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Ligand Conformations and Spin States in Open Metallocenes of the First Row Transition Metals Having U-Shaped 2,4-Dimethylpentadienyl Ligands

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Supporting Information

Tables S1 to S36: Atomic coordinates of the optimized structures for the $(2,4\text{-}Me_2C_5H_5)_2M$ (M =Ti, V, Cr, Mn, Fe, Co, Ni) complexes.

Tables S37 to S72: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $(2,4\text{-}Me_2C_5H_5)_2M$ (M =Ti, V, Cr, Mn, Fe, Co, Ni) complexes.

Tables S73 to S79: The distances (in Å) of M-C bonds for the $(2,4\text{-}Me_2C_5H_5)_2M$ (M = Ti, V, Cr, Mn, Fe, Co, Ni) complexes;

Tables S80 to S86: Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO and LUMO energies (in hartree), HOMO-LUMO gaps (in eV), the χ angles for the $(2,4\text{-}Me_2C_5H_5)_2M$ (M = Ti, V, Cr, Mn, Fe, Co, Ni) complexes by the B3LYP* method;

Table S87: The comparison of the relative energies (ΔE in kcal/mol) and the conformation angle (χ) for the simpler model systems $(C_5H_7)_2M$ (M = Ti, V, Cr, Mn, Fe, Co, Ni) predicted by the B3LYP* and M06L methods.

Figures S1-S7: The optimized $(C_5H_7)_2M$ structures (M = Ti, V, Cr, Mn, Fe, Co, Ni) by the B3LYP* method.

Complete Gaussian09 reference (Reference 38).

Table S1. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Ti** structure **Ti-1S.**

	B3LYP*		
	x	Y	z
6	1.519845	1.993330	0.447277
1	1.276219	2.127400	1.500072
1	1.629869	2.928207	-0.102406
6	2.097398	-0.475978	0.471445
6	0.194574	-0.261246	2.131070
1	-0.560673	-0.823706	2.682330
1	0.462650	0.685478	2.600583
6	2.254746	0.865079	-0.015953
1	2.665507	-1.221262	-0.089517
6	1.158751	-1.027904	1.399414
6	-0.194574	-0.261246	-2.131070
1	-0.462650	0.685478	-2.600583
1	0.560673	-0.823707	-2.682330
6	-2.097398	-0.475978	-0.471445
6	-1.519844	1.993330	-0.447277
1	-1.629869	2.928207	0.102406
1	-1.276219	2.127400	-1.500072
6	-1.158751	-1.027904	-1.399414
1	-2.665507	-1.221262	0.089517
6	-2.254746	0.865079	0.015953
6	1.094736	-2.543524	1.493720
1	0.065813	-2.884969	1.670136
1	1.701586	-2.888482	2.345581
1	1.472514	-3.037989	0.588622
6	3.164732	1.048478	-1.219743
1	2.774301	1.821462	-1.895133
1	3.287705	0.120568	-1.793234
1	4.160959	1.378912	-0.885920
6	-3.164732	1.048479	1.219743
1	-4.160958	1.378912	0.885920
1	-2.774301	1.821462	1.895133
1	-3.287705	0.120568	1.793234
6	-1.094736	-2.543524	-1.493720
1	-1.701586	-2.888482	-2.345581
1	-1.472514	-3.037989	-0.588622
1	-0.065813	-2.884969	-1.670135
22	0.000000	0.382270	0.000000

Table S2. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Ti** structure **Ti-2S.**

	B3LYP*		
	x	y	z
6	-1.517213	1.573580	1.256655
1	-0.939046	2.088607	2.019964
1	-2.538848	1.343546	1.559561
6	-0.000270	1.916874	-0.731638
6	1.516800	1.573997	1.256627
1	2.538501	1.344240	1.559520
1	0.938521	2.088907	2.019933
6	-1.295253	1.798896	-0.132949
1	-0.000292	1.983404	-1.822375
6	1.294756	1.799229	-0.132978
6	-1.516800	-1.573979	1.256632
1	-0.938528	-2.088895	2.019938
1	-2.538500	-1.344216	1.559523
6	0.000267	-1.916881	-0.731633
6	1.517212	-1.573576	1.256658
1	2.538847	-1.343538	1.559558
1	0.939057	-2.088618	2.019967
6	-1.294758	-1.799223	-0.132974
1	0.000288	-1.983418	-1.822370
6	1.295251	-1.798899	-0.132948
22	0.000005	-0.000004	0.571693
6	-2.488848	1.794765	-1.072428
1	-3.290628	1.145589	-0.696687
1	-2.226685	1.470309	-2.088577
1	-2.904089	2.812557	-1.139710
6	2.488330	1.795377	-1.072484
1	3.290266	1.146384	-0.696760
1	2.903335	2.813265	-1.139775
1	2.226219	1.470859	-2.088627
6	2.488844	-1.794772	-1.072428
1	2.904094	-2.812562	-1.139696
1	3.290620	-1.145584	-0.696698
1	2.226678	-1.470333	-2.088582
6	-2.488333	-1.795374	-1.072479
1	-2.903340	-2.813262	-1.139765
1	-2.226222	-1.470862	-2.088624
1	-3.290267	-1.146377	-0.696759

Table S3. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Ti** structure **Ti-3S.**

	B3LYP*		
	x	y	z
6	-1.015170	1.504903	-1.392859
1	-1.121421	0.947441	-2.319818
1	-0.647611	2.523572	-1.531747
6	-2.319902	-0.000013	0.162687
6	-1.015165	-1.504916	-1.392860
1	-0.647581	-2.523576	-1.531746
1	-1.121436	-0.947456	-2.319816
6	-1.898447	1.292321	-0.288701
1	-2.928165	-0.000011	1.069864
6	-1.898431	-1.292345	-0.288691
6	1.015203	-1.504914	1.392865
1	1.121442	-0.947434	2.319811
1	0.647645	-2.523582	1.531762
6	2.319892	0.000015	-0.162700
6	1.015177	1.504909	1.392875
1	0.647607	2.523572	1.531776
1	1.121449	0.947441	2.319827
6	1.898447	-1.292322	0.288689
1	2.928136	0.000022	-1.069889
6	1.898432	1.292342	0.288699
22	-0.000007	0.000002	0.000005
6	-2.345172	-2.489854	0.532827
1	-1.584497	-3.280828	0.523677
1	-3.261737	-2.914516	0.093200
1	-2.559019	-2.226419	1.577232
6	-2.345209	2.489829	0.532807
1	-1.584541	3.280809	0.523666
1	-2.559068	2.226394	1.577210
1	-3.261772	2.914482	0.093168
6	2.345168	2.489856	-0.532814
1	3.261746	2.914502	-0.093202
1	1.584502	3.280838	-0.523640
1	2.558990	2.226429	-1.577226
6	2.345199	-2.489822	-0.532835
1	3.261791	-2.914451	-0.093234
1	2.559007	-2.226386	-1.577248
1	1.584552	-3.280821	-0.523658

Table S4. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Ti** structure **Ti-1T.**

	B3LYP*		
	x	y	z
6	-1.555539	1.758632	1.236275
1	-0.896369	2.151758	2.004103
1	-2.584982	1.595823	1.555744
6	0.000000	1.926177	-0.744850
6	1.555539	1.758632	1.236275
1	2.584982	1.595823	1.555744
1	0.896369	2.151758	2.004103
6	-1.296810	1.888052	-0.135167
1	0.000000	1.951058	-1.836804
6	1.296810	1.888052	-0.135167
6	-1.555539	-1.758632	1.236275
1	-0.896369	-2.151758	2.004103
1	-2.584982	-1.595823	1.555744
6	0.000000	-1.926177	-0.744850
6	1.555539	-1.758632	1.236275
1	2.584982	-1.595823	1.555744
1	0.896369	-2.151758	2.004103
6	-1.296810	-1.888052	-0.135167
1	0.000000	-1.951058	-1.836804
6	1.296810	-1.888052	-0.135167
22	0.000000	0.000000	0.645310
6	-2.477467	1.832700	-1.092379
1	-3.336985	1.323301	-0.638301
1	-2.226124	1.328294	-2.034754
1	-2.793663	2.858931	-1.335425
6	2.477467	1.832700	-1.092379
1	3.336985	1.323301	-0.638301
1	2.793663	2.858931	-1.335425
1	2.226124	1.328294	-2.034754
6	2.477467	-1.832700	-1.092379
1	2.793663	-2.858931	-1.335425
1	3.336985	-1.323301	-0.638301
1	2.226124	-1.328294	-2.034754
6	-2.477467	-1.832700	-1.092379
1	-2.793663	-2.858931	-1.335425
1	-2.226124	-1.328294	-2.034754
1	-3.336985	-1.323301	-0.638301

Table S5. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Ti** structure **Ti-2T.**

	B3LYP*		
	x	y	z
6	1.221426	1.393405	1.553645
1	2.084996	1.481546	0.901340
1	1.452770	1.120094	2.583932
6	-0.543653	2.316980	0.000000
6	1.221426	1.393405	-1.553645
1	1.452770	1.120094	-2.583932
1	2.084996	1.481546	-0.901340
6	0.000000	2.036194	1.297001
1	-1.542456	2.758771	0.000000
6	0.000000	2.036194	-1.297001
6	-1.221426	-1.393405	-1.553645
1	-2.084996	-1.481546	-0.901340
1	-1.452770	-1.120094	-2.583932
6	0.543653	-2.316980	0.000000
6	-1.221426	-1.393405	1.553645
1	-1.452770	-1.120094	2.583932
1	-2.084996	-1.481546	0.901340
6	0.000000	-2.036194	-1.297001
1	1.542456	-2.758771	0.000000
6	0.000000	-2.036194	1.297001
22	0.000000	0.000000	0.000000
6	-0.908992	2.335289	-2.479033
1	-1.971758	2.236821	-2.221590
1	-0.690026	1.672097	-3.325364
1	-0.737580	3.369606	-2.816086
6	-0.908992	2.335289	2.479033
1	-0.690026	1.672097	3.325364
1	-1.971758	2.236821	2.221590
1	-0.737580	3.369606	2.816086
6	0.908992	-2.335289	2.479033
1	0.737580	-3.369606	2.816086
1	0.690026	-1.672097	3.325364
1	1.971758	-2.236821	2.221590
6	0.908992	-2.335289	-2.479033
1	0.737580	-3.369606	-2.816086
1	1.971758	-2.236821	-2.221590
1	0.690026	-1.672097	-3.325364

Table S6. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Ti** structure **Ti-3T.**

	B3LYP*		
	x	y	z
6	-1.791796	0.031963	-1.857363
1	-1.568613	-0.938700	-2.287539
1	-1.949858	0.830087	-2.583220
6	-2.056603	-0.627059	0.568541
6	-0.477527	-2.357531	-0.383609
1	0.263196	-3.120537	-0.139628
1	-0.853133	-2.390220	-1.401083
6	-2.340517	0.198736	-0.570726
1	-2.482675	-0.277151	1.511237
6	-1.185176	-1.768512	0.680092
6	0.477527	2.357531	-0.383610
1	0.853133	2.390220	-1.401084
1	-0.263196	3.120537	-0.139630
6	2.056603	0.627059	0.568540
6	1.791796	-0.031964	-1.857364
1	1.949857	-0.830088	-2.583220
1	1.568613	0.938699	-2.287540
6	1.185177	1.768513	0.680091
1	2.482676	0.277152	1.511237
6	2.340517	-0.198737	-0.570727
6	-0.926872	-2.277307	2.091623
1	0.060828	-2.750510	2.168972
1	-1.676634	-3.042586	2.346673
1	-0.995074	-1.482025	2.846688
6	-3.156857	1.453074	-0.301513
1	-2.853591	2.270318	-0.968263
1	-3.066378	1.797294	0.737692
1	-4.220648	1.244940	-0.495131
6	3.156857	-1.453074	-0.301513
1	4.220648	-1.244940	-0.495132
1	2.853591	-2.270318	-0.968263
1	3.066378	-1.797293	0.737692
6	0.926872	2.277308	2.091622
1	1.676635	3.042587	2.346671
1	0.995075	1.482027	2.846687
1	-0.060827	2.750511	2.168971
22	0.000000	0.000000	-0.281695

Table S7. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$V** structure **V-1D.**

	B3LYP*		
	x	y	z
6	1.497258	-1.555114	1.242908
1	0.914259	-2.091966	1.985975
1	2.514716	-1.327849	1.563778
6	0.000042	-1.823232	-0.759725
6	-1.497200	-1.555176	1.242896
1	-2.514669	-1.327952	1.563758
1	-0.914188	-2.092014	1.985963
6	1.289464	-1.732344	-0.150964
1	0.000048	-1.854767	-1.852237
6	-1.289388	-1.732392	-0.150977
6	1.497198	1.555173	1.242902
1	0.914186	2.092008	1.985971
1	2.514667	1.327948	1.563766
6	-0.000042	1.823234	-0.759719
6	-1.497260	1.555111	1.242911
1	-2.514718	1.327845	1.563779
1	-0.914261	2.091959	1.985981
6	1.289388	1.732393	-0.150970
1	-0.000046	1.854772	-1.852231
6	-1.289464	1.732345	-0.150960
6	2.488069	-1.720769	-1.082094
1	3.314634	-1.131744	-0.665256
1	2.246953	-1.330206	-2.079804
1	2.856383	-2.751509	-1.203938
6	-2.487986	-1.720860	-1.082117
1	-3.314572	-1.131860	-0.665286
1	-2.856265	-2.751612	-1.203959
1	-2.246875	-1.330292	-2.079826
6	-2.488068	1.720773	-1.082092
1	-2.856381	2.751513	-1.203933
1	-3.314633	1.131747	-0.665255
1	-2.246952	1.330211	-2.079802
6	2.487987	1.720863	-1.082108
1	2.856267	2.751616	-1.203947
1	2.246878	1.330298	-2.079819
1	3.314573	1.131862	-0.665279
23	0.000000	-0.000001	0.616620

Table S8. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$V** structure **V-2D.**

	B3LYP*		
	x	y	z
6	0.951411	-1.495316	-1.390749
1	1.031602	-0.924520	-2.311354
1	0.575781	-2.510454	-1.532060
6	2.271837	0.000000	0.145841
6	0.951411	1.495316	-1.390750
1	0.575780	2.510453	-1.532061
1	1.031601	0.924518	-2.311354
6	1.845346	-1.290010	-0.302961
1	2.880483	0.000001	1.053133
6	1.845345	1.290010	-0.302962
6	-0.951415	1.495317	1.390752
1	-1.031606	0.924518	2.311355
1	-0.575786	2.510455	1.532065
6	-2.271835	0.000000	-0.145844
6	-0.951416	-1.495317	1.390751
1	-0.575787	-2.510455	1.532063
1	-1.031607	-0.924519	2.311355
6	-1.845345	1.290010	0.302961
1	-2.880477	0.000001	-1.053139
6	-1.845346	-1.290010	0.302960
6	2.296319	2.486721	0.516270
1	1.553171	3.293206	0.480458
1	3.231515	2.885957	0.092674
1	2.481604	2.229972	1.567687
6	2.296320	-2.486720	0.516271
1	1.553172	-3.293205	0.480460
1	2.481606	-2.229970	1.567688
1	3.231515	-2.885957	0.092675
6	-2.296318	-2.486719	-0.516274
1	-3.231519	-2.885952	-0.092686
1	-1.553174	-3.293208	-0.480455
1	-2.481594	-2.229971	-1.567693
6	-2.296317	2.486720	-0.516273
1	-3.231518	2.885952	-0.092685
1	-2.481591	2.229973	-1.567692
1	-1.553173	3.293209	-0.480453
23	0.000001	0.000000	0.000003

Table S9. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$V** structure **V-3D.**

	B3LYP*		
	x	y	z
6	-1.498580	-1.970447	0.535082
1	-1.225331	-2.097418	1.580769
1	-1.641994	-2.909388	-0.000993
6	-2.010113	0.506003	0.530790
6	-0.047075	0.239539	2.088968
1	0.761641	0.772291	2.592830
1	-0.322400	-0.696740	2.573155
6	-2.221126	-0.836688	0.077130
1	-2.578817	1.259991	-0.018683
6	-1.013608	1.035978	1.406134
6	0.047055	0.239560	-2.088952
1	0.322367	-0.696716	-2.573153
1	-0.761663	0.772319	-2.592806
6	2.010115	0.505996	-0.530796
6	1.498555	-1.970453	-0.535076
1	1.641972	-2.909392	0.001002
1	1.225318	-2.097427	-1.580767
6	1.013603	1.035986	-1.406124
1	2.578836	1.259977	0.018668
6	2.221123	-0.836696	-0.077136
6	-0.907772	2.547692	1.503022
1	0.135637	2.862760	1.637590
1	-1.469318	2.898446	2.382963
1	-1.313646	3.057226	0.619423
6	-3.169942	-1.017019	-1.096685
1	-2.816221	-1.808346	-1.771029
1	-3.292303	-0.095605	-1.680442
1	-4.161536	-1.321647	-0.726896
6	3.169956	-1.017031	1.096663
1	4.161545	-1.321658	0.726858
1	2.816247	-1.808360	1.771011
1	3.292327	-0.095618	1.680422
6	0.907784	2.547702	-1.503004
1	1.469342	2.898455	-2.382939
1	1.313657	3.057228	-0.619400
1	-0.135620	2.862782	-1.637579
23	0.000005	-0.430604	-0.000004

Table S10. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$V** structure **V-1Q.**

	B3LYP*		
	x	y	z
6	-1.898444	-0.409930	-1.839687
1	-1.589597	-1.385965	-2.194755
1	-2.230595	0.278838	-2.617616
6	-1.812193	-0.809253	0.650588
6	-0.102606	-2.371701	-0.340892
1	0.775795	-2.983813	-0.129697
1	-0.571642	-2.559926	-1.299516
6	-2.322510	-0.161189	-0.524367
1	-2.199212	-0.433763	1.600398
6	-0.778500	-1.801731	0.749746
6	0.102605	2.371703	-0.340893
1	0.571625	2.559922	-1.299526
1	-0.775801	2.983806	-0.129693
6	1.812196	0.809254	0.650583
6	1.898447	0.409936	-1.839691
1	2.230590	-0.278833	-2.617621
1	1.589620	1.385980	-2.194755
6	0.778505	1.801735	0.749741
1	2.199213	0.433764	1.600394
6	2.322508	0.161182	-0.524370
6	-0.304605	-2.143166	2.154536
1	0.758669	-2.416990	2.160540
1	-0.868418	-3.012432	2.527167
1	-0.459521	-1.316448	2.860451
6	-3.272620	1.001370	-0.285978
1	-3.190514	1.748475	-1.085467
1	-3.093868	1.497251	0.677494
1	-4.308393	0.627836	-0.285762
6	3.272598	-1.001393	-0.285981
1	4.308378	-0.627878	-0.285756
1	3.190484	-1.748492	-1.085475
1	3.093830	-1.497276	0.677487
6	0.304617	2.143175	2.154533
1	0.868432	3.012443	2.527158
1	0.459538	1.316460	2.860450
1	-0.758657	2.416997	2.160541
23	0.000002	0.000004	-0.486680

Table S11. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$V** structure **V-2Q.**

	B3LYP*		
	x	y	z
6	-0.982247	-1.258489	1.674579
1	-1.064268	-0.495134	2.439121
1	-0.544422	-2.198794	2.012996
6	-2.267872	-0.147115	-0.195224
6	-1.305612	1.728181	1.175766
1	-1.052725	2.789787	1.181379
1	-1.299212	1.250658	2.148956
6	-1.778921	-1.294396	0.519490
1	-2.806023	-0.363352	-1.119888
6	-2.040966	1.240011	0.082876
6	1.305612	1.728180	-1.175766
1	1.299212	1.250657	-2.148956
1	1.052726	2.789786	-1.181378
6	2.267872	-0.147117	0.195223
6	0.982245	-1.258490	-1.674579
1	0.544418	-2.198794	-2.012995
1	1.064266	-0.495135	-2.439121
6	2.040967	1.240010	-0.082876
1	2.806024	-0.363354	1.119887
6	1.778920	-1.294398	-0.519490
6	-2.497421	2.227045	-0.979329
1	-1.830832	3.097964	-1.019056
1	-3.505353	2.593085	-0.728743
1	-2.539735	1.773195	-1.978081
6	-2.033273	-2.641083	-0.138829
1	-1.272987	-3.377094	0.152314
1	-2.054264	-2.570813	-1.234207
1	-3.008850	-3.027685	0.194794
6	2.033271	-2.641085	0.138828
1	3.008848	-3.027687	-0.194794
1	1.272984	-3.377095	-0.152314
1	2.054262	-2.570814	1.234207
6	2.497424	2.227043	0.979329
1	3.505355	2.593082	0.728742
1	2.539738	1.773193	1.978080
1	1.830835	3.097962	1.019056
23	0.000000	0.122026	0.000001

Table S12. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Cr** structure **Cr-1S.**

	B3LYP*		
	x	y	z
6	-1.443542	1.951049	-0.573986
1	-1.131948	2.078194	-1.608413
1	-1.594312	2.890609	-0.039495
6	-1.948082	-0.515235	-0.583036
6	0.067647	-0.226929	-2.043964
1	0.907000	-0.745811	-2.513300
1	-0.185704	0.716479	-2.525130
6	-2.177643	0.823761	-0.137087
1	-2.528030	-1.273712	-0.049418
6	-0.918005	-1.034476	-1.419032
6	-0.067647	-0.226929	2.043964
1	0.185704	0.716479	2.525130
1	-0.907000	-0.745811	2.513300
6	1.948082	-0.515236	0.583036
6	1.443542	1.951049	0.573986
1	1.594312	2.890609	0.039495
1	1.131948	2.078194	1.608413
6	0.918005	-1.034476	1.419032
1	2.528030	-1.273712	0.049418
6	2.177643	0.823761	0.137087
6	-0.799613	-2.544774	-1.523599
1	0.249327	-2.852191	-1.626951
1	-1.329553	-2.887413	-2.426001
1	-1.234084	-3.064971	-0.660425
6	-3.159514	1.000978	1.010120
1	-2.849795	1.821690	1.670700
1	-3.267101	0.091219	1.614529
1	-4.150797	1.261621	0.607468
6	3.159514	1.000978	-1.010120
1	4.150797	1.261621	-0.607468
1	2.849795	1.821690	-1.670700
1	3.267101	0.091219	-1.614529
6	0.799613	-2.544774	1.523599
1	1.329553	-2.887413	2.426001
1	1.234084	-3.064971	0.660425
1	-0.249327	-2.852191	1.626951
24	0.000000	0.436504	0.000000

Table S13. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Cr** structure **Cr-1T.**

	B3LYP*		
	x	y	z
6	1.446922	-1.500398	1.258233
1	0.899326	-2.065913	2.004117
1	2.450647	-1.218289	1.579744
6	0.000021	-1.859163	-0.758116
6	-1.446898	-1.500425	1.258225
1	-2.450630	-1.218334	1.579730
1	-0.899296	-2.065932	2.004112
6	1.280053	-1.721583	-0.141458
1	0.000025	-1.937065	-1.848460
6	-1.280017	-1.721606	-0.141466
6	1.446897	1.500422	1.258231
1	0.899294	2.065926	2.004119
1	2.450628	1.218329	1.579736
6	-0.000020	1.859166	-0.758111
6	-1.446924	1.500394	1.258236
1	-2.450649	1.218284	1.579744
1	-0.899328	2.065907	2.004122
6	1.280017	1.721606	-0.141459
1	-0.000023	1.937070	-1.848455
6	-1.280053	1.721583	-0.141455
6	2.495335	-1.727168	-1.049677
1	3.301726	-1.104152	-0.642731
1	2.267896	-1.383910	-2.068192
1	2.888536	-2.753666	-1.119326
6	-2.495293	-1.727212	-1.049692
1	-3.301694	-1.104203	-0.642754
1	-2.888481	-2.753715	-1.119338
1	-2.267852	-1.383956	-2.068208
6	-2.495333	1.727171	-1.049674
1	-2.888534	2.753669	-1.119321
1	-3.301725	1.104154	-0.642731
1	-2.267893	1.383915	-2.068191
6	2.495294	1.727215	-1.049683
1	2.888482	2.753719	-1.119325
1	2.267855	1.383963	-2.068201
1	3.301695	1.104205	-0.642747
24	0.000000	-0.000001	0.507073

Table S14. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Cr** structure **Cr-2T.**

	B3LYP*		
	x	y	z
6	1.235910	1.125917	1.464014
1	2.130296	1.390132	0.909840
1	1.435918	0.753271	2.470302
6	-0.530225	2.153091	0.000000
6	1.235910	1.125917	-1.464014
1	1.435918	0.753271	-2.470302
1	2.130296	1.390132	-0.909840
6	0.000000	1.809686	1.284029
1	-1.534059	2.582695	0.000000
6	0.000000	1.809686	-1.284029
6	-1.235910	-1.125917	-1.464014
1	-2.130296	-1.390132	-0.909840
1	-1.435918	-0.753271	-2.470302
6	0.530225	-2.153091	0.000000
6	-1.235910	-1.125917	1.464014
1	-1.435918	-0.753271	2.470302
1	-2.130296	-1.390132	0.909840
6	0.000000	-1.809686	-1.284029
1	1.534059	-2.582695	0.000000
6	0.000000	-1.809686	1.284029
6	-0.874539	2.099293	-2.489956
1	-0.699501	1.371013	-3.291780
1	-0.617167	3.092435	-2.891181
1	-1.944598	2.097432	-2.243644
6	-0.874539	2.099293	2.489956
1	-0.699501	1.371013	3.291780
1	-1.944598	2.097432	2.243644
1	-0.617167	3.092435	2.891181
6	0.874539	-2.099293	2.489956
1	0.617167	-3.092435	2.891181
1	0.699501	-1.371013	3.291780
1	1.944598	-2.097432	2.243644
6	0.874539	-2.099293	-2.489956
1	0.617167	-3.092435	-2.891181
1	1.944598	-2.097432	-2.243644
1	0.699501	-1.371013	-3.291780
24	0.000000	0.000000	0.000000

Table S15. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Cr** structure **Cr-3T.**

	B3LYP*		
	x	y	z
6	-1.436807	-1.930975	0.531828
1	-1.223961	-2.128585	1.578120
1	-1.554428	-2.831710	-0.072792
6	-1.922583	0.537574	0.627542
6	0.006607	0.078842	2.168563
1	0.855544	0.538653	2.678617
1	-0.312468	-0.862091	2.607422
6	-2.150969	-0.779719	0.101410
1	-2.472150	1.337795	0.126394
6	-0.911521	0.968100	1.540338
6	-0.006623	0.078844	-2.168536
1	0.312463	-0.862063	-2.607448
1	-0.855566	0.538663	-2.678573
6	1.922590	0.537570	-0.627546
6	1.436799	-1.930978	-0.531835
1	1.554408	-2.831710	0.072792
1	1.223961	-2.128585	-1.578129
6	0.911522	0.968107	-1.540327
1	2.472170	1.337786	-0.126402
6	2.150966	-0.779724	-0.101412
6	-0.711392	2.465610	1.702237
1	0.352287	2.709048	1.829119
1	-1.232937	2.810510	2.608578
1	-1.101144	3.037577	0.849793
6	-3.114792	-0.901008	-1.065403
1	-2.778882	-1.670256	-1.772934
1	-3.233116	0.043738	-1.612160
1	-4.105780	-1.206187	-0.693696
6	3.114789	-0.901023	1.065400
1	4.105764	-1.206250	0.693698
1	2.778852	-1.670241	1.772951
1	3.233151	0.043731	1.612135
6	0.711406	2.465617	-1.702232
1	1.232934	2.810506	-2.608586
1	1.101180	3.037587	-0.849799
1	-0.352273	2.709064	-1.829094
24	0.000002	-0.367417	-0.000008

Table S16. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Cr** structure **Cr-1P.**

	B3LYP*		
	x	y	z
6	-0.227145	1.857659	1.878211
1	0.819806	1.972966	2.144982
1	-0.921524	1.927318	2.716201
6	0.000000	1.885255	-0.620748
6	2.457777	1.916729	0.044201
1	3.491867	1.764258	-0.264968
1	2.305096	2.269525	1.059388
6	-0.720602	2.136010	0.580551
1	-0.593185	1.950791	-1.536999
6	1.446247	1.743816	-0.855082
6	-2.457777	-1.916729	0.044201
1	-2.305096	-2.269525	1.059388
1	-3.491867	-1.764258	-0.264968
6	0.000000	-1.885255	-0.620748
6	0.227145	-1.857659	1.878211
1	0.921524	-1.927318	2.716201
1	-0.819806	-1.972966	2.144982
6	-1.446247	-1.743816	-0.855082
1	0.593185	-1.950791	-1.536999
6	0.720602	-2.136010	0.580551
6	1.796992	1.373254	-2.288476
1	2.874903	1.210047	-2.408714
1	1.494568	2.179783	-2.973793
1	1.268304	0.462558	-2.606124
6	-2.196879	2.471371	0.439675
1	-2.786918	2.049392	1.263855
1	-2.614335	2.114995	-0.511208
1	-2.319202	3.565000	0.470907
6	2.196879	-2.471371	0.439675
1	2.319202	-3.565000	0.470907
1	2.786918	-2.049392	1.263855
1	2.614335	-2.114995	-0.511208
6	-1.796992	-1.373254	-2.288476
1	-1.494568	-2.179783	-2.973793
1	-1.268304	-0.462558	-2.606124
1	-2.874903	-1.210047	-2.408714
24	0.000000	0.000000	0.631374

Table S17. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-1D.**

	B3LYP*		
	x	y	z
6	1.420937	-1.479977	1.246522
1	0.876820	-2.070849	1.974082
1	2.419482	-1.195247	1.585450
6	0.000016	-1.792744	-0.779797
6	-1.420922	-1.479996	1.246514
1	-2.419472	-1.195279	1.585436
1	-0.876801	-2.070863	1.974076
6	1.273994	-1.670405	-0.154965
1	0.000019	-1.847639	-1.872641
6	-1.273968	-1.670421	-0.154972
6	1.420920	1.479992	1.246520
1	0.876799	2.070857	1.974083
1	2.419470	1.195275	1.585443
6	-0.000015	1.792747	-0.779792
6	-1.420938	1.479973	1.246525
1	-2.419484	1.195243	1.585451
1	-0.876822	2.070843	1.974087
6	1.273968	1.670422	-0.154966
1	-0.000017	1.847645	-1.872635
6	-1.273993	1.670405	-0.154961
6	2.497084	-1.677434	-1.051874
1	3.319772	-1.099324	-0.613837
1	2.290851	-1.291749	-2.059463
1	2.854187	-2.714299	-1.155244
6	-2.497053	-1.677465	-1.051889
1	-3.319749	-1.099364	-0.613858
1	-2.854143	-2.714334	-1.155260
1	-2.290818	-1.291780	-2.059477
6	-2.497083	1.677437	-1.051872
1	-2.854186	2.714302	-1.155239
1	-3.319771	1.099326	-0.613838
1	-2.290849	1.291756	-2.059461
6	2.497054	1.677469	-1.051881
1	2.854145	2.714338	-1.155248
1	2.290820	1.291787	-2.059471
1	3.319750	1.099365	-0.613851
25	0.000000	-0.000001	0.529069

Table S18. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-2D.**

	B3LYP*		
	x	y	z
6	1.442763	0.864242	-1.411953
1	0.880726	0.972609	-2.332344
1	2.444313	0.453815	-1.556291
6	0.000000	2.167795	0.159505
6	-1.442763	0.864242	-1.411954
1	-2.444313	0.453814	-1.556292
1	-0.880725	0.972609	-2.332344
6	1.279860	1.740617	-0.310883
1	-0.000001	2.751477	1.083314
6	-1.279860	1.740617	-0.310884
6	-1.442763	-0.864242	1.411954
1	-0.880725	-0.972609	2.332344
1	-2.444313	-0.453815	1.556293
6	0.000000	-2.167795	-0.159505
6	1.442763	-0.864243	1.411954
1	2.444313	-0.453815	1.556292
1	0.880726	-0.972609	2.332344
6	-1.279860	-1.740617	0.310884
1	0.000000	-2.751476	-1.083314
6	1.279860	-1.740617	0.310883
6	-2.489940	2.166701	0.499574
1	-3.312528	1.448344	0.394269
1	-2.853026	3.134115	0.117723
1	-2.261021	2.285232	1.566965
6	2.489940	2.166701	0.499575
1	3.312528	1.448345	0.394271
1	2.261020	2.285232	1.566966
1	2.853025	3.134116	0.117725
6	2.489940	-2.166701	-0.499575
1	2.853025	-3.134116	-0.117725
1	3.312528	-1.448345	-0.394270
1	2.261020	-2.285232	-1.566966
6	-2.489940	-2.166701	-0.499574
1	-2.853026	-3.134115	-0.117724
1	-2.261021	-2.285231	-1.566965
1	-3.312528	-1.448345	-0.394269
25	0.000000	0.000000	0.000000

Table S19. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-3D.**

	B3LYP*		
	x	y	z
6	1.389450	1.909680	0.600174
1	1.134643	2.102688	1.637127
1	1.535165	2.815695	0.008161
6	1.846516	-0.555770	0.677947
6	-0.127222	-0.071272	2.125284
1	-1.015333	-0.506072	2.589694
1	0.193277	0.860423	2.580297
6	2.115500	0.763362	0.189244
1	2.405755	-1.358117	0.188753
6	0.789296	-0.977959	1.537193
6	0.127222	-0.071272	-2.125284
1	-0.193277	0.860423	-2.580297
1	1.015333	-0.506072	-2.589694
6	-1.846516	-0.555770	-0.677947
6	-1.389450	1.909680	-0.600174
1	-1.535165	2.815695	-0.008161
1	-1.134643	2.102688	-1.637127
6	-0.789296	-0.977959	-1.537193
1	-2.405755	-1.358117	-0.188753
6	-2.115500	0.763362	-0.189244
6	0.564506	-2.471436	1.693904
1	-0.504285	-2.699739	1.802111
1	1.064212	-2.819825	2.611263
1	0.965499	-3.049815	0.851727
6	3.127209	0.893717	-0.936038
1	2.826065	1.674864	-1.646182
1	3.265759	-0.044459	-1.488842
1	4.101986	1.188742	-0.516786
6	-3.127209	0.893717	0.936038
1	-4.101986	1.188742	0.516786
1	-2.826065	1.674864	1.646182
1	-3.265759	-0.044459	1.488842
6	-0.564506	-2.471436	-1.693904
1	-1.064211	-2.819825	-2.611263
1	-0.965499	-3.049815	-0.851727
1	0.504285	-2.699739	-1.802111
25	0.000000	0.391495	0.000000

Table S20. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-1Q.**

	B3LYP*		
	x	y	z
6	-2.228391	-0.326123	1.288427
1	-2.264911	0.353103	2.137434
1	-2.651921	-1.307824	1.512581
6	-1.759696	1.271816	-0.580015
6	-0.281704	1.912001	1.389613
1	0.635159	2.432813	1.672390
1	-0.996336	1.793148	2.199165
6	-2.461620	0.165096	-0.051540
1	-1.918817	1.475023	-1.642177
6	-0.678384	2.019175	0.028636
6	0.364665	-2.040780	1.076289
1	1.082419	-1.784445	1.854069
1	-0.358294	-2.806383	1.356721
6	1.446540	-0.751491	-0.754509
6	3.283156	-0.544470	0.989641
1	4.188588	-0.036103	1.321326
1	2.949174	-1.383643	1.594176
6	0.647597	-1.848440	-0.308095
1	1.356569	-0.537722	-1.825156
6	2.660079	-0.154317	-0.151083
6	-3.352202	-0.637912	-0.981915
1	-3.196971	-1.717443	-0.842731
1	-3.177119	-0.397315	-2.039194
1	-4.411145	-0.437348	-0.756861
6	0.072588	2.967555	-0.890839
1	1.062283	3.209758	-0.484533
1	-0.485147	3.914806	-0.967903
1	0.194190	2.568703	-1.907472
6	3.265245	0.965788	-0.978797
1	3.607906	0.576842	-1.950602
1	4.124966	1.420822	-0.471687
1	2.529021	1.751755	-1.191497
6	-0.108900	-2.667718	-1.337138
1	0.490902	-3.549607	-1.612355
1	-0.298691	-2.097429	-2.256632
1	-1.068198	-3.031753	-0.944683
25	-0.264299	-0.095634	0.512543

Table S21. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-2Q.**

	B3LYP*		
	x	y	z
6	0.387083	-1.610095	-1.355513
1	0.915011	-1.123611	-2.173701
1	-0.399159	-2.295953	-1.673837
6	1.875613	-0.892944	0.538099
6	3.149729	0.150896	-1.392119
1	3.868070	0.897675	-1.730952
1	2.759835	-0.527545	-2.146411
6	0.985569	-1.837657	-0.077823
1	2.058108	-1.067128	1.602687
6	2.832885	0.053537	-0.074090
6	-0.387082	1.610095	1.355513
1	-0.915010	1.123610	2.173701
1	0.399160	2.295952	1.673836
6	-1.875613	0.892944	-0.538098
6	-3.149729	-0.150895	1.392120
1	-3.868071	-0.897674	1.730953
1	-2.759835	0.527547	2.146411
6	-0.985569	1.837657	0.077823
1	-2.058109	1.067128	-1.602687
6	-2.832885	-0.053537	0.074091
6	3.513706	0.971385	0.926755
1	4.170392	1.694024	0.426873
1	4.124470	0.382375	1.628450
1	2.775152	1.521511	1.527245
6	0.467470	-2.983448	0.776210
1	-0.559425	-3.261613	0.503073
1	0.491087	-2.742550	1.847974
1	1.102994	-3.869362	0.622041
6	-3.513705	-0.971385	-0.926754
1	-4.124470	-0.382376	-1.628449
1	-4.170392	-1.694024	-0.426872
1	-2.775152	-1.521512	-1.527243
6	-0.467470	2.983448	-0.776210
1	-1.102994	3.869362	-0.622040
1	-0.491088	2.742551	-1.847974
1	0.559424	3.261613	-0.503073
25	0.000000	0.000000	-0.000001

Table S22. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-3Q.**

	B3LYP*		
	x	y	z
6	1.493589	1.881086	0.350797
1	1.358199	2.169864	1.392890
1	1.593129	2.745138	-0.311182
6	2.095618	-0.536965	0.568494
6	0.224695	-0.118786	2.236688
1	-0.579975	-0.572624	2.816615
1	0.514499	0.878980	2.549083
6	2.310859	0.735166	0.010859
1	2.663514	-1.353721	0.116162
6	1.059633	-0.963019	1.495156
6	-0.224695	-0.118787	-2.236688
1	-0.514499	0.878980	-2.549082
1	0.579976	-0.572624	-2.816615
6	-2.095618	-0.536965	-0.568494
6	-1.493589	1.881086	-0.350798
1	-1.593130	2.745139	0.311181
1	-1.358199	2.169864	-1.392890
6	-1.059633	-0.963019	-1.495156
1	-2.663514	-1.353722	-0.116162
6	-2.310859	0.735166	-0.010859
6	0.870954	-2.466982	1.619954
1	-0.129981	-2.710377	1.999330
1	1.601545	-2.869060	2.339609
1	1.022309	-2.991297	0.667210
6	3.292884	0.862953	-1.137826
1	2.842072	1.411600	-1.977055
1	3.630692	-0.114948	-1.505846
1	4.178213	1.433689	-0.817368
6	-3.292884	0.862952	1.137826
1	-4.178213	1.433688	0.817368
1	-2.842073	1.411601	1.977055
1	-3.630692	-0.114948	1.505846
6	-0.870954	-2.466983	-1.619953
1	-1.601545	-2.869060	-2.339608
1	-1.022309	-2.991297	-0.667210
1	0.129981	-2.710377	-1.999330
25	0.000000	0.448964	0.000000

Table S23. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-1X.**

	B3LYP*		
	x	y	z
6	2.014083	1.851132	0.252988
1	1.809747	2.018818	1.309100
1	2.147269	2.770843	-0.322627
6	2.657205	-0.589977	0.379980
6	0.684630	-0.270814	1.928796
1	-0.066968	-0.814448	2.508167
1	0.995298	0.662599	2.398364
6	2.754759	0.720584	-0.164775
1	3.300666	-1.345484	-0.074753
6	1.652342	-1.069058	1.252561
6	-0.684630	-0.270815	-1.928796
1	-0.995297	0.662598	-2.398364
1	0.066968	-0.814449	-2.508167
6	-2.657205	-0.589977	-0.379980
6	-2.014083	1.851132	-0.252989
1	-2.147269	2.770843	0.322625
1	-1.809748	2.018818	-1.309102
6	-1.652342	-1.069059	-1.252561
1	-3.300665	-1.345484	0.074753
6	-2.754759	0.720584	0.164774
6	1.514735	-2.576463	1.382987
1	0.457221	-2.874815	1.349845
1	1.907364	-2.902963	2.358484
1	2.056687	-3.117233	0.596512
6	3.645446	0.883199	-1.385183
1	3.218500	1.609242	-2.090574
1	3.809583	-0.064946	-1.913258
1	4.627409	1.274500	-1.075855
6	-3.645445	0.883200	1.385183
1	-4.627407	1.274501	1.075856
1	-3.218498	1.609243	2.090574
1	-3.809581	-0.064945	1.913259
6	-1.514736	-2.576463	-1.382987
1	-1.907369	-2.902964	-2.358482
1	-2.056685	-3.117233	-0.596509
1	-0.457221	-2.874815	-1.349847
25	-0.000001	0.727382	0.000000

Table S24. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2Fe$** structure **Fe-1S.**

	B3LYP*		
	x	y	z
6	-0.666819	1.288286	1.674308
1	-0.578240	2.340594	1.416422
1	-0.372401	1.078257	2.705858
6	-2.014413	0.514988	-0.226430
6	0.000000	1.850027	-0.947019
1	0.667552	2.002085	-1.799690
1	0.056366	2.642750	-0.212294
6	-1.755005	0.507775	1.170429
1	-2.806865	-0.144724	-0.588043
6	-1.177753	1.106918	-1.234250
6	0.000000	-1.850027	-0.947019
1	-0.056366	-2.642750	-0.212294
1	-0.667552	-2.002085	-1.799690
6	2.014413	-0.514988	-0.226430
6	0.666819	-1.288286	1.674308
1	0.372401	-1.078257	2.705858
1	0.578240	-2.340594	1.416422
6	1.177753	-1.106918	-1.234250
1	2.806865	0.144724	-0.588043
6	1.755005	-0.507775	1.170429
6	-1.536163	0.780877	-2.672847
1	-0.680120	0.919252	-3.342894
1	-2.323303	1.475258	-3.006852
1	-1.923368	-0.240443	-2.794226
6	-2.581655	-0.396269	2.060112
1	-1.982368	-0.783078	2.893669
1	-3.001851	-1.248931	1.509681
1	-3.416112	0.176722	2.495431
6	2.581655	0.396269	2.060112
1	3.416112	-0.176722	2.495431
1	1.982368	0.783078	2.893669
1	3.001851	1.248931	1.509681
6	1.536163	-0.780877	-2.672847
1	2.323303	-1.475258	-3.006852
1	1.923368	0.240443	-2.794226
1	0.680120	-0.919252	-3.342894
26	0.000000	0.000000	0.136702

Table S25. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Fe** structure **Fe-2S.**

	B3LYP*		
	x	y	z
6	-1.368247	-0.668870	-1.815464
1	-0.985222	-1.596069	-2.225775
1	-1.735933	0.023218	-2.576573
6	-1.478337	-1.117615	0.656588
6	0.572998	-2.065846	-0.353950
1	1.610626	-2.353599	-0.172132
1	0.131915	-2.559746	-1.214086
6	-2.025884	-0.583468	-0.551940
1	-2.004204	-0.860507	1.580005
6	-0.193995	-1.733379	0.792615
6	-0.572998	2.065846	-0.353950
1	-0.131915	2.559746	-1.214086
1	-1.610626	2.353599	-0.172132
6	1.478337	1.117615	0.656588
6	1.368247	0.668869	-1.815464
1	1.735933	-0.023218	-2.576573
1	0.985222	1.596068	-2.225775
6	0.193995	1.733379	0.792615
1	2.004204	0.860507	1.580005
6	2.025884	0.583467	-0.551940
6	0.358329	-1.945100	2.189113
1	1.452108	-1.850569	2.196480
1	0.119229	-2.964424	2.531088
1	-0.060151	-1.238283	2.917950
6	-3.281808	0.258915	-0.421787
1	-3.320994	1.035153	-1.195795
1	-3.378329	0.735697	0.563529
1	-4.158683	-0.391792	-0.566430
6	3.281808	-0.258915	-0.421787
1	4.158683	0.391792	-0.566430
1	3.320994	-1.035153	-1.195795
1	3.378329	-0.735697	0.563529
6	-0.358329	1.945100	2.189112
1	-0.119229	2.964425	2.531087
1	0.060151	1.238283	2.917950
1	-1.452108	1.850569	2.196480
26	0.000000	0.000000	-0.369947

Table S26. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2Fe$** structure **Fe-1T.**

	B3LYP*		
	x	y	z
6	-0.190985	-1.984130	1.177576
1	-0.925759	-1.716704	1.936359
1	0.559446	-2.702178	1.509256
6	-1.326239	-0.859675	-0.723243
6	-3.147366	-0.551723	1.035490
1	-4.094667	-0.083789	1.303950
1	-2.730181	-1.243675	1.761441
6	-0.479135	-1.885436	-0.213444
1	-1.246650	-0.711995	-1.805413
6	-2.577652	-0.290587	-0.168330
6	2.281243	-0.125679	1.203877
1	2.315700	0.597833	2.014851
1	2.778221	-1.067094	1.451867
6	1.562562	1.342820	-0.664066
6	0.203381	1.969129	1.389182
1	-0.722238	2.439708	1.725272
1	0.950785	1.834469	2.162392
6	2.373917	0.301872	-0.161922
1	1.611859	1.511691	-1.742969
6	0.506640	2.057151	0.017983
6	0.317528	-2.724065	-1.194276
1	1.284484	-3.032745	-0.775133
1	0.495283	-2.191420	-2.138118
1	-0.247915	-3.639346	-1.430489
6	-3.301984	0.630548	-1.136161
1	-4.185138	1.086674	-0.672030
1	-3.633478	0.064615	-2.020918
1	-2.646095	1.433107	-1.498382
6	-0.388729	2.908326	-0.868000
1	0.066376	3.904758	-0.984028
1	-1.375594	3.052511	-0.411372
1	-0.518860	2.482756	-1.872021
6	3.233954	-0.479511	-1.137395
1	4.278028	-0.136033	-1.071702
1	2.901994	-0.359767	-2.177477
1	3.234046	-1.550589	-0.892710
26	0.286444	-0.070270	0.549375

Table S27. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2Fe$** structure **Fe-2T.**

	B3LYP*		
	x	y	z
6	-1.518940	0.571842	-1.871252
1	-1.984728	-0.370285	-2.150372
1	-1.331941	1.234479	-2.718591
6	-1.718795	0.444387	0.617463
6	-2.104693	-1.984297	-0.042992
1	-2.132948	-3.024097	0.283913
1	-2.340170	-1.802402	-1.085074
6	-1.730534	1.184482	-0.599113
1	-1.686966	1.050353	1.527686
6	-1.866455	-0.995888	0.869676
6	2.104699	1.984297	-0.042995
1	2.340173	1.802400	-1.085078
1	2.132957	3.024096	0.283909
6	1.718795	-0.444386	0.617460
6	1.518935	-0.571843	-1.871254
1	1.331936	-1.234481	-2.718593
1	1.984722	0.370284	-2.150375
6	1.866457	0.995889	0.869673
1	1.686967	-1.050351	1.527684
6	1.730532	-1.184482	-0.599115
6	-1.699841	-1.381390	2.331393
1	-1.698654	-2.470418	2.461447
1	-2.527636	-0.967336	2.927089
1	-0.765583	-0.979411	2.748509
6	-1.707857	2.700937	-0.503590
1	-1.074622	3.139208	-1.286500
1	-1.345933	3.049589	0.472489
1	-2.727993	3.090133	-0.645904
6	1.707856	-2.700937	-0.503591
1	2.727991	-3.090133	-0.645906
1	1.074619	-3.139209	-1.286499
1	1.345933	-3.049588	0.472489
6	1.699846	1.381392	2.331390
1	2.527639	0.967334	2.927086
1	0.765586	0.979417	2.748506
1	1.698664	2.470420	2.461443
26	-0.000001	-0.000001	-0.564934

Table S28. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2Fe$** structure **Fe-1P.**

	B3LYP*		
	x	y	z
6	-1.712503	1.919896	-0.443270
1	-1.481342	2.032660	-1.497110
1	-1.774066	2.857294	0.111541
6	-2.303131	-0.534312	-0.416211
6	-0.404389	-0.259711	-2.060387
1	0.373351	-0.800500	-2.603710
1	-0.703804	0.672698	-2.530993
6	-2.411302	0.808498	0.066386
1	-2.891490	-1.279326	0.122381
6	-1.322164	-1.045341	-1.311237
6	0.404389	-0.259711	2.060387
1	0.703804	0.672698	2.530993
1	-0.373351	-0.800499	2.603711
6	2.303131	-0.534312	0.416211
6	1.712503	1.919896	0.443270
1	1.774066	2.857294	-0.111541
1	1.481343	2.032660	1.497110
6	1.322164	-1.045341	1.311237
1	2.891490	-1.279326	-0.122381
6	2.411302	0.808498	-0.066386
6	-1.185630	-2.557093	-1.392788
1	-0.136769	-2.851735	-1.530857
1	-1.743226	-2.926704	-2.267209
1	-1.577809	-3.063741	-0.501407
6	-3.244118	1.008812	1.322469
1	-2.863899	1.849683	1.917268
1	-3.265763	0.112992	1.957033
1	-4.281195	1.249913	1.041602
6	3.244118	1.008811	-1.322469
1	4.281195	1.249913	-1.041602
1	2.863900	1.849683	-1.917268
1	3.265763	0.112992	-1.957033
6	1.185629	-2.557093	1.392788
1	1.743226	-2.926704	2.267209
1	1.577809	-3.063741	0.501408
1	0.136768	-2.851734	1.530857
26	0.000000	0.469405	0.000000

Table S29. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Co** structure **Co-1D.**

	B3LYP*		
	x	y	z
6	-0.335285	1.969613	-0.874427
1	-0.750771	2.048349	-1.874569
1	0.497805	2.654120	-0.698246
6	-2.166444	0.708404	0.286851
6	-1.611806	-0.337077	-1.943708
1	-1.642657	-1.273724	-2.504750
1	-1.531025	0.549512	-2.561558
6	-1.176130	1.727982	0.260523
1	-2.709940	0.566799	1.223302
6	-2.282144	-0.337347	-0.690822
6	3.437677	-1.203954	-0.518174
1	3.148820	-2.176646	-0.122393
1	4.313334	-1.170998	-1.167302
6	1.578587	-0.041635	0.699212
6	0.324227	-2.020153	0.026521
1	-0.439516	-2.768965	0.241315
1	0.968795	-2.241356	-0.823931
6	2.759135	-0.074756	-0.210719
1	1.633764	0.769113	1.435599
6	0.745893	-1.151215	1.067674
6	-0.931221	2.510127	1.537894
1	0.138418	2.723406	1.668068
1	-1.299529	1.988494	2.431525
1	-1.445197	3.481790	1.475145
6	-3.102830	-1.553619	-0.298527
1	-2.727360	-2.458546	-0.792657
1	-4.141945	-1.407704	-0.632982
1	-3.120232	-1.723170	0.786577
6	0.153947	-1.244297	2.457698
1	0.828962	-1.830209	3.101946
1	-0.821881	-1.747870	2.452781
1	0.038611	-0.253930	2.917940
6	3.233439	1.268715	-0.726792
1	3.371292	1.979094	0.103686
1	2.491160	1.709463	-1.406033
1	4.187355	1.175451	-1.260715
27	-0.175946	-0.071007	-0.386369

Table S30. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Co** structure **Co-2D.**

	B3LYP*		
	x	y	z
6	-3.141308	-0.010713	1.379719
1	-2.725928	0.666531	2.121825
1	-3.906097	-0.706162	1.726406
6	-1.780189	0.917388	-0.547189
6	-0.280118	1.566024	1.338775
1	0.535507	2.210518	1.668613
1	-0.812813	1.063275	2.142914
6	-2.792454	0.027563	0.069009
1	-1.954968	1.095616	-1.612485
6	-0.869416	1.832665	0.072697
6	3.141421	0.010595	-1.379670
1	2.726056	-0.666673	-2.121764
1	3.906248	0.706004	-1.726350
6	1.780161	-0.917375	0.547196
6	0.280126	-1.565972	-1.338803
1	-0.535496	-2.210451	-1.668678
1	0.812847	-1.063203	-2.142914
6	2.792486	-0.027603	-0.068979
1	1.954906	-1.095606	1.612498
6	0.869389	-1.832639	-0.072715
6	-0.289522	2.947475	-0.780870
1	0.746719	3.176967	-0.498964
1	-0.885359	3.861932	-0.635602
1	-0.315402	2.700723	-1.850874
6	-3.502569	-0.875911	-0.922887
1	-4.200332	-1.556321	-0.419270
1	-2.783177	-1.471875	-1.501883
1	-4.074392	-0.272477	-1.645046
6	0.289461	-2.947451	0.780825
1	0.885282	-3.861918	0.635548
1	-0.746781	-3.176917	0.498905
1	0.315336	-2.700718	1.850833
6	3.502561	0.875904	0.922915
1	4.074325	0.272492	1.645139
1	2.783146	1.471912	1.501839
1	4.200370	1.556274	0.419308
27	-0.000006	0.000014	-0.000005

Table S31. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Co** structure **Co-3D.**

	B3LYP*		
	x	y	z
6	1.318161	-0.936419	-1.872372
1	2.011551	-0.134879	-2.114166
1	0.971947	-1.506790	-2.735189
6	1.468707	-0.849274	0.620115
6	3.111402	0.996104	0.042970
1	3.636944	1.898568	0.356416
1	3.346016	0.615758	-0.947466
6	1.286292	-1.573978	-0.599074
1	1.177730	-1.393275	1.524096
6	2.261501	0.368019	0.896625
6	-3.111381	-0.996125	0.042977
1	-3.346001	-0.615779	-0.947456
1	-3.636910	-1.898597	0.356422
6	-1.468708	0.849272	0.620128
6	-1.318175	0.936433	-1.872361
1	-0.971969	1.506811	-2.735175
1	-2.011562	0.134890	-2.114157
6	-2.261487	-0.368031	0.896634
1	-1.177731	1.393270	1.524110
6	-1.286305	1.573984	-0.599059
6	2.083956	0.909393	2.304755
1	2.643690	1.841435	2.450315
1	2.443569	0.176330	3.043481
1	1.023789	1.097205	2.527384
6	0.739430	-2.988408	-0.506876
1	0.074751	-3.218264	-1.350357
1	0.189173	-3.157601	0.428267
1	1.576036	-3.703550	-0.537889
6	-0.739452	2.988417	-0.506855
1	-1.576063	3.703554	-0.537858
1	-0.074780	3.218283	-1.350340
1	-0.189189	3.157607	0.428285
6	-2.083935	-0.909406	2.304763
1	-2.443564	-0.176353	3.043490
1	-1.023765	-1.097199	2.527393
1	-2.643651	-1.841460	2.450319
27	-0.000002	0.000006	-0.589783

Table S32. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Co** structure **Co-1Q.**

	B3LYP*		
	x	y	z
6	1.074862	1.497607	1.370938
1	1.076895	0.891353	2.268673
1	0.686304	2.508450	1.505367
6	2.421830	0.000000	-0.139070
6	1.074862	-1.497607	1.370939
1	0.686304	-2.508449	1.505367
1	1.076895	-0.891353	2.268673
6	1.958175	1.278608	0.298867
1	3.063960	0.000000	-1.021638
6	1.958175	-1.278608	0.298867
6	-1.074862	-1.497607	-1.370938
1	-1.076895	-0.891353	-2.268673
1	-0.686304	-2.508450	-1.505367
6	-2.421830	0.000000	0.139070
6	-1.074863	1.497607	-1.370938
1	-0.686304	2.508450	-1.505367
1	-1.076895	0.891353	-2.268673
6	-1.958175	-1.278608	-0.298867
1	-3.063960	0.000000	1.021638
6	-1.958175	1.278608	-0.298867
6	2.361821	-2.470430	-0.553350
1	1.622627	-3.278076	-0.479770
1	3.321038	-2.869649	-0.188557
1	2.487337	-2.204038	-1.611111
6	2.361821	2.470431	-0.553350
1	1.622626	3.278076	-0.479771
1	2.487337	2.204038	-1.611111
1	3.321038	2.869649	-0.188557
6	-2.361821	2.470430	0.553350
1	-3.321038	2.869649	0.188557
1	-1.622627	3.278076	0.479771
1	-2.487337	2.204038	1.611111
6	-2.361821	-2.470431	0.553350
1	-3.321038	-2.869649	0.188557
1	-2.487337	-2.204038	1.611111
1	-1.622626	-3.278076	0.479771
27	0.000000	0.000000	0.000000

Table S33. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Co** structure **Co-2Q.**

	B3LYP*		
	x	y	z
6	1.693556	1.896276	0.418991
1	1.439327	2.037482	1.464885
1	1.780526	2.821630	-0.153192
6	2.288501	-0.551982	0.474141
6	0.327965	-0.242203	2.031221
1	-0.471970	-0.766727	2.557866
1	0.605727	0.707152	2.481106
6	2.412366	0.774584	-0.037719
1	2.895826	-1.310506	-0.023363
6	1.270592	-1.040730	1.338911
6	-0.327965	-0.242203	-2.031221
1	-0.605727	0.707152	-2.481107
1	0.471970	-0.766728	-2.557866
6	-2.288501	-0.551982	-0.474141
6	-1.693556	1.896276	-0.418991
1	-1.780525	2.821631	0.153191
1	-1.439327	2.037482	-1.464886
6	-1.270592	-1.040731	-1.338910
1	-2.895826	-1.310505	0.023363
6	-2.412366	0.774584	0.037719
6	1.120985	-2.549870	1.437373
1	0.066736	-2.833676	1.554539
1	1.654533	-2.910567	2.330457
1	1.531150	-3.072321	0.563458
6	3.285734	0.944971	-1.269511
1	2.912225	1.756729	-1.907561
1	3.345941	0.027471	-1.869528
1	4.307660	1.215970	-0.961462
6	-3.285733	0.944972	1.269511
1	-4.307660	1.215971	0.961462
1	-2.912225	1.756730	1.907561
1	-3.345941	0.027472	1.869528
6	-1.120985	-2.549870	-1.437373
1	-1.654534	-2.910567	-2.330456
1	-1.531150	-3.072321	-0.563457
1	-0.066736	-2.833677	-1.554538
27	0.000000	0.514155	0.000000

Table S34. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Ni** structure **Ni-1S.**

	B3LYP*		
	x	y	z
6	2.052894	1.295598	1.396463
1	1.286844	0.877112	2.044617
1	2.599346	2.156617	1.783463
6	1.669847	-0.340851	-0.518872
6	0.986869	-1.816951	1.346783
1	0.694118	-2.812722	1.680547
1	1.297029	-1.132725	2.137179
6	2.301581	0.832158	0.148862
1	1.829952	-0.338205	-1.602172
6	1.446748	-1.652837	0.017473
6	-1.989284	2.527580	0.887308
1	-2.693725	1.937675	1.471284
1	-1.823122	3.556536	1.207135
6	-1.549071	0.668123	-0.753876
6	-2.021457	-0.750273	1.218958
1	-2.405146	-1.692279	1.610706
1	-1.846126	0.029276	1.959407
6	-1.367988	2.037445	-0.211282
1	-1.505268	0.636541	-1.848177
6	-2.214946	-0.449781	-0.154427
6	3.327617	1.537413	-0.721499
1	3.754336	2.411767	-0.213916
1	2.873122	1.876101	-1.666120
1	4.148125	0.854993	-0.991775
6	1.444383	-2.834765	-0.935257
1	0.753161	-3.621484	-0.605513
1	2.454963	-3.271329	-0.972947
1	1.175133	-2.534076	-1.956793
6	-2.870255	-1.479219	-1.055769
1	-3.927754	-1.208518	-1.203207
1	-2.839992	-2.485168	-0.616619
1	-2.397911	-1.511308	-2.046942
6	-0.465931	2.929979	-1.038736
1	-0.828088	2.988116	-2.077388
1	0.555535	2.528073	-1.068370
1	-0.426763	3.947699	-0.630928
28	-0.258350	-0.650515	0.208919

Table S35. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Ni** structure **Ni-2S.**

	B3LYP*		
	x	y	z
6	2.035923	2.406729	1.860969
1	2.716129	2.435369	1.011172
1	2.470241	2.568879	2.847906
6	0.015590	2.018384	0.411128
6	1.641093	0.752563	-0.958454
1	1.950035	0.412508	-1.947285
1	2.381715	0.627873	-0.170084
6	0.704579	2.212659	1.713519
1	-0.960827	2.513063	0.364487
6	0.593288	1.706392	-0.862731
6	-2.035923	-2.406729	-1.860969
1	-2.716129	-2.435369	-1.011172
1	-2.470241	-2.568879	-2.847906
6	-0.015590	-2.018384	-0.411128
6	-1.641093	-0.752563	0.958454
1	-1.950035	-0.412508	1.947285
1	-2.381715	-0.627873	0.170084
6	-0.704579	-2.212659	-1.713519
1	0.960827	-2.513063	-0.364487
6	-0.593288	-1.706392	0.862731
6	-0.120244	2.162998	-2.121118
1	0.017478	1.454959	-2.948972
1	0.290715	3.134473	-2.438014
1	-1.196751	2.299159	-1.951047
6	-0.212823	2.265490	2.919327
1	0.348072	2.463189	3.841278
1	-0.763915	1.321619	3.037323
1	-0.965911	3.059999	2.798370
6	0.120244	-2.162998	2.121118
1	-0.290715	-3.134473	2.438014
1	-0.017478	-1.454959	2.948972
1	1.196751	-2.299159	1.951047
6	0.212823	-2.265490	-2.919327
1	0.965911	-3.059999	-2.798370
1	0.763915	-1.321619	-3.037323
1	-0.348072	-2.463189	-3.841278
28	0.000000	0.000000	0.000000

Table S36. Optimized coordinates for the **(2,4-$Me_2C_5H_5)_2$Ni** structure **Ni-3S.**

	B3LYP*		
	x	y	z
6	1.508995	-1.962798	-0.646443
1	1.397042	-1.907988	-1.722259
1	1.398240	-2.964362	-0.226307
6	2.220587	0.389480	-0.171660
6	0.594554	0.490224	-2.068917
1	-0.103969	1.134803	-2.606389
1	0.813595	-0.446580	-2.565678
6	2.223505	-1.019485	0.107201
1	2.768757	1.009022	0.542643
6	1.471180	1.108101	-1.157864
6	-0.404494	-0.285388	1.882381
1	-0.907954	-1.235367	2.061619
1	0.469494	-0.082972	2.505451
6	-2.452012	0.556034	0.718884
6	-1.489178	-1.215072	-0.681041
1	-1.512769	-1.303272	-1.777612
1	-1.504646	-2.242718	-0.278750
6	-1.087466	0.779367	1.272629
1	-3.263858	1.192883	1.085974
6	-2.673413	-0.422568	-0.183163
6	1.512628	2.624429	-1.088011
1	0.564789	3.061116	-1.428766
1	2.302697	2.995274	-1.759157
1	1.727937	2.996348	-0.078267
6	2.893636	-1.459523	1.397366
1	2.390457	-2.339416	1.818866
1	2.902092	-0.666227	2.156753
1	3.938226	-1.741973	1.195137
6	-4.044241	-0.761499	-0.717029
1	-4.296778	-1.812037	-0.500093
1	-4.075061	-0.653331	-1.813085
1	-4.825835	-0.123114	-0.282365
6	-0.702631	2.217334	1.561056
1	-1.388359	2.633730	2.318614
1	-0.786126	2.853399	0.669839
1	0.318226	2.296903	1.957470
28	0.151568	-0.317355	-0.093785

Table S37. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Ti$** structure **Ti-1S**.

B3LYP*		
56(0)	789(1)	1460(23)
62(2)	809(3)	1463(11)
87(0)	810(12)	1470(1)
130(3)	844(3)	1470(11)
132(0)	856(44)	1474(16)
137(0)	859(0)	1476(1)
138(0)	867(4)	1478(29)
148(0)	874(0)	1491(0)
157(1)	876(6)	1494(2)
177(0)	879(2)	1506(8)
183(0)	984(4)	1506(6)
200(0)	985(2)	1510(34)
207(4)	998(1)	1513(21)
263(1)	998(0)	3016(14)
285(7)	1005(35)	3017(57)
296(1)	1006(0)	3017(71)
303(2)	1030(14)	3018(0)
355(0)	1034(11)	3079(24)
374(2)	1036(42)	3080(1)
384(2)	1041(0)	3083(1)
399(1)	1073(2)	3083(21)
405(3)	1074(2)	3106(0)
416(0)	1210(3)	3108(28)
433(1)	1210(1)	3112(1)
443(2)	1294(0)	3112(29)
488(15)	1294(2)	3119(0)
508(2)	1382(5)	3120(6)
553(2)	1382(8)	3140(15)
561(0)	1390(0)	3140(13)
577(6)	1391(0)	3146(4)
593(0)	1394(1)	3146(1)
598(2)	1396(2)	3195(8)
645(4)	1399(43)	3195(14)
673(11)	1412(10)	3220(4)
674(0)	1460(21)	3220(0)

Table S38. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Ti$** structure **Ti-2S**.

B3LYP*					
46(	0)	797(	0)	1461(	24)
93(	0)	799(	1)	1461(	0)
114(	0)	827(	2)	1470(	47)
135(	6)	846(	20)	1473(	4)
136(	0)	857(	46)	1476(	6)
143(	1)	863(	1)	1477(	1)
145(	0)	871(	1)	1487(	23)
177(	1)	877(	11)	1491(	0)
191(	0)	878(	0)	1501(	2)
204(	5)	885(	8)	1511(	0)
208(	5)	980(	0)	1516(	29)
212(	0)	986(	5)	1520(	11)
230(	0)	996(	14)	1523(	51)
239(	0)	1000(	1)	3017(	0)
263(	6)	1005(	24)	3017(	26)
274(	1)	1011(	1)	3018(	79)
304(	5)	1028(	34)	3019(	32)
338(	6)	1034(	0)	3079(	0)
366(	1)	1034(	43)	3080(	42)
369(	0)	1041(	1)	3081(	0)
381(	6)	1069(	0)	3081(	8)
384(	1)	1071(	3)	3109(	2)
408(	0)	1207(	4)	3109(	0)
428(	3)	1207(	0)	3111(	35)
439(	0)	1296(	0)	3111(	23)
483(	36)	1298(	1)	3136(	0)
507(	0)	1378(	0)	3137(	6)
539(	1)	1384(	7)	3139(	1)
560(	3)	1389(	1)	3140(	28)
586(	10)	1390(	0)	3148(	1)
592(	0)	1397(	3)	3150(	8)
597(	0)	1398(	2)	3212(	0)
641(	0)	1403(	37)	3214(	28)
697(	6)	1418(	33)	3236(	1)
712(	5)	1457(	0)	3238(	2)

Table S39. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Ti$** structure **Ti-3S**.

B3LYP*		
53(0)	791(0)	1461(52)
54(3)	799(1)	1469(2)
84(0)	810(46)	1469(0)
134(0)	819(0)	1470(0)
155(0)	855(47)	1470(20)
155(4)	859(0)	1474(28)
159(0)	868(0)	1479(0)
163(0)	873(1)	1486(0)
169(0)	878(8)	1488(2)
188(0)	883(0)	1505(0)
188(1)	982(0)	1510(10)
207(3)	982(5)	1510(0)
223(0)	997(14)	1510(67)
239(0)	1000(0)	3016(0)
263(4)	1006(0)	3017(73)
265(0)	1007(30)	3017(70)
307(1)	1031(0)	3017(0)
333(8)	1036(24)	3083(0)
342(0)	1038(43)	3083(46)
345(0)	1041(0)	3083(0)
361(6)	1067(0)	3083(0)
408(0)	1070(2)	3114(0)
409(1)	1201(0)	3114(39)
425(0)	1203(2)	3115(0)
440(3)	1295(0)	3115(16)
473(0)	1296(4)	3126(0)
511(7)	1373(0)	3127(16)
532(10)	1375(7)	3133(24)
561(0)	1392(0)	3134(0)
578(0)	1393(0)	3147(10)
600(0)	1394(3)	3148(0)
601(0)	1396(7)	3209(0)
639(0)	1399(61)	3210(17)
660(6)	1411(0)	3235(4)
690(0)	1455(0)	3236(0)

Table S40. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Ti$** structure **Ti-1T**.

B3LYP*		
16(0)	768(0)	1462(25)
89(0)	776(73)	1463(0)
97(0)	800(0)	1466(90)
106(0)	810(17)	1475(4)
116(0)	829(59)	1476(4)
118(0)	835(0)	1477(0)
125(4)	869(5)	1484(21)
143(1)	878(2)	1498(0)
151(0)	881(0)	1507(127)
169(2)	882(7)	1528(0)
181(0)	986(3)	1536(70)
191(0)	988(1)	1554(26)
198(0)	989(0)	1561(90)
216(0)	991(5)	3022(0)
248(0)	1014(30)	3022(8)
259(4)	1017(1)	3023(47)
271(1)	1033(24)	3024(27)
324(3)	1035(4)	3087(0)
340(5)	1036(0)	3087(47)
340(0)	1036(22)	3089(1)
345(1)	1065(0)	3089(4)
388(9)	1068(2)	3116(0)
392(3)	1221(0)	3116(0)
443(0)	1221(0)	3118(26)
446(0)	1288(4)	3118(27)
510(14)	1291(2)	3141(1)
525(0)	1382(0)	3142(29)
545(0)	1386(38)	3145(0)
562(2)	1389(0)	3145(1)
580(0)	1393(0)	3154(0)
595(24)	1393(12)	3154(3)
596(1)	1399(0)	3229(0)
600(0)	1429(1)	3230(34)
697(1)	1436(30)	3256(0)
705(4)	1459(0)	3257(1)

Table S41. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Ti$** structure **Ti-2T**.

B3LYP*					
20(	0)	774(	0)	1461(	91)
64(	0)	785(	2)	1469(	0)
71(	1)	786(	0)	1470(	20)
113(	2)	794(	150)	1471(	2)
116(	0)	834(	0)	1471(	0)
118(	0)	836(	45)	1476(	25)
118(	1)	873(	2)	1479(	0)
119(	0)	879(	0)	1496(	0)
131(	0)	880(	0)	1500(	162)
176(	0)	884(	6)	1526(	0)
183(	6)	987(	3)	1527(	52)
197(	0)	988(	0)	1553(	0)
197(	0)	989(	5)	1553(	99)
206(	0)	989(	0)	3022(	0)
243(	0)	1014(	32)	3022(	45)
261(	2)	1015(	0)	3022(	43)
279(	5)	1035(	30)	3022(	0)
296(	0)	1036(	0)	3088(	0)
334(	1)	1038(	19)	3088(	0)
349(	0)	1038(	0)	3088(	0)
350(	6)	1065(	2)	3089(	46)
391(	0)	1065(	0)	3118(	30)
397(	14)	1219(	0)	3118(	0)
443(	0)	1220(	0)	3118(	0)
447(	0)	1289(	0)	3118(	23)
513(	0)	1290(	9)	3139(	0)
531(	5)	1382(	52)	3139(	4)
546(	7)	1383(	0)	3142(	33)
559(	0)	1391(	15)	3143(	0)
587(	0)	1391(	0)	3149(	0)
588(	27)	1392(	0)	3149(	0)
601(	1)	1397(	0)	3225(	0)
602(	0)	1428(	31)	3226(	31)
695(	7)	1431(	0)	3252(	1)
700(	0)	1459(	0)	3253(	0)

Table S42. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Ti$** structure **Ti-3T**.

B3LYP*		
38(0)	768(1)	1462(26)
63(0)	770(36)	1470(7)
68(0)	785(32)	1471(2)
120(2)	808(5)	1472(9)
123(0)	826(49)	1472(1)
131(2)	830(0)	1478(9)
135(0)	862(19)	1479(19)
139(2)	872(0)	1490(48)
142(0)	878(3)	1492(15)
161(0)	880(1)	1520(26)
165(2)	987(4)	1522(14)
197(0)	987(0)	1541(37)
198(0)	988(2)	1544(47)
235(0)	989(2)	3017(18)
247(1)	1011(40)	3018(35)
256(2)	1013(1)	3020(52)
282(2)	1029(29)	3020(2)
322(1)	1033(10)	3080(23)
326(1)	1036(22)	3081(2)
346(0)	1038(1)	3085(9)
362(0)	1065(1)	3085(17)
382(1)	1065(1)	3109(27)
408(5)	1213(1)	3109(3)
439(0)	1214(1)	3114(23)
442(0)	1288(0)	3115(4)
509(7)	1290(2)	3140(11)
521(1)	1383(35)	3140(2)
542(0)	1384(10)	3144(2)
555(1)	1390(3)	3144(18)
585(11)	1392(5)	3151(0)
593(0)	1395(0)	3151(2)
601(6)	1397(0)	3235(6)
608(7)	1421(9)	3236(15)
687(0)	1425(16)	3256(1)
687(2)	1459(84)	3256(1)

Table S43. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2V$** structure **V-1D**.

B3LYP*		
42(0)	819(0)	1459(27)
125(0)	824(10)	1460(0)
132(0)	843(6)	1472(44)
137(5)	851(12)	1474(3)
139(0)	861(37)	1478(8)
144(0)	880(2)	1479(0)
152(1)	881(2)	1488(22)
201(0)	883(0)	1499(0)
209(0)	883(11)	1508(4)
213(3)	897(10)	1522(0)
224(6)	979(0)	1527(28)
231(1)	986(5)	1528(26)
232(0)	994(19)	1534(54)
243(0)	999(0)	3019(0)
280(3)	1008(17)	3019(20)
281(0)	1012(2)	3021(64)
309(13)	1030(32)	3021(30)
340(4)	1032(0)	3082(0)
360(0)	1033(39)	3082(42)
364(1)	1039(2)	3085(0)
385(12)	1066(0)	3085(9)
386(1)	1070(1)	3114(1)
410(0)	1212(1)	3114(0)
428(3)	1212(0)	3118(23)
439(0)	1297(1)	3119(21)
485(31)	1299(2)	3133(0)
506(0)	1381(0)	3134(15)
536(1)	1387(9)	3135(2)
559(2)	1390(1)	3136(42)
594(9)	1390(0)	3143(1)
595(0)	1398(4)	3144(8)
598(0)	1398(6)	3213(0)
635(0)	1415(16)	3215(30)
715(3)	1426(29)	3242(0)
727(5)	1458(0)	3244(3)

Table S44. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2V$** structure **V-2D**.

B3LYP*		
49(2)	814(0)	1465(52)
94(0)	822(1)	1469(0)
101(0)	830(0)	1470(0)
135(0)	834(61)	1470(0)
155(0)	864(36)	1471(18)
157(0)	865(0)	1474(25)
158(3)	873(0)	1481(0)
163(0)	882(2)	1497(0)
171(0)	884(8)	1499(9)
208(0)	892(0)	1514(0)
213(6)	984(0)	1516(22)
218(0)	984(4)	1525(0)
227(0)	996(13)	1525(66)
241(0)	998(0)	3019(0)
270(0)	1009(0)	3019(63)
281(1)	1010(26)	3019(58)
326(5)	1033(0)	3019(0)
344(0)	1036(21)	3085(0)
351(0)	1038(41)	3085(0)
354(3)	1040(0)	3085(0)
362(12)	1067(0)	3085(47)
406(0)	1069(1)	3116(35)
421(0)	1208(0)	3116(0)
427(0)	1210(0)	3116(0)
443(3)	1296(0)	3117(15)
485(0)	1298(7)	3129(0)
516(7)	1380(0)	3129(22)
533(10)	1381(11)	3135(35)
556(0)	1392(0)	3136(0)
597(0)	1394(0)	3143(8)
602(1)	1394(11)	3143(0)
603(0)	1397(8)	3214(0)
649(0)	1412(39)	3216(20)
701(8)	1419(0)	3243(3)
713(0)	1459(0)	3244(0)

Table S45. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2V$** structure **V-3D**.

B3LYP*		
65(2)	810(5)	1461(19)
87(0)	833(3)	1463(20)
116(0)	842(21)	1470(2)
127(2)	852(3)	1470(11)
132(0)	863(27)	1473(12)
136(0)	875(0)	1476(5)
143(1)	880(12)	1479(28)
151(0)	885(2)	1501(3)
153(2)	886(4)	1502(5)
186(0)	890(1)	1515(11)
201(0)	984(2)	1515(11)
214(1)	985(2)	1521(36)
222(4)	1000(6)	1524(23)
271(0)	1000(0)	3018(11)
294(6)	1006(24)	3019(34)
305(2)	1006(1)	3019(60)
316(1)	1032(12)	3020(17)
359(2)	1033(12)	3081(24)
378(2)	1035(40)	3084(1)
389(3)	1039(1)	3085(1)
399(2)	1072(1)	3085(21)
411(4)	1073(1)	3109(1)
419(0)	1214(1)	3112(21)
434(1)	1215(0)	3113(1)
444(1)	1294(1)	3113(26)
492(14)	1294(4)	3119(0)
510(2)	1384(11)	3119(15)
548(3)	1386(7)	3135(25)
564(0)	1390(3)	3135(20)
586(6)	1392(0)	3140(3)
597(0)	1395(3)	3140(0)
606(3)	1396(5)	3196(12)
670(2)	1410(21)	3196(16)
696(9)	1420(8)	3221(4)
719(0)	1459(11)	3222(0)

Table S46. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2V$** structure **V-1Q**.

B3LYP*		
37(0)	792(33)	1462(23)
72(0)	796(0)	1467(6)
83(0)	812(44)	1469(0)
124(0)	821(15)	1472(13)
126(0)	840(2)	1472(1)
131(1)	840(65)	1479(8)
136(0)	874(2)	1481(13)
141(0)	879(0)	1497(98)
142(3)	880(4)	1497(27)
171(1)	883(3)	1528(24)
172(0)	987(5)	1529(11)
200(0)	987(1)	1554(36)
216(0)	990(2)	1556(54)
237(1)	991(0)	3021(12)
247(0)	1013(32)	3021(29)
258(4)	1014(1)	3022(38)
293(4)	1035(23)	3022(4)
323(4)	1037(6)	3086(25)
338(1)	1038(16)	3086(0)
348(1)	1038(2)	3088(4)
367(0)	1063(2)	3088(23)
388(1)	1064(1)	3112(25)
398(8)	1217(0)	3113(6)
441(0)	1217(0)	3117(23)
443(0)	1289(1)	3117(1)
523(3)	1291(4)	3140(17)
526(1)	1384(39)	3140(4)
552(0)	1384(9)	3143(1)
558(1)	1390(2)	3143(22)
600(12)	1392(8)	3149(1)
606(2)	1396(0)	3149(0)
608(0)	1398(0)	3246(5)
615(4)	1431(6)	3246(15)
709(1)	1434(22)	3270(2)
717(2)	1458(72)	3270(1)

Table S47. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2V$** structure **V-2Q**.

B3LYP*		
15(0)	797(21)	1461(84)
86(1)	809(0)	1470(17)
89(0)	810(0)	1471(0)
115(1)	823(106)	1471(3)
118(1)	843(0)	1472(2)
133(1)	846(36)	1480(1)
135(0)	874(2)	1482(20)
143(0)	879(0)	1496(7)
145(0)	882(5)	1501(112)
180(0)	883(0)	1528(0)
186(1)	988(0)	1529(32)
201(0)	989(5)	1555(2)
209(0)	991(2)	1556(78)
227(1)	991(0)	3022(26)
247(0)	1014(31)	3022(25)
262(4)	1016(0)	3023(15)
297(10)	1036(27)	3023(23)
310(1)	1037(0)	3089(12)
336(1)	1039(1)	3089(0)
349(0)	1039(19)	3089(34)
368(2)	1064(1)	3089(0)
386(0)	1065(0)	3117(22)
398(8)	1217(0)	3117(12)
441(0)	1218(0)	3118(10)
442(0)	1291(0)	3118(9)
525(0)	1292(6)	3139(3)
529(3)	1384(41)	3140(13)
555(2)	1385(1)	3145(0)
557(0)	1391(13)	3145(23)
605(1)	1392(1)	3154(6)
605(14)	1394(1)	3154(1)
607(1)	1399(0)	3243(1)
609(1)	1430(30)	3243(20)
711(0)	1433(0)	3268(3)
716(3)	1459(3)	3268(0)

Table S48. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Cr$** structure **Cr-1S**.

B3LYP*		
66(2)	837(8)	1463(15)
98(0)	855(2)	1466(14)
128(0)	858(3)	1470(5)
129(2)	859(42)	1471(10)
142(0)	876(2)	1475(11)
147(4)	890(16)	1479(4)
147(0)	891(2)	1481(29)
160(0)	900(0)	1513(5)
179(1)	906(2)	1513(5)
188(0)	907(7)	1525(22)
212(0)	984(2)	1527(23)
227(1)	985(2)	1536(31)
234(3)	998(10)	1538(20)
279(0)	999(0)	3020(9)
298(5)	1007(16)	3021(51)
314(3)	1008(1)	3021(11)
329(0)	1029(10)	3022(33)
360(5)	1033(41)	3084(24)
373(0)	1036(13)	3087(1)
393(11)	1037(0)	3087(22)
401(2)	1070(0)	3087(1)
423(8)	1074(0)	3109(12)
425(0)	1218(0)	3110(0)
434(2)	1220(1)	3113(6)
446(1)	1292(2)	3113(4)
489(12)	1292(6)	3115(5)
515(2)	1385(10)	3116(13)
540(4)	1388(9)	3123(43)
566(0)	1389(11)	3123(45)
590(6)	1393(5)	3130(2)
598(0)	1397(2)	3131(7)
611(4)	1397(2)	3193(14)
698(1)	1423(8)	3193(19)
715(6)	1428(6)	3220(0)
754(0)	1459(11)	3221(4)

Table S49. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Cr$** structure **Cr-1T**.

B3LYP*		
7(0)	841(0)	1459(27)
124(0)	852(7)	1460(0)
125(1)	860(14)	1472(38)
138(0)	864(6)	1475(4)
141(3)	868(21)	1477(8)
146(0)	878(0)	1479(0)
157(1)	887(3)	1490(19)
207(0)	890(3)	1490(0)
213(0)	890(0)	1501(1)
222(2)	912(13)	1524(0)
235(2)	976(0)	1527(15)
238(4)	983(5)	1531(8)
239(0)	994(20)	1534(39)
245(0)	1000(1)	3017(0)
287(6)	1009(12)	3018(23)
288(0)	1014(2)	3019(70)
314(6)	1029(33)	3020(30)
335(10)	1031(0)	3080(0)
355(0)	1032(37)	3080(40)
362(0)	1041(2)	3082(0)
376(9)	1062(0)	3083(13)
380(0)	1067(1)	3113(3)
406(0)	1203(0)	3113(0)
426(0)	1204(1)	3117(24)
428(0)	1300(1)	3117(19)
494(17)	1303(2)	3134(0)
496(0)	1375(0)	3134(2)
538(0)	1384(3)	3136(42)
553(1)	1389(0)	3138(34)
597(1)	1390(1)	3141(1)
597(0)	1398(6)	3144(9)
635(8)	1399(5)	3227(0)
644(0)	1410(17)	3229(16)
741(2)	1422(22)	3253(3)
748(2)	1457(0)	3255(6)

Table S50. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Cr$** structure **Cr-2T**.

B3LYP*		
41(2)	829(0)	1466(45)
111(0)	837(2)	1469(3)
115(1)	846(0)	1470(0)
144(0)	853(61)	1470(0)
161(0)	864(0)	1471(20)
173(0)	867(22)	1475(20)
177(0)	872(0)	1482(0)
180(4)	879(1)	1498(0)
191(0)	881(9)	1499(10)
208(1)	893(0)	1514(0)
217(4)	982(4)	1518(14)
235(0)	983(0)	1529(0)
237(1)	997(16)	1529(52)
245(0)	998(0)	3018(0)
278(0)	1011(0)	3019(63)
300(7)	1012(23)	3019(54)
322(9)	1032(0)	3019(0)
347(0)	1036(22)	3085(0)
350(0)	1038(36)	3085(0)
354(2)	1039(0)	3085(0)
380(3)	1066(0)	3085(44)
404(0)	1068(1)	3116(0)
426(0)	1205(0)	3116(38)
429(3)	1208(0)	3117(0)
440(1)	1299(0)	3117(13)
496(0)	1301(7)	3132(0)
509(8)	1381(9)	3133(31)
547(3)	1381(0)	3137(31)
558(0)	1391(0)	3137(0)
600(1)	1394(11)	3149(12)
601(0)	1395(0)	3149(0)
614(0)	1397(9)	3225(0)
664(0)	1413(34)	3226(14)
729(0)	1419(0)	3251(8)
731(2)	1458(0)	3251(0)

Table S51. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **(2,4-$Me_2C_5H_5)_2$Cr** structure **Cr-3T**.

B3LYP*		
58(1)	837(8)	1462(11)
103(0)	838(1)	1464(13)
105(0)	847(23)	1469(2)
140(0)	862(0)	1470(13)
142(0)	870(19)	1475(10)
144(3)	874(1)	1478(8)
160(0)	878(12)	1480(18)
169(0)	887(0)	1501(6)
171(0)	888(7)	1501(4)
202(2)	898(3)	1512(3)
204(1)	983(3)	1513(7)
215(0)	983(2)	1527(33)
220(2)	999(11)	1528(13)
273(0)	1000(0)	3018(65)
291(1)	1008(2)	3018(7)
298(6)	1009(20)	3018(11)
310(9)	1033(12)	3019(38)
356(1)	1034(12)	3082(23)
359(2)	1038(33)	3083(0)
383(1)	1041(0)	3084(21)
389(5)	1068(0)	3084(4)
397(0)	1069(1)	3109(24)
421(4)	1209(1)	3109(3)
430(0)	1209(0)	3113(2)
438(1)	1296(1)	3114(24)
501(10)	1297(4)	3127(1)
505(2)	1381(10)	3127(23)
551(1)	1383(5)	3135(7)
556(0)	1389(2)	3135(34)
598(0)	1393(0)	3142(7)
600(1)	1395(6)	3142(3)
630(6)	1395(5)	3216(7)
670(0)	1412(21)	3217(10)
725(1)	1420(12)	3238(2)
741(1)	1462(22)	3239(5)

Table S52. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **(2,4-$Me_2C_5H_5)_2$Cr** structure **Cr-1P**.

B3LYP*					
26(	2)	782(	25)	1463(	59)
32(	0)	806(	11)	1467(	15)
49(	0)	830(	8)	1469(	1)
55(	0)	831(	1)	1471(	5)
64(	0)	854(	10)	1472(	0)
85(	1)	854(	192)	1483(	18)
99(	0)	859(	11)	1484(	5)
127(	0)	864(	7)	1496(	90)
144(	0)	886(	0)	1497(	16)
153(	0)	886(	4)	1522(	12)
163(	0)	974(	0)	1525(	91)
165(	0)	975(	0)	1628(	79)
172(	6)	993(	5)	1629(	20)
222(	0)	993(	1)	3020(	37)
226(	0)	1017(	10)	3020(	1)
256(	0)	1018(	0)	3023(	35)
283(	3)	1039(	25)	3023(	0)
293(	5)	1040(	0)	3079(	1)
341(	2)	1048(	2)	3079(	34)
352(	1)	1048(	1)	3089(	0)
355(	4)	1068(	4)	3090(	20)
370(	2)	1069(	1)	3115(	1)
399(	39)	1226(	5)	3115(	23)
445(	0)	1227(	0)	3118(	32)
447(	0)	1276(	29)	3118(	2)
514(	4)	1277(	6)	3130(	14)
517(	3)	1386(	20)	3130(	19)
570(	6)	1387(	24)	3143(	2)
576(	2)	1392(	3)	3143(	1)
576(	3)	1394(	12)	3154(	2)
580(	5)	1400(	4)	3154(	3)
641(	22)	1400(	3)	3233(	15)
646(	17)	1434(	1)	3233(	8)
704(	3)	1434(	6)	3256(	2)
705(	1)	1461(	36)	3256(	3)

Table S53. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-1D**.

B3LYP*					
-2(	0)	859(	0)	1457(	27)
124(	0)	865(	26)	1461(	0)
147(	1)	868(	20)	1475(	25)
149(	3)	868(	4)	1478(	4)
154(	0)	889(	0)	1479(	19)
160(	0)	890(	0)	1480(	0)
164(	1)	908(	3)	1492(	18)
228(	2)	908(	1)	1499(	0)
229(	0)	918(	0)	1508(	2)
231(	0)	933(	16)	1536(	0)
238(	0)	975(	0)	1540(	11)
241(	2)	984(	3)	1542(	22)
256(	3)	991(	18)	1547(	39)
259(	0)	998(	2)	3019(	0)
295(	3)	1012(	9)	3019(	18)
298(	0)	1018(	2)	3021(	59)
325(	23)	1028(	0)	3021(	28)
336(	0)	1031(	37)	3081(	42)
351(	1)	1035(	29)	3081(	0)
371(	15)	1036(	2)	3085(	14)
379(	0)	1058(	0)	3085(	1)
385(	2)	1067(	0)	3115(	0)
409(	0)	1207(	0)	3117(	0)
427(	0)	1209(	0)	3119(	4)
428(	0)	1300(	2)	3122(	6)
496(	0)	1302(	5)	3122(	0)
504(	12)	1379(	0)	3123(	0)
538(	0)	1388(	5)	3126(	53)
546(	1)	1389(	0)	3127(	2)
598(	0)	1390(	0)	3127(	69)
599(	0)	1399(	8)	3131(	29)
655(	0)	1399(	8)	3226(	0)
664(	5)	1423(	5)	3228(	15)
774(	0)	1430(	20)	3255(	5)
774(	2)	1456(	0)	3256(	7)

Table S54. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Mn$** structure **Mn-2D**.

B3LYP*		
38(2)	857(0)	1468(40)
124(0)	857(6)	1470(3)
144(1)	859(0)	1470(0)
165(0)	866(64)	1472(0)
173(0)	877(0)	1473(15)
182(0)	878(0)	1478(18)
184(0)	889(24)	1486(0)
186(4)	890(8)	1511(0)
194(0)	902(4)	1512(15)
224(1)	910(0)	1524(0)
227(3)	984(3)	1527(27)
240(0)	984(0)	1548(50)
243(1)	994(15)	1548(0)
245(0)	996(0)	3020(0)
281(0)	1015(0)	3020(53)
307(12)	1017(21)	3020(45)
324(0)	1036(21)	3020(0)
334(16)	1036(0)	3086(0)
346(0)	1037(34)	3086(0)
360(0)	1037(0)	3086(0)
402(3)	1065(0)	3086(46)
403(0)	1067(0)	3117(29)
428(0)	1210(0)	3117(0)
439(6)	1211(1)	3118(0)
439(1)	1298(0)	3118(9)
510(0)	1302(10)	3129(0)
512(9)	1384(13)	3130(50)
546(2)	1386(0)	3132(48)
549(0)	1392(0)	3133(0)
604(3)	1394(14)	3138(12)
606(0)	1395(0)	3139(0)
644(0)	1398(9)	3230(0)
676(0)	1427(30)	3231(15)
759(0)	1428(0)	3257(10)
774(4)	1461(0)	3258(0)

Table S55. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Mn$** structure **Mn-3D**.

B3LYP*					
58(	1)	855(	3)	1464(	11)
116(	0)	856(	9)	1466(	11)
132(	0)	862(	38)	1469(	2)
149(	3)	866(	0)	1471(	16)
155(	0)	884(	0)	1476(	9)
170(	1)	886(	4)	1480(	6)
171(	0)	888(	9)	1482(	19)
175(	1)	911(	2)	1511(	8)
177(	0)	913(	11)	1512(	7)
212(	1)	919(	2)	1523(	13)
219(	2)	983(	2)	1524(	12)
225(	0)	983(	2)	1540(	30)
228(	2)	998(	13)	1541(	14)
277(	1)	999(	0)	3020(	54)
296(	2)	1010(	13)	3020(	5)
300(	2)	1011(	1)	3021(	10)
318(	18)	1031(	15)	3022(	35)
349(	1)	1036(	32)	3084(	22)
365(	6)	1036(	13)	3086(	1)
388(	2)	1039(	0)	3086(	3)
393(	5)	1065(	0)	3086(	23)
403(	0)	1070(	0)	3114(	7)
428(	7)	1213(	0)	3114(	11)
430(	1)	1214(	1)	3115(	4)
439(	1)	1296(	2)	3115(	2)
501(	9)	1297(	6)	3121(	37)
511(	2)	1383(	11)	3121(	0)
545(	1)	1386(	8)	3126(	25)
555(	0)	1390(	4)	3126(	60)
601(	0)	1393(	2)	3130(	4)
601(	1)	1396(	6)	3131(	2)
639(	5)	1397(	5)	3219(	7)
689(	0)	1425(	9)	3219(	12)
754(	1)	1429(	11)	3243(	2)
762(	1)	1462(	14)	3243(	6)

Table S56. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-1Q**.

B3LYP*		
15(0)	820(10)	1462(26)
39(0)	829(3)	1464(24)
75(0)	851(1)	1467(22)
91(0)	855(26)	1471(0)
111(0)	859(4)	1474(11)
140(1)	871(9)	1478(24)
148(1)	872(27)	1486(5)
158(1)	877(14)	1488(1)
177(0)	885(8)	1494(26)
185(0)	900(10)	1508(18)
186(1)	970(1)	1511(23)
208(0)	981(1)	1527(10)
220(1)	990(5)	1650(51)
236(1)	996(9)	3015(33)
257(1)	1004(5)	3016(12)
268(1)	1016(4)	3017(47)
290(0)	1030(28)	3023(23)
316(4)	1033(24)	3077(6)
324(2)	1038(5)	3078(29)
351(1)	1049(1)	3079(6)
371(1)	1068(3)	3091(9)
380(3)	1069(1)	3104(7)
401(1)	1199(1)	3104(8)
427(0)	1226(9)	3109(25)
440(1)	1277(16)	3117(17)
492(7)	1290(3)	3119(16)
508(21)	1374(3)	3125(13)
544(2)	1383(7)	3130(13)
559(2)	1388(0)	3138(8)
571(5)	1392(1)	3138(2)
591(3)	1395(11)	3150(5)
645(10)	1398(5)	3203(9)
675(8)	1403(27)	3222(11)
706(4)	1432(1)	3231(4)
719(2)	1458(4)	3244(5)

Table S57. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-2Q**.

B3LYP*		
31(2)	811(0)	1460(86)
42(0)	824(2)	1465(21)
43(1)	837(0)	1466(0)
67(0)	843(4)	1470(10)
87(0)	857(0)	1470(0)
89(2)	858(29)	1481(0)
130(1)	872(113)	1484(19)
136(0)	874(0)	1485(0)
166(0)	884(0)	1486(40)
167(0)	885(23)	1504(0)
168(0)	971(2)	1505(29)
174(1)	971(0)	1644(106)
210(6)	990(0)	1645(0)
224(0)	990(12)	3018(49)
228(0)	1016(15)	3018(0)
276(0)	1016(0)	3021(42)
325(6)	1034(45)	3021(0)
336(0)	1036(0)	3081(0)
350(0)	1049(3)	3081(27)
353(1)	1049(0)	3082(0)
369(0)	1063(0)	3082(22)
375(0)	1067(4)	3106(0)
393(1)	1222(0)	3106(28)
437(0)	1222(15)	3118(35)
445(7)	1274(0)	3118(0)
511(39)	1276(31)	3123(0)
519(0)	1380(21)	3123(35)
562(1)	1380(0)	3133(0)
564(0)	1390(0)	3133(10)
579(11)	1392(14)	3148(0)
587(0)	1397(0)	3148(7)
668(0)	1398(13)	3216(0)
688(3)	1431(4)	3217(18)
708(0)	1431(0)	3244(12)
709(12)	1460(0)	3244(0)

Table S58. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **(2,4-$Me_2C_5H_5)_2$Mn** structure **Mn-3Q**.

B3LYP*		
44(0)	806(5)	1463(18)
67(0)	807(20)	1465(0)
90(1)	845(2)	1465(11)
94(2)	847(49)	1471(18)
105(0)	863(1)	1471(16)
125(2)	868(1)	1478(17)
140(0)	873(2)	1486(2)
149(1)	879(0)	1490(0)
157(0)	884(3)	1493(3)
167(0)	918(3)	1517(73)
176(0)	982(2)	1528(4)
198(2)	983(0)	1552(28)
199(0)	995(5)	1553(12)
218(1)	997(0)	3017(67)
231(0)	1004(20)	3017(8)
245(0)	1006(5)	3019(11)
254(5)	1034(37)	3019(39)
309(4)	1035(6)	3079(2)
320(1)	1037(8)	3079(20)
362(1)	1039(3)	3082(23)
364(0)	1072(2)	3084(2)
415(1)	1073(0)	3106(13)
419(1)	1206(1)	3106(5)
432(0)	1207(0)	3110(0)
439(0)	1286(5)	3111(42)
486(1)	1286(5)	3114(22)
494(0)	1377(7)	3116(1)
547(2)	1382(6)	3137(10)
552(0)	1388(1)	3138(22)
580(1)	1392(2)	3144(1)
587(2)	1393(9)	3144(0)
637(7)	1394(5)	3187(2)
675(1)	1413(26)	3187(17)
705(0)	1418(3)	3248(1)
716(4)	1459(22)	3248(6)

Table S59. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Mn$** structure **Mn-1X**.

B3LYP*		
19(0)	795(14)	1460(39)
33(0)	798(6)	1467(16)
42(0)	812(0)	1471(7)
50(0)	812(67)	1472(16)
61(0)	846(208)	1472(1)
74(2)	850(20)	1477(15)
82(0)	886(1)	1477(2)
112(1)	886(32)	1501(58)
115(2)	888(72)	1502(40)
123(2)	891(15)	1521(66)
131(0)	991(1)	1526(161)
184(6)	991(1)	1542(103)
185(0)	1007(1)	1545(21)
196(0)	1007(1)	3019(7)
215(4)	1013(0)	3020(37)
220(1)	1014(2)	3020(38)
241(20)	1031(30)	3020(1)
280(0)	1032(0)	3082(22)
305(45)	1033(9)	3084(2)
356(0)	1034(11)	3086(0)
358(0)	1076(2)	3086(23)
397(1)	1076(2)	3106(4)
401(34)	1207(3)	3106(0)
447(0)	1208(1)	3112(32)
448(0)	1291(25)	3112(4)
522(5)	1292(2)	3114(1)
528(3)	1372(67)	3114(4)
572(0)	1373(60)	3116(4)
573(5)	1385(1)	3116(30)
614(6)	1388(1)	3150(15)
615(0)	1388(3)	3150(10)
624(36)	1390(5)	3185(9)
627(31)	1434(29)	3185(16)
697(1)	1436(16)	3205(9)
705(3)	1459(42)	3205(2)

Table S60. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Fe$** structure **Fe-1S**.

B3LYP*		
39(0)	868(3)	1463(31)
128(1)	868(11)	1468(1)
137(0)	876(2)	1469(0)
151(1)	877(14)	1469(9)
165(0)	888(3)	1478(8)
167(2)	898(3)	1485(1)
180(0)	913(0)	1488(21)
184(0)	923(10)	1498(0)
226(0)	938(6)	1504(4)
230(1)	940(2)	1527(10)
234(0)	980(2)	1529(14)
241(3)	984(2)	1538(23)
264(0)	996(17)	1543(5)
276(4)	997(1)	3016(45)
302(3)	1017(12)	3017(24)
341(9)	1018(1)	3020(17)
347(1)	1032(3)	3021(31)
352(9)	1036(12)	3080(23)
381(2)	1038(32)	3080(0)
397(7)	1039(5)	3083(1)
417(2)	1066(0)	3084(23)
423(2)	1069(0)	3106(8)
429(1)	1204(0)	3109(28)
430(3)	1206(0)	3114(11)
458(15)	1303(0)	3115(11)
502(0)	1305(4)	3117(12)
510(8)	1380(0)	3118(23)
547(0)	1381(9)	3125(36)
550(1)	1389(1)	3130(10)
601(0)	1395(6)	3141(27)
606(0)	1396(11)	3141(2)
706(4)	1397(4)	3198(14)
723(2)	1416(14)	3200(8)
800(1)	1421(0)	3254(4)
802(4)	1463(10)	3254(13)

Table S61. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Fe$** structure **Fe-2S**.

B3LYP*					
50(	1)	866(	12)	1463(	2)
121(	0)	868(	4)	1468(	3)
127(	0)	873(	2)	1470(	10)
154(	0)	874(	22)	1472(	3)
165(	0)	893(	2)	1473(	11)
178(	0)	895(	0)	1480(	10)
186(	5)	914(	5)	1484(	9)
199(	0)	914(	3)	1500(	12)
201(	1)	918(	14)	1508(	8)
225(	1)	946(	5)	1521(	14)
231(	0)	981(	2)	1525(	2)
236(	2)	982(	1)	1542(	14)
242(	0)	995(	15)	1543(	11)
283(	1)	997(	2)	3017(	17)
311(	2)	1016(	1)	3018(	33)
317(	8)	1018(	14)	3019(	44)
347(	14)	1034(	18)	3019(	6)
368(	1)	1035(	7)	3081(	30)
373(	0)	1037(	24)	3082(	8)
395(	11)	1039(	4)	3082(	14)
422(	6)	1062(	0)	3083(	1)
423(	4)	1065(	0)	3110(	19)
427(	0)	1205(	1)	3112(	6)
433(	1)	1206(	0)	3117(	3)
447(	13)	1300(	2)	3117(	2)
506(	5)	1302(	4)	3123(	31)
514(	3)	1379(	11)	3124(	13)
552(	0)	1383(	3)	3127(	35)
554(	0)	1391(	5)	3128(	39)
604(	0)	1393(	0)	3133(	8)
604(	0)	1394(	8)	3134(	8)
704(	5)	1396(	6)	3218(	6)
729(	0)	1423(	6)	3218(	9)
788(	1)	1423(	12)	3243(	5)
810(	0)	1461(	30)	3243(	16)

Table S62. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Fe$** structure **Fe-1T**.

B3LYP*					
19(	0)	829(	19)	1461(	15)
30(	0)	839(	4)	1466(	35)
78(	0)	860(	16)	1467(	7)
92(	0)	862(	7)	1472(	1)
127(	0)	867(	15)	1474(	16)
136(	0)	872(	35)	1482(	19)
146(	3)	880(	7)	1487(	7)
157(	1)	884(	4)	1499(	22)
173(	0)	887(	2)	1501(	15)
183(	0)	915(	7)	1514(	18)
193(	1)	968(	1)	1525(	40)
200(	0)	982(	2)	1547(	20)
217(	1)	990(	2)	1651(	44)
242(	1)	999(	4)	3018(	9)
249(	1)	1008(	7)	3019(	47)
270(	1)	1016(	3)	3020(	18)
295(	2)	1031(	24)	3022(	25)
318(	2)	1035(	18)	3081(	23)
329(	1)	1036(	8)	3083(	3)
354(	1)	1049(	1)	3084(	21)
368(	2)	1066(	2)	3089(	7)
395(	2)	1069(	0)	3107(	6)
403(	2)	1209(	0)	3108(	4)
435(	0)	1229(	9)	3113(	10)
443(	1)	1277(	15)	3114(	40)
498(	6)	1292(	6)	3120(	16)
508(	14)	1380(	3)	3123(	11)
543(	1)	1385(	10)	3132(	5)
558(	3)	1389(	1)	3134(	20)
574(	5)	1392(	3)	3140(	2)
594(	1)	1395(	13)	3151(	5)
657(	10)	1398(	6)	3207(	8)
658(	6)	1423(	12)	3214(	13)
706(	1)	1434(	1)	3248(	6)
739(	1)	1459(	6)	3257(	3)

Table S63. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Fe$** structure **Fe-2T**.

B3LYP*		
10(0)	838(3)	1464(35)
45(1)	842(3)	1466(12)
58(0)	848(92)	1469(0)
72(0)	858(0)	1470(5)
80(0)	861(7)	1470(2)
97(0)	876(60)	1482(5)
129(1)	877(2)	1484(15)
150(0)	884(0)	1503(76)
155(0)	887(4)	1506(3)
157(0)	897(3)	1513(2)
159(0)	977(3)	1515(32)
172(2)	977(0)	1625(19)
216(5)	989(5)	1625(69)
228(1)	990(0)	3021(48)
242(0)	1016(9)	3021(1)
284(0)	1017(2)	3023(0)
308(6)	1037(33)	3023(37)
323(3)	1039(0)	3084(28)
360(1)	1044(3)	3084(0)
366(0)	1047(2)	3087(1)
369(2)	1066(5)	3087(25)
405(3)	1069(0)	3113(16)
422(1)	1225(5)	3113(1)
441(1)	1225(0)	3119(23)
448(3)	1278(25)	3119(6)
511(11)	1279(3)	3125(20)
511(1)	1384(12)	3125(39)
558(1)	1387(14)	3129(5)
569(1)	1391(1)	3129(8)
587(7)	1394(12)	3155(5)
591(0)	1398(8)	3155(1)
651(3)	1398(0)	3218(2)
674(3)	1434(7)	3218(17)
710(0)	1434(2)	3271(2)
716(0)	1461(37)	3271(6)

Table S64. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Fe$** structure **Fe-1P**.

B3LYP*		
35(0)	797(1)	1459(47)
49(0)	804(0)	1462(19)
74(0)	808(75)	1470(3)
75(0)	811(0)	1472(14)
86(0)	836(102)	1476(0)
86(0)	842(5)	1478(13)
89(0)	877(12)	1479(32)
115(1)	881(0)	1493(48)
133(1)	881(5)	1494(66)
136(1)	887(4)	1515(2)
152(0)	986(2)	1517(25)
187(1)	986(3)	1543(41)
187(0)	999(2)	1546(27)
216(10)	999(1)	3022(23)
218(0)	1010(0)	3022(8)
225(0)	1010(10)	3022(27)
240(7)	1031(25)	3023(34)
271(0)	1033(6)	3086(21)
295(9)	1034(9)	3088(1)
345(0)	1034(12)	3088(22)
355(1)	1066(1)	3089(3)
391(10)	1067(1)	3113(2)
393(1)	1210(1)	3115(2)
442(0)	1210(0)	3115(25)
445(0)	1293(10)	3115(24)
498(3)	1293(0)	3127(0)
508(1)	1376(43)	3127(14)
560(0)	1377(35)	3142(2)
561(3)	1386(4)	3142(12)
596(0)	1389(1)	3152(8)
600(2)	1391(2)	3152(5)
635(18)	1392(3)	3219(6)
649(8)	1428(10)	3219(12)
707(0)	1429(11)	3251(7)
717(1)	1459(45)	3251(0)

Table S65. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Co$** structure **Co-1D**.

B3LYP*		
23(0)	839(1)	1460(22)
54(0)	847(32)	1463(9)
91(0)	848(1)	1466(2)
105(0)	865(15)	1469(6)
116(0)	877(2)	1473(6)
134(0)	881(8)	1478(22)
152(1)	892(10)	1481(6)
166(2)	900(33)	1483(4)
177(0)	906(39)	1494(31)
180(1)	912(4)	1514(26)
194(1)	971(1)	1516(1)
219(1)	983(2)	1535(24)
230(0)	996(1)	1660(29)
242(2)	997(9)	3016(24)
272(2)	1013(1)	3019(19)
284(2)	1015(4)	3021(25)
328(0)	1032(30)	3021(19)
340(1)	1034(12)	3080(14)
352(2)	1036(10)	3085(9)
358(6)	1052(1)	3085(8)
371(1)	1060(1)	3086(12)
400(2)	1064(2)	3090(20)
413(3)	1198(0)	3110(16)
431(0)	1223(11)	3112(16)
431(0)	1283(13)	3117(9)
501(24)	1295(9)	3118(33)
504(5)	1369(32)	3121(12)
554(1)	1377(4)	3124(4)
557(1)	1389(2)	3128(17)
583(6)	1391(2)	3136(5)
603(2)	1392(16)	3149(9)
693(20)	1398(8)	3211(11)
704(8)	1423(21)	3217(10)
742(3)	1427(1)	3229(8)
766(1)	1455(55)	3250(6)

Table S66. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Co$** structure **Co-2D**.

B3LYP*					
25(	1)	834(	0)	1461(	0)
42(	0)	843(	9)	1465(	29)
44(	0)	858(	0)	1466(	0)
77(	1)	870(	15)	1470(	8)
92(	0)	870(	0)	1471(	0)
108(	1)	880(	1)	1481(	0)
131(	1)	883(	98)	1484(	21)
143(	0)	885(	0)	1490(	0)
160(	0)	886(	0)	1493(	41)
162(	0)	886(	34)	1518(	31)
167(	0)	971(	0)	1519(	0)
173(	2)	971(	1)	1652(	86)
224(	3)	992(	9)	1653(	0)
225(	0)	992(	0)	3020(	40)
236(	1)	1016(	0)	3020(	0)
282(	0)	1016(	10)	3021(	42)
325(	7)	1037(	33)	3021(	0)
338(	0)	1039(	0)	3083(	0)
353(	0)	1049(	3)	3083(	28)
356(	0)	1049(	0)	3086(	8)
371(	3)	1065(	0)	3086(	12)
378(	0)	1067(	4)	3111(	0)
417(	7)	1226(	0)	3111(	19)
438(	0)	1227(	15)	3118(	34)
444(	7)	1276(	0)	3118(	0)
516(	28)	1277(	31)	3121(	0)
519(	0)	1383(	25)	3122(	50)
563(	2)	1386(	0)	3136(	0)
566(	0)	1391(	0)	3136(	16)
588(	6)	1392(	13)	3147(	8)
596(	0)	1398(	0)	3147(	0)
691(	0)	1399(	13)	3223(	0)
701(	11)	1432(	2)	3224(	26)
723(	0)	1433(	0)	3242(	0)
739(	2)	1461(	48)	3242(	9)

Table S67. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Co$** structure **Co-3D**.

B3LYP*		
25(0)	839(11)	1463(35)
31(1)	853(0)	1467(13)
49(0)	854(1)	1467(6)
80(0)	871(3)	1470(0)
87(0)	873(2)	1470(6)
107(0)	880(7)	1481(19)
123(2)	881(122)	1485(4)
147(0)	885(1)	1494(54)
158(0)	887(6)	1497(3)
165(0)	895(7)	1517(1)
167(0)	974(1)	1517(29)
170(1)	974(0)	1647(14)
218(4)	991(8)	1648(71)
231(1)	993(0)	3020(2)
235(0)	1017(7)	3020(37)
288(0)	1017(2)	3021(39)
324(6)	1039(30)	3021(2)
345(1)	1040(0)	3080(30)
353(1)	1048(2)	3080(1)
354(1)	1050(1)	3087(0)
369(1)	1065(6)	3087(21)
395(3)	1068(0)	3111(14)
426(3)	1225(1)	3111(2)
440(0)	1225(8)	3118(16)
446(4)	1277(32)	3118(22)
516(22)	1277(3)	3121(30)
517(5)	1385(11)	3122(25)
566(2)	1385(12)	3138(1)
569(0)	1391(0)	3139(12)
586(4)	1393(13)	3148(5)
598(1)	1399(2)	3148(2)
689(14)	1400(10)	3228(22)
696(6)	1433(0)	3228(6)
729(0)	1433(3)	3247(2)
730(1)	1461(27)	3247(5)

Table S68. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **(2,4-$Me_2C_5H_5)_2$Co** structure **Co-1Q**.

B3LYP*					
27(	0)	805(	0)	1462(	85)
70(	0)	806(	0)	1470(	0)
73(	0)	808(	56)	1471(	18)
82(	0)	816(	0)	1472(	0)
88(	0)	821(	0)	1472(	2)
97(	0)	834(	142)	1480(	17)
101(	0)	878(	0)	1484(	0)
114(	0)	881(	14)	1497(	0)
127(	0)	884(	5)	1501(	181)
140(	0)	889(	0)	1526(	0)
177(	0)	987(	0)	1526(	0)
181(	0)	987(	6)	1558(	0)
190(	1)	993(	1)	1560(	75)
190(	0)	994(	0)	3023(	0)
209(	0)	1015(	18)	3023(	47)
231(	0)	1016(	0)	3024(	36)
253(	1)	1034(	20)	3024(	0)
254(	0)	1035(	0)	3090(	0)
268(	39)	1036(	0)	3090(	0)
338(	2)	1036(	20)	3090(	0)
341(	0)	1063(	3)	3090(	44)
390(	13)	1064(	0)	3118(	0)
395(	0)	1215(	0)	3119(	36)
442(	0)	1215(	0)	3119(	0)
446(	0)	1296(	0)	3119(	17)
508(	0)	1297(	14)	3140(	0)
511(	0)	1381(	57)	3140(	17)
551(	7)	1382(	0)	3143(	22)
559(	0)	1390(	0)	3144(	0)
597(	2)	1391(	14)	3154(	9)
601(	0)	1391(	0)	3154(	0)
622(	0)	1396(	0)	3245(	0)
635(	16)	1432(	0)	3246(	20)
720(	2)	1434(	31)	3273(	3)
723(	0)	1459(	0)	3273(	0)

Table S69. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Co$** structure **Co-2Q**.

B3LYP*					
32(	0)	806(	19)	1460(	41)
48(	0)	807(	1)	1462(	14)
61(	0)	813(	62)	1470(	3)
70(	0)	819(	0)	1472(	12)
78(	0)	843(	78)	1476(	0)
82(	0)	849(	4)	1478(	12)
91(	0)	881(	8)	1480(	27)
109(	0)	885(	1)	1495(	68)
130(	1)	885(	16)	1500(	82)
144(	0)	893(	5)	1521(	6)
156(	0)	987(	2)	1523(	20)
187(	0)	988(	3)	1548(	44)
190(	2)	999(	0)	1551(	27)
223(	3)	1000(	2)	3022(	34)
226(	0)	1011(	0)	3022(	5)
228(	0)	1011(	9)	3022(	13)
245(	11)	1030(	22)	3023(	32)
274(	0)	1033(	0)	3086(	19)
299(	14)	1033(	15)	3088(	1)
351(	0)	1035(	14)	3088(	21)
358(	0)	1067(	1)	3089(	3)
395(	11)	1068(	2)	3114(	3)
397(	1)	1213(	1)	3115(	2)
444(	0)	1214(	0)	3115(	22)
446(	0)	1293(	11)	3116(	21)
502(	3)	1293(	1)	3126(	18)
512(	1)	1377(	44)	3126(	0)
560(	4)	1379(	35)	3136(	3)
564(	0)	1385(	5)	3136(	15)
596(	0)	1389(	5)	3150(	10)
600(	2)	1391(	1)	3150(	6)
632(	21)	1392(	1)	3217(	9)
669(	7)	1432(	12)	3217(	14)
724(	0)	1433(	9)	3242(	5)
728(	2)	1459(	36)	3242(	0)

Table S70. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Ni$** structure **Ni-1S**.

B3LYP*		
39(0)	830(18)	1461(33)
46(0)	841(4)	1463(26)
55(0)	862(0)	1466(5)
86(1)	874(11)	1469(6)
104(1)	879(12)	1472(1)
107(1)	886(55)	1478(18)
128(0)	889(6)	1480(13)
159(0)	897(34)	1482(11)
160(1)	900(4)	1488(12)
166(3)	914(3)	1517(12)
171(1)	961(1)	1523(15)
191(0)	970(0)	1660(36)
207(0)	992(6)	1664(19)
218(0)	994(1)	3011(22)
229(0)	1015(4)	3018(15)
257(4)	1016(3)	3019(29)
299(0)	1034(26)	3021(25)
328(3)	1039(10)	3067(20)
343(5)	1050(0)	3084(13)
353(2)	1052(2)	3085(6)
368(0)	1065(2)	3090(10)
387(3)	1067(1)	3102(9)
422(4)	1227(5)	3107(4)
440(1)	1229(10)	3112(6)
442(5)	1275(11)	3113(34)
505(3)	1280(12)	3115(29)
512(17)	1381(10)	3122(20)
559(1)	1385(5)	3125(6)
572(5)	1390(13)	3133(3)
591(5)	1392(5)	3141(4)
595(6)	1396(5)	3145(4)
701(8)	1397(10)	3211(6)
708(2)	1427(1)	3221(13)
749(5)	1432(0)	3232(5)
754(11)	1460(19)	3239(11)

Table S71. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **(2,4-$Me_2C_5H_5)_2$Ni** structure **Ni-2S**.

B3LYP*					
34(	1)	832(	0)	1460(	0)
37(	0)	841(	9)	1463(	0)
48(	0)	861(	0)	1464(	25)
69(	0)	874(	9)	1470(	0)
95(	0)	879(	0)	1470(	7)
102(	2)	883(	2)	1478(	0)
138(	1)	886(	0)	1480(	26)
146(	0)	888(	54)	1488(	0)
157(	0)	900(	0)	1488(	26)
158(	0)	901(	76)	1514(	20)
159(	0)	970(	0)	1517(	0)
167(	3)	970(	0)	1661(	77)
211(	2)	992(	10)	1661(	0)
215(	0)	993(	0)	3019(	49)
228(	1)	1014(	0)	3019(	0)
278(	0)	1014(	7)	3019(	35)
331(	0)	1036(	31)	3019(	0)
335(	4)	1040(	0)	3078(	0)
347(	5)	1050(	0)	3078(	34)
350(	5)	1050(	2)	3085(	17)
354(	0)	1064(	2)	3085(	0)
394(	0)	1064(	0)	3103(	17)
427(	7)	1225(	0)	3104(	0)
435(	0)	1226(	17)	3113(	0)
441(	11)	1279(	36)	3113(	44)
509(	32)	1280(	0)	3117(	48)
510(	0)	1379(	15)	3117(	0)
556(	2)	1382(	0)	3132(	14)
559(	0)	1390(	0)	3132(	0)
591(	5)	1391(	19)	3139(	8)
599(	0)	1398(	0)	3139(	0)
700(	0)	1398(	16)	3221(	0)
704(	15)	1428(	1)	3221(	21)
733(	0)	1428(	0)	3231(	13)
751(	7)	1459(	46)	3231(	0)

Table S72. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(2,4\text{-}Me_2C_5H_5)_2Ni$** structure **Ni-3S**.

B3LYP*		
36(0)	832(15)	1457(6)
61(0)	851(1)	1459(11)
110(0)	861(16)	1465(25)
119(0)	864(20)	1466(8)
132(1)	872(4)	1470(11)
143(0)	882(1)	1471(11)
148(0)	883(1)	1482(15)
152(1)	893(10)	1484(9)
183(1)	909(6)	1499(14)
191(0)	957(4)	1531(1)
196(0)	985(2)	1535(11)
206(1)	989(3)	1563(16)
212(1)	995(1)	1698(14)
220(1)	999(7)	2998(20)
249(4)	1007(6)	3004(58)
272(1)	1013(14)	3005(38)
283(2)	1037(14)	3023(24)
318(0)	1039(8)	3024(21)
332(1)	1042(9)	3051(16)
343(2)	1064(0)	3058(25)
371(0)	1087(25)	3073(20)
385(4)	1118(6)	3088(10)
396(2)	1171(3)	3089(9)
439(0)	1221(0)	3097(22)
455(1)	1267(3)	3108(7)
486(5)	1296(5)	3112(19)
498(0)	1345(6)	3115(11)
530(1)	1383(7)	3116(34)
558(1)	1384(9)	3119(12)
594(1)	1389(4)	3135(17)
622(1)	1392(5)	3136(19)
667(0)	1396(3)	3141(1)
704(3)	1399(5)	3203(7)
756(1)	1433(4)	3250(7)
769(3)	1439(3)	3273(3)

Table S73. Titanium–carbon distances (in Å) for the **(2,4-$Me_2C_5H_5)_2$Ti** structures. The *italics* indicates the distances too long to be bonded.

	Ti-1S	Ti-2S	Ti-3S	Ti-1T	Ti-2T	Ti-3T
TiC1	2.260	2.291	2.288	2.421	2.418	2.386
TiC2	2.306	2.326	2.315	2.420	2.414	2.367
TiC3	2.315	2.318	2.326	2.375	2.380	2.312
TiC4	2.300	2.326	2.315	2.420	2.414	2.336
TiC5	2.235	2.291	2.288	2.421	2.418	2.408
TiC6	*3.456*	*3.481*	*3.462*	*3.538*	*3.525*	*3.475*
TiC7	*3.463*	*3.481*	*3.462*	*3.538*	*3.525*	*3.417*
TiC8	2.235	2.291	2.288	2.421	2.418	2.408
TiC9	2.300	2.326	2.315	2.420	2.414	2.336
TiC10	2.315	2.318	2.326	2.375	2.380	2.312
TiC11	2.306	2.326	2.315	2.420	2.414	2.367
TiC12	2.260	2.291	2.288	2.421	2.418	2.386
TiC13	*3.463*	*3.481*	*3.462*	*3.538*	*3.525*	*3.417*
TiC14	*3.456*	*3.481*	*3.462*	*3.538*	*3.525*	*3.475*

Table S74. Vanadium–carbon distances (in Å) for the **(2,4-$Me_2C_5H_5)_2$V** structures. The *italics* indicates the distances too long to be bonded.

	V-1D	V-2D	V-3D	V-1Q	V-2Q
VC1	2.214	2.248	2.253	2.367	2.382
VC2	2.259	2.292	2.272	2.328	2.333
VC3	2.280	2.284	2.277	2.287	2.292
VC4	2.271	2.292	2.272	2.320	2.329
VC5	2.194	2.248	2.253	2.378	2.381
VC6	*3.405*	*3.469*	*3.424*	*3.428*	*3.433*
VC7	*3.457*	*3.469*	*3.424*	*3.415*	*3.410*
VC8	2.194	2.248	2.253	2.378	2.381
VC9	2.271	2.292	2.272	2.320	2.329
VC10	2.280	2.284	2.277	2.287	2.292
VC11	2.259	2.292	2.272	2.328	2.333
VC12	2.214	2.248	2.253	2.367	2.382
VC13	*3.457*	*3.469*	*3.424*	*3.415*	*3.410*
VC14	*3.405*	*3.469*	*3.424*	*3.428*	*3.433*

Table S75. Chromium–carbon distances (in Å) for the **(2,4-$Me_2C_5H_5)_2$Cr** structures. The *italics* indicates the distances too long to be bonded.

	Cr-1T	Cr-2T	Cr-3T	Cr-1P	Cr-1S
CrC1	2.189	2.222	2.216	2.249	2.170
CrC2	2.192	2.219	2.241	2.255	2.216
CrC3	2.216	2.217	2.249	2.263	2.245
CrC4	2.233	2.219	2.241	2.710	2.241
CrC5	2.214	2.222	2.216	*3.172*	2.150
CrC6	*3.335*	*3.372*	*3.411*	*3.312*	*3.365*
CrC7	*3.381*	*3.372*	*3.411*	*3.693*	*3.442*
CrC8	2.214	2.222	2.216	*3.172*	2.150
CrC9	2.233	2.219	2.241	2.710	2.241
CrC10	2.216	2.217	2.249	2.263	2.245
CrC11	2.192	2.219	2.241	2.255	2.216
CrC12	2.189	2.222	2.216	2.249	2.170
CrC13	*3.381*	*3.372*	*3.411*	*3.693*	*3.442*
CrC14	*3.335*	*3.372*	*3.411*	*3.312*	*3.365*

Table S76. Manganese–carbon distances (in Å) for the **(2,4-$Me_2C_5H_5)_2$Mn** structures. The *italics* indicates the distances too long to be bonded.

	Mn-1D	Mn-2D	Mn-3D	Mn-1X	Mn-1Q	Mn-2Q	Mn-3Q
MnC1	2.144	2.196	2.174	2.320	*3.447*	2.099	2.124
MnC2	2.156	2.183	2.209	*2.760*	*2.834*	2.329	2.284
MnC3	2.183	2.174	2.220	*2.990*	2.146	2.385	2.302
MnC4	2.205	2.183	2.209	*2.743*	2.087	2.313	2.209
MnC5	2.179	2.196	2.174	2.277	2.140	2.319	2.191
MnC6	*3.303*	*3.338*	*3.398*	*3.903*	*3.761*	*3.508*	*3.473*
MnC7	*3.374*	*3.338*	*3.398*	*3.889*	*3.118*	*3.448*	*3.386*
MnC8	2.179	2.196	2.174	2.277	2.140	2.319	2.121
MnC9	2.205	2.183	2.209	*2.743*	2.087	2.313	2.139
MnC10	2.183	2.174	2.220	*2.990*	2.146	2.385	2.228
MnC11	2.156	2.183	2.209	*2.760*	*2.834*	2.329	2.999
MnC12	2.144	2.196	2.174	2.320	*3.447*	2.099	*3.607*
MnC13	*3.374*	*3.338*	*3.398*	*3.889*	*3.118*	*3.448*	*3.172*
MnC14	*3.303*	*3.338*	*3.398*	*3.903*	*3.761*	*3.508*	*3.976*

Table S77. Iron–carbon distances (in Å) for the **(2,4-$Me_2C_5H_5)_2$Fe** structures. The *italics* indicates the distances too long to be bonded.

	Fe-1S	Fe-2S	Fe-1T	Fe-2T	Fe-1P
FeC1	2.100	2.114	2.083	2.207	2.288
FeC2	2.116	2.099	2.097	2.204	2.246
FeC3	2.119	2.111	2.133	2.258	2.547
FeC4	2.096	2.119	2.556	2.237	2.400
FeC5	2.144	2.144	*2.939*	2.100	2.223
FeC6	*3.292*	*3.244*	*3.196*	*3.367*	*3.545*
FeC7	*3.234*	*3.296*	*3.631*	*3.421*	*3.536*
FeC8	2.144	2.144	*2.939*	*3.501*	2.223
FeC9	2.096	2.119	2.556	*2.961*	2.400
FeC10	2.119	2.111	2.133	2.201	2.547
FeC11	2.116	2.099	2.097	2.113	2.246
FeC12	2.100	2.114	2.083	2.070	2.288
FeC13	*3.234*	*3.296*	*3.631*	*4.026*	*3.536*
FeC14	*3.292*	*3.244*	*3.196*	*3.176*	*3.545*

Table S78. Cobalt–carbon distances (in Å) for the **(2,4-$Me_2C_5H_5)_2$Co** structures. The *italics* indicates the distances too long to be bonded.

	Co-1D	Co-2D	Co-3D	Co-1Q	Co-2Q
CoC1	2.064	2.079	2.104	2.226	2.297
CoC2	2.033	2.030	2.158	2.427	2.358
CoC3	2.084	2.076	2.241	2.569	2.426
CoC4	2.731	2.793	2.145	2.413	2.358
CoC5	*3.328*	*3.431*	2.135	2.192	2.297
CoC6	*3.080*	*3.063*	*3.307*	*3.549*	*3.462*
CoC7	*3.681*	*3.727*	*3.282*	*3.565*	*3.462*
CoC8	*3.328*	*3.431*	*3.789*	2.192	2.297
CoC9	2.731	2.793	*2.940*	2.413	2.358
CoC10	2.084	2.076	2.063	2.569	2.426
CoC11	2.033	2.030	2.032	2.427	2.358
CoC12	2.064	2.079	2.054	2.226	2.297
CoC13	*3.681*	*3.727*	*3.679*	*3.565*	*3.462*
CoC14	*3.080*	*3.063*	*3.094*	*3.549*	*3.462*

Table S79. Nickel–carbon distances (in Å) for the **(2,4-$Me_2C_5H_5)_2$Ni** structures. The *italics* indicates the distances too long to be bonded.

	Ni-1S	**Ni-2S**	**Ni-3S**
NiC1	*3. 661*	2. 034	2. 204
NiC2	2. 886	2. 000	2. 197
NiC3	2. 060	2. 081	2. 188
NiC4	2. 002	*2. 938*	2. 215
NiC5	2. 044	*3. 682*	2. 179
NiC6	*3. 701*	*3. 018*	*3. 324*
NiC7	*3. 032*	*3. 797*	*3. 390*
NiC8	2. 044	2. 051	2. 053
NiC9	2. 002	1. 987	2. 146
NiC10	2. 060	2. 084	*2. 864*
NiC11	2. 886	*2. 959*	*2. 828*
NiC12	*3. 661*	*3. 246*	1. 960
NiC13	*3. 032*	*2. 997*	*3. 145*
NiC14	*3. 701*	*4. 303*	*4. 265*

Table S80. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO and LUMO energies (in hartree), HOMO-LUMO gaps (in eV), the χ angles for the $(2,4\text{-}Me_2C_5H_5)_2Ti$ structures by B3LYP* method.

	Ti-1S(C_2)	**Ti-2S(C_{2v})**	**Ti-3S(C_{2h})**	**Ti-1T(C_{2v})**	**Ti-2T(C_{2h})**	**Ti-3T(C_2)**
–HOMO(α)	0.15886	0.15672	0.16392	0.13541	0.14163	0.13789
–LUMO(α)	0.05983	0.05871	0.06883	0.04267	0.05054	0.05558
gap/eV	2.69	2.67	2.59	2.52	2.48	2.24
E+1395	-0.74922	-0.73988	-0.73547	-0.72322	-0.72290	-0.72012
ΔE	0.0	5.9	8.7	16.4	16.6	18.3
χ	89.8°	0.0°	180.0°	0.0°	180.0°	57.1°

Table S81. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO and LUMO energies (in hartree), HOMO-LUMO gaps (in eV), the χ angles for the $(2,4\text{-}Me_2C_5H_5)_2V$ structures by B3LYP* method.

	V-1D (C_2)	**V-2D(C_{2v})**	**V-3D (C_{2h})**	**V-1Q (C_2)**	**V-2Q (C_2)**
–HOMO(α)	0.17600	0.17343	0.18452	0.15894	0.16064
–LUMO(α)	0.05380	0.06176	0.07617	0.01523	0.01672
gap/eV	3.33	3.04	2.95	3.91	3.92
E+1490	-0.27451	-0.26170	-0.25979	-0.26243	-0.26176
ΔE	0.0	8.0	9.2	7.6	8.0
χ	88.4°	0.0°	180.0°	57.7°	157.3°

Table S82. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO and LUMO energies (in hartree), HOMO-LUMO gaps (in eV), the χ angles for the $(2,4\text{-}Me_2C_5H_5)_2Cr$ structures by B3LYP* method.

	Cr-1T (C_2)	**Cr-2T (C_{2h})**	**Cr-3T(C_{2v})**	**Cr-1P (C_2)**	**Cr-1S (C_2)**
–HOMO(α)	0.17766	0.18647	0.17136	0.16173	0.14644
–LUMO(α)	0.02350	0.02542	0.02918	0.03937	0.05645
gap/eV	4.19	4.38	3.87	3.33	2.45
E+1490	-0.73232	-0.72781	-0.71936	-0.71125	-0.70358
ΔE	0.0	2.8	8.1	13.2	18.0
χ	83.3°	180.0°	0.0°	68.1°	87.8°

Table S83. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO and LUMO energies (in hartree), HOMO-LUMO gaps (in eV), the χ angles for the $(2,4\text{-}Me_2C_5H_5)_2Mn$ structures by B3LYP* method.

	Mn-1D (C_2)	**Mn-2D (C_{2h})**	**Mn-3D (C_{2v})**	**Mn-1X (C_2)**	**Mn-1Q (C_i)**	**Mn-2Q (C_2)**	**Mn-3Q (C_1)**
–HOMO(α)	0.17907	0.18793	0.17643	0.16036	0.18494	0.14672	0.17478
–LUMO(α)	0.02209	0.02415	0.02839	0.03364	0.04555	0.05427	0.05407
gap/eV	4.27	4.46	4.03	3.45	3.79	2.52	3.28
E+1697	-0.23598	-0.23083	-0.22204	-0.23290	-0.23214	-0.23002	-0.22852
ΔE	0.0	3.2	8.7	1.9	2.4	3.7	4.7
χ	82.8°	180.0°	0.0°	78.0°	180.0°	83.8°	4.1°

Table S84. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO and LUMO energies (in hartree), HOMO-LUMO gaps (in eV), the χ angles for the $(2,4\text{-}Me_2C_5H_5)_2Fe$ structures by B3LYP* method.

	Fe-1S(C_2)	**Fe-2S(C_2)**	**Fe-1T(C_2)**	**Fe-2T(C_1)**	**Fe-1P(C_2)**
–HOMO(α)	0.18018	0.18339	0.17271	0.17799	0.15578
–LUMO(α)	0.02262	0.02450	0.04744	0.05297	0.02184
gap/eV	4.29	4.32	3.41	3.40	3.64
E+1809	-0.95840	-0.95048	-0.94642	-0.93999	-0.93391
ΔE	0.0	5.0	7.5	11.6	15.4
χ	60.4°	145.6°	71.8°	0.5°	87.3°

Table S85. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO and LUMO energies (in hartree), HOMO-LUMO gaps (in eV), the χ angles for the $(2,4\text{-}Me_2C_5H_5)_2Co$ structures by B3LYP* method.

	Co-1D (C_2)	**Co-2D (C_i)**	**Co-3D (C_1)**	**Co-1Q (C_2)**	**Co-2Q (C_{2h})**
–HOMO(α)	0.18322	0.18633	0.17000	0.15463	0.15853
–LUMO(α)	0.05052	0.04547	0.05025	0.02384	0.01848
gap/eV	3.61	3.83	3.26	3.56	3.81
E+1928	-1.01094	-1.01024	-1.00566	-0.99082	-0.98217
ΔE	0.0	0.4	3.3	12.6	18.1
χ	112.8°	180.0°	66.9°	95.5°	180.0°

Table S86. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO and LUMO energies (in hartree), HOMO-LUMO gaps (in eV), the χ angles for the $(2,4\text{-}Me_2C_5H_5)_2Ni$ structures by B3LYP* method.

	Ni-1S (C_i)	**Ni-2S (C_1)**	**Ni-3S (C_1)**
–HOMO(α)	0.18762	0.18587	0.17958
–LUMO(α)	0.04296	0.04484	0.04220
gap/eV	4.30	3.84	3.74
E+2054	-0.56832	-0.56174	-0.54776
ΔE	0.0	4.1	12.9
χ	180.0°	1.3°	74.4°

The simpler model systems $(C_5H_7)_2M$ have been studied with the B3LYP* method, as well as the M06-L method. The differences between the relative energies and the conformation angle from the two methods are quite small (Table S87).

Table S87. The comparison of the relative energies (ΔE in kcal/mol) and the conformation angle (χ) for the simpler model systems $(C_5H_7)_2M$ (M = Ti, V, Cr, Mn, Fe, Co, Ni) predicted by the B3LYP* and M06L methods.

	ΔE (in kcal/mol)		χ (in degrees)	
	B3LYP*	M06L	B3LYP*	M06L
Ti-1S	0.0	0.0	0.0°	0.0°
Ti-2S	3.6	4.2	180.0°	180.0°
Ti-1T	13.3	17.9	0.0°	0.0°
Ti-2T	14.1	19.4	180.0°	155.2°
V-1D	0.0	0.0	0.0°	0.0°
V-2D	3.0	4.6	180.0°	180.0°
V-1Q	2.7	2.6	50.9°	47.8°
V-2Q	3.3	2.9	134.4°	131.1°
Cr-1S	23.7	27.7	0.0°	0.0°
Cr-2S	26.3	32.6	180.0°	180.0°
Cr-1T	0.0	0.0	180.0°	180.0°
Cr-2T	3.4	3.6	0.0°	0.0°
Cr-1P	12.0	16.3	69.8°	62.2°
Cr-2P	12.4	16.8	180.0°	180.0°
Mn-1D	0.0	0.0	180.0°	180.0°
Mn-2D	2.8	2.4	0.0°	0.0°
Mn-1Q	0.3	-0.5	0.0°	0.0°
Mn-2Q	0.01	-0.1	179.5°	178.3°
Mn-1X	1.97	0.8	64.0°	52.3°
Fe-1S	0.0	0.0	51.6°	48.0°
Fe-2S	4.4	3.4	137.9°	132.6°
Co-1D	0.0	0.0	59.7°	51.7°
Co-2D	1.5	0.8	180.0°	158.1°
Ni-1S	0.0	0.0	180.0°	180.0°
Ni-2S	2.0	1.1	0.0°	0.0°

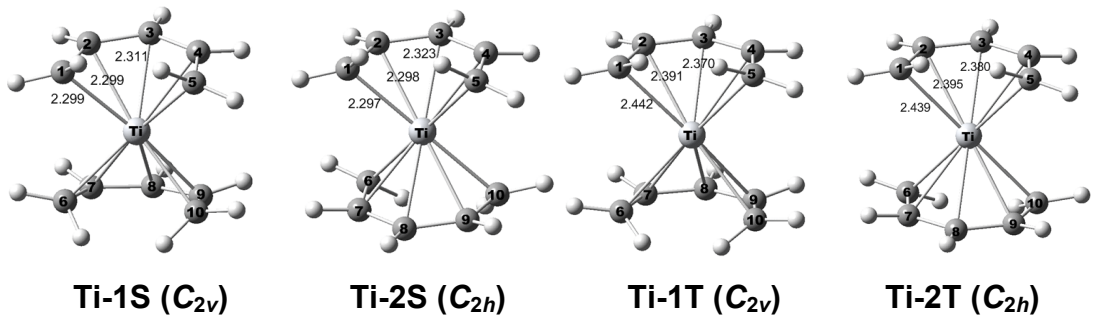

Figure S1. The optimized $(C_5H_7)_2Ti$ structures by the B3LYP* method.

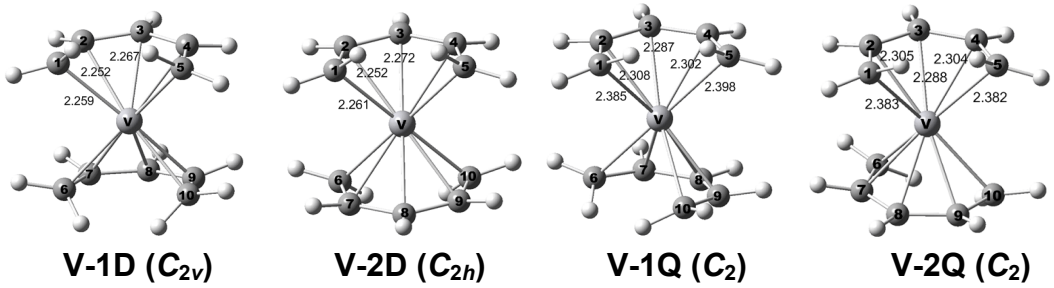

Figure S2. The optimized $(C_5H_7)_2V$ structures.

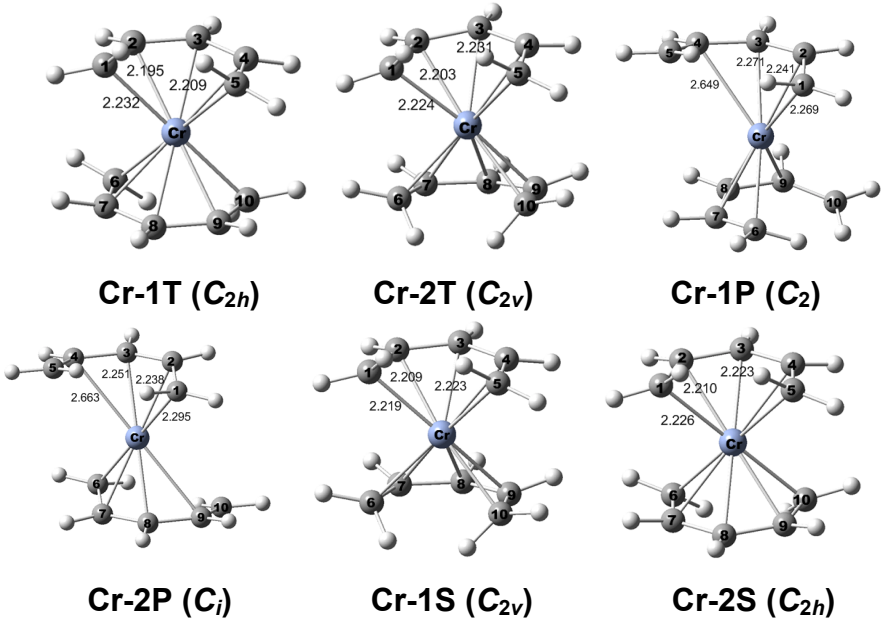

Figure S3. The optimized $(C_5H_7)_2Cr$ structures.

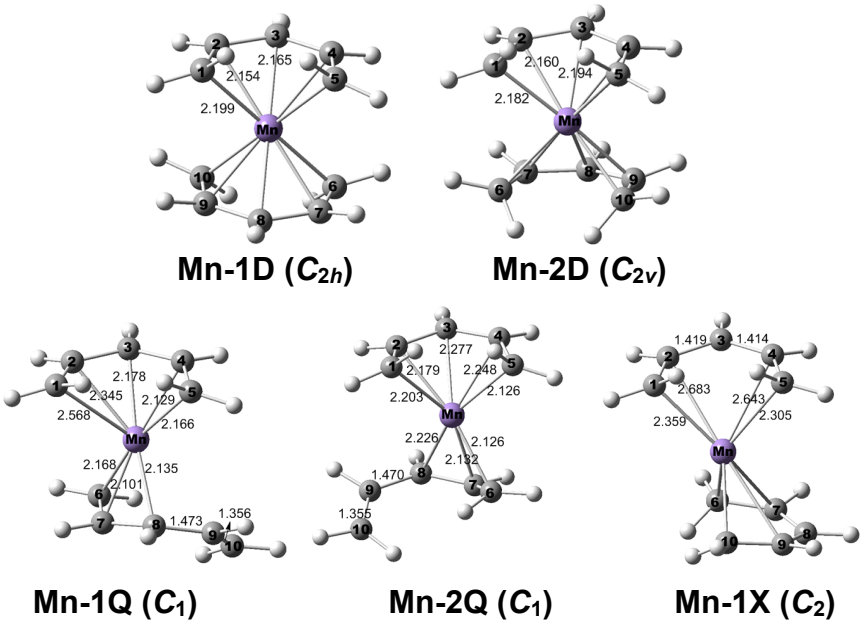

Figure S4. The optimized $(C_5H_7)_2Mn$ structures.

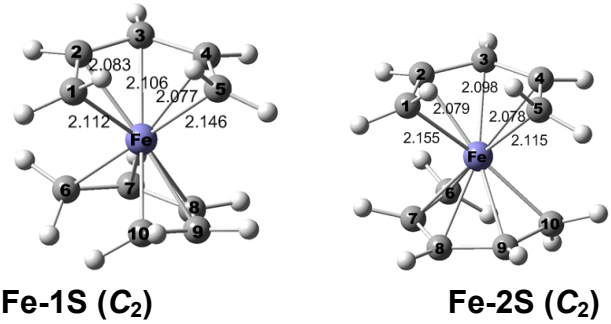

Figure S5. The optimized $(C_5H_7)_2Fe$ structures.

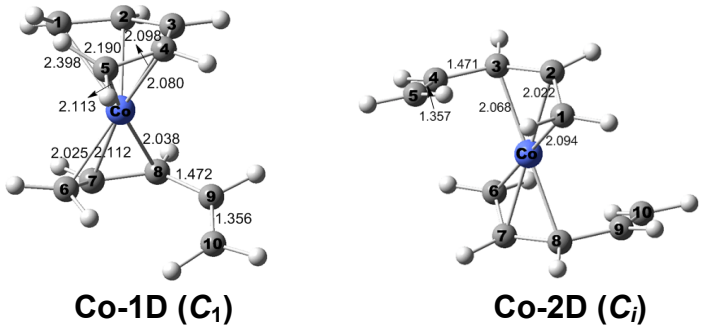

Figure S6. The optimized $(C_5H_7)_2Co$ structures.

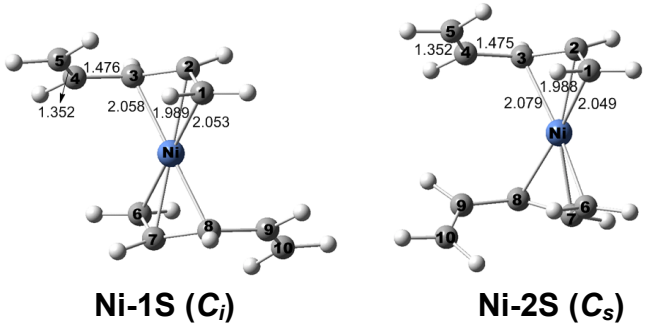

Figure S7. The optimized $(C_5H_7)_2Ni$ structures.

Complete Gaussian 09 reference (Reference 38)

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