116000000	2.921106000000	0.225426000000
H	2.859840000000	3.302033000000	-0.792694000000
H	2.166079000000	3.302467000000	0.826868000000

H	3.913875000000	3.357849000000	0.618634000000
C	-2.938385000000	2.966203000000	-0.293426000000
H	-2.082305000000	3.317984000000	-0.868975000000
H	-3.835859000000	3.410511000000	-0.734619000000
H	-2.841785000000	3.368486000000	0.720009000000
C	-2.990985000000	-2.920826000000	-0.225790000000
H	-2.165892000000	-3.302070000000	-0.827230000000
H	-2.859653000000	-3.301730000000	0.792331000000
H	-3.913682000000	-3.357703000000	-0.618995000000
C	0.992973000000	-0.046121000000	-3.139168000000
H	0.692366000000	-0.058256000000	-4.192181000000
H	1.618014000000	0.834582000000	-2.978877000000
H	1.604732000000	-0.931438000000	-2.954757000000
C	-0.993280000000	0.046956000000	3.138752000000
H	-1.618771000000	-0.833352000000	2.978030000000
H	-0.692682000000	0.058430000000	4.191774000000
H	-1.604582000000	0.932673000000	2.954757000000
C	5.053685000000	-1.482877000000	-1.163370000000
H	4.976083000000	-2.561785000000	-1.041498000000
H	5.000152000000	-1.265583000000	-2.236064000000
H	6.053440000000	-1.182571000000	-0.833757000000
C	5.075840000000	1.365874000000	-1.202270000000
H	6.069984000000	1.121634000000	-0.812788000000
H	5.067902000000	1.057501000000	-2.253103000000
H	4.968334000000	2.448742000000	-1.175179000000
C	-5.054203000000	1.482870000000	1.162960000000
H	-5.000561000000	1.265700000000	2.235673000000
H	-4.976834000000	2.561782000000	1.040972000000
H	-6.053913000000	1.182320000000	0.833434000000
C	-5.075941000000	-1.365891000000	1.201880000000
H	-5.068114000000	-1.057457000000	2.252695000000
H	-6.070111000000	-1.121857000000	0.812333000000
H	-4.968233000000	-2.448741000000	1.174852000000

Low-spin eclipsed $[\text{Cr}^{(1,2,3,4,5,6,7\text{-MeIndenyl)}_2]$ ($S = 1$), $E = -2289.95611508$ a.u., $\nu_1 = 20.2908$ cm^{-1}

Cr	0.539111480000	0.529780970000	0.376188760000
C	-0.237898230000	0.265442130000	2.369662000000
C	1.186290020000	0.437136260000	2.392619910000
C	1.792133470000	-0.625733130000	1.632275030000
C	0.726742460000	-1.499149110000	1.182626070000
C	0.735789940000	-2.678728330000	0.375419150000
C	-0.475155480000	-3.236273410000	0.012384830000
C	-1.720239720000	-2.664447360000	0.449674770000
C	-1.759218520000	-1.565433760000	1.283748130000
C	-0.524956630000	-0.945458880000	1.648928240000
C	-0.557120690000	2.035263230000	-0.633397720000
C	0.760518570000	2.519055750000	-0.311516550000
C	1.728389610000	1.697711290000	-0.982699410000

C	1.014812860000	0.735574420000	-1.780782370000
C	1.468235480000	-0.342078400000	-2.603432190000
C	0.528831660000	-1.213171080000	-3.122915110000
C	-0.876774530000	-1.011175430000	-2.906613020000
C	-1.346816070000	0.058504130000	-2.171124480000
C	-0.400811730000	0.935887930000	-1.562173820000
C	1.929017360000	1.466269040000	3.186156550000
H	2.865622770000	1.748355450000	2.701641200000
H	1.340659280000	2.375826860000	3.313927970000
H	2.176712230000	1.089874000000	4.186074370000
C	1.060662230000	3.756566050000	0.474922940000
H	1.069562740000	4.642421080000	-0.171671200000
H	0.314483340000	3.926982370000	1.253041340000
H	2.034037190000	3.696456130000	0.963436300000
C	-3.048724660000	-1.044460890000	1.866738820000
H	-2.898556610000	-0.728900470000	2.898935510000
H	-3.433038420000	-0.178202090000	1.316296850000
H	-3.828280470000	-1.804214280000	1.870679690000
C	-2.822044650000	0.330488460000	-2.028298130000
H	-3.226276100000	-0.122339740000	-1.116463520000
H	-3.015765660000	1.400512680000	-1.979503090000
H	-3.387789700000	-0.063554280000	-2.871388840000
C	-1.841219070000	-1.981328760000	-3.546046110000
H	-2.805973590000	-1.987077020000	-3.042977010000
H	-2.017043210000	-1.740975900000	-4.601792170000
H	-1.455770130000	-3.001075520000	-3.518677400000
C	-2.993805030000	-3.327327120000	-0.018020130000
H	-3.181409210000	-4.269473140000	0.510399730000
H	-3.864056870000	-2.689366150000	0.120353390000
H	-2.937631080000	-3.569055180000	-1.080891510000
C	0.933453900000	-2.410383640000	-3.947668100000
H	0.650493820000	-3.339321440000	-3.442387180000
H	0.436150750000	-2.415054350000	-4.922214880000
H	2.005485790000	-2.457527910000	-4.119868920000
C	-0.560233990000	-4.482172870000	-0.833932620000
H	-1.146628100000	-5.259723930000	-0.334768740000
H	-1.058763320000	-4.279997160000	-1.786582180000
H	0.414976540000	-4.901191680000	-1.065806780000
C	2.061861860000	-3.266348660000	-0.029945100000
H	1.981081200000	-4.307852850000	-0.332622650000
H	2.495670970000	-2.713738720000	-0.869024450000
H	2.771965460000	-3.222123870000	0.795428910000
C	2.940976520000	-0.451614780000	-2.908606650000
H	3.493988720000	-0.948388230000	-2.103628620000
H	3.130818440000	-1.007220370000	-3.824895490000
H	3.376799690000	0.539165100000	-3.034765560000
C	3.277471390000	-0.801637650000	1.501959060000
H	3.662287700000	-1.530712130000	2.224692350000
H	3.576114800000	-1.132355450000	0.507918850000
H	3.786668610000	0.143361050000	1.697064650000

C	3.208237950000	1.916582600000	-0.863278440000
H	3.769951040000	0.984685930000	-0.844820040000
H	3.592619230000	2.523467760000	-1.691223120000
H	3.434958520000	2.452002130000	0.060444540000
C	-1.188427040000	1.202255340000	3.055388760000
H	-2.104756240000	1.357658280000	2.489145710000
H	-1.466972600000	0.834215640000	4.049587140000
H	-0.720726540000	2.178797240000	3.192941300000
C	-1.820575320000	2.686249670000	-0.150879080000
H	-2.244145690000	3.357708880000	-0.907081020000
H	-2.589043080000	1.960857260000	0.115662500000
H	-1.619784330000	3.287924130000	0.736876280000

Low-spin staggered $[\text{Cr}^{(1,2,3,4,5,6,7\text{-MeIndenyl})_2}]$ ($S = 1$), $E = -2289.95430388$ a.u., $\nu_1 = 11.8756 \text{ cm}^{-1}$

Cr	-0.001327722170	-0.128800210916	0.002287418251
C	-0.785390141949	-1.347862886375	-1.553369301632
C	-0.021697602443	-0.261868857488	-2.108743737194
C	-0.635933950834	0.978125361477	-1.724134410396
C	-1.824796704508	0.666210082806	-0.975383633474
C	-2.784816212863	1.497887728052	-0.321928701205
C	-3.728102725947	0.898865385706	0.490339263528
C	-3.821271849710	-0.529581142980	0.608207437178
C	-2.962866002288	-1.363420396933	-0.083986218888
C	-1.917651881565	-0.772233719950	-0.858837967293
C	0.630904877137	1.080638109766	1.660268551649
C	0.020888963803	-0.136549394798	2.117614989593
C	0.788003876720	-1.250803410917	1.626630602911
C	1.918033753238	-0.713523572972	0.898765144204
C	2.965575035115	-1.345888283670	0.160429802942
C	3.821733813405	-0.551510506138	-0.579278129973
C	3.723551639581	0.881107544029	-0.546063649450
C	2.778019313083	1.523891429084	0.229336810493
C	1.820545039545	0.728998491428	0.930599148765
C	3.111433257431	-2.844484181641	0.238135379940
H	2.875624887292	-3.198122436345	1.241087673057
H	2.436164214083	-3.357488539032	-0.454997968144
H	4.124917148147	-3.169616272807	0.010520407304
C	2.773917972456	3.021726625868	0.408416213952
H	2.105400056024	3.524501133388	-0.298570793593
H	2.441386643104	3.281519801358	1.412628370334
H	3.769684097763	3.443701554308	0.277575093557
C	-2.785266580390	2.982559422356	-0.589059546129
H	-2.118207107182	3.528252363104	0.086827164767
H	-2.453504151718	3.183554279089	-1.606958629565
H	-3.782327887168	3.408487415838	-0.483142831443
C	-3.103589851943	-2.864483440541	-0.071226605454
H	-2.861337775262	-3.277916198971	-1.049383934553
H	-2.430737319814	-3.331947427073	0.655730370317

H	-4.117434114772	-3.178333592201	0.170403018711
C	1.174213608656	-0.391605718550	-2.999301845155
H	1.890461479115	0.411676478805	-2.818122546669
H	1.699230215061	-1.331666360693	-2.826643049152
H	0.887781569824	-0.356391605356	-4.057166724915
C	-1.173512661725	-0.217893900767	3.015870666684
H	-1.891420224239	0.572658763445	2.790749111753
H	-1.697045573368	-1.167165787107	2.897364002202
H	-0.885697767891	-0.122406448299	4.069637928057
C	4.893233796491	-1.145197764108	-1.459959490458
H	4.935289333459	-2.229324998588	-1.395259504963
H	4.712381024927	-0.894031223194	-2.510732225783
H	5.884667922930	-0.755049582491	-1.210309133918
C	4.705693648516	1.667534048379	-1.380358772236
H	5.724560108971	1.602672830801	-0.981690339823
H	4.744543901506	1.279207334791	-2.401515336292
H	4.438987087389	2.719919144107	-1.446256462138
C	-4.712797594764	1.729825382305	1.277042994982
H	-4.749499090424	1.402882829364	2.319547948905
H	-4.450170658752	2.785289264053	1.279760041459
H	-5.731624866064	1.637296230454	0.883760200280
C	-4.889684012120	-1.073991884063	1.523840961346
H	-4.709152637462	-0.759403137408	2.557454771041
H	-5.882995354418	-0.703778192877	1.252227855293
H	-4.927058677216	-2.160229814767	1.524315964804
C	-0.078609995958	2.318888507996	-2.102728394597
H	-0.529352769906	2.701557402738	-3.026020940810
H	-0.231553861878	3.065123462917	-1.324410136921
H	0.996580100558	2.239707012946	-2.273892114937
C	-0.459061155604	-2.794264480781	-1.787512763528
H	-0.608910122104	-3.407298882165	-0.899519544382
H	-1.067645130359	-3.221088338866	-2.593353820144
H	0.585421187189	-2.898828850113	-2.085193935431
C	0.467671024589	-2.681755840508	1.948025872061
H	0.619228913628	-3.347037077147	1.098746225555
H	1.078762519033	-3.056428447580	2.777558640117
H	-0.576108720720	-2.772153550496	2.252883148909
C	0.072088616319	2.440185228093	1.963139210096
H	0.526539539076	2.875896121674	2.860766487343
H	0.220237795755	3.141225065795	1.142863302301
H	-1.002175523426	2.370074521354	2.144198945994

High-spin eclipsed $[\text{Cr}(\text{}^{1,2,3,4,5,6,7\text{-Me}}\text{Indenyl})_2]$ ($S = 2$), $E = -2289.94988659$ a.u., $\nu_1 = 22.9311$ cm^{-1}

Cr	0.640004132262	0.736625837818	0.530077480883
C	-0.244446615869	0.196684511318	2.529054195344
C	1.169641116713	0.252567251687	2.658403894102
C	1.761717472234	-0.723378520598	1.805365963562
C	0.684573188250	-1.528441671474	1.250313026591

C	0.678695911474	-2.648204106740	0.388092948806
C	-0.548795307539	-3.206222255226	0.036317503045
C	-1.772987698135	-2.626334222992	0.459484258336
C	-1.794230105159	-1.517897866948	1.303086562961
C	-0.558926371987	-0.956621553017	1.702536794600
C	-0.530534516548	2.113428452495	-0.789397628961
C	0.761277432149	2.680774645004	-0.583134825518
C	1.749158170968	1.808870762840	-1.113534502074
C	1.053299366508	0.733926468363	-1.804970621687
C	1.526525977617	-0.380024930374	-2.538760668634
C	0.590758030296	-1.222283173021	-3.136313762196
C	-0.802444908165	-1.025606569609	-2.950952239801
C	-1.289807793919	0.049308493202	-2.210601186056
C	-0.362377727451	0.945178568428	-1.635664736374
C	1.923667899187	1.213183612852	3.529148579141
H	2.884420844349	1.490695876025	3.092000457432
H	1.359662740853	2.132580572704	3.694324805001
H	2.123615049167	0.771902850214	4.512195285629
C	1.031400679389	3.980273447730	0.115416876034
H	0.264909897965	4.201686123003	0.860143885780
H	1.995197672134	3.974043480532	0.627093116272
H	1.040482124609	4.811413072193	-0.598935564509
C	-3.096096199469	-0.954795941367	1.817183905784
H	-3.009748372435	-0.665971423132	2.864032752311
H	-3.413588105545	-0.064974368128	1.260630271748
H	-3.901359340752	-1.684729581213	1.749568782780
C	-2.774262512991	0.262627287214	-2.061283793166
H	-3.157260430080	-0.208959883249	-1.149807627490
H	-3.020302253202	1.321580294463	-2.014536319044
H	-3.322828904397	-0.160799459334	-2.902363464730
C	-1.779600311346	-2.000943871678	-3.565613206086
H	-2.610088365654	-2.205263488129	-2.889006728901
H	-2.207788899809	-1.618345827575	-4.500512045886
H	-1.307422132977	-2.954596871532	-3.795461858599
C	-3.072292502219	-3.236473246661	-0.015552640462
H	-3.475846323648	-3.958427605302	0.705114765381
H	-3.837183765327	-2.475621264326	-0.175743886465
H	-2.941220258617	-3.763313097104	-0.959716267879
C	1.053910116616	-2.354378816141	-4.024307230773
H	0.961545063436	-3.330192848130	-3.532798970001
H	0.460237843408	-2.400742968678	-4.940022051532
H	2.093820586718	-2.234553851848	-4.322187749679
C	-0.588745034352	-4.464571032506	-0.798060646865
H	-1.326902013414	-5.170565603137	-0.410821291930
H	-0.857496681876	-4.257064876415	-1.839742606556
H	0.372961570554	-4.974467109558	-0.803193266763
C	1.961804095060	-3.239879586127	-0.139639875131
H	2.240493851099	-4.154395950159	0.396756321433
H	1.867807666076	-3.496661649203	-1.195717796084
H	2.788665221477	-2.543194159021	-0.051559172105

C	3.006352591259	-0.648526914708	-2.669350076918
H	3.218287056280	-1.718113825673	-2.662298815404
H	3.421369586112	-0.238496666330	-3.597540232820
H	3.559536849408	-0.207807323957	-1.844166595324
C	3.243618378379	-0.971432963520	1.734659765772
H	3.497323685807	-1.970483163393	2.101252741259
H	3.647339446271	-0.882785814082	0.723030026702
H	3.776429422132	-0.251337554242	2.357274245663
C	3.220371669998	2.122926736548	-1.124129030088
H	3.823404117867	1.400571440616	-0.567278855976
H	3.611141216360	2.156605790909	-2.144917206124
H	3.398244318346	3.101293301166	-0.675370238316
C	-1.193274543207	1.091850976012	3.274863530328
H	-2.043898654902	1.393691590802	2.663934169399
H	-1.588074564371	0.607025146054	4.175129627854
H	-0.684890065098	2.002349809961	3.597926481622
C	-1.810598729660	2.764750097687	-0.347868495584
H	-2.279318837020	3.332734035389	-1.159713084157
H	-2.540190876788	2.037961188084	0.009468224773
H	-1.621628994861	3.465445914244	0.467523806318

High-spin staggered [Cr(^{1,2,3,4,5,6,7}-MeIndenyl)₂] (S = 2), E = -2289.94827429 a.u., ν_1 = 8.5851 cm⁻¹

Cr	-0.000852000000	0.034006000000	0.000751000000
C	-0.797595000000	-1.152313000000	-1.728949000000
C	-0.165681000000	0.012309000000	-2.247808000000
C	-0.828598000000	1.168659000000	-1.749037000000
C	-1.998864000000	0.720252000000	-1.013879000000
C	-2.996550000000	1.428737000000	-0.300860000000
C	-3.896066000000	0.697026000000	0.471379000000
C	-3.888071000000	-0.725438000000	0.472310000000
C	-2.968147000000	-1.446460000000	-0.287539000000
C	-1.980971000000	-0.722924000000	-1.002344000000
C	0.840547000000	1.219950000000	1.708151000000
C	0.167650000000	0.087536000000	2.248188000000
C	0.787858000000	-1.099916000000	1.769891000000
C	1.972194000000	-0.706583000000	1.025949000000
C	2.945136000000	-1.464393000000	0.329253000000
C	3.869989000000	-0.780586000000	-0.456668000000
C	3.910893000000	0.640853000000	-0.487652000000
C	3.017336000000	1.409110000000	0.257573000000
C	2.007615000000	0.735879000000	0.989267000000
C	2.983282000000	-2.968305000000	0.454346000000
H	2.593924000000	-3.287047000000	1.418819000000
H	2.391786000000	-3.468556000000	-0.321541000000
H	4.003346000000	-3.345717000000	0.380153000000
C	3.111385000000	2.915250000000	0.295493000000
H	2.585944000000	3.386882000000	-0.543241000000
H	2.683149000000	3.308964000000	1.213785000000

H	4.148001000000	3.251366000000	0.258406000000
C	-3.083960000000	2.933148000000	-0.389432000000
H	-2.514127000000	3.432557000000	0.403232000000
H	-2.699189000000	3.289247000000	-1.342412000000
H	-4.116341000000	3.274997000000	-0.312937000000
C	-3.013072000000	-2.953404000000	-0.364712000000
H	-2.585268000000	-3.306817000000	-1.299789000000
H	-2.460507000000	-3.430374000000	0.453146000000
H	-4.037417000000	-3.324519000000	-0.323421000000
C	1.055594000000	0.019605000000	-3.117321000000
H	1.654578000000	0.917478000000	-2.960021000000
H	1.699128000000	-0.837137000000	-2.912736000000
H	0.779320000000	-0.015733000000	-4.177095000000
C	-1.051984000000	0.138908000000	3.118569000000
H	-1.668892000000	1.010412000000	2.895122000000
H	-1.678771000000	-0.743236000000	2.982130000000
H	-0.773161000000	0.189678000000	4.177046000000
C	4.872620000000	-1.536163000000	-1.295685000000
H	5.882666000000	-1.487194000000	-0.871389000000
H	4.609212000000	-2.586579000000	-1.403067000000
H	4.935453000000	-1.113754000000	-2.301725000000
C	4.957613000000	1.290827000000	-1.359421000000
H	5.964020000000	0.934613000000	-1.118246000000
H	4.786706000000	1.054123000000	-2.415670000000
H	4.957704000000	2.374644000000	-1.272065000000
C	-4.922640000000	1.399441000000	1.327278000000
H	-4.699729000000	2.457390000000	1.450784000000
H	-5.932339000000	1.318137000000	0.907179000000
H	-4.963525000000	0.958671000000	2.326609000000
C	-4.913324000000	-1.428857000000	1.328026000000
H	-4.758240000000	-1.200639000000	2.388469000000
H	-5.931714000000	-1.109154000000	1.085628000000
H	-4.869790000000	-2.510445000000	1.225526000000
C	-0.416582000000	2.575480000000	-2.077831000000
H	-1.029792000000	3.000783000000	-2.880574000000
H	-0.492514000000	3.241687000000	-1.218135000000
H	0.619779000000	2.597123000000	-2.418469000000
C	-0.335676000000	-2.550604000000	-2.026673000000
H	-0.406591000000	-3.204531000000	-1.157250000000
H	-0.918135000000	-3.009265000000	-2.834032000000
H	0.707806000000	-2.542802000000	-2.345740000000
C	0.319827000000	-2.485125000000	2.114737000000
H	0.389643000000	-3.168048000000	1.267922000000
H	0.900502000000	-2.918059000000	2.937396000000
H	-0.723909000000	-2.463842000000	2.432213000000
C	0.435671000000	2.639032000000	1.990715000000
H	1.055645000000	3.090305000000	2.773866000000
H	0.505998000000	3.275208000000	1.107919000000
H	-0.597915000000	2.674467000000	2.338688000000

S6 Standardized analysis of the ΔH and ΔS effect over $T_{1/2}$

To analyze the relative weights that ΔH and ΔS have over the tuning of $T_{1/2}$, one must calculate the standardized multilinear regression coefficients. To do so, first we have to autoscale both quantities, a process that consists on removing the average value and dividing among the standard deviation of the sample for each entry in the dataset. Once this is done, the relationship $T_{1/2} = \Delta H / \Delta S$ can be linearized using logarithms, and the corresponding standardized regression coefficients can be extracted.

The results for the model are provided below

Linear function: $\ln(T_{1/2}) = a_1 \cdot \ln(\Delta H) - a_2 \cdot \ln(\Delta S) + b$

Eclipsed configuration:

$$\ln(T_{1/2}) = 0.516909725 \cdot \ln(\Delta H) - 0.331840085 \cdot \ln(\Delta S) + 5.467609061$$

$$R^2 = 0.998879253$$

Staggered configuration:

$$\ln(T_{1/2}) = 0.974318895 \cdot \ln(\Delta H) - 0.200565399 \cdot \ln(\Delta S) + 4.472974499$$

$$R^2 = 0.999993287$$

The ratio between a_1 and a_2 gives us information about the relevant weight of such quantities in tuning $T_{1/2}$