Alkyne Dichotomy and Hydrogen Migration in Binuclear Cyclopentadienylmetal Alkyne Complexes

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Supporting Information

Tables S1 to S11: Atomic coordinates of the optimized structures for the **cmp-n (n=1~6)** and **TS-n (n=1~5)** complexes in **Figure 15;**

Tables S12 to S22: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **cmp-n (n=1~6)** and **TS-n (n=1~5)** complexes in **Figure 15**;

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Tables S33 to S46: Atomic coordinates of the optimized structures for the $\mathbf{Cp_2M_2C_2(NMe_2)_2}$ (M= Ni, Co, Fe) complexes;

Tables S47 to S58: Atomic coordinates of the optimized structures for the $\mathbf{Cp_2M_2(MeC_2NMe_2)}$ (M= Ni, Co, Fe) complexes;

Tables S59 to S83: Atomic coordinates of the optimized structures for the $\mathbf{Cp_2M_2C_2Me_2}$(M= Ni, Co, Fe) complexes.

Tables S84 to S97: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $\mathbf{Cp_2M_2C_2(NMe_2)_2}$ (M= Ni, Co,

Fe)complexes;

Tables S98 to S109: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2M_2(MeC_2NMe_2)$** (M= Ni, Co, Fe) complexes;

Tables S110 to S134: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2M_2C_2Me_2$**(M= Ni, Co, Fe) complexes.

Table S1. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-1**.

	M06L		
	x	y	z
C	-0.261614	2.169194	-1.035817
C	-0.080105	0.791831	-0.899891
N	-0.355309	2.945956	0.023046
C	-0.573194	4.371245	-0.135972
C	-0.306235	2.517743	1.420811
H	0.387889	3.145486	1.982829
H	-1.291412	2.611188	1.884428
H	0.236191	4.939386	0.329455
H	-1.508814	4.673802	0.341804
H	-0.616362	4.597563	-1.195963
H	0.014101	1.481781	1.466927
C	0.032904	-0.195463	-2.049760
H	0.999886	-0.804730	-2.080010
H	-0.767874	-1.012064	-2.075860
H	-0.027794	0.300803	-3.013288
C	2.594379	0.444647	0.901041
C	3.304218	-0.106947	-0.189202
H	3.950734	0.427644	-0.866524
C	3.010346	-1.505952	-0.235519
H	3.384268	-2.199814	-0.972927
C	1.839945	-0.606447	1.511307
H	1.189053	-0.504100	2.366375
C	2.129360	-1.824338	0.819863
H	1.735725	-2.800751	1.050499
C	-1.820356	-0.691991	1.482877
C	-1.551046	-2.037645	1.073236
H	-0.846708	-2.710167	1.535956
C	-2.352289	-2.309897	-0.053868
H	-2.363246	-3.229044	-0.618301
C	-2.828325	-0.156301	0.624716
H	-3.248171	0.835827	0.676065
C	-3.132305	-1.143139	-0.339364
H	-3.829719	-1.037232	-1.155685
H	-1.368952	-0.187203	2.322585
H	2.590102	1.481649	1.197835
Co	-1.131083	-0.671845	-0.383346
Co	1.273089	-0.399672	-0.383479

Table S2. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-2**.

	M06L		
	x	y	z
C	1.956757	-1.216095	-0.925102
C	0.728385	-0.559560	-0.900237
N	2.333086	-2.040891	0.024085
C	3.644639	-2.661582	-0.040913
C	1.574590	-2.423149	1.219317
H	2.206863	-2.296283	2.099885
H	0.687309	-1.802499	1.303055
H	3.550931	-3.749901	-0.038387
H	4.247442	-2.376920	0.824958
H	4.135801	-2.339268	-0.952755
H	1.275197	-3.471723	1.168266
C	-0.202247	-0.058418	-1.863780
H	-0.157291	-0.292777	-2.922490
H	-0.423323	1.079402	-1.815511
H	-0.573734	-2.061511	-0.588864
C	-2.399912	-1.697652	0.972794
C	-3.047664	-1.543431	-0.301915
H	-3.390788	-2.343128	-0.936924
C	-3.181998	-0.159768	-0.548197
H	-3.607334	0.285744	-1.433203
C	-2.117481	-0.416457	1.481453
H	-1.632129	-0.197986	2.419881
C	-2.587542	0.541328	0.526367
H	-2.528965	1.613390	0.622154
C	1.456240	1.577947	1.319783
C	0.179794	2.215693	1.388705
H	-0.580967	2.023403	2.128689
C	0.070117	3.104405	0.294699
H	-0.780707	3.723412	0.058203
C	2.148784	2.101683	0.186926
H	3.125429	1.801716	-0.156863
C	1.284640	3.022880	-0.451664
H	1.495844	3.551388	-1.368082
H	1.827530	0.831297	2.004056
H	-2.159949	-2.635792	1.447105
Co	0.424633	1.171730	-0.333702
Co	-1.168758	-0.728126	-0.339676

Table S3. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-3**.

	M06L		
	x	y	z
C	1.927852	-1.169293	-1.001484
C	0.533103	-0.897321	-1.016459
N	2.407221	-1.916342	-0.007853
C	3.826182	-2.205700	0.036161
C	1.636167	-2.472063	1.103331
H	1.104724	-3.382168	0.812915
H	2.299792	-2.720290	1.929702
H	4.009214	-3.283575	0.033104
H	4.283953	-1.792975	0.940577
H	4.290328	-1.761119	-0.838592
H	0.899982	-1.745075	1.451412
C	-0.310853	-0.083784	-1.862905
H	-0.694998	-0.343385	-2.844850
H	0.152238	0.962031	-2.044008
H	-0.135177	-1.675522	-0.456107
C	-2.540460	-1.576392	0.953710
C	-3.138653	-1.434443	-0.336434
H	-3.423778	-2.236235	-0.998043
C	-3.283036	-0.046499	-0.578778
H	-3.668195	0.405133	-1.479009
C	-2.343374	-0.293892	1.517946
H	-1.922173	-0.083312	2.488100
C	-2.778981	0.660932	0.551906
H	-2.740574	1.734216	0.653479
C	1.433276	1.285257	1.376407
C	0.238326	2.062712	1.323284
H	-0.603768	1.974661	1.989648
C	0.341581	2.934407	0.213947
H	-0.409787	3.632745	-0.119129
C	2.305258	1.730412	0.333910
H	3.270662	1.314906	0.094262
C	1.625112	2.728073	-0.388718
H	1.990696	3.226877	-1.272744
H	1.651739	0.511047	2.095536
H	-2.264034	-2.512762	1.415594
Co	0.524272	0.987357	-0.373825
Co	-1.330582	-0.474218	-0.261428

Table S4. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-4**.

	M06L		
	x	y	z
C	-1.587911	1.174009	-0.972801
C	-0.218591	0.975073	-1.208070
N	-2.124777	2.134687	-0.132238
C	-3.516207	1.954449	0.212203
C	-1.295180	2.625743	0.944741
H	-0.442250	3.182177	0.556323
H	-1.878078	3.303822	1.563697
H	-3.939396	2.897569	0.556523
H	-3.663053	1.204748	1.001161
H	-4.072260	1.631921	-0.666645
H	-0.907882	1.808964	1.571674
C	0.359791	-0.196984	-1.747747
H	0.511401	-0.539389	-2.763612
H	-2.285329	0.828736	-1.727996
H	0.484779	1.720755	-0.652541
C	2.789388	1.270763	0.971263
C	3.405847	0.972257	-0.288520
H	3.866291	1.685309	-0.953398
C	3.299328	-0.421144	-0.494976
H	3.644537	-0.966764	-1.358101
C	2.320294	0.073318	1.546623
H	1.809783	-0.024451	2.491159
C	2.601587	-0.978644	0.619953
H	2.345916	-2.018909	0.744285
C	-1.825609	-1.226767	1.410920
C	-0.603338	-1.929002	1.344002
H	0.180192	-1.906832	2.084732
C	-0.567151	-2.657099	0.117205
H	0.244132	-3.279536	-0.224634
C	-2.549446	-1.523812	0.213810
H	-3.519522	-1.129951	-0.049252
C	-1.789863	-2.423548	-0.570889
H	-2.076563	-2.837734	-1.523716
H	-2.159301	-0.598211	2.221260
H	2.684185	2.257123	1.397862
Co	-0.739019	-0.672882	-0.291598
Co	1.446731	0.365703	-0.298380

Table S5. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-5**.

	M06L		
	x	y	z
C	-0.947198	1.412123	-1.182373
C	0.426757	1.147121	-1.626089
N	-1.217167	1.731153	0.177814
C	-2.583143	2.173873	0.457753
C	-0.248902	2.488224	0.974696
H	-0.440074	3.559438	0.859726
H	-0.355487	2.219917	2.024909
H	-2.687344	3.237863	0.229415
H	-2.815966	2.024130	1.510455
H	-3.284636	1.604760	-0.145670
H	0.752424	2.242150	0.636480
C	0.280199	-0.285967	-1.672623
H	0.122224	-0.961431	-2.512278
H	-1.745576	1.682710	-1.873630
H	0.940240	1.771930	-2.356664
C	2.933419	0.894640	0.753854
C	3.394110	0.161893	-0.383730
H	3.948377	0.568787	-1.214859
C	3.022781	-1.202323	-0.212134
H	3.231130	-2.006754	-0.899594
C	2.235845	-0.001149	1.589332
H	1.741075	0.245722	2.516794
C	2.288483	-1.302018	0.989722
H	1.849541	-2.201444	1.393696
C	-2.468386	-0.967654	1.227310
C	-1.243753	-1.675062	1.324326
H	-0.613483	-1.752475	2.194780
C	-0.995108	-2.237802	0.046543
H	-0.115791	-2.791918	-0.239689
C	-3.003545	-1.124387	-0.077779
H	-3.936733	-0.719746	-0.436876
C	-2.084049	-1.899033	-0.818960
H	-2.177067	-2.189092	-1.853064
H	-2.915127	-0.384816	2.019602
H	3.079562	1.949707	0.927561
Co	-1.081815	-0.234041	-0.167311
Co	1.374327	0.022471	-0.290648

Table S6. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-6**.

	M06L		
	x	y	z
C	0.487485	1.880989	-0.223466
C	0.673758	1.388592	-1.551728
N	-0.870010	1.690238	0.299766
C	-1.849797	2.576266	-0.350908
C	-0.889960	1.893348	1.750320
H	-0.619742	2.925010	2.004220
H	-1.883982	1.687960	2.143018
H	-1.624133	3.628147	-0.143312
H	-2.850387	2.350160	0.015908
H	-1.817889	2.405534	-1.423339
H	-0.175077	1.212203	2.207974
C	0.009761	0.149254	-1.686617
H	0.090599	-0.413347	-2.615109
H	0.983603	2.783640	0.134450
H	1.326480	1.860641	-2.280223
C	2.579662	0.065157	1.400798
C	3.335105	0.252369	0.208170
H	3.972993	1.094054	-0.011451
C	3.096352	-0.860333	-0.639999
H	3.510946	-1.007992	-1.624758
C	1.865447	-1.152277	1.284300
H	1.196356	-1.567919	2.021196
C	2.179853	-1.722159	0.013140
H	1.786076	-2.643750	-0.385060
C	-1.890213	-1.370360	1.351461
C	-1.261558	-2.196200	0.383810
H	-0.436573	-2.867376	0.562300
C	-1.889347	-1.976060	-0.872604
H	-1.608817	-2.442599	-1.803674
C	-2.897791	-0.633720	0.672517
H	-3.530032	0.119403	1.121288
C	-2.921758	-1.010780	-0.695680
H	-3.596004	-0.640481	-1.450870
H	-1.649988	-1.308937	2.401295
H	2.542697	0.743388	2.239011
Co	-1.080014	-0.248831	-0.204085
Co	1.328568	0.120908	-0.220815

Table S7. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-1**.

M06L			
	x	y	z
C	1.344267	1.772813	-1.010435
C	0.368077	0.775273	-0.943565
N	1.632115	2.538884	0.023735
C	2.684822	3.530020	-0.084166
C	1.019517	2.476747	1.348667
H	1.795960	2.470990	2.116097
H	0.380087	3.344239	1.529140
H	3.495277	3.311804	0.616667
H	2.300611	4.525651	0.151636
H	3.067664	3.518034	-1.099113
H	0.427626	1.570021	1.420886
C	-0.054362	-0.166667	-1.940802
H	0.162789	-0.044549	-2.994022
H	-1.139247	-0.560440	-1.923718
H	1.429795	-1.232991	-1.846260
C	2.085959	-1.191053	1.197536
C	2.517807	-2.070115	0.183747
H	3.485668	-2.070088	-0.289337
C	1.444788	-2.987441	-0.095856
H	1.470716	-3.782191	-0.823257
C	0.742893	-1.522804	1.516379
H	0.132460	-1.030595	2.255506
C	0.358625	-2.653619	0.731035
H	-0.598263	-3.149184	0.755043
C	-1.995695	0.573911	1.452469
C	-2.563335	-0.676706	1.045694
H	-2.430404	-1.619125	1.554292
C	-3.304068	-0.466431	-0.131887
H	-3.837002	-1.216325	-0.693886
C	-2.398111	1.562755	0.514995
H	-2.132004	2.607396	0.531935
C	-3.170645	0.912968	-0.483294
H	-3.589158	1.383071	-1.359542
H	-1.407161	0.739952	2.341229
H	2.656779	-0.378549	1.617867
Co	-1.308277	0.104185	-0.385231
Co	0.879380	-1.044082	-0.497377

Table S8. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-2**.

	M06L		
	x	y	z
C	1.935592	-1.232570	-0.953454
C	0.677809	-0.626380	-0.928706
N	2.344483	-2.026733	0.012975
C	3.676719	-2.601096	-0.050524
C	1.607917	-2.409747	1.222255
H	2.285806	-2.376691	2.076205
H	0.780083	-1.725173	1.384418
H	3.624399	-3.692024	-0.021654
H	4.278713	-2.273804	0.801012
H	4.145907	-2.283589	-0.975571
H	1.217273	-3.426265	1.142381
C	-0.242925	-0.061994	-1.863014
H	-0.280554	-0.313149	-2.918332
H	-0.344083	1.098106	-1.841746
H	-0.409919	-1.898921	-0.424900
C	-2.459094	-1.684380	0.934847
C	-3.069814	-1.510395	-0.350214
H	-3.388982	-2.297110	-1.013373
C	-3.198500	-0.118376	-0.569074
H	-3.593816	0.347728	-1.457402
C	-2.211195	-0.412324	1.493631
H	-1.765228	-0.215743	2.455842
C	-2.656012	0.561816	0.548262
H	-2.600084	1.632108	0.666107
C	1.496502	1.492140	1.309366
C	0.229493	2.146687	1.395014
H	-0.532620	1.950435	2.132117
C	0.133004	3.057260	0.317989
H	-0.708786	3.692682	0.092945
C	2.200237	2.032965	0.190730
H	3.174586	1.728925	-0.155809
C	1.349637	2.976737	-0.428152
H	1.569051	3.524149	-1.331532
H	1.857360	0.725284	1.976744
H	-2.217293	-2.631167	1.391626
Co	0.453468	1.136363	-0.349113
Co	-1.206039	-0.656389	-0.305837

Table S9. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-3**.

	M06L		
	x	y	z
C	1.906807	-1.224579	-1.006328
C	0.493377	-1.047624	-0.950301
N	2.523995	-1.818897	0.019476
C	3.952000	-2.040248	-0.046235
C	1.892471	-2.155680	1.288459
H	1.337601	-3.096067	1.235033
H	2.645932	-2.255387	2.068352
H	4.196606	-3.091276	0.128064
H	4.480694	-1.445349	0.705672
H	4.296911	-1.753207	-1.034599
H	1.195673	-1.361895	1.573086
C	-0.296177	-0.136257	-1.715153
H	-0.463567	-0.042874	-2.781261
H	1.670986	0.621029	-1.524513
H	-0.097690	-1.757644	-0.264356
C	-2.934196	-1.724696	0.072864
C	-3.297304	-0.651933	-0.777452
H	-3.642061	-0.733638	-1.795079
C	-3.046053	0.553206	-0.067702
H	-3.180436	1.553072	-0.448974
C	-2.526839	-1.188769	1.340893
H	-2.198282	-1.761121	2.194000
C	-2.595504	0.209476	1.252134
H	-2.322015	0.910505	2.025384
C	1.902375	1.596781	1.084928
C	0.557779	1.600649	1.514453
H	0.163010	1.085029	2.375484
C	-0.187497	2.420844	0.609340
H	-1.241826	2.635009	0.672339
C	1.987480	2.388970	-0.092699
H	2.882561	2.568855	-0.665082
C	0.695783	2.917984	-0.377133
H	0.439011	3.566089	-1.198325
H	2.715178	1.048747	1.535525
H	-2.955468	-2.771470	-0.188471
Co	0.665113	0.855514	-0.426173
Co	-1.354661	-0.496065	-0.223050

Table S10. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-4**.

	M06L		
	x	y	z
C	-1.156467	1.319288	-1.077231
C	0.224078	1.142779	-1.533735
N	-1.443199	1.946309	0.140313
C	-2.821582	2.243674	0.443296
C	-0.464437	2.786421	0.788543
H	-0.452636	3.797174	0.363954
H	-0.693807	2.860849	1.851299
H	-3.127757	3.215734	0.039493
H	-2.975918	2.265788	1.522508
H	-3.461688	1.475524	0.013430
H	0.521141	2.338637	0.660300
C	0.290861	-0.266224	-1.742183
H	0.387949	-0.879244	-2.634957
H	-1.976957	1.316569	-1.791717
H	0.807515	1.933626	-2.016242
C	2.895542	1.085423	0.514453
C	3.364319	0.183739	-0.487457
H	3.868285	0.462123	-1.399417
C	3.027301	-1.131483	-0.079114
H	3.237501	-2.042662	-0.616093
C	2.291648	0.333786	1.555656
H	1.856542	0.725123	2.461774
C	2.351053	-1.031319	1.169306
H	1.941835	-1.860560	1.726978
C	-2.389034	-1.017902	1.189982
C	-1.165838	-1.710899	1.410574
H	-0.580357	-1.698927	2.315579
C	-0.854677	-2.406107	0.216473
H	0.021240	-3.009968	0.039140
C	-2.854194	-1.308933	-0.114960
H	-3.754335	-0.927638	-0.571259
C	-1.899221	-2.142775	-0.734811
H	-1.939233	-2.522642	-1.742893
H	-2.876801	-0.366577	1.899860
H	2.987863	2.160677	0.479586
Co	-0.920103	-0.441994	-0.198939
Co	1.337729	0.021824	-0.271293

Table S11. Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-5**.

	M06L		
	x	y	z
C	-0.561145	2.296430	-0.680816
C	0.695780	1.830140	-0.902466
N	-1.433162	1.616442	0.240997
C	-2.837566	1.959121	-0.016897
C	-1.074346	1.951991	1.637605
H	-1.226849	3.018132	1.838789
H	-1.701871	1.367976	2.307967
H	-3.016099	3.030599	0.128375
H	-3.477849	1.403061	0.663226
H	-3.091967	1.685568	-1.037826
H	-0.032238	1.682285	1.793901
C	0.107294	0.391976	-1.489012
H	-0.000506	0.463142	-2.573281
H	-0.975254	3.204151	-1.123801
H	1.334307	2.446979	-1.532298
C	3.241875	0.711990	0.477288
C	3.382465	-0.161812	-0.634814
H	3.892317	0.062120	-1.558287
C	2.715341	-1.370985	-0.313021
H	2.624646	-2.237679	-0.948570
C	2.518039	0.044787	1.501686
H	2.275953	0.435696	2.476844
C	2.178679	-1.239459	0.998668
H	1.609707	-1.990470	1.523105
C	-2.495321	-1.266040	0.933320
C	-1.254780	-1.893926	1.174904
H	-0.768567	-2.003854	2.130860
C	-0.768006	-2.342924	-0.089312
H	0.171127	-2.840452	-0.269309
C	-2.815489	-1.362122	-0.458629
H	-3.716443	-1.003895	-0.931753
C	-1.742753	-2.034477	-1.083018
H	-1.649913	-2.245719	-2.136771
H	-3.104641	-0.780651	1.682981
H	3.607092	1.726370	0.526659
Co	-1.026280	-0.341063	-0.180447
Co	1.379569	0.199338	-0.226246

Table S12. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-1**.

M06L		
37(0)	802(13)	1387(4)
48(0)	810(27)	1395(4)
49(0)	814(5)	1398(0)
76(0)	820(3)	1414(10)
99(0)	821(0)	1423(37)
115(1)	823(6)	1442(0)
131(0)	827(1)	1443(0)
161(2)	832(13)	1465(0)
172(8)	867(1)	1466(1)
175(0)	877(1)	1475(1)
194(1)	880(0)	1479(38)
205(0)	884(1)	1486(12)
274(2)	889(3)	1492(4)
285(2)	959(16)	1543(21)
333(2)	1013(5)	1554(30)
363(0)	1014(11)	1562(50)
371(5)	1026(0)	2560(7)
376(3)	1030(2)	2569(3)
393(0)	1032(12)	3023(75)
408(1)	1047(6)	3032(81)
416(4)	1069(0)	3096(22)
426(1)	1070(0)	3108(9)
440(1)	1073(1)	3147(1)
444(1)	1077(1)	3184(1)
504(1)	1093(1)	3186(3)
514(10)	1119(117)	3219(1)
549(33)	1140(29)	3222(2)
581(5)	1142(6)	3222(0)
592(1)	1155(4)	3224(0)
600(5)	1226(1)	3236(10)
603(3)	1249(9)	3237(10)
609(6)	1271(0)	3243(8)
775(25)	1272(0)	3245(8)
777(5)	1304(3)	3252(4)
789(5)	1384(3)	3252(4)

Table S13. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-2**.

M06L		
25(0)	796(24)	1394(10)
51(1)	806(19)	1394(1)
60(1)	809(2)	1396(2)
70(0)	819(13)	1402(2)
79(2)	819(18)	1412(6)
97(2)	826(2)	1425(29)
112(4)	831(10)	1448(1)
141(0)	836(41)	1452(3)
154(1)	839(1)	1462(1)
175(0)	843(12)	1471(3)
184(5)	870(9)	1473(1)
206(3)	886(1)	1482(2)
259(2)	891(1)	1484(34)
296(4)	893(1)	1492(8)
341(4)	899(0)	1574(111)
347(3)	935(67)	1637(3)
368(2)	1011(5)	1954(62)
372(0)	1020(8)	2437(1)
395(5)	1023(4)	3028(56)
399(2)	1030(4)	3036(100)
419(9)	1032(36)	3103(21)
444(8)	1040(5)	3116(9)
453(10)	1072(1)	3151(5)
458(20)	1074(1)	3170(1)
474(12)	1076(0)	3186(4)
541(6)	1080(1)	3224(1)
574(23)	1092(0)	3225(0)
593(1)	1143(17)	3228(1)
598(3)	1145(14)	3232(1)
602(2)	1154(55)	3241(8)
608(2)	1156(10)	3243(8)
623(3)	1219(1)	3245(4)
662(56)	1272(0)	3249(7)
769(2)	1275(0)	3255(2)
783(12)	1378(4)	3259(5)

Table S14. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-3**.

M06L		
8(0)	801(17)	1391(0)
40(2)	808(13)	1394(10)
56(0)	813(23)	1396(3)
58(0)	820(4)	1406(122)
73(1)	825(1)	1418(10)
92(1)	828(4)	1445(1)
122(2)	829(4)	1446(1)
131(3)	833(18)	1462(1)
148(5)	837(10)	1463(23)
167(2)	881(0)	1468(0)
174(3)	886(0)	1483(12)
200(0)	889(0)	1484(43)
250(2)	890(2)	1488(3)
264(3)	901(1)	1504(1)
319(2)	972(36)	1527(73)
352(4)	1016(11)	1654(4)
370(4)	1019(5)	2374(1)
384(6)	1029(6)	2470(2)
396(2)	1031(6)	3013(93)
403(4)	1036(10)	3024(59)
427(6)	1057(68)	3084(30)
435(0)	1072(1)	3102(12)
447(8)	1072(5)	3143(8)
464(8)	1074(1)	3143(12)
508(2)	1077(3)	3177(4)
541(1)	1092(1)	3216(3)
584(5)	1142(25)	3226(0)
591(2)	1144(12)	3226(1)
593(3)	1147(18)	3227(1)
601(1)	1149(21)	3238(7)
612(3)	1243(2)	3240(7)
618(7)	1270(0)	3243(8)
771(1)	1273(0)	3249(4)
777(1)	1333(28)	3253(4)
791(1)	1387(18)	3256(3)

Table S15. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-4**.

M06L		
28(0)	802(28)	1388(1)
59(0)	813(17)	1394(6)
69(0)	816(47)	1395(3)
85(0)	823(3)	1397(2)
91(1)	824(6)	1429(41)
99(1)	829(5)	1440(10)
135(1)	832(6)	1443(13)
155(15)	836(23)	1448(0)
159(8)	851(14)	1467(1)
191(2)	880(6)	1468(1)
212(1)	884(1)	1472(20)
223(2)	886(4)	1479(16)
248(0)	886(2)	1486(4)
281(2)	889(0)	1505(15)
326(2)	955(9)	1516(45)
348(4)	1010(8)	1597(118)
365(6)	1016(4)	2392(7)
381(9)	1033(13)	2977(28)
392(37)	1037(3)	2991(69)
397(4)	1070(4)	3096(28)
426(6)	1072(3)	3097(22)
451(34)	1073(3)	3149(9)
493(7)	1076(31)	3156(21)
536(3)	1078(1)	3163(5)
557(15)	1080(75)	3180(10)
577(4)	1115(6)	3218(2)
590(0)	1141(21)	3218(3)
595(4)	1144(11)	3226(2)
600(2)	1155(39)	3229(0)
606(0)	1193(10)	3238(11)
647(4)	1239(7)	3240(8)
715(12)	1270(0)	3243(12)
773(3)	1275(0)	3245(5)
780(6)	1329(7)	3254(5)
794(6)	1351(64)	3255(4)

Table S16. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-5**.

M06L		
31(0)	797(9)	1316(11)
56(0)	807(13)	1356(26)
82(0)	810(29)	1391(0)
92(1)	818(9)	1394(4)
132(1)	823(2)	1396(5)
154(2)	830(1)	1401(2)
161(0)	835(3)	1408(4)
188(1)	838(19)	1441(2)
211(2)	851(29)	1445(2)
221(1)	873(2)	1449(2)
244(2)	877(8)	1465(1)
247(1)	878(1)	1471(1)
284(1)	892(2)	1473(1)
318(3)	898(2)	1485(6)
344(3)	996(49)	1489(7)
350(4)	1010(11)	1506(9)
360(3)	1017(3)	3021(78)
379(3)	1022(19)	3037(76)
388(6)	1031(8)	3081(38)
412(10)	1036(6)	3089(48)
426(1)	1039(9)	3106(45)
448(17)	1070(0)	3123(11)
472(1)	1071(1)	3130(9)
504(2)	1073(1)	3174(7)
574(5)	1078(0)	3178(9)
590(2)	1102(21)	3211(1)
595(1)	1115(1)	3213(4)
598(0)	1141(19)	3218(2)
603(3)	1148(10)	3230(1)
610(1)	1166(18)	3231(16)
704(0)	1179(10)	3234(16)
758(24)	1196(11)	3240(7)
773(2)	1269(0)	3246(7)
790(5)	1275(0)	3249(5)
794(14)	1287(22)	3259(2)

Table S17. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **cmp-6**.

M06L		
31(0)	797(9)	1316(11)
56(0)	807(13)	1356(26)
82(0)	810(29)	1391(0)
92(1)	818(9)	1394(4)
132(1)	823(2)	1396(5)
154(2)	830(1)	1401(2)
161(0)	835(3)	1408(4)
188(1)	838(19)	1441(2)
211(2)	851(29)	1445(2)
221(1)	873(2)	1449(2)
244(2)	877(8)	1465(1)
247(1)	878(1)	1471(1)
284(1)	892(2)	1473(1)
318(3)	898(2)	1485(6)
344(3)	996(49)	1489(7)
350(4)	1010(11)	1506(9)
360(3)	1017(3)	3021(78)
379(3)	1022(19)	3037(76)
388(6)	1031(8)	3081(38)
412(10)	1036(6)	3089(48)
426(1)	1039(9)	3106(45)
448(17)	1070(0)	3123(11)
472(1)	1071(1)	3130(9)
504(2)	1073(1)	3174(7)
574(5)	1078(0)	3178(9)
590(2)	1102(21)	3211(1)
595(1)	1115(1)	3213(4)
598(0)	1141(19)	3218(2)
603(3)	1148(10)	3230(1)
610(1)	1166(18)	3231(16)
704(0)	1179(10)	3234(16)
758(24)	1196(11)	3240(7)
773(2)	1269(0)	3246(7)
790(5)	1275(0)	3249(5)
794(14)	1287(22)	3259(2)

Table S18. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-1**.

M06L		
-341(46)	789(8)	1389(6)
31(0)	804(17)	1394(1)
40(0)	812(5)	1396(2)
48(0)	819(38)	1401(8)
60(1)	821(10)	1415(10)
90(0)	823(19)	1424(52)
109(1)	826(4)	1444(1)
137(2)	831(4)	1449(1)
147(3)	835(12)	1468(1)
164(3)	836(2)	1475(4)
173(1)	882(2)	1477(1)
185(6)	887(1)	1483(38)
223(1)	891(0)	1486(16)
264(1)	894(2)	1496(7)
274(5)	939(11)	1562(118)
338(4)	995(83)	1674(14)
343(6)	1011(5)	2060(25)
363(2)	1013(9)	2471(6)
375(1)	1030(3)	3022(84)
384(2)	1036(4)	3033(85)
400(12)	1040(7)	3094(24)
418(2)	1055(70)	3107(10)
427(5)	1071(0)	3179(2)
457(3)	1072(3)	3185(3)
498(10)	1077(3)	3190(1)
531(3)	1078(7)	3221(1)
563(38)	1090(1)	3226(0)
583(7)	1143(17)	3234(0)
594(3)	1145(13)	3235(1)
598(4)	1151(71)	3236(9)
603(1)	1154(4)	3245(6)
622(9)	1229(4)	3250(6)
642(24)	1271(0)	3253(7)
694(35)	1275(0)	3253(1)
784(2)	1368(36)	3263(4)

Table S19. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-2**.

M06L		
-321(15)	799(6)	1394(6)
24(0)	804(4)	1395(11)
52(1)	807(39)	1396(2)
57(1)	815(13)	1399(2)
64(0)	818(12)	1418(2)
74(1)	825(3)	1424(42)
98(0)	831(5)	1447(0)
136(1)	833(11)	1452(1)
145(1)	838(17)	1464(1)
156(1)	840(21)	1468(0)
181(0)	862(5)	1477(1)
200(8)	887(1)	1484(4)
244(3)	891(1)	1486(37)
275(0)	895(3)	1492(8)
288(5)	898(0)	1567(117)
349(2)	952(92)	1682(5)
365(3)	1015(5)	2028(57)
373(6)	1018(11)	2396(0)
383(2)	1023(7)	3026(77)
396(2)	1029(6)	3037(73)
423(6)	1033(17)	3100(21)
429(7)	1036(5)	3118(10)
447(11)	1071(1)	3148(6)
449(1)	1074(1)	3169(2)
480(6)	1075(0)	3185(4)
500(11)	1080(1)	3225(1)
562(19)	1090(1)	3226(0)
592(1)	1143(19)	3228(1)
597(8)	1144(12)	3231(1)
600(1)	1152(15)	3241(9)
603(1)	1156(46)	3242(7)
606(2)	1222(0)	3246(6)
686(16)	1272(0)	3248(6)
687(25)	1274(0)	3256(2)
779(6)	1382(3)	3258(5)

Table S20. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-3**.

M06L		
-502(54)	804(3)	1389(6)
29(0)	807(33)	1395(66)
58(0)	815(3)	1397(20)
67(1)	823(12)	1398(19)
80(0)	826(18)	1399(5)
84(1)	829(4)	1422(11)
109(0)	834(5)	1433(29)
127(3)	834(15)	1442(1)
133(1)	842(27)	1450(3)
154(1)	850(11)	1469(2)
170(0)	870(35)	1475(3)
193(12)	889(1)	1479(57)
214(4)	892(1)	1483(26)
240(1)	897(2)	1487(11)
265(6)	928(5)	1501(2)
326(3)	972(18)	1530(68)
351(3)	1009(10)	1817(16)
375(0)	1020(2)	2523(1)
384(13)	1028(81)	3010(60)
395(15)	1037(10)	3017(97)
409(7)	1040(3)	3083(33)
425(9)	1055(38)	3090(11)
432(6)	1073(1)	3137(15)
474(12)	1074(5)	3174(9)
517(2)	1079(2)	3176(5)
554(8)	1082(0)	3222(0)
580(3)	1100(1)	3226(1)
591(0)	1143(14)	3227(1)
600(5)	1146(8)	3236(2)
604(1)	1150(1)	3239(6)
606(1)	1162(33)	3244(5)
676(3)	1253(4)	3246(4)
751(11)	1270(33)	3250(8)
774(10)	1272(0)	3256(3)
799(4)	1278(0)	3262(5)

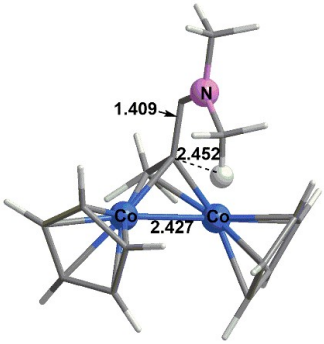
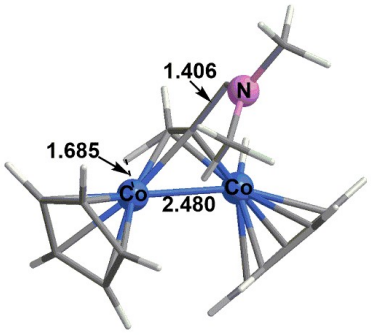
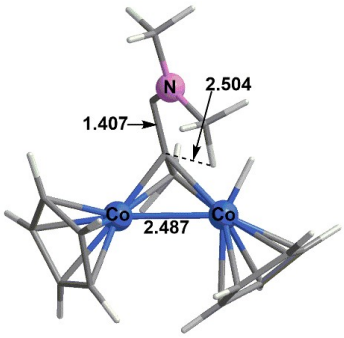
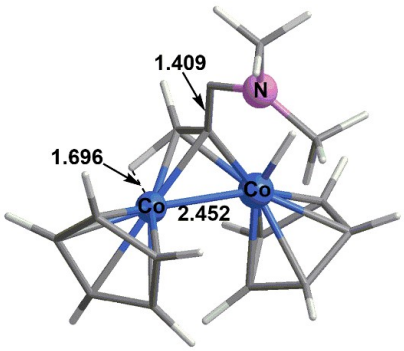
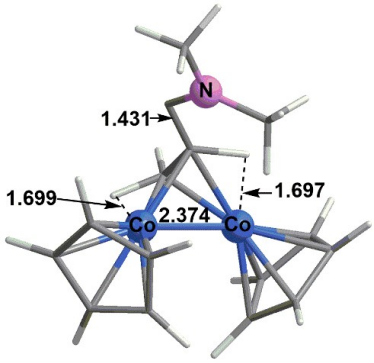
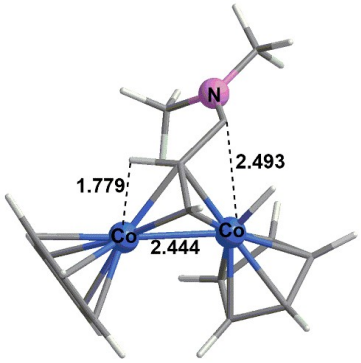
Table S21. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-4**.

M06L		
-192(28)	792(33)	1350(22)
25(0)	801(15)	1384(101)
47(0)	808(21)	1388(9)
77(0)	816(5)	1393(2)
84(1)	822(5)	1394(3)
101(1)	824(1)	1400(1)
131(2)	828(5)	1417(4)
135(0)	832(1)	1445(0)
151(2)	835(14)	1447(2)
197(1)	856(33)	1450(1)
209(2)	874(1)	1461(0)
216(0)	878(2)	1469(0)
226(1)	882(0)	1471(0)
258(2)	891(1)	1483(3)
318(0)	1003(3)	1492(9)
335(2)	1016(7)	1517(15)
356(0)	1017(8)	3001(49)
361(6)	1029(3)	3008(187)
381(4)	1036(26)	3025(71)
391(4)	1039(88)	3093(28)
421(2)	1065(8)	3097(4)
433(4)	1069(5)	3111(22)
469(17)	1071(0)	3125(27)
487(5)	1073(0)	3141(4)
556(1)	1077(1)	3153(10)
581(9)	1108(9)	3213(1)
589(6)	1129(11)	3217(5)
594(3)	1142(22)	3217(2)
600(8)	1146(8)	3228(1)
612(9)	1153(48)	3233(12)
694(2)	1176(15)	3237(14)
712(2)	1228(10)	3238(4)
744(28)	1270(0)	3246(6)
772(2)	1275(0)	3248(7)
782(6)	1337(39)	3254(4)

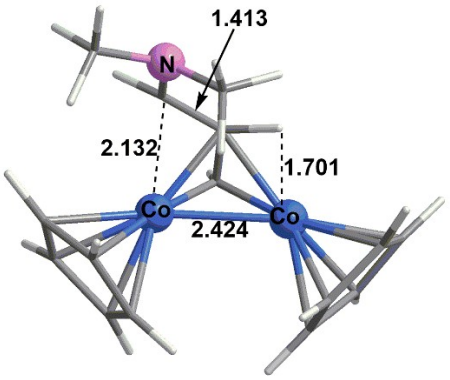
Table S22. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **TS-5**.

M06L		
-317(4)	791(11)	1327(19)
27(0)	802(29)	1391(2)
65(0)	810(12)	1394(0)
75(0)	817(5)	1396(2)
106(0)	825(16)	1398(1)
129(1)	827(14)	1414(3)
145(3)	830(5)	1442(0)
158(1)	832(21)	1445(0)
196(2)	843(20)	1450(1)
209(1)	860(9)	1463(0)
218(2)	877(4)	1468(0)
240(1)	881(1)	1474(2)
273(0)	884(1)	1479(2)
295(0)	888(3)	1492(10)
319(2)	946(3)	1495(7)
346(1)	982(47)	1540(13)
360(5)	1013(7)	3009(61)
365(3)	1019(6)	3015(104)
385(4)	1029(20)	3083(8)
399(6)	1030(16)	3084(28)
409(4)	1035(2)	3120(38)
428(3)	1057(11)	3124(7)
442(1)	1070(1)	3131(7)
492(39)	1073(2)	3165(2)
522(15)	1074(1)	3177(6)
575(7)	1076(1)	3201(7)
589(4)	1112(2)	3221(2)
595(3)	1142(23)	3224(2)
596(0)	1145(11)	3225(0)
599(1)	1149(1)	3236(8)
678(1)	1186(3)	3239(14)
746(15)	1215(4)	3240(12)
757(0)	1270(0)	3242(12)
768(1)	1274(0)	3252(6)
785(18)	1280(5)	3253(3)

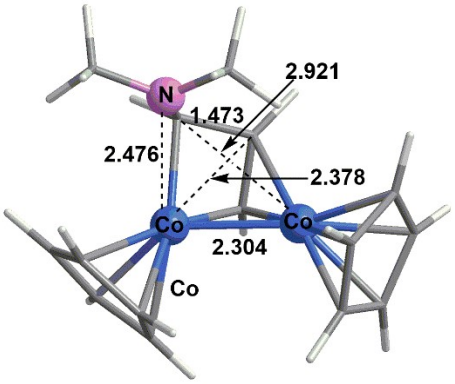
Tables S23: The optimized structures of the **cmp-n (n=1~6)**and**TS-n (n=1~5)**complexes in Figure 15.

cmp-1, TS-1	
 **cmp-1**	 **TS-1**
cmp-2, TS-2	
 **cmp-2**	 **TS-2**
cmp-3, TS-3	
 **cmp-3**	 **TS-3**

cmp-4, TS-4

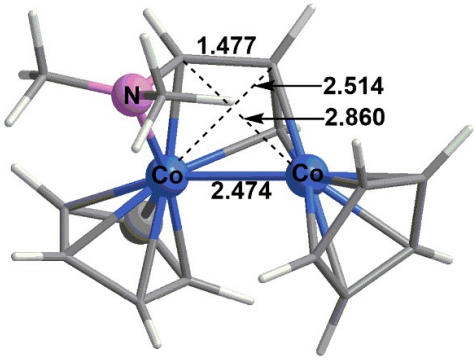


cmp-4

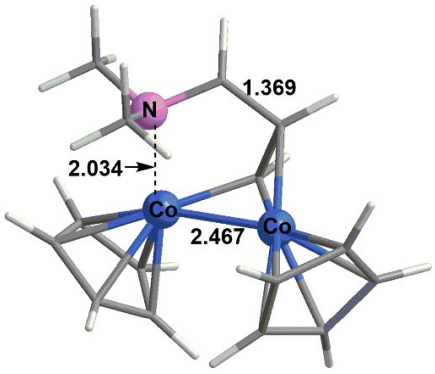


TS-4

cmp-5, TS-5

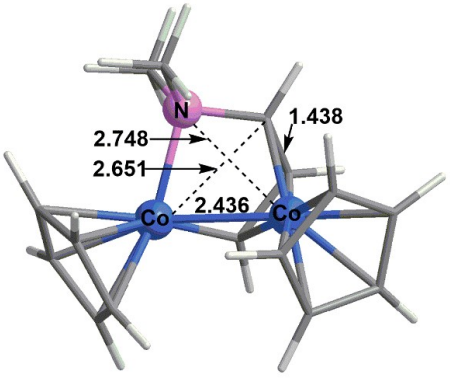


cmp-5



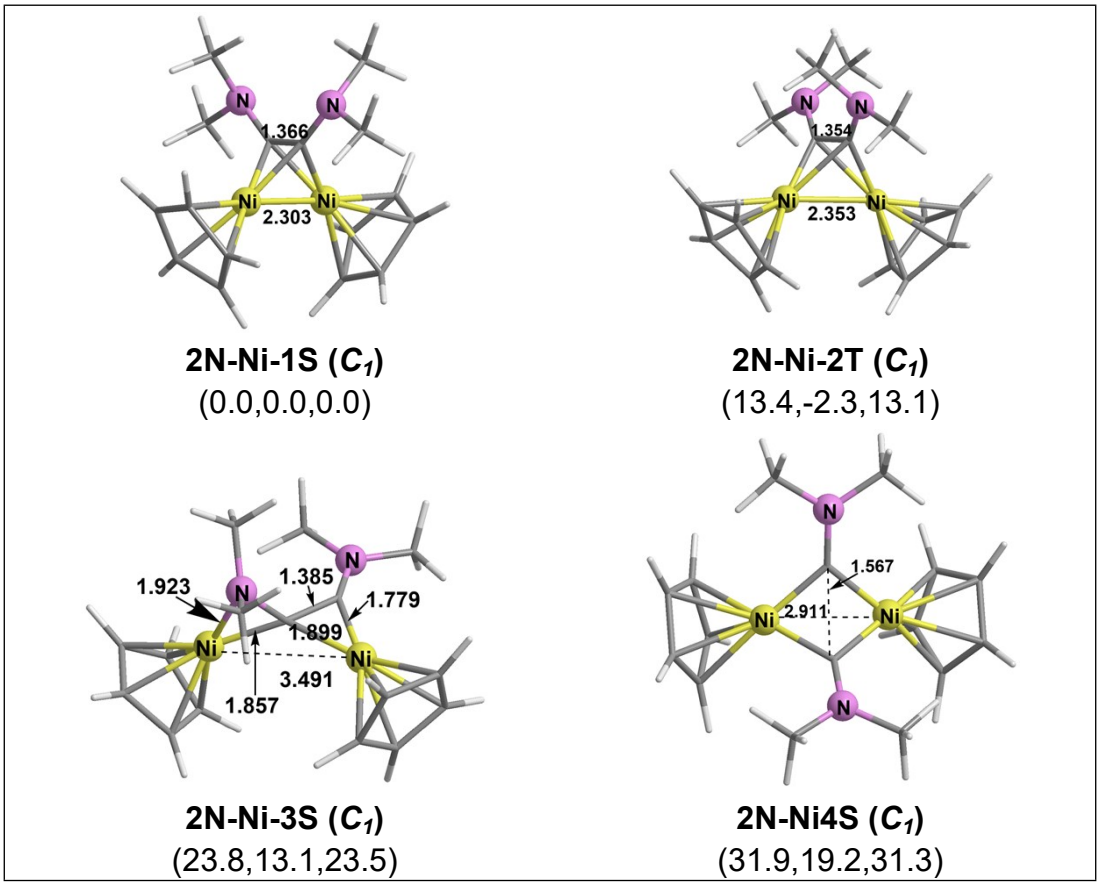
TS-5

cmp-6

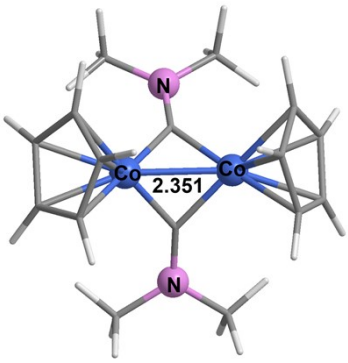


cmp-6

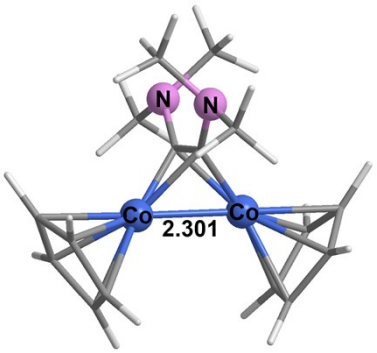
Tables S24: All theoptimized structures of the $Cp_2Ni_2C_2(NMe_2)_2$complexes. The numbers in parentheses in the second line are the relative energies (ΔE in kcal/mol) predicted by M06-L/DZP, ωB97xD/DZP, and M06-L with the def2-TZVP basis set for the transition metal.



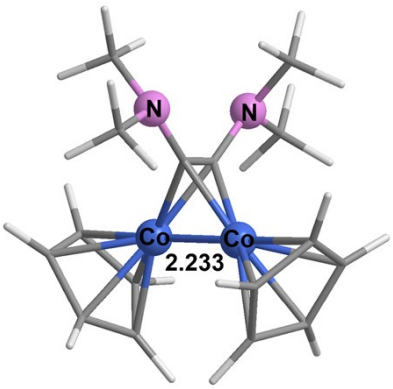
Tables S25: All theoptimized structures of the $Cp_2Co_2C_2(NMe_2)_2$complexes.



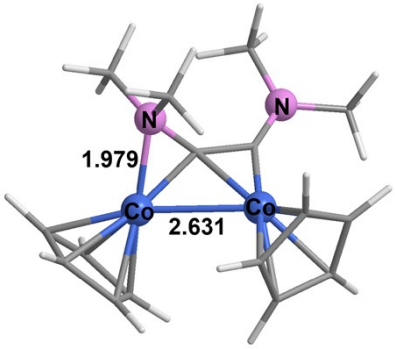
2N-Co-1S (C_{2v})
(0.0,0.0.,0.0)



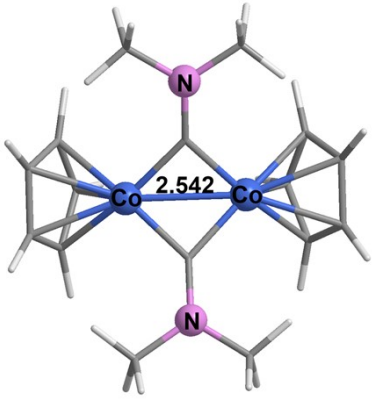
2N-Co-2T (C_1)
(3.2,-7.5,3.7)



2N-Co-3S (C_2)
(4.1,1.8,4.8)

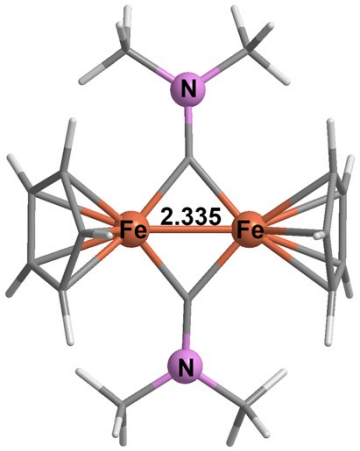


2N-Co-4S (C_1)
(19.8,17.8,20.6)

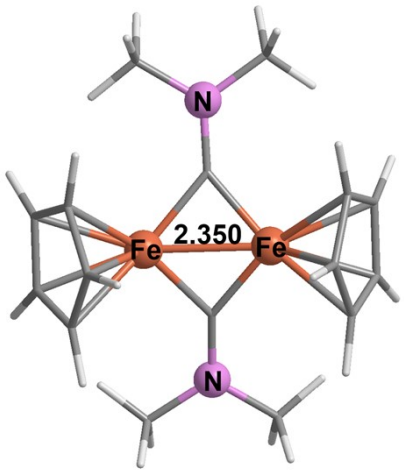


2N-Co-5T (C_{2v})
(23.7,12.8,24.9)

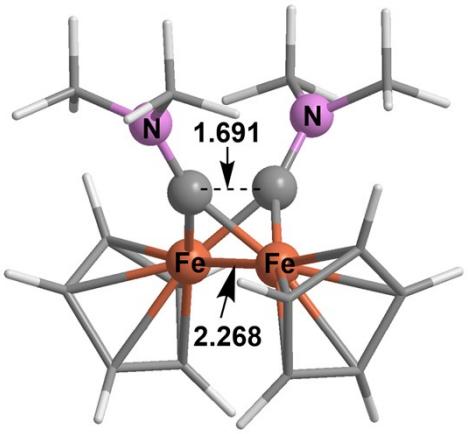
Tables S26: All the optimized structures of the $Cp_2Fe_2C_2(NMe_2)_2$complexes.



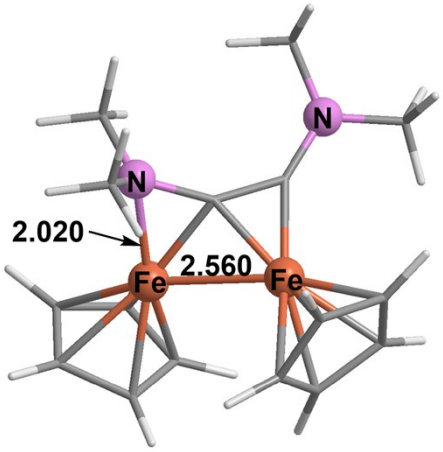
2N-Fe-1S (C_1)
(0.0,0.0,0.0)



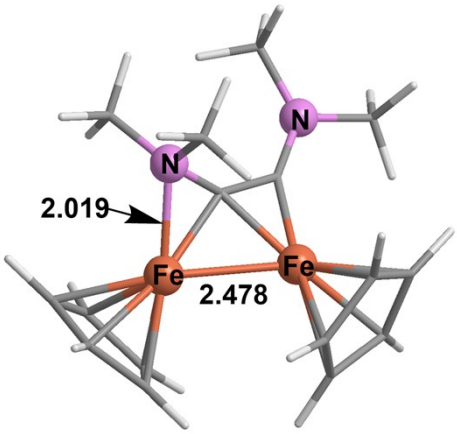
2N-Fe-2T (C_1)
(2.3,-8.0,2.7)



2N-Fe-3S (C_1)
(14.6,12.0,14.7)

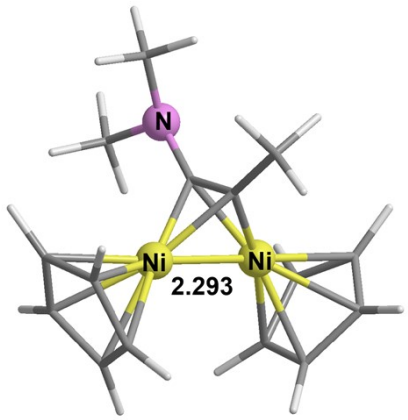


2N-Fe-4T (C_1)
(16.4,-13.7,,16.1)

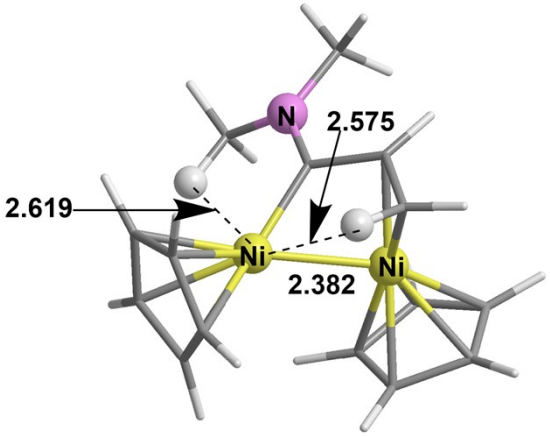


2N-Fe-5S (C_1)
(19.6,-0.1,19.0)

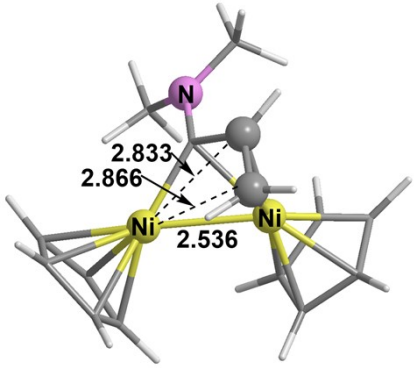
Tables S27: All theoptimized structures of the **$Cp_2Ni_2(MeC_2NMe_2)$**complexes.



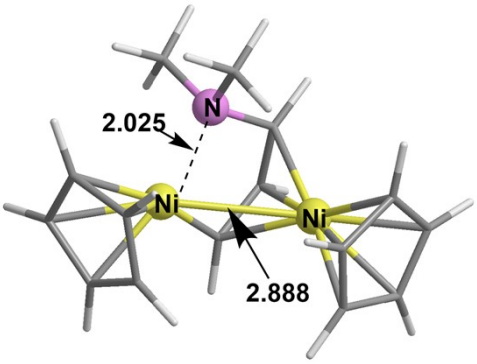
1N-Ni-1S (C_1)
(0.0,0.0,0.0)



1N-Ni-2S (C_1)
(6.9,-2.6,6.9)

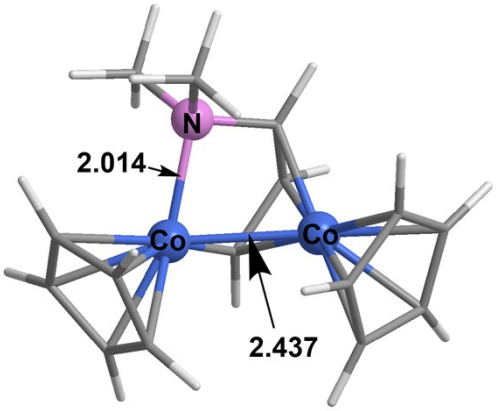


1N-Ni-3T (C_1)
(10.7,-7.3,10.1)

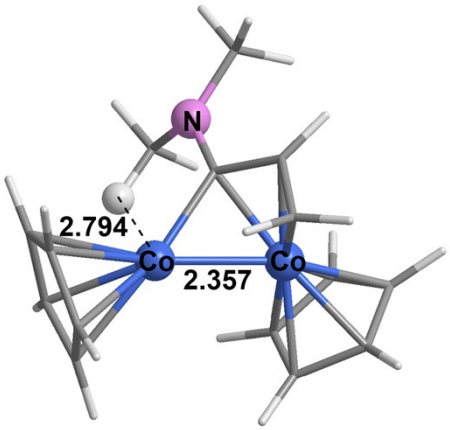


1N-Ni-4S (C_1)
(11.4-7.9,10.7)

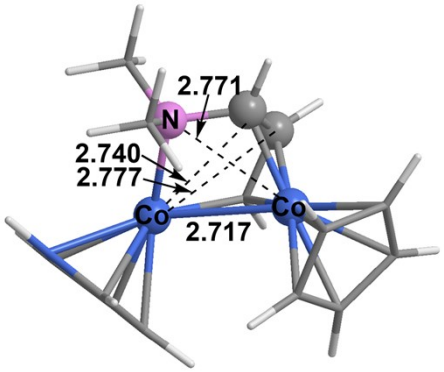
Tables S28: All theoptimized structures of the **$Cp_2Co_2(MeC_2NMe_2)$**complexes.



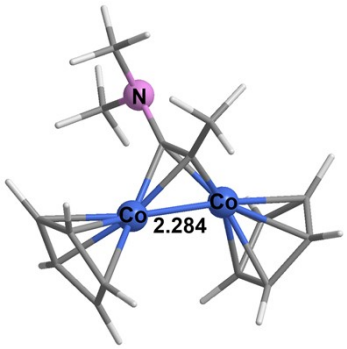
1N-Co-1S (C_1)
(0.0,0.0,0.0)



1N-Co-2T (C_1)
(11.8,3.9,11.7)

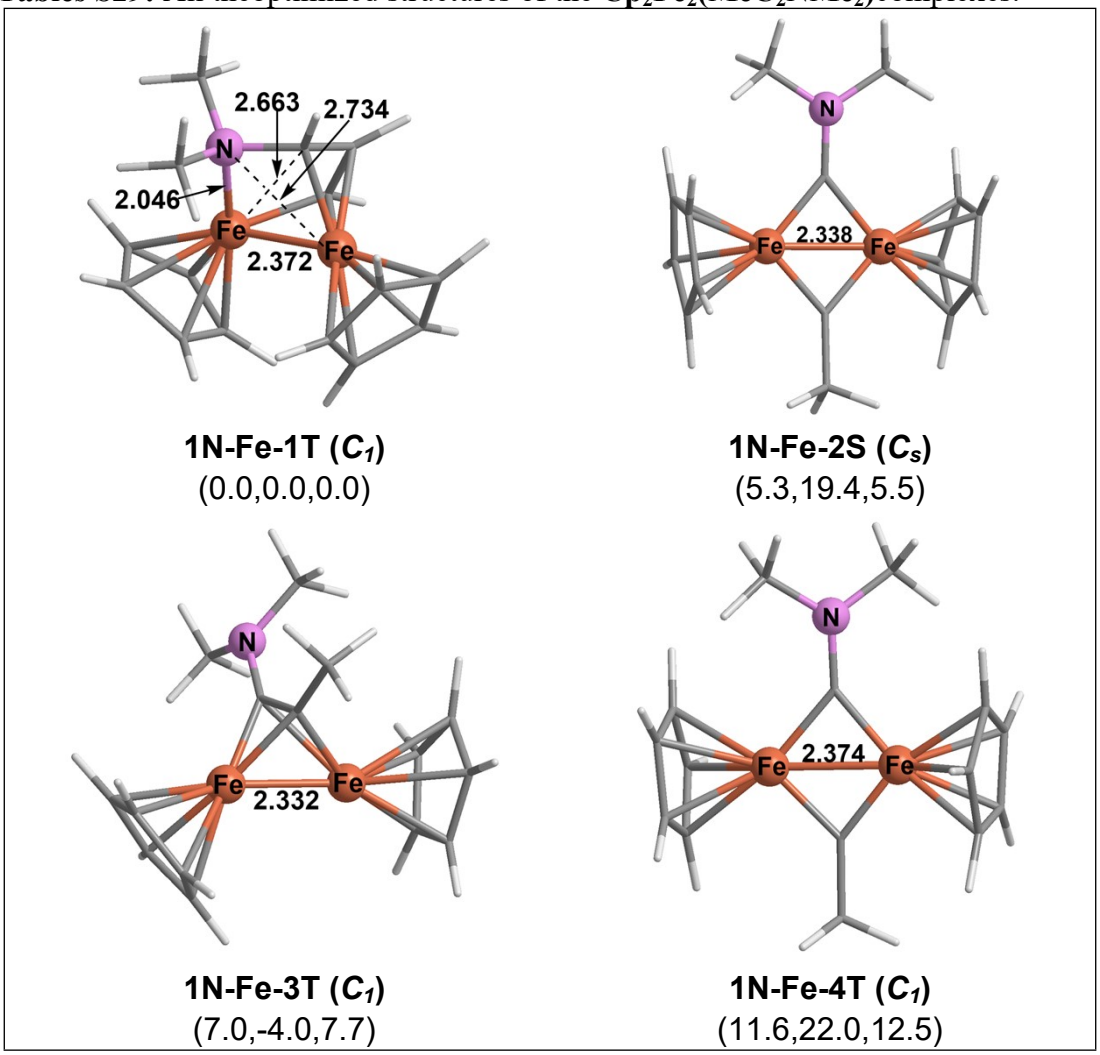


1N-Co-3T (C_1)
(12.0,-2.5,11.5)

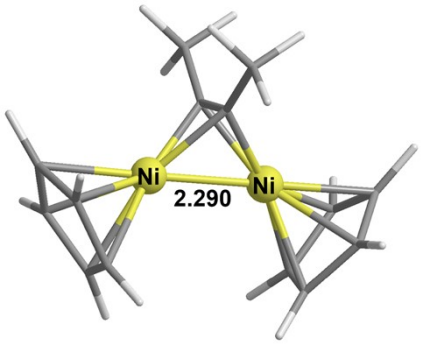


1N-Co-4T (C_1)
(15.3,9.1,14.9)

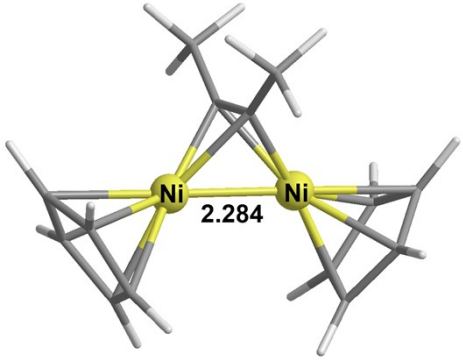
Tables S29: All theoptimized structures of the **$Cp_2Fe_2(MeC_2NMe_2)$**complexes.



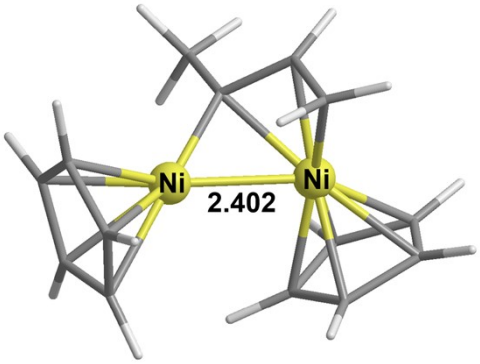
Tables S30: All theoptimized structures of the $Cp_2Ni_2C_2Me_2$complexes.



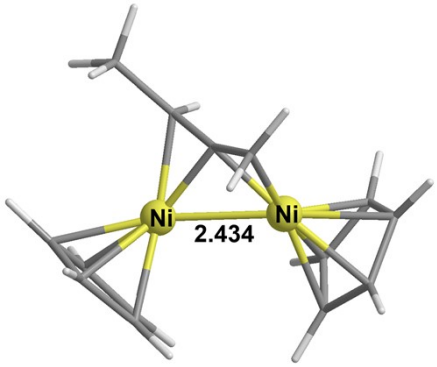
0N-Ni-1S (C_1)
(0.0,0.0,0.0)



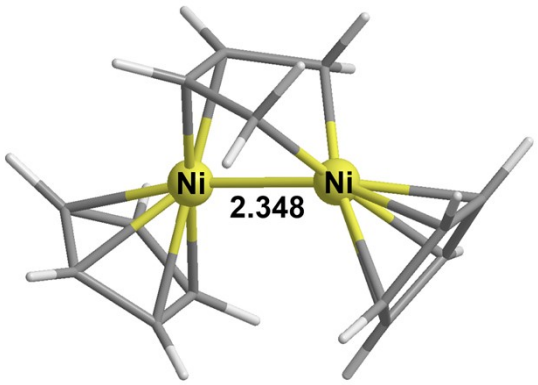
0N-Ni-2T (C_1)
(13.5,-3.1,13.2)



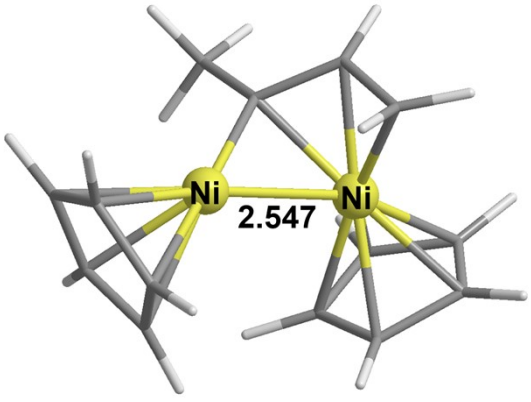
0N-Ni-3S (C_1)
(13.6,1.4,13.5)



0N-Ni-4S (C_1)
(14.7,6.9,14.6)

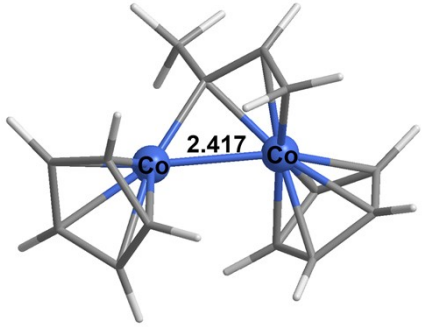


0N-Ni-5S (C_s)
(15.5,9.2,15.8)

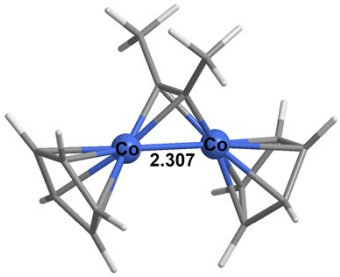


0N-Ni-6T (C_1)
(15.9,-2.9,15.2)

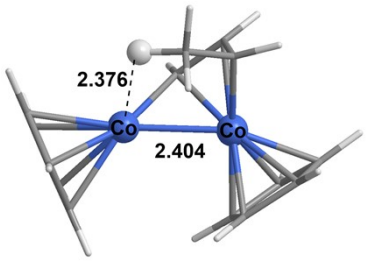
Tables S31: All theoptimized structuresof the $Cp_2Co_2C_2Me_2$complexes.



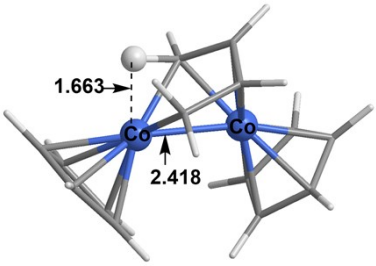
0N-Co-1T (C_1)
(0.0,0.0,0.0)



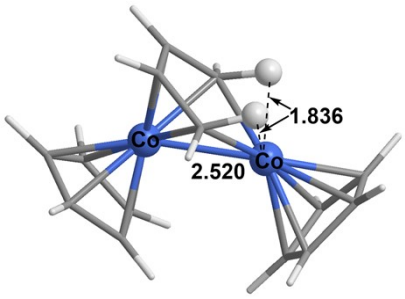
0N-Co-2T (C_{2v})
(0.7,12.4,0.3)



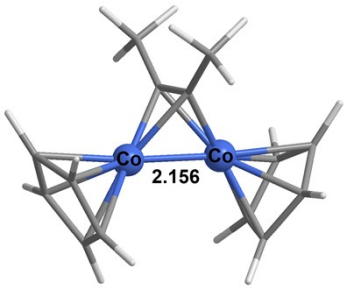
0N-Co-3T (C_1)
(3.0,3.3,2.8)



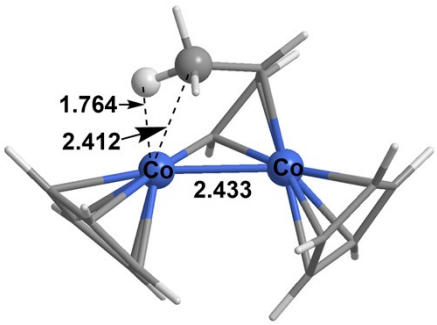
0N-Co-4S (C_1)
(3.0,19.6,3.5)



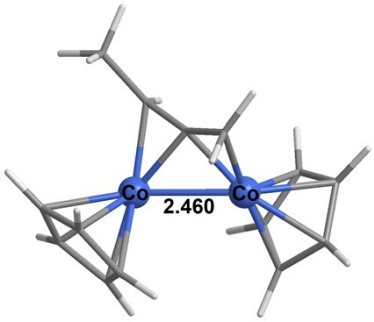
0N-Co-5T (C_s)
(3.5,9.0,4.0)



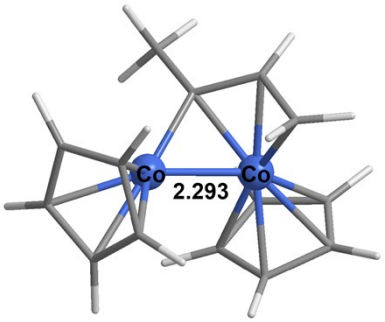
0N-Co-6S (C_1)
(4.4,20.8,4.5)



0N-Co-7S (C_1)
(4.5,18.3,4.7)

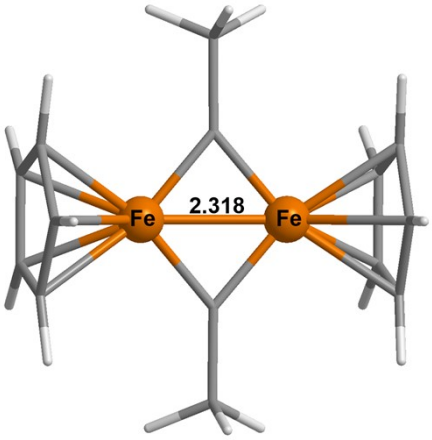


0N-Co-8T (C_1)
(9.6,16.7,9.5)

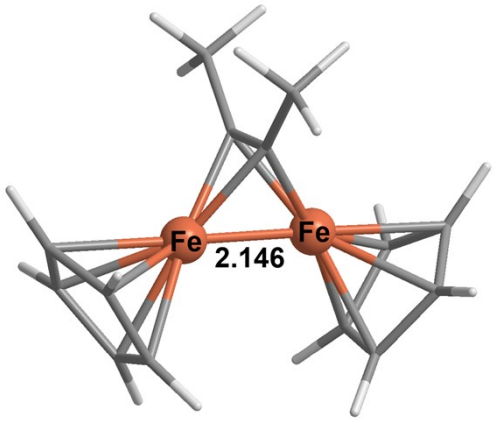


0N-Co-9S (*C_1*)
(10.0,25.1,10.3)

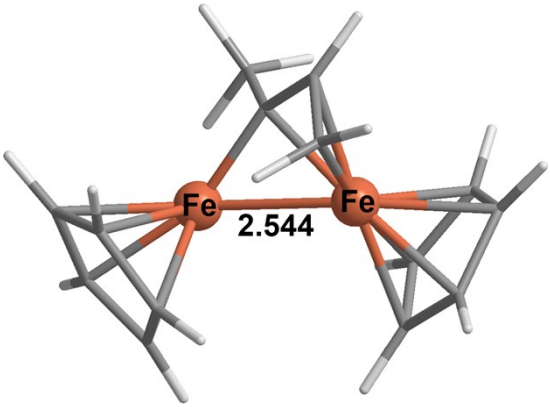
Tables S32: All theoptimized structures of the **$Cp_2Fe_2C_2Me_2$**complexes.



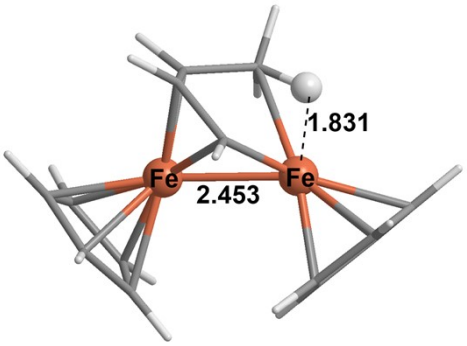
0N-Fe-1S (C_2)
(0.0,0.0,0.0)



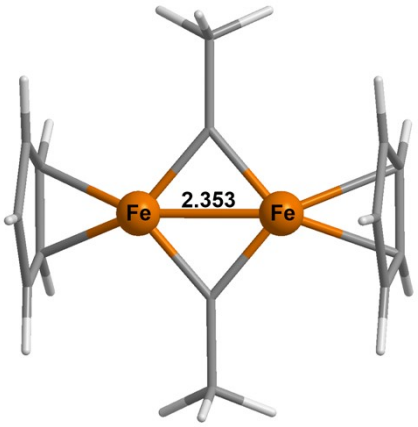
0N-Fe-2T (C_1)
(10.6,-6.2,10.1)



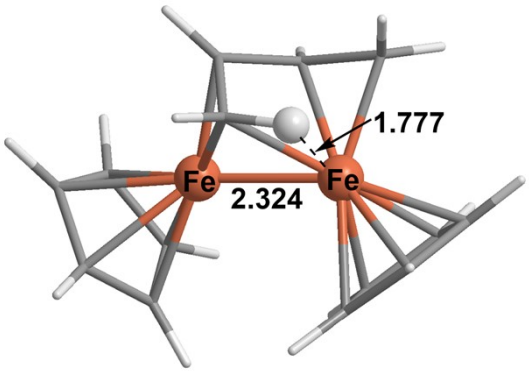
0N-Fe-3T (C_1)
(11.8,-10.0,11.5)



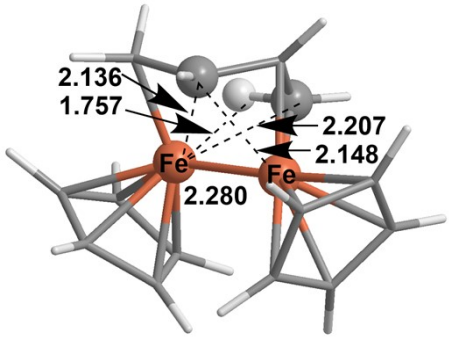
0N-Fe-4T (C_1)
(12.5,-8.3,11.9)



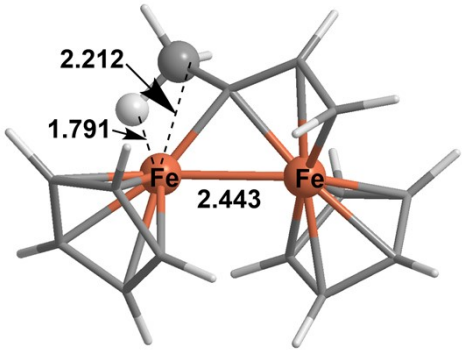
0N-Fe-5T (C_1)
(12.8,23.4,14.3)



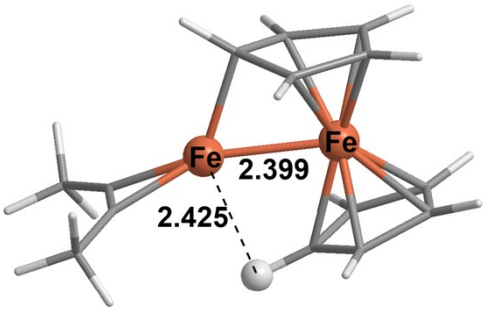
0N-Fe-6T (C_1)
(13.7,-5.8,13.8)



0N-Fe-7S (C_1)
(13.8,5.8,13.3)



0N-Fe-8S (C_1)
(13.8,0.3,13.3)



0N-Fe-9T (C_s)
(16.9,6.8,16.6)

0N-Fe-10T (C_1)
(21.4,-0.5,20.7)

Tables S33 : Optimized coordinates for the **$Cp_2Ni_2(MeC_2NMe_2)_2$**structure **2N-Ni-1S**

	M06L/DZP				M06L/Def2TZVPP				wB97xd/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.029584	0.972158	-0.688008	C	-0.031421	0.973483	-0.683819	C	0.012431	1.006636	-0.683172
C	0.035702	0.968623	0.685244	C	0.038193	0.969953	0.680385	C	-0.012429	1.006623	0.683188
N	-0.229402	1.889916	-1.693957	N	-0.232601	1.864413	-1.700223	N	-0.245963	1.877701	-1.705077
C	-0.400714	1.335401	-3.025390	C	-0.383064	1.302054	-3.025568	C	-0.308249	1.285847	-3.031018
C	-1.160203	2.965693	-1.387168	C	-1.129453	2.970129	-1.422771	C	-1.281986	2.866449	-1.443018
H	-1.045337	3.776892	-2.113976	H	-0.983866	3.761059	-2.158761	H	-1.235140	3.659931	-2.196493
H	-2.208717	2.619502	-1.413471	H	-2.18255	2.658939	-1.456171	H	-2.286235	2.410042	-1.466141
H	-0.276223	2.122721	-3.776472	H	-0.24323	2.079343	-3.776801	H	-0.238530	2.071143	-3.791661
H	-1.397893	0.879315	-3.158360	H	-1.375398	0.853705	-3.171924	H	-1.246283	0.724910	-3.179897
H	0.353630	0.561419	-3.188057	H	0.365743	0.527099	-3.172259	H	0.529862	0.594853	-3.148829
H	-0.962186	3.353597	-0.384259	H	-0.931512	3.36991	-0.430883	H	-1.131731	3.305702	-0.453094
C	-2.422084	-1.729458	-0.847551	C	-2.416445	-1.721771	-0.845198	C	-2.200278	-1.969489	-0.684222
C	-3.145638	-0.560779	-0.483456	C	-3.135409	-0.557855	-0.489496	C	-2.995961	-0.793087	-0.742909
H	-3.635985	0.127104	-1.162543	H	-3.626135	0.121288	-1.168717	H	-3.360796	-0.310423	-1.641565
C	-3.095769	-0.440958	0.942937	C	-3.090891	-0.434377	0.928831	C	-3.190292	-0.334914	0.597060
H	-3.544522	0.353409	1.527805	H	-3.545093	0.35476	1.507548	H	-3.746580	0.546407	0.893687
C	-1.940783	-2.340249	0.355444	C	-1.941538	-2.325222	0.354525	C	-1.955690	-2.276296	0.696991
H	-1.334000	-3.237162	0.408665	H	-1.345018	-3.222401	0.412692	H	-1.380810	-3.117548	1.064730
C	-2.375521	-1.560401	1.461351	C	-2.376938	-1.546301	1.450207	C	-2.576841	-1.277769	1.486941
H	-2.168735	-1.759559	2.505702	H	-2.182455	-1.746288	2.491619	H	-2.572326	-1.220698	2.568726
C	2.184787	-2.064197	0.594575	C	2.19052	-2.043336	0.605358	C	2.200266	-1.969512	0.684189
C	2.964577	-0.888379	0.771795	C	2.963922	-0.870723	0.763392	C	2.995953	-0.793116	0.742894
H	3.294619	-0.475684	1.717971	H	3.30445	-0.452946	1.697504	H	3.360786	-0.310466	1.641558
C	3.200335	-0.323438	-0.519603	C	3.189815	-0.323311	-0.528689	C	3.190282	-0.334920	-0.597067
H	3.755055	0.584344	-0.726468	H	3.7453	0.57508	-0.748228	H	3.746570	0.546407	-0.893676
C	1.974745	-2.253546	-0.811032	C	1.972317	-2.246906	-0.788965	C	1.955674	-2.276297	-0.697028
H	1.407361	-3.058513	-1.263157	H	1.412884	-3.058622	-1.226664	H	1.380791	-3.117541	-1.064779
C	2.606456	-1.187085	-1.498398	C	2.594945	-1.193988	-1.488505	C	2.576828	-1.277759	-1.486964
H	2.620835	-1.035158	-2.570973	H	2.609605	-1.059675	-2.558324	H	2.572311	-1.220674	-2.568748
H	1.809694	-2.705943	1.382942	H	1.829885	-2.678345	1.399081	H	1.851182	-2.546988	1.531492
H	-2.250024	-2.088637	-1.855019	H	-2.249259	-2.087315	-1.845857	H	-1.851197	-2.546953	-1.531534
Ni	1.137422	-0.397687	-0.179213	Ni	1.134248	-0.391531	-0.17699	Ni	1.126307	-0.368023	-0.192906
Ni	-1.146016	-0.384155	0.171953	Ni	-1.142821	-0.377019	0.169332	Ni	-1.126315	-0.368016	0.192894
N	0.249643	1.879034	1.697639	N	0.252083	1.853015	1.704251	N	0.245984	1.877657	1.705115
C	1.269194	2.881112	1.423052	C	1.2543	2.874157	1.462867	C	1.282019	2.866397	1.443079
H	1.189541	3.702031	2.143580	H	1.153185	3.675484	2.194889	H	1.235177	3.659869	2.196565
H	2.287124	2.456029	1.487640	H	2.273182	2.468012	1.533344	H	2.286263	2.409978	1.466203
H	1.136912	3.277820	0.412535	H	1.129802	3.289447	0.465156	H	1.131777	3.305667	0.453160
C	0.336206	1.317101	3.034379	C	0.303189	1.284469	3.034963	C	0.308268	1.285766	3.031040
H	1.287482	0.780756	3.198520	H	1.24235	0.74521	3.218767	H	1.246294	0.724811	3.179897
H	0.254689	2.115775	3.779189	H	0.210364	2.076045	3.778341	H	0.238566	2.071043	3.791704

H	-0.484613	0.609303	3.176689	H	-0.520821	0.584913	3.156757	H	-0.529853	0.594782	3.148837

Tables S34 : Optimized coordinates for the $Cp_2Ni_2(MeC_2NMe_2)_2$structure **2N-Ni-2T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.200117	1.123194	0.652601	C	0.160566	1.106023	0.657868	C	0.343163	1.173278	0.588125
C	-0.200121	1.123196	-0.652600	C	-0.160567	1.106024	-0.657867	C	-0.343151	1.173278	-0.588126
N	0.079821	2.009301	1.687898	N	0.01465	1.973581	1.69575	N	0.434138	2.064404	1.615213
C	0.427602	1.529800	3.011933	C	0.324687	1.488614	3.022347	C	1.092898	1.615545	2.829018
C	-1.053857	2.919725	1.651622	C	-1.091878	2.909106	1.632603	C	-0.696173	2.958221	1.820146
H	-1.993271	2.412581	1.931451	H	-2.047082	2.427419	1.880097	H	-1.545255	2.430004	2.284253
H	-0.887036	3.750110	2.345681	H	-0.927465	3.726303	2.334744	H	-0.398583	3.789228	2.468531
H	-0.381207	0.923110	3.454525	H	-0.492549	0.88476	3.439241	H	0.422199	0.999137	3.449587
H	0.628233	2.376584	3.676958	H	0.505662	2.328384	3.693264	H	1.420872	2.480218	3.416719
H	1.323113	0.907802	2.940052	H	1.217468	0.869799	2.977593	H	1.963792	1.014789	2.557816
H	-1.172199	3.319422	0.641157	H	-1.170907	3.319611	0.628344	H	-1.026387	3.360945	0.858900
C	-0.079827	2.009304	-1.687895	N	-0.014651	1.973583	-1.695748	C	-0.434118	2.064402	-1.615218
C	-0.427608	1.529805	-3.011931	C	-0.324689	1.488618	-3.022346	C	-1.092880	1.615541	-2.829022
H	0.381201	0.923119	-3.454525	H	0.492547	0.884765	-3.439242	H	-0.422185	0.999125	-3.449586
C	-1.323118	0.907805	-2.940051	H	-1.217469	0.869803	-2.977592	C	-1.963779	1.014794	-2.557819
H	-0.628243	2.376591	-3.676954	H	-0.505664	2.328389	-3.693261	H	-1.420845	2.480214	-3.416729
C	1.053849	2.919730	-1.651618	C	1.091877	2.909108	-1.6326	C	0.696200	2.958208	-1.820154
H	1.172191	3.319425	-0.641152	H	1.170906	3.319611	-0.62834	H	1.026416	3.360934	-0.858910
C	1.993264	2.412590	-1.931450	H	2.047081	2.427422	-1.880095	C	1.545279	2.429981	-2.284257
H	0.887025	3.750117	-2.345674	H	0.927463	3.726306	-2.33474	H	0.398619	3.789214	-2.468544
C	1.176516	-0.374308	0.085655	Ni	1.171946	-0.371621	0.105839	C	1.189681	-0.366040	-0.047879
C	-1.176515	-0.374310	-0.085656	Ni	-1.171945	-0.371622	-0.10584	C	-1.189686	-0.366030	0.047881
H	2.918139	-0.897936	-1.043772	C	2.929413	-0.879112	-0.992554	H	2.822523	-0.962218	-1.330023
C	2.028454	-2.015990	-0.948081	C	2.06098	-2.004547	-0.904619	C	1.902310	-2.043219	-1.156720
H	1.534941	-2.509333	-1.776918	H	1.594585	-2.511023	-1.73459	H	1.322002	-2.517826	-1.938516
C	1.893011	-2.347620	0.427329	C	1.911597	-2.329065	0.462155	C	1.884453	-2.381083	0.226072
H	1.271507	-3.136199	0.835548	H	1.305454	-3.125745	0.863694	H	1.276959	-3.151196	0.685937
C	3.347721	-0.556755	0.268087	C	3.333837	-0.527746	0.315945	C	3.380219	-0.645227	-0.059921
H	4.011966	0.257780	0.529887	H	3.984913	0.289869	0.581229	H	4.101935	0.137449	0.141050
H	2.692982	-1.431628	1.180453	C	2.683506	-1.403144	1.217969	H	2.787359	-1.508182	0.904891
H	2.795559	-1.419601	2.259499	H	2.775981	-1.389357	2.29277	H	2.991689	-1.511955	1.969266
Ni	-2.692980	-1.431630	-1.180455	C	-2.683506	-1.403144	-1.21797	Ni	-2.787370	-1.508164	-0.904888
Ni	-1.893005	-2.347622	-0.427337	C	-1.911597	-2.329065	-0.462156	Ni	-1.884472	-2.381069	-0.226064
N	-1.271500	-3.136198	-0.835561	H	-1.305454	-3.125745	-0.863695	N	-1.276983	-3.151189	-0.685925
C	-2.028446	-2.015999	0.948075	C	-2.060979	-2.004549	0.904617	C	-1.902330	-2.043200	1.156727
H	-1.534931	-2.509344	1.776909	H	-1.594585	-2.511024	1.734588	H	-1.322027	-2.517809	1.938526
H	-3.347719	-0.556762	-0.268084	C	-3.333836	-0.527747	-0.315945	H	-3.380226	-0.645201	0.059919
H	-4.011967	0.257773	-0.529879	H	-3.984913	0.289868	-0.581229	H	-4.101936	0.137479	-0.141057

C	-2.918134	-0.897947	1.043773	C	-2.929412	-0.879113	0.992554	C	-2.822535	-0.962191	1.330024
H	-3.216784	-0.403425	1.961313	H	-3.236634	-0.3905	1.904292	H	-3.059609	-0.475561	2.268810
H	3.216790	-0.403409	-1.961310	H	3.236635	-0.390498	-1.904292	H	3.059599	-0.475593	-2.268812
H	-2.795559	-1.419598	-2.259501	H	-2.775981	-1.389357	-2.292771	H	-2.991698	-1.511940	-1.969264

Tables S35 : Optimized coordinates for the **$Cp_2Ni_2(MeC_2NMe_2)_2$**structure **2N-Ni -3S**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	0.828216	1.305650	0.010627	C	0.822187	1.291217	0.012368	C	0.806920	1.284486	0.037096
C	-0.040115	0.291138	0.409585	C	-0.041737	0.280944	0.400533	C	-0.038162	0.225491	0.406875
N	0.737271	2.588256	-0.318773	N	0.755203	2.569323	-0.305418	N	0.703220	2.560514	-0.264845
C	1.890414	3.311230	-0.824058	C	1.921375	3.279964	-0.789311	C	1.859428	3.300160	-0.750011
C	-0.523771	3.313861	-0.301505	C	-0.487021	3.321697	-0.283053	C	-0.561632	3.284889	-0.234709
H	-0.580460	4.006406	0.549059	H	-0.530484	4.002447	0.571269	H	-0.617373	3.947151	0.638439
H	-0.624129	3.899184	-1.222709	H	-0.56961	3.9188	-1.19242	H	-0.649344	3.896772	-1.139481
H	2.092547	4.197460	-0.210405	H	2.129364	4.150366	-0.163521	H	2.019861	4.196729	-0.139409
H	1.716974	3.641321	-1.856312	H	1.762676	3.628818	-1.812426	H	1.705469	3.606463	-1.792289
H	2.754833	2.645602	-0.797120	H	2.774058	2.607647	-0.766569	H	2.733870	2.650688	-0.686907
H	-1.345885	2.589984	-0.249251	H	-1.324376	2.624547	-0.242617	H	-1.383523	2.563297	-0.215443
C	-0.769805	0.094180	1.648136	N	-0.76623	0.070109	1.635342	C	-0.763154	-0.000080	1.635911
C	-1.051284	1.271368	2.474031	C	-1.062684	1.231028	2.471391	C	-1.010606	1.142533	2.519641
H	-1.790024	1.015981	3.240020	H	-1.809984	0.964505	3.218205	H	-1.749899	0.862634	3.276643
C	-0.134174	1.626315	2.969118	H	-0.16049	1.578534	2.987186	C	-0.080965	1.448711	3.020758
H	-1.459683	2.068434	1.851515	H	-1.459795	2.034118	1.859818	H	-1.407341	1.979239	1.944341
C	-0.335224	-1.045792	2.463121	C	-0.342335	-1.077528	2.437349	C	-0.354935	-1.188876	2.395180
H	0.577559	-0.791628	3.024587	H	0.557673	-0.833541	3.012583	H	0.563852	-0.981574	2.961921
C	-1.130430	-1.320369	3.164225	H	-1.141371	-1.35878	3.1233	C	-1.159023	-1.474407	3.081711
H	-0.119264	-1.888805	1.804252	H	-0.12039	-1.91073	1.777751	H	-0.161381	-2.004186	1.697531
C	3.559692	-0.631639	-1.055864	C	3.538748	-0.628418	-1.075326	C	3.644167	-0.485684	-0.985308
C	2.567308	-1.560292	-1.484026	C	2.562064	-1.575483	-1.470132	C	2.725325	-1.413029	-1.558114
H	2.192256	-1.677793	-2.493086	H	2.181946	-1.721445	-2.468363	H	2.419664	-1.453959	-2.596330
C	2.120935	-2.275567	-0.335444	C	2.147376	-2.274687	-0.309666	C	2.231894	-2.231176	-0.505442
H	1.342202	-3.030445	-0.323005	H	1.392952	-3.045724	-0.274949	H	1.490623	-3.015521	-0.605653
C	3.751926	-0.799653	0.350545	C	3.751201	-0.766485	0.323141	C	3.773741	-0.781077	0.410774
H	4.440920	-0.237533	0.969388	H	4.440778	-0.189064	0.918198	H	4.415711	-0.263649	1.113632
C	2.861692	-1.814896	0.798620	C	2.891382	-1.78462	0.798735	C	2.894693	-1.854195	0.710113
H	2.762623	-2.176753	1.815379	H	2.817222	-2.132115	1.816993	H	2.752708	-2.314769	1.680545
H	-3.187489	0.381546	-1.382707	C	-3.32307	0.429665	-1.219273	H	-3.381322	0.455619	-1.192613
H	-3.879600	-0.208333	-0.296713	C	-3.883113	-0.349585	-0.186421	H	-3.926766	-0.367705	-0.176155
Ni	-4.609655	0.280310	0.338564	H	-4.607357	-0.013857	0.540109	Ni	-4.654192	-0.064533	0.568506
Ni	-3.462130	-1.581026	-0.185222	C	-3.3625	-1.679239	-0.282429	Ni	-3.396778	-1.698679	-0.330068
N	-3.825213	-2.289343	0.550817	H	-3.627766	-2.504083	0.360507	N	-3.649824	-2.552427	0.287849
C	-2.294882	-0.615620	-1.907838	C	-2.389577	-0.399923	-1.906939	C	-2.429900	-0.340373	-1.909769

H	-1.606032	-0.476945	-2.733842	H	-1.779043	-0.103741	-2.746304	H	-1.821335	-0.006707	-2.742323
H	-2.516243	-1.846983	-1.204232	C	-2.460194	-1.720028	-1.358639	H	-2.497657	-1.690506	-1.417573
H	-2.015116	-2.788502	-1.393157	H	-1.898551	-2.57612	-1.697106	H	-1.917579	-2.528425	-1.784365
C	-3.296616	1.397153	-1.745419	H	-3.547726	1.460841	-1.441695	C	-3.610041	1.499837	-1.370215
H	4.089102	0.071254	-1.688571	H	4.04983	0.063877	-1.725987	H	4.190688	0.280863	-1.522637
H	-1.764106	-0.291228	0.038615	Ni	-1.76551	-0.289107	0.032606	H	-1.779348	-0.287883	0.046978
H	1.730490	-0.226925	-0.040155	Ni	1.724618	-0.232051	-0.044656	H	1.742150	-0.213779	-0.039613

Tables S36 : Optimized coordinates for the **$Cp_2Ni_2(MeC_2NMe_2)_2$**structure **2N-Ni -4S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.000001	-1.054155	-0.470652	C	0.000000	-0.783299	-0.587653	C	0.000001	-1.070062	-0.494148
C	0.000000	1.054162	-0.470644	C	0.000003	0.783297	-0.587657	C	0.000001	1.070064	-0.494144
N	-0.000001	-2.208513	-1.134891	N	0.000000	-1.801881	-1.483868	N	0.000001	-2.186682	-1.195709
C	-1.220604	-2.914455	-1.500740	C	-1.226703	-2.492684	-1.817996	C	-1.220347	-2.870919	-1.612363
C	1.220603	-2.914456	-1.500737	C	1.226703	-2.492683	-1.817995	C	1.220348	-2.870920	-1.612362
H	1.338436	-3.829459	-0.904419	H	1.453707	-3.298391	-1.110797	H	1.300820	-3.845867	-1.114544
H	1.186861	-3.200235	-2.559419	H	1.145597	-2.928530	-2.814450	H	1.205116	-3.034951	-2.697011
H	-1.338445	-3.829452	-0.904416	H	-1.453695	-3.298404	-1.110809	H	-1.300821	-3.845865	-1.114544
H	-1.186853	-3.200243	-2.559420	H	-1.145602	-2.928516	-2.814458	H	-1.205115	-3.034951	-2.697012
H	-2.070956	-2.254088	-1.324660	H	-2.052265	-1.783369	-1.793581	H	-2.076695	-2.252055	-1.348861
H	2.070954	-2.254092	-1.324642	H	2.052262	-1.783363	-1.793597	H	2.076696	-2.252058	-1.348860
C	0.000000	2.208520	-1.134883	N	0.000005	1.801875	-1.483877	C	0.000001	2.186687	-1.195700
C	1.220601	2.914462	-1.500736	C	1.226709	2.492678	-1.818002	C	1.220349	2.870926	-1.612350
H	1.338419	3.829482	-0.904442	H	1.453703	3.298395	-1.110812	H	1.300821	3.845871	-1.114527
C	2.070958	2.254112	-1.324617	H	2.052270	1.783362	-1.793590	C	2.076696	2.252062	-1.348851
H	1.186867	3.200213	-2.559427	H	1.145609	2.928513	-2.814463	H	1.205117	3.034962	-2.696999
C	-1.220603	2.914464	-1.500729	C	-1.226699	2.492670	-1.818014	C	-1.220347	2.870925	-1.612352
H	-2.070957	2.254107	-1.324627	H	-2.052254	1.783345	-1.793627	H	-2.076694	2.252061	-1.348853
C	-1.338429	3.829472	-0.904419	H	-1.453715	3.298374	-1.110816	C	-1.300821	3.845870	-1.114529
H	-1.186864	3.200234	-2.559415	H	-1.145585	2.928520	-2.814467	H	-1.205114	3.034961	-2.697000
C	-1.395220	0.000001	0.128696	Ni	-1.455313	0.000004	0.206854	C	-1.377072	0.000000	0.123494
C	1.395223	0.000001	0.128692	Ni	1.455311	-0.000002	0.206861	C	1.377072	0.000000	0.123496
H	-3.505785	0.703786	0.167091	C	-3.516020	0.704424	0.401090	H	-3.487296	0.703224	0.266836
C	-2.742387	1.144593	1.298541	C	-2.694699	1.144053	1.473254	C	-2.676749	1.144084	1.368544
H	-2.552946	2.177645	1.568841	H	-2.498091	2.170981	1.738847	H	-2.482526	2.176482	1.635994
C	-2.324071	-0.000003	2.034983	C	-2.210944	-0.000066	2.161015	C	-2.239634	-0.000002	2.091763
H	-1.736950	0.000000	2.944772	H	-1.574364	-0.000128	3.030906	H	-1.616994	-0.000003	2.977645
C	-3.505782	-0.703796	0.167091	C	-3.516071	-0.704307	0.401027	C	-3.487295	-0.703227	0.266835
H	-3.986371	-1.342942	-0.564760	H	-4.039104	-1.340922	-0.295544	H	-4.004637	-1.342251	-0.439393
H	-2.742384	-1.144600	1.298543	C	-2.694774	-1.144089	1.473146	H	-2.676748	-1.144088	1.368542
H	-2.552943	-2.177652	1.568841	H	-2.498234	-2.171054	1.738644	H	-2.482524	-2.176486	1.635991
Ni	3.505781	0.703801	0.167105	C	3.516051	0.704350	0.401059	Ni	3.487294	0.703227	0.266842

Ni	2.742376	1.144587	1.298559	C	2.694743	1.144080	1.473191	Ni	2.676746	1.144082	1.368551
N	2.552932	2.177635	1.568871	H	2.498177	2.171032	1.738719	N	2.482520	2.176478	1.636005
C	2.324065	-0.000021	2.034983	C	2.210939	0.000024	2.161023	C	2.239632	-0.000008	2.091766
H	1.736940	-0.000036	2.944770	H	1.574358	0.000044	3.030913	H	1.616991	-0.000012	2.977646
H	3.505790	-0.703781	0.167086	C	3.516038	-0.704381	0.401081	H	3.487297	-0.703223	0.266836
H	3.986387	-1.342913	-0.564772	H	4.039045	-1.341062	-0.295449	H	4.004640	-1.342244	-0.439393
C	2.742388	-1.144605	1.298527	C	2.694723	-1.144062	1.473228	C	2.676749	-1.144090	1.368541
H	2.552954	-2.177663	1.568809	H	2.498140	-2.171003	1.738790	H	2.482526	-2.176489	1.635986
H	-3.986373	1.342929	-0.564764	H	-4.039010	1.341139	-0.295421	H	-4.004639	1.342248	-0.439391
H	3.986368	1.342958	-0.564738	H	4.039069	1.341000	-0.295492	H	4.004636	1.342256	-0.439382

Tables S37 : Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)_2$**structure **2N-Co-1S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	1.107447	0.000000	0.608786	C	1.086526	0.000000	0.618282	C	1.067677	0.000000	0.629181
C	-1.107447	0.000000	0.608786	C	-1.086526	0.000000	0.618282	C	-1.067677	0.000000	0.629181
N	2.189339	0.000000	1.380900	N	2.142671	0.000000	1.410632	N	2.115057	0.000000	1.439476
C	2.859014	1.226028	1.785819	C	2.806496	1.222285	1.828681	C	2.755341	1.227201	1.889403
C	2.859014	-1.226028	1.785819	C	2.806496	-1.222285	1.828681	C	2.755341	-1.227201	1.889403
H	3.791414	-1.375545	1.223622	H	3.740567	-1.374338	1.279984	H	3.721066	-1.375199	1.387343
H	3.107112	-1.186126	2.853773	H	3.044645	-1.175224	2.893132	H	2.929934	-1.185140	2.971977
H	3.791414	1.375545	1.223622	H	3.740567	1.374338	1.279984	H	3.721066	1.375199	1.387343
H	3.107112	1.186126	2.853773	H	3.044645	1.175224	2.893132	H	2.929934	1.185140	2.971977
H	2.187075	2.063711	1.595769	H	2.143390	2.059881	1.641031	H	2.096422	2.063704	1.659871
H	2.187075	-2.063711	1.595769	H	2.143390	-2.059881	1.641031	H	2.096422	-2.063704	1.659871
N	-2.189339	0.000000	1.380900	N	-2.142671	0.000000	1.410632	N	-2.115057	0.000000	1.439476
C	-2.859014	-1.226028	1.785819	C	-2.806496	-1.222285	1.828681	C	-2.755341	-1.227201	1.889403
H	-3.791414	-1.375545	1.223622	H	-3.740567	-1.374338	1.279984	H	-3.721066	-1.375199	1.387343
H	-2.187075	-2.063711	1.595769	H	-2.143390	-2.059881	1.641031	H	-2.096422	-2.063704	1.659871
H	-3.107112	-1.186126	2.853773	H	-3.044645	-1.175224	2.893132	H	-2.929934	-1.185140	2.971977
C	-2.859014	1.226028	1.785819	C	-2.806496	1.222285	1.828681	C	-2.755341	1.227201	1.889403
H	-2.187075	2.063711	1.595769	H	-2.143390	2.059881	1.641031	H	-2.096422	2.063704	1.659871
H	-3.791414	1.375545	1.223622	H	-3.740567	1.374338	1.279984	H	-3.721066	1.375199	1.387343
H	-3.107112	1.186126	2.853773	H	-3.044645	1.175224	2.893132	H	-2.929934	1.185140	2.971977
Co	0.000000	1.179772	-0.227050	Co	0.000000	1.175377	-0.237457	Co	0.000000	1.174266	-0.247178
Co	0.000000	-1.179772	-0.227050	Co	0.000000	-1.175377	-0.237457	Co	0.000000	-1.174266	-0.247178
C	-0.712185	3.136047	-0.304081	C	-0.708395	3.123032	-0.336752	C	-0.711544	3.138446	-0.377875
C	-1.154090	2.421088	-1.463456	C	-1.148046	2.399985	-1.481225	C	-1.154396	2.384369	-1.510105
H	-2.184046	2.225637	-1.737764	H	-2.173026	2.210311	-1.758166	H	-2.183595	2.183490	-1.780628
C	0.000000	1.986240	-2.175023	C	0.000000	1.957700	-2.182397	C	0.000000	1.928915	-2.208141
H	0.000000	1.387411	-3.078072	H	0.000000	1.356470	-3.077644	H	0.000000	1.303714	-3.092243
C	0.712185	3.136047	-0.304081	C	0.708395	3.123032	-0.336752	C	0.711544	3.138446	-0.377875
H	1.345471	3.628694	0.424671	H	1.338372	3.626170	0.379419	H	1.344632	3.652933	0.334647
C	1.154090	2.421088	-1.463456	C	1.148046	2.399985	-1.481225	C	1.154396	2.384369	-1.510105

H	2.184046	2.225637	-1.737764	H	2.173026	2.210311	-1.758166	H	2.183595	2.183490	-1.780628
C	-0.712185	-3.136047	-0.304081	C	-0.708395	-3.123032	-0.336752	C	-0.711544	-3.138446	-0.377875
C	-1.154090	-2.421088	-1.463456	C	-1.148046	-2.399985	-1.481225	C	-1.154396	-2.384369	-1.510105
H	-2.184046	-2.225637	-1.737764	H	-2.173026	-2.210311	-1.758166	H	-2.183595	-2.183490	-1.780628
C	0.000000	-1.986240	-2.175023	C	0.000000	-1.957700	-2.182397	C	0.000000	-1.928915	-2.208141
H	0.000000	-1.387411	-3.078072	H	0.000000	-1.356470	-3.077644	H	0.000000	-1.303714	-3.092243
C	0.712185	-3.136047	-0.304081	C	0.708395	-3.123032	-0.336752	C	0.711544	-3.138446	-0.377875
H	1.345471	-3.628694	0.424671	H	1.338372	-3.626170	0.379419	H	1.344632	-3.652933	0.334647
C	1.154090	-2.421088	-1.463456	C	1.148046	-2.399985	-1.481225	C	1.154396	-2.384369	-1.510105
H	2.184046	-2.225637	-1.737764	H	2.173026	-2.210311	-1.758166	H	2.183595	-2.183490	-1.780628
H	-1.345471	3.628694	0.424671	H	-1.338372	3.626170	0.379419	H	-1.344632	3.652933	0.334647
H	-1.345471	-3.628694	0.424671	H	-1.338372	-3.626170	0.379419	H	-1.344632	-3.652933	0.334647

Tables S38 : Optimized coordinates for the$Cp_2Co_2(MeC_2NMe_2)_2$structure **2N-Co-2T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.012968	0.947721	-0.696436	C	0.007292	0.936208	-0.702398	C	1.063845	-0.826976	-0.553247
C	-0.010423	0.936222	0.709166	C	-0.008895	0.935656	0.703104	C	0.330624	-0.916018	0.618538
N	0.108612	1.949551	-1.646207	N	0.143404	1.931164	-1.658723	N	1.702035	-1.689895	-1.352397
C	0.087644	1.499465	-3.026668	C	0.152901	1.467109	-3.034593	C	2.428523	-1.214152	-2.512886
C	1.154224	2.925618	-1.372865	C	1.183830	2.909427	-1.374169	C	1.412446	-3.114007	-1.309129
H	2.162435	2.509837	-1.553014	H	2.195417	2.491464	-1.529514	H	0.823907	-3.415984	-2.187486
H	1.021953	3.803141	-2.015042	H	1.065516	3.780365	-2.027920	H	2.342220	-3.697484	-1.300555
H	1.019903	0.979066	-3.310290	H	1.092500	0.946866	-3.293688	H	1.886079	-1.444763	-3.441597
H	-0.046971	2.356489	-3.695352	H	0.029646	2.316817	-3.714702	H	3.419475	-1.683063	-2.565966
H	-0.746424	0.806581	-3.164208	H	-0.675775	0.770044	-3.182926	H	2.546024	-0.132338	-2.428189
H	1.103745	3.237937	-0.325407	H	1.112814	3.232682	-0.331206	H	0.837822	-3.339409	-0.407527
N	-2.529487	-1.331719	-1.428779	N	-2.558560	-1.275422	-1.432991	N	1.664125	2.499817	-0.958982
C	-3.187338	-0.414273	-0.557531	C	-3.197449	-0.381492	-0.524481	C	2.509956	2.096639	0.118531
H	-3.732890	0.471327	-0.862307	H	-3.741707	0.516202	-0.794472	H	3.532135	1.749050	0.031466
H	-2.990239	-0.857960	0.790526	H	-2.978679	-0.862691	0.806147	H	1.762573	2.206155	1.331105
H	-3.371149	-0.378572	1.684498	H	-3.342270	-0.407267	1.719545	H	2.118887	1.954606	2.322422
C	-1.906714	-2.330523	-0.624157	C	-1.927981	-2.299892	-0.668421	C	0.394825	2.853814	-0.413055
H	-1.298909	-3.153447	-0.981817	H	-1.329914	-3.114442	-1.059903	H	-0.469450	3.185233	-0.975033
H	-2.198268	-2.039921	0.741641	H	-2.192152	-2.046097	0.709313	H	0.456320	2.674429	1.004690
H	-1.833667	-2.596705	1.597093	H	-1.814601	-2.628337	1.541889	H	-0.355522	2.838959	1.702044
Co	1.960087	-2.286323	0.658420	Co	1.931255	-2.297272	0.667984	Co	-3.066513	1.177691	-0.142864
Co	2.594852	-1.256747	1.412667	Co	2.561495	-1.272367	1.432224	Co	-3.334002	0.082587	0.720853
C	2.582965	-1.155581	2.491264	C	2.536288	-1.173077	2.510730	C	-3.523420	0.145147	1.786199
C	3.219417	-0.362637	0.494376	C	3.199346	-0.378054	0.523424	C	-3.275079	-1.111470	-0.048769
H	3.764861	0.536806	0.755956	H	3.743169	0.519974	0.793182	H	-3.425541	-2.117411	0.325598
C	2.205795	-2.034745	-0.723065	C	2.194446	-2.043245	-0.709862	C	-2.848461	0.664997	-1.456110
H	1.822600	-2.622147	-1.549416	H	1.816904	-2.625777	-1.542236	H	-2.635841	1.250509	-2.342633

C	2.986135	-0.847752	-0.832498	C	2.980137	-0.859278	-0.807098	C	-2.981732	-0.754537	-1.398677
H	3.338227	-0.394388	-1.751460	H	3.343057	-0.403667	-1.720669	H	-2.892088	-1.438137	-2.234597
C	1.370050	-3.102112	1.059528	C	1.333915	-3.112209	1.059770	C	-3.024416	2.220913	0.148253
H	-2.485168	-1.263379	-2.509152	H	-2.532854	-1.176108	-2.511485	H	1.930662	2.518724	-2.008691
C	1.159035	-0.391694	0.106071	C	1.151296	-0.404421	0.114929	C	-1.261346	-0.144748	-0.191725
C	-1.144301	-0.418872	-0.113712	C	-1.149939	-0.406779	-0.115235	C	0.827560	0.871535	0.038434
H	-0.153056	1.920271	1.674363	H	-0.147182	1.929651	1.660109	H	0.465602	-1.817098	1.693798
C	-0.157837	1.444379	3.046304	C	-0.157191	1.464478	3.035595	C	-0.315513	-1.431847	2.859077
H	-0.034983	2.288538	3.733404	H	-0.035420	2.313778	3.716483	H	-0.257263	-2.218004	3.620475
C	-1.095620	0.919796	3.302917	C	-1.096393	0.942961	3.293572	C	0.037291	-0.481623	3.299269
H	0.672804	0.747910	3.186158	H	0.672162	0.768234	3.183994	H	-1.362207	-1.305070	2.568047
C	-1.196199	2.898332	1.399484	C	-1.188697	2.906722	1.375485	C	1.854937	-2.084799	2.045317
H	-2.206347	2.476068	1.551591	H	-2.199838	2.487250	1.529680	H	2.365407	-1.176463	2.414204
H	-1.079505	3.763408	2.061234	H	-1.072101	3.777298	2.030024	H	1.896602	-2.854349	2.823877
H	-1.126701	3.231135	0.359530	H	-1.117296	3.230886	0.332832	H	2.406765	-2.447286	1.173106

Tables S39 : Optimized coordinates for the $Cp_2Co_2(MeC_2NMe_2)_2$structure **2N-Co-3S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.252065	1.014934	-0.643139	C	-0.250612	1.011420	-0.639622	C	-0.379987	1.040592	-0.581390
C	0.252060	1.014932	0.643139	C	0.250652	1.011414	0.639621	C	0.379974	1.040597	0.581389
N	-0.319560	1.992109	-1.608617	N	-0.327225	1.971750	-1.608230	N	-0.629830	2.037247	-1.496826
C	-0.768765	1.579239	-2.924060	C	-0.817381	1.572487	-2.907831	C	-1.343947	1.630999	-2.693825
C	0.761161	2.964944	-1.629136	C	0.719445	2.973884	-1.643980	C	0.460562	2.969509	-1.746752
H	1.673539	2.554312	-2.096357	H	1.625785	2.600972	-2.140161	H	1.252347	2.510695	-2.363361
H	0.456665	3.853787	-2.192966	H	0.376379	3.856153	-2.185769	H	0.080642	3.855478	-2.267919
H	0.022957	1.054448	-3.487322	H	-0.048771	1.056549	-3.499651	H	-0.707722	1.036815	-3.371977
H	-1.082961	2.452905	-3.505920	H	-1.145679	2.448161	-3.468712	H	-1.700631	2.516176	-3.232974
H	-1.617838	0.900467	-2.812802	H	-1.660432	0.898193	-2.781317	H	-2.204507	1.022486	-2.406989
H	1.012145	3.259024	-0.605961	H	0.989208	3.265044	-0.630880	H	0.908647	3.280551	-0.799071
N	-2.625509	-1.335520	-1.019545	C	-2.616021	-1.346840	-0.991563	N	-2.638286	-1.434682	-0.791982
C	-3.189635	-0.436989	-0.064741	C	-3.177963	-0.447372	-0.048953	C	-3.190523	-0.518967	0.151304
H	-3.791921	0.436366	-0.283173	H	-3.792721	0.410222	-0.271319	H	-3.839571	0.318731	-0.071203
H	-2.736141	-0.845715	1.224020	C	-2.722122	-0.840440	1.234829	H	-2.667990	-0.859660	1.432427
H	-2.937879	-0.335856	2.159407	H	-2.929888	-0.330652	2.162959	H	-2.854321	-0.325735	2.356411
C	-1.870638	-2.336495	-0.310147	C	-1.856906	-2.330965	-0.279622	C	-1.816581	-2.373963	-0.082468
H	-1.320033	-3.155052	-0.759088	H	-1.310688	-3.149910	-0.720633	H	-1.254657	-3.185247	-0.527635
H	-1.947775	-2.036143	1.074915	C	-1.931665	-2.021035	1.094765	H	-1.837074	-2.018931	1.290539
H	-1.449758	-2.569696	1.875388	H	-1.438054	-2.547503	1.896009	H	-1.284071	-2.502269	2.086035
Co	1.870637	-2.336500	0.310106	C	1.856832	-2.331019	0.279624	Co	1.816620	-2.373933	0.082492
Co	2.625491	-1.335543	1.019546	C	2.615967	-1.346913	0.991569	Co	2.638320	-1.434627	0.791980
C	2.747444	-1.281316	2.095537	H	2.745738	-1.307275	2.062010	C	2.802398	-1.424335	1.862834
C	3.189635	-0.436985	0.064778	C	3.177941	-0.447464	0.048962	C	3.190532	-0.518920	-0.151329

H	3.791916	0.436364	0.283246	H	3.792726	0.410113	0.271328	H	3.839571	0.318791	0.071156
C	1.947800	-2.036108	-1.074946	C	1.931612	-2.021095	-1.094763	C	1.837092	-2.018925	-1.290522
H	1.449798	-2.569638	-1.875443	H	1.437996	-2.547555	-1.896010	H	1.284088	-2.502286	-2.086003
C	2.736168	-0.845675	-1.224003	C	2.722105	-0.840524	-1.234824	C	2.667990	-0.859644	-1.432440
H	2.937923	-0.335789	-2.159371	H	2.929895	-0.330747	-2.162953	H	2.854301	-0.325732	-2.356435
C	1.320024	-3.155071	0.759013	H	1.310584	-3.149944	0.720635	C	1.254713	-3.185216	0.527680
H	-2.747484	-1.281266	-2.095532	H	-2.745810	-1.307205	-2.062002	H	-2.802351	-1.424410	-1.862838
C	1.117795	-0.463841	-0.021761	Co	1.115774	-0.460306	-0.032415	C	1.108754	-0.443473	-0.142849
C	-1.117793	-0.463844	0.021759	Co	-1.115798	-0.460273	0.032408	C	-1.108746	-0.443488	0.142847
H	0.319553	1.992104	1.608622	N	0.327285	1.971730	1.608236	H	0.629800	2.037254	1.496827
C	0.768762	1.579227	2.924061	C	0.817424	1.572454	2.907838	C	1.343923	1.631016	2.693825
H	1.082948	2.452893	3.505930	H	1.145763	2.448116	3.468713	H	1.700588	2.516198	3.232979
C	-0.022953	1.054421	3.487318	H	0.048790	1.056556	3.499662	C	0.707710	1.036815	3.371974
H	1.617845	0.900467	2.812799	H	1.660444	0.898120	2.781329	H	2.204497	1.022522	2.406988
C	-0.761178	2.964927	1.629151	C	-0.719323	2.973928	1.643972	C	-0.460609	2.969495	1.746756
H	-1.673550	2.554283	2.096374	H	-1.625674	2.601087	2.140186	H	-1.252387	2.510663	2.363362
H	-0.456690	3.853771	2.192984	H	-0.376194	3.856195	2.185724	H	-0.080707	3.855469	2.267927
H	-1.012170	3.259010	0.605979	H	-0.989090	3.265067	0.630867	H	-0.908700	3.280534	0.799076

Tables S40 : Optimized coordinates for the $Cp_2Co_2(MeC_2NMe_2)_2$structure **2N-Co-4S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	1.433421	0.872098	-0.454602	C	1.420477	0.895748	-0.429036	C	1.359657	0.945858	-0.414304
C	0.163352	0.920310	0.089414	C	0.154075	0.911382	0.104845	C	0.126142	0.878834	0.214990
N	2.369076	1.759673	-0.823379	N	2.338596	1.787559	-0.800762	N	2.217007	1.887506	-0.817677
C	3.697927	1.303573	-1.174824	C	3.668262	1.352382	-1.161838	C	3.547319	1.508196	-1.254188
C	2.196986	3.185101	-0.630527	C	2.144812	3.211590	-0.640808	C	1.962119	3.306771	-0.662694
H	2.605477	3.526168	0.333912	H	2.553502	3.580909	0.307020	H	2.420389	3.706855	0.254006
H	2.706847	3.738346	-1.427427	H	2.639506	3.751031	-1.449791	H	2.372612	3.855736	-1.518542
H	4.409248	1.439133	-0.346459	H	4.383819	1.513312	-0.348577	H	4.304791	1.768274	-0.500637
H	4.075569	1.857387	-2.042911	H	4.023951	1.900582	-2.036338	H	3.802669	2.016189	-2.193008
H	3.644779	0.240462	-1.418524	H	3.637356	0.290875	-1.391748	H	3.561800	0.428228	-1.411734
H	1.131643	3.425758	-0.662163	H	1.082056	3.436960	-0.671213	H	0.885026	3.479181	-0.624222
N	-0.625657	1.486846	1.164533	N	-0.653169	1.467309	1.165876	N	-0.717125	1.424198	1.240057
C	-1.030872	2.887412	1.039868	C	-1.079175	2.857823	1.045563	C	-1.140073	2.817925	1.103905
H	-1.939265	3.067010	1.625799	H	-1.996000	3.015844	1.614912	H	-2.060352	2.976960	1.676293
H	-0.243789	3.566053	1.405428	H	-0.315724	3.544078	1.429232	H	-0.369208	3.508832	1.477376
H	-1.244323	3.103163	-0.010586	H	-1.278279	3.081518	0.000010	H	-1.346932	3.027077	0.051528
C	-0.271852	1.133071	2.542499	C	-0.336139	1.104976	2.546237	C	-0.418760	1.066672	2.629928
H	0.541527	1.774064	2.918497	H	0.457475	1.743989	2.950720	H	0.370593	1.712702	3.043086
H	-1.146626	1.255549	3.190603	H	-1.224786	1.218075	3.168084	H	-1.325724	1.175943	3.234682
H	0.056075	0.090811	2.555904	H	-0.005433	0.070059	2.567190	H	-0.084701	0.028787	2.656738
Co	1.918673	-2.484292	-0.688142	C	1.963842	-2.433666	-0.695040	Co	2.108257	-2.342414	-0.705506

Co	0.566469	-2.790848	-0.370600	C	0.622680	-2.765884	-0.391292	Co	0.770538	-2.749106	-0.448040
C	-0.184122	-3.153978	-1.063370	H	-0.112968	-3.133387	-1.089003	C	0.063577	-3.118068	-1.180706
C	0.363055	-2.508703	1.023752	C	0.409345	-2.513602	0.998850	C	0.511993	-2.562151	0.950164
H	-0.570131	-2.619994	1.564194	H	-0.516945	-2.656788	1.532409	H	-0.426571	-2.760359	1.452140
C	2.551624	-2.001069	0.503623	C	2.579053	-1.962411	0.500755	C	2.673769	-1.885682	0.527201
H	3.581637	-1.673400	0.588261	H	3.600112	-1.627524	0.597767	H	3.676280	-1.497905	0.662430
C	1.594693	-2.044927	1.566659	C	1.622653	-2.038942	1.551712	C	1.692543	-2.051019	1.554168
H	1.769222	-1.746023	2.594023	H	1.788068	-1.762308	2.581354	H	1.816734	-1.793477	2.599204
C	-2.114327	-0.856969	-1.688658	C	-2.103135	-0.868148	-1.694172	C	-2.040983	-0.886597	-1.755983
H	-2.647159	0.464952	-1.749948	C	-2.645481	0.441055	-1.745173	H	-2.604074	0.417824	-1.785801
C	-2.466319	1.193595	-2.530844	H	-2.483643	1.170405	-2.522868	C	-2.413861	1.182253	-2.529016
C	-3.397422	0.675595	-0.554852	C	-3.391627	0.634367	-0.553982	C	-3.390984	0.561979	-0.605324
H	-3.892421	1.598493	-0.269787	H	-3.897530	1.544335	-0.266129	H	-3.923573	1.457052	-0.302776
C	-2.608030	-1.486566	-0.486164	C	-2.584454	-1.506691	-0.500932	C	-2.560903	-1.580997	-0.604117
H	-2.381544	-2.496281	-0.161651	H	-2.354033	-2.513603	-0.189192	H	-2.326160	-2.600548	-0.322452
C	-3.405074	-0.546338	0.209306	C	-3.386853	-0.585943	0.197447	C	-3.406212	-0.693135	0.099475
H	-3.902522	-0.702184	1.158874	H	-3.887325	-0.755959	1.137403	H	-3.942068	-0.903058	1.017067
C	-1.456321	-1.314254	-2.418431	H	-1.450897	-1.315011	-2.427585	C	-1.343711	-1.294722	-2.477255
H	2.378889	-2.570179	-1.665269	H	2.430219	-2.502709	-1.665036	H	2.598982	-2.344897	-1.671105
H	-1.471514	0.178978	-0.071685	Co	-1.472118	0.160284	-0.075292	H	-1.458887	0.091752	-0.031285
H	0.962393	-0.796006	0.021056	Co	0.982470	-0.781876	0.031469	H	1.016225	-0.747704	0.053026

Tables S41 : Optimized coordinates for the$Cp_2Co_2(MeC_2NMe_2)_2$structure **2N-Co-5T**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	-1.259078	0.000000	-0.473384	C	-1.260811	0.000000	-0.475714	C	0.584568	-0.026591	1.115555
C	1.259078	0.000000	-0.473384	C	1.260811	0.000000	-0.475714	C	0.584568	-0.026591	-1.115555
N	-2.546403	0.000000	-0.826229	N	-2.538745	0.000000	-0.826864	N	1.364935	-0.021954	2.176624
C	-3.315523	1.218346	-1.034872	C	-3.312234	1.215413	-1.023287	C	1.857390	-1.250373	2.792549
C	-3.315523	-1.218346	-1.034872	C	-3.312234	-1.215413	-1.023287	C	1.810471	1.196432	2.846339
H	-4.027603	-1.388970	-0.214892	H	-3.993246	-1.395944	-0.186235	H	1.532535	1.169511	3.907779
H	-3.887700	-1.143654	-1.968114	H	-3.913429	-1.130195	-1.930471	H	2.901697	1.293664	2.776550
H	-4.027603	1.388970	-0.214892	H	-3.993246	1.395944	-0.186235	H	1.399173	-1.397295	3.779324
H	-3.887700	1.143654	-1.968114	H	-3.913429	1.130195	-1.930471	H	2.946069	-1.197100	2.919084
H	-2.629711	2.062816	-1.098070	H	-2.635756	2.056483	-1.120382	H	1.602577	-2.085221	2.140569
H	-2.629711	-2.062816	-1.098070	H	-2.635756	-2.056483	-1.120382	H	1.337550	2.053839	2.366330
N	2.546403	0.000000	-0.826229	N	2.538745	0.000000	-0.826864	N	1.364935	-0.021954	-2.176624
C	3.315523	-1.218346	-1.034872	C	3.312234	-1.215413	-1.023287	C	1.810471	1.196432	-2.846339
H	4.027603	-1.388970	-0.214892	H	3.993246	-1.395944	-0.186235	H	1.532535	1.169511	-3.907779
H	2.629711	-2.062816	-1.098070	H	2.635756	-2.056483	-1.120382	H	1.337550	2.053839	-2.366330
H	3.887700	-1.143654	-1.968114	H	3.913429	-1.130195	-1.930471	H	2.901697	1.293664	-2.776550
C	3.315523	1.218346	-1.034872	C	3.312234	1.215413	-1.023287	C	1.857390	-1.250373	-2.792549
H	2.629711	2.062816	-1.098070	H	2.635756	2.056483	-1.120382	H	1.602577	-2.085221	-2.140569
H	4.027603	1.388970	-0.214892	H	3.993246	1.395944	-0.186235	H	1.399173	-1.397295	-3.779324

H	3.887700	1.143654	-1.968114	H	3.913429	1.130195	-1.930471	H	2.946069	-1.197100	-2.919084
Co	0.000000	1.278772	-0.028475	Co	0.000000	1.271108	-0.031538	Co	-0.234883	-1.234591	0.000000
Co	0.000000	-1.278772	-0.028475	Co	0.000000	-1.271108	-0.031538	Co	-0.033428	1.381864	0.000000
C	0.707854	3.315057	-0.043740	C	0.703511	3.300788	-0.042360	C	-0.388485	-3.298721	-0.705365
C	1.145078	2.625823	1.132848	C	1.138714	2.614073	1.126759	C	-1.498370	-2.503887	-1.149963
H	2.175657	2.436928	1.411788	H	2.164323	2.432097	1.407624	H	-1.769549	-2.312594	-2.181277
C	0.000000	2.229249	1.877418	C	0.000000	2.217264	1.865997	C	-2.205579	-2.056672	0.000000
H	0.000000	1.673181	2.806543	H	0.000000	1.670751	2.794946	H	-3.091497	-1.433253	0.000000
C	-0.707854	3.315057	-0.043740	C	-0.703511	3.300788	-0.042360	C	-0.388485	-3.298721	0.705365
H	-1.343227	3.769207	-0.795288	H	-1.335555	3.759937	-0.785752	H	0.322331	-3.812676	1.341669
C	-1.145078	2.625823	1.132848	C	-1.138714	2.614073	1.126759	C	-1.498370	-2.503887	1.149963
H	-2.175657	2.436928	1.411788	H	-2.164323	2.432097	1.407624	H	-1.769549	-2.312594	2.181277
C	0.707854	-3.315057	-0.043740	C	0.703511	-3.300788	-0.042360	C	-0.559293	3.346507	-0.712084
C	1.145078	-2.625823	1.132848	C	1.138714	-2.614073	1.126759	C	-1.534566	2.397289	-1.146957
H	2.175657	-2.436928	1.411788	H	2.164323	-2.432097	1.407624	H	-1.761326	2.152560	-2.178189
C	0.000000	-2.229249	1.877418	C	0.000000	-2.217264	1.865997	C	-2.166320	1.838781	0.000000
H	0.000000	-1.673181	2.806543	H	0.000000	-1.670751	2.794946	H	-2.942504	1.084914	0.000000
C	-0.707854	-3.315057	-0.043740	C	-0.703511	-3.300788	-0.042360	C	-0.559293	3.346507	0.712084
H	-1.343227	-3.769207	-0.795288	H	-1.335555	-3.759937	-0.785752	H	0.058996	3.964707	1.352679
C	-1.145078	-2.625823	1.132848	C	-1.138714	-2.614073	1.126759	C	-1.534566	2.397289	1.146957
H	-2.175657	-2.436928	1.411788	H	-2.164323	-2.432097	1.407624	H	-1.761326	2.152560	2.178189
H	1.343227	3.769207	-0.795288	H	1.335555	3.759937	-0.785752	H	0.322331	-3.812676	-1.341669
H	1.343227	-3.769207	-0.795288	H	1.335555	-3.759937	-0.785752	H	0.058996	3.964707	-1.352679

Table S42. Optimized coordinates for the **$Cp_2Fe_2(MeC_2NMe_2)_2$**structure **2N-Fe -1S**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	-0.000036	-1.383009	-0.246615	C	-0.000039	-1.382199	-0.256630	C	-0.000058	-1.360909	-0.283998
C	0.000036	1.383010	-0.246611	C	0.000040	1.382200	-0.256625	C	0.000059	1.360910	-0.283992
N	-0.000080	-2.713759	-0.485177	N	-0.000081	-2.703624	-0.496986	N	-0.000123	-2.691549	-0.520947
C	-1.214757	-3.495402	-0.638337	C	-1.211173	-3.488138	-0.643930	C	-1.213424	-3.474305	-0.688725
C	1.214541	-3.495501	-0.638286	C	1.210961	-3.488233	-0.643832	C	1.213104	-3.474458	-0.688550
H	1.498993	-4.013880	0.289887	H	1.492581	-3.997497	0.283706	H	1.469714	-4.035458	0.221991
H	1.059683	-4.259040	-1.409608	H	1.055080	-4.254473	-1.404250	H	1.071641	-4.197828	-1.500380
H	-1.499311	-4.013734	0.289831	H	-1.492879	-3.997423	0.283571	H	-1.470150	-4.035394	0.221730
H	-1.059916	-4.258974	-1.409630	H	-1.055309	-4.254355	-1.404374	H	-1.071994	-4.197586	-1.500641
H	-2.033360	-2.849662	-0.949973	H	-2.029267	-2.854325	-0.960500	H	-2.041426	-2.823015	-0.954424
H	2.033217	-2.849824	-0.949856	H	2.029119	-2.854496	-0.960389	H	2.041196	-2.823296	-0.954288
N	0.000078	2.713760	-0.485168	N	0.000081	2.703625	-0.496977	N	0.000123	2.691551	-0.520939
C	1.214755	3.495406	-0.638320	C	1.211173	3.488139	-0.643917	C	1.213425	3.474310	-0.688702
H	1.499306	4.013731	0.289853	H	1.492879	3.997421	0.283585	H	1.470150	4.035383	0.221762
H	2.033360	2.849671	-0.949960	H	2.029267	2.854328	-0.960489	H	2.041427	2.823024	-0.954412
H	1.059913	4.258985	-1.409607	H	1.055310	4.254360	-1.404358	H	1.071996	4.197604	-1.500606
C	-1.214543	3.495500	-0.638279	C	-1.210962	3.488234	-0.643820	C	-1.213104	3.474457	-0.688550

H	-2.033221	2.849821	-0.949839	H	-2.029120	2.854497	-0.960378	H	-2.041192	2.823293	-0.954296
H	-1.498991	4.013888	0.289890	H	-1.492582	3.997494	0.283720	H	-1.469724	4.035454	0.221991
H	-1.059688	4.259033	-1.409609	H	-1.055082	4.254476	-1.404235	H	-1.071637	4.197830	-1.500376
Fe	-1.172066	0.000032	-0.015684	Fe	-1.167325	0.000035	-0.018107	Fe	-1.167612	0.000053	-0.032786
Fe	1.172067	-0.000032	-0.015684	Fe	1.167325	-0.000035	-0.018107	Fe	1.167612	-0.000052	-0.032780
C	-3.093351	0.711912	-0.451813	C	-3.084791	0.707850	-0.435827	C	-3.127748	0.710201	-0.384601
C	-2.689124	1.147380	0.848860	C	-2.672544	1.141400	0.853857	C	-2.666030	1.147589	0.895668
H	-2.561260	2.172101	1.173199	H	-2.552136	2.160737	1.179375	H	-2.538780	2.171059	1.220808
C	-2.419611	0.000041	1.646213	C	-2.397276	0.000042	1.644164	C	-2.375704	0.000063	1.681684
H	-2.063754	0.000007	2.668534	H	-2.042391	0.000013	2.661813	H	-1.971578	0.000020	2.685701
C	-3.093403	-0.711698	-0.451841	C	-3.084834	-0.707649	-0.435852	C	-3.127815	-0.709902	-0.384635
H	-3.384808	-1.338200	-1.286830	H	-3.389838	-1.330161	-1.261708	H	-3.453660	-1.332407	-1.208621
C	-2.689209	-1.147246	0.848814	C	-2.672614	-1.141270	0.853817	C	-2.666137	-1.147397	0.895611
H	-2.561427	-2.171990	1.173114	H	-2.552268	-2.160627	1.179298	H	-2.538978	-2.170895	1.220698
C	3.093404	0.711701	-0.451838	C	3.084834	0.707650	-0.435848	C	3.127815	0.709902	-0.384628
C	2.689209	1.147243	0.848819	C	2.672614	1.141268	0.853822	C	2.666138	1.147393	0.895620
H	2.561426	2.171986	1.173124	H	2.552268	2.160623	1.179307	H	2.538982	2.170891	1.220710
C	2.419612	-0.000047	1.646213	C	2.397275	-0.000047	1.644166	C	2.375705	-0.000068	1.681690
H	2.063755	-0.000018	2.668535	H	2.042390	-0.000022	2.661815	H	1.971580	-0.000026	2.685707
C	3.093353	-0.711909	-0.451816	C	3.084791	-0.707848	-0.435827	C	3.127747	-0.710201	-0.384597
H	3.384711	-1.338460	-1.286784	H	3.389759	-1.330406	-1.261663	H	3.453536	-1.332775	-1.208553
C	2.689126	-1.147383	0.848856	C	2.672543	-1.141402	0.853855	C	2.666029	-1.147592	0.895670
H	2.561264	-2.172106	1.173191	H	2.552135	-2.160740	1.179370	H	2.538778	-2.171063	1.220808
H	-3.384708	1.338466	-1.286779	H	-3.389758	1.330410	-1.261661	H	-3.453539	1.332777	-1.208554
H	3.384807	1.338207	-1.286824	H	3.389840	1.330166	-1.261702	H	3.453660	1.332409	-1.208612

Table S43. Optimized coordinates for the **$Cp_2Fe_2(MeC_2NMe_2)_2$**structure **2N-Fe -2T**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	0.053601	-1.360433	-0.428536	C	-0.056123	1.35577	-0.445883	C	0.074398	-1.358451	-0.098473
C	0.053544	1.360440	-0.428527	C	-0.056117	-1.355771	-0.445881	C	0.074347	1.358457	-0.098464
N	0.031128	-2.671674	-0.719798	N	-0.033849	2.655502	-0.74445	N	0.033544	-2.693648	-0.203486
C	-1.192494	-3.439673	-0.864442	C	1.185893	3.427025	-0.881538	C	-0.885618	-3.523718	0.555785
C	1.239826	-3.465137	-0.858673	C	-1.239822	3.448659	-0.886985	C	1.015750	-3.428461	-0.982157
H	1.420806	-4.089335	0.028857	H	-1.426213	4.064162	-0.001145	H	1.776164	-3.899442	-0.341796
H	1.147701	-4.132052	-1.725049	H	-1.141244	4.119227	-1.742888	H	0.515632	-4.218678	-1.556821
H	-1.381523	-4.074288	0.014405	H	1.370513	4.05299	-0.002222	H	-1.511148	-2.887013	1.180841
H	-1.117651	-4.096053	-1.740727	H	1.110134	4.087502	-1.74779	H	-0.325961	-4.213647	1.202848
H	-2.032347	-2.759666	-0.999505	H	2.025821	2.757606	-1.021001	H	-1.523844	-4.122249	-0.109773
H	2.089847	-2.801933	-1.008101	H	-2.086463	2.793317	-1.047548	H	1.504131	-2.741372	-1.673219
N	0.031014	2.671678	-0.719797	N	-0.033838	-2.655502	-0.74445	N	0.033436	2.693653	-0.203471
C	1.239678	3.465200	-0.858639	C	-1.239808	-3.448663	-0.886984	C	1.015600	3.428514	-0.982149
H	1.420601	4.089406	0.028896	H	-1.426197	-4.064166	-0.001144	H	1.775940	3.899612	-0.341786
H	2.089734	2.802037	-1.008042	H	-2.086451	-2.793325	-1.047548	H	1.504076	2.741432	-1.673149

H	1.147544	4.132110	-1.725017	H	-1.141227	-4.119233	-1.742886	H	0.515428	4.218648	-1.556882
C	-1.192642	3.439617	-0.864476	C	1.185908	-3.42702	-0.88154	C	-0.885783	3.523681	0.555774
H	-2.032461	2.759568	-0.999538	H	2.025833	-2.757597	-1.021003	H	-1.524036	4.122164	-0.109802
H	-1.381714	4.074242	0.014355	H	1.370531	-4.052984	-0.002224	H	-1.511285	2.886951	1.180833
H	-1.117816	4.095983	-1.740773	H	1.11015	-4.087498	-1.747791	H	-0.326174	4.213655	1.202832
Fe	-1.189201	-0.000024	-0.127131	Fe	1.183398	0.000003	-0.128194	Fe	-1.201528	-0.000022	0.152150
Fe	1.166456	0.000026	0.011465	Fe	-1.162956	-0.000003	0.008698	Fe	1.214584	0.000025	-0.012437
C	-3.198000	0.712883	-0.175291	C	3.189025	-0.708962	-0.149811	C	-2.927046	-0.000063	-1.315078
C	-2.625838	1.144373	1.065454	C	2.605586	-1.138266	1.077202	C	-2.976352	1.144181	-0.481068
H	-2.464272	2.173126	1.365574	H	2.447141	-2.162069	1.376233	H	-2.932080	2.172522	-0.817954
C	-2.317624	-0.000037	1.841017	C	2.288556	0.000004	1.843753	C	-3.137040	0.709764	0.874440
H	-1.820369	-0.000019	2.802913	H	1.789526	0.000002	2.799418	H	-3.252795	1.349794	1.741403
C	-3.197967	-0.713023	-0.175282	C	3.189022	0.708974	-0.149811	C	-2.976309	-1.144302	-0.481059
H	-3.605606	-1.350311	-0.951230	H	3.610163	1.343001	-0.913438	H	-2.931993	-2.172644	-0.817937
C	-2.625786	-1.144471	1.065469	C	2.605582	1.138275	1.077203	C	-3.137014	-0.709881	0.874445
H	-2.464175	-2.173213	1.365602	H	2.447132	2.162077	1.376236	H	-3.252740	-1.349910	1.741412
C	3.140295	0.709199	-0.212596	C	-3.132313	-0.705238	-0.173446	C	3.102930	0.709247	-0.629536
C	2.606424	1.146646	1.045183	C	-2.575821	-1.140939	1.065495	C	2.837493	1.148915	0.708529
H	2.449599	2.175343	1.348232	H	-2.42103	-2.164651	1.366961	H	2.758989	2.176801	1.039752
C	2.283983	0.000029	1.821519	C	-2.23689	-0.000004	1.829457	C	2.685539	0.000066	1.530772
H	1.842981	0.000011	2.810466	H	-1.784619	-0.000003	2.808021	H	2.446468	0.000080	2.587016
C	3.140322	-0.709067	-0.212609	C	-3.132315	0.705226	-0.173447	C	3.102949	-0.709167	-0.629515
H	3.519386	-1.336005	-1.011092	H	-3.533781	1.328422	-0.956121	H	3.287285	-1.340618	-1.489378
C	2.606467	-1.146559	1.045160	C	-2.575824	1.14093	1.065494	C	2.837525	-1.148803	0.708564
H	2.449681	-2.175268	1.348190	H	-2.421037	2.164642	1.36696	H	2.759047	-2.176681	1.039818
H	-3.605664	1.350144	-0.951249	H	3.610168	-1.342986	-0.91344	H	-2.774876	-0.000063	-2.387550
H	3.519337	1.336167	-1.011066	H	-3.533777	-1.328436	-0.956121	H	3.287245	1.340676	-1.489420

Table S44. Optimized coordinates for the **$Cp_2Fe_2(MeC_2NMe_2)_2$**structure **2N-Fe-3S**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	-0.000004	0.647402	-0.851299	C	-0.000004	0.656523	-0.845261	C	-0.000002	0.653937	-0.914083
C	0.000003	0.647364	0.851305	C	0.000004	0.656511	0.845255	C	0.000002	0.653927	0.914086
N	-0.000006	1.760497	-1.621403	N	-0.000006	1.755373	-1.621475	N	-0.000005	1.707913	-1.740434
C	1.233442	2.280683	-2.171069	C	1.230130	2.282836	-2.164503	C	1.233882	2.230266	-2.296451
C	-1.233461	2.280708	-2.171029	C	-1.230144	2.282828	-2.164508	C	-1.233894	2.230256	-2.296455
H	-1.205042	3.377637	-2.196302	H	-1.194524	3.374269	-2.189503	H	-1.216066	3.327960	-2.291146
H	-1.419251	1.921538	-3.195363	H	-1.419568	1.929404	-3.184595	H	-1.387040	1.891769	-3.331672
H	1.205040	3.377612	-2.196351	H	1.194500	3.374277	-2.189504	H	1.216042	3.327970	-2.291147
H	1.419196	1.921500	-3.195405	H	1.419564	1.929409	-3.184587	H	1.387038	1.891775	-3.331664
H	2.062934	1.954318	-1.536435	H	2.057956	1.965129	-1.533636	H	2.067019	1.879532	-1.684230
H	-2.062940	1.954352	-1.536373	H	-2.057971	1.965109	-1.533648	H	-2.067031	1.879510	-1.684242
C	-2.829165	-0.948307	-1.153123	C	-2.814748	-0.956917	-1.146757	C	-2.814350	-0.945212	-1.152554

C	-3.219704	-0.203887	-0.000008	C	-3.209239	-0.220461	0.000004	C	-3.218644	-0.210615	0.000007
H	-3.710479	0.764055	-0.000011	H	-3.713483	0.734339	0.000004	H	-3.727242	0.746748	0.000012
C	-2.829170	-0.948305	1.153107	C	-2.814739	-0.956912	1.146766	C	-2.814342	-0.945219	1.152561
H	-2.966053	-0.646344	2.185244	H	-2.960861	-0.660536	2.173715	H	-2.960313	-0.647825	2.183976
C	-2.241803	-2.176203	-0.707294	C	-2.218658	-2.172344	-0.703190	C	-2.193177	-2.155884	-0.708235
H	-1.819343	-2.946140	-1.341907	H	-1.799128	-2.939422	-1.335081	H	-1.756703	-2.916065	-1.344286
C	-2.241806	-2.176200	0.707286	C	-2.218653	-2.172340	0.703200	C	-2.193173	-2.155888	0.708231
H	-1.819353	-2.946136	1.341905	H	-1.799117	-2.939414	1.335093	H	-1.756694	-2.916072	1.344275
C	2.241774	-2.176221	0.707252	C	2.218634	-2.172368	0.703144	C	2.193155	-2.155919	0.708169
C	2.829120	-0.948337	1.153133	C	2.814710	-0.956956	1.146772	C	2.814315	-0.945269	1.152566
H	2.965958	-0.646401	2.185283	H	2.960804	-0.660619	2.173735	H	2.960260	-0.647919	2.183998
C	3.219704	-0.203886	0.000055	C	3.209239	-0.220460	0.000049	C	3.218644	-0.210615	0.000054
H	3.710484	0.764054	0.000101	H	3.713483	0.734339	0.000098	H	3.727242	0.746748	0.000111
C	2.241832	-2.176180	-0.707329	C	2.218677	-2.172316	-0.703246	C	2.193196	-2.155853	-0.708298
H	1.819400	-2.946098	-1.341984	H	1.799160	-2.939367	-1.335179	H	1.756734	-2.916003	-1.344393
C	2.829214	-0.948273	-1.153095	C	2.814777	-0.956872	-1.146751	C	2.814377	-0.945162	-1.152548
H	2.966144	-0.646285	-2.185218	H	2.960934	-0.660462	-2.173685	H	2.960380	-0.647718	-2.183945
H	1.819291	-2.946175	1.341830	H	1.799085	-2.939470	1.334995	H	1.756663	-2.916133	1.344168
H	-2.966046	-0.646342	-2.185259	H	-2.960877	-0.660546	-2.173706	H	-2.960328	-0.647812	-2.183966
Fe	1.139013	-0.497846	-0.000026	Fe	1.133841	-0.493016	-0.000015	Fe	1.115311	-0.460861	-0.000008
Fe	-1.139015	-0.497844	-0.000015	Fe	-1.133841	-0.493016	-0.000004	Fe	-1.115311	-0.460861	-0.000001
N	0.000009	1.760409	1.621475	N	0.000006	1.755347	1.621488	N	0.000005	1.707891	1.740452
C	1.233465	2.280641	2.171075	C	1.230144	2.282789	2.164536	C	1.233893	2.230229	2.296478
H	1.205036	3.377570	2.196330	H	1.194523	3.374230	2.189559	H	1.216069	3.327934	2.291170
H	1.419270	1.921491	3.195413	H	1.419568	1.929338	3.184613	H	1.387034	1.891740	3.331695
H	2.062938	1.954281	1.536415	H	2.057971	1.965088	1.533667	H	2.067032	1.879482	1.684268
C	-1.233440	2.280633	2.171100	C	-1.230130	2.282797	2.164530	C	-1.233881	2.230239	2.296473
H	-1.419215	1.921494	3.195447	H	-1.419564	1.929343	3.184605	H	-1.387033	1.891745	3.331687
H	-1.205024	3.377564	2.196340	H	-1.194500	3.374237	2.189559	H	-1.216045	3.327943	2.291172
H	-2.062926	1.954255	1.536465	H	-2.057956	1.965106	1.533655	H	-2.067020	1.879504	1.684256

Table S45. Optimized coordinates for the **$Cp_2Fe_2(MeC_2NMe_2)_2$**structure **2N-Fe-4T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	1.430160	0.902795	-0.335397	C	1.430212	0.912921	-0.318324	C	1.512807	0.911678	-0.270583
C	0.292523	0.911411	0.421527	C	0.289198	0.910038	0.417918	C	0.320212	0.920810	0.381188
N	2.347996	1.750203	-0.832892	N	2.349468	1.752009	-0.803277	N	2.467133	1.777849	-0.645155
C	3.553389	1.214068	-1.432447	C	3.544022	1.221752	-1.421424	C	3.639245	1.301395	-1.353771
C	2.382247	3.165154	-0.526916	C	2.375072	3.171308	-0.53242	C	2.340193	3.209381	-0.457422
H	1.396421	3.494229	-0.195548	H	1.411853	3.492197	-0.15084	H	1.702177	3.674918	-1.223207
H	3.111767	3.395705	0.265099	H	3.14345	3.428628	0.205418	H	1.915053	3.422375	0.529228
H	4.409142	1.263998	-0.741462	H	4.408987	1.287837	-0.752237	H	4.561340	1.538730	-0.804495
H	3.815789	1.776408	-2.337676	H	3.782754	1.776558	-2.331817	H	3.709866	1.749378	-2.355307
H	3.374543	0.168593	-1.691876	H	3.374899	0.177715	-1.66938	H	3.554311	0.218211	-1.457186

H	2.662212	3.743447	-1.416561	H	2.592666	3.733378	-1.443963	H	3.328630	3.678354	-0.506507
N	-0.712019	1.664004	1.110069	N	-0.716458	1.654022	1.104426	N	-0.708933	1.746625	0.950302
C	-0.988781	3.043705	0.714601	C	-1.014407	3.025751	0.710397	C	-0.957354	3.073410	0.382216
H	-2.011130	3.311664	1.003192	H	-2.040989	3.271658	0.984042	H	-1.988124	3.373552	0.599294
H	-0.295413	3.748354	1.199916	H	-0.347375	3.740175	1.205317	H	-0.273903	3.823330	0.804431
H	-0.898824	3.127772	-0.371637	H	-0.91163	3.118408	-0.368234	H	-0.820273	3.027434	-0.700180
C	-0.788940	1.456573	2.560465	C	-0.810154	1.442655	2.548938	C	-0.772663	1.740188	2.416632
H	-0.060611	2.089762	3.088219	H	-0.098333	2.078095	3.086011	H	-0.009194	2.409296	2.839036
H	-1.796591	1.696625	2.918250	H	-1.818739	1.675385	2.892805	H	-1.764566	2.069230	2.746690
H	-0.563840	0.407298	2.770401	H	-0.583271	0.400599	2.763671	H	-0.585597	0.724833	2.772663
C	1.953938	-2.414687	-0.664979	C	1.962464	-2.395239	-0.663974	C	2.013533	-2.453731	-0.706018
C	0.629079	-2.811739	-0.310529	C	0.644676	-2.794736	-0.317465	C	0.680120	-2.862838	-0.421950
H	-0.121386	-3.189366	-0.996946	H	-0.097022	-3.173639	-1.003883	H	-0.049800	-3.195484	-1.150674
C	0.450331	-2.612114	1.094318	C	0.462959	-2.605252	1.08001	C	0.458400	-2.725747	0.980925
H	-0.449803	-2.818112	1.661649	H	-0.429835	-2.825244	1.643401	H	-0.463540	-2.943071	1.506305
C	2.595763	-1.944384	0.523189	C	2.596824	-1.933644	0.521653	C	2.623224	-2.064350	0.530421
H	3.599374	-1.539909	0.591885	H	3.598088	-1.538574	0.596736	H	3.632200	-1.690643	0.656317
C	1.663257	-2.057889	1.605511	C	1.666846	-2.055037	1.594738	C	1.662007	-2.240033	1.568720
H	1.844185	-1.758418	2.631801	H	1.846523	-1.770765	2.62028	H	1.810298	-2.009406	2.616881
C	-1.927331	-1.010565	-1.643305	C	-1.933164	-1.002835	-1.648071	C	-2.109700	-0.996444	-1.626152
C	-2.475674	0.284481	-1.915889	C	-2.490733	0.284002	-1.898889	C	-2.723423	0.282511	-1.767294
H	-2.183347	0.948627	-2.720412	H	-2.221945	0.952325	-2.701634	H	-2.559725	0.990477	-2.570644
C	-3.408223	0.575648	-0.891999	C	-3.407182	0.556654	-0.866087	C	-3.543774	0.486763	-0.623796
H	-3.952761	1.507271	-0.776567	H	-3.959674	1.476103	-0.738943	H	-4.115273	1.382232	-0.405040
C	-2.592607	-1.542346	-0.478251	C	-2.57619	-1.547252	-0.485709	C	-2.618541	-1.604822	-0.426848
H	-2.444065	-2.529310	-0.054815	H	-2.418941	-2.533741	-0.078804	H	-2.357511	-2.588378	-0.056249
C	-3.509854	-0.554023	-0.026813	C	-3.490682	-0.576589	-0.017473	C	-3.512082	-0.692532	0.179766
H	-4.144647	-0.620623	0.849629	H	-4.114569	-0.657768	0.859593	H	-4.039773	-0.837387	1.115404
H	-1.194372	-1.531087	-2.248326	H	-1.212559	-1.512974	-2.266534	H	-1.414923	-1.451231	-2.321355
H	2.384961	-2.451294	-1.658723	H	2.396781	-2.43301	-1.650561	H	2.480815	-2.439347	-1.683279
Fe	-1.444565	0.129961	0.007464	Fe	-1.44326	0.127601	-0.001131	Fe	-1.468237	0.167043	0.016140
Fe	0.925753	-0.813716	0.151449	Fe	0.934385	-0.808084	0.153769	Fe	0.982348	-0.832910	0.145230

Table S46. Optimized coordinates for the **$Cp_2Fe_2(MeC_2NMe_2)_2$**structure **2N-Fe-5S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	1.572811	0.698834	-0.466059	C	1.558395	0.739093	-0.424893	C	1.524351	0.826101	-0.398657
C	0.328412	0.915937	0.061799	C	0.319923	0.914083	0.108271	C	0.303136	0.898189	0.205176
N	2.658904	1.428658	-0.769154	N	2.622309	1.476807	-0.746559	N	2.524515	1.645022	-0.754342
C	3.913807	0.764213	-1.054514	C	3.876289	0.833281	-1.066456	C	3.806399	1.074364	-1.124397
C	2.718608	2.855130	-0.524376	C	2.666888	2.905878	-0.529357	C	2.501292	3.068136	-0.476657
H	1.721415	3.284660	-0.649971	H	1.668632	3.321052	-0.64186	H	1.496381	3.460178	-0.649570
H	3.076064	3.091485	0.490865	H	3.040889	3.163867	0.468636	H	2.796435	3.293644	0.559925
H	4.578750	0.744263	-0.177437	H	4.565406	0.832415	-0.214823	H	4.534378	1.143896	-0.301932

H	4.441284	1.275001	-1.869430	H	4.367681	1.346509	-1.895334	H	4.221462	1.592337	-1.998687
H	3.698379	-0.264592	-1.351046	H	3.675671	-0.196488	-1.349746	H	3.651485	0.021392	-1.366952
H	3.397192	3.333224	-1.239806	H	3.322289	3.377146	-1.262862	H	3.191396	3.589528	-1.149366
N	-0.482261	1.726519	0.939347	N	-0.530902	1.719251	0.940479	N	-0.639408	1.706309	0.932452
C	-0.757361	3.104001	0.536457	C	-0.822851	3.084484	0.522302	C	-0.947218	3.046861	0.438005
H	-1.679358	3.454894	1.013404	H	-1.767934	3.410977	0.957556	H	-1.934818	3.352636	0.800462
H	0.061410	3.780673	0.828517	H	-0.039954	3.779866	0.844606	H	-0.204416	3.779953	0.784799
H	-0.887000	3.136765	-0.548689	H	-0.909076	3.115044	-0.561497	H	-0.962419	3.029141	-0.654227
C	-0.200504	1.603899	2.371930	C	-0.321888	1.606421	2.382462	C	-0.488894	1.667934	2.390512
H	0.684158	2.198425	2.653421	H	0.532604	2.213326	2.706135	H	0.339958	2.315503	2.714633
H	-1.063082	1.952219	2.950871	H	-1.213406	1.943923	2.912142	H	-1.417844	2.002910	2.865448
H	-0.011611	0.551335	2.598101	H	-0.130445	0.56486	2.628345	H	-0.274272	0.641143	2.694304
C	1.570476	-2.721450	-0.576498	C	1.643544	-2.656734	-0.588847	C	1.844173	-2.580719	-0.635534
C	0.188728	-2.872929	-0.249710	C	0.270421	-2.849862	-0.2804	C	0.476268	-2.860219	-0.343837
H	-0.584568	-3.204978	-0.934471	H	-0.483355	-3.185998	-0.976094	H	-0.259544	-3.205911	-1.060508
C	-0.018284	-2.470455	1.104294	C	0.045115	-2.497265	1.075893	C	0.231717	-2.582809	1.036731
H	-0.954173	-2.494560	1.650021	H	-0.886865	-2.56835	1.612967	H	-0.702246	-2.720724	1.567073
C	2.231664	-2.204098	0.578173	C	2.279133	-2.161527	0.579352	C	2.454486	-2.107503	0.565393
H	3.281629	-1.946290	0.657488	H	3.318525	-1.889592	0.677193	H	3.479925	-1.776987	0.676911
C	1.249785	-2.024076	1.608206	C	1.290886	-2.038703	1.600254	C	1.458914	-2.096124	1.591257
H	1.440373	-1.635755	2.603082	H	1.464213	-1.68135	2.604113	H	1.608025	-1.761872	2.611297
C	-2.150224	-0.793611	-1.614295	C	-2.114672	-0.816687	-1.625144	C	-2.105948	-0.862734	-1.658407
C	-2.421780	0.615789	-1.714254	C	-2.423644	0.578105	-1.713052	C	-2.500958	0.519436	-1.687046
H	-2.072148	1.281919	-2.495019	H	-2.099132	1.256629	-2.486996	H	-2.203870	1.252761	-2.426789
C	-3.228803	0.982638	-0.593400	C	-3.242099	0.908728	-0.599279	C	-3.356513	0.749000	-0.566383
H	-3.549017	1.993189	-0.358767	H	-3.597927	1.901018	-0.361832	H	-3.786899	1.704362	-0.287781
C	-2.768416	-1.264164	-0.418190	C	-2.721457	-1.313879	-0.444426	C	-2.695811	-1.455334	-0.512210
H	-2.703511	-2.277419	-0.034719	H	-2.639577	-2.32574	-0.076543	H	-2.545160	-2.475878	-0.181090
C	-3.444202	-0.169458	0.222592	C	-3.427079	-0.249605	0.199181	C	-3.472188	-0.460643	0.173211
H	-4.026583	-0.215190	1.134917	H	-4.013554	-0.321457	1.101408	H	-4.041935	-0.605471	1.082831
H	-1.560493	-1.383338	-2.306098	H	-1.514229	-1.381645	-2.319958	H	-1.439721	-1.348910	-2.359351
H	2.024658	-2.943492	-1.534583	H	2.109512	-2.844777	-1.542909	H	2.322138	-2.687005	-1.601523
Fe	-1.435152	0.207650	0.002349	Fe	-1.439686	0.183604	-0.004407	Fe	-1.476970	0.127141	0.035809
Fe	0.771361	-0.896876	0.001307	Fe	0.798484	-0.88047	0.029205	Fe	0.889916	-0.862508	0.058437

Tables S47 : Optimized coordinates for the **$Cp_2Ni_2(MeC_2NMe_2)$**structure **1N-Ni-1S**

	M06L/DZPDZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.125327	1.244795	0.073134	C	-0.12141	1.242222	0.084897	C	-0.107444	1.266059	0.122114
C	-0.043649	0.660247	1.307108	C	-0.042151	0.654278	1.307208	C	-0.060466	0.655770	1.327869
N	-0.342286	2.469613	-0.504317	N	-0.333792	2.454209	-0.496925	N	-0.380281	2.466277	-0.471590
C	-0.591886	2.472822	-1.933519	C	-0.548653	2.470777	-1.92668	C	-0.523077	2.436338	-1.917494
C	-1.142939	3.416202	0.252339	C	-1.09471	3.432051	0.251984	C	-1.345934	3.306884	0.218717
H	-1.055772	4.412090	-0.194453	H	-0.968887	4.417789	-0.195634	H	-1.336176	4.311193	-0.217908

H	-2.211847	3.139154	0.270911	H	-2.168355	3.199269	0.267879	H	-2.368731	2.899548	0.145403
H	-0.418100	3.474159	-2.342306	H	-0.346503	3.466104	-2.322993	H	-0.430752	3.450701	-2.320958
H	-1.626094	2.171269	-2.176460	H	-1.577615	2.1952	-2.194423	H	-1.496056	2.015836	-2.222820
H	0.089909	1.766359	-2.414601	H	0.126108	1.75848	-2.396899	H	0.268735	1.810310	-2.336448
H	-0.782175	3.465210	1.282388	H	-0.738234	3.471344	1.278527	H	-1.075720	3.384198	1.275128
C	-0.078274	0.997871	2.753327	C	-0.077005	0.97178	2.749989	C	-0.091301	0.934114	2.792730
H	-1.045829	1.440947	3.025895	H	-1.038114	1.412086	3.029387	H	-1.054973	1.377887	3.073695
H	0.071746	0.116379	3.383001	H	0.069469	0.087601	3.368753	H	0.043609	0.015946	3.370651
H	0.701887	1.728155	3.004934	H	0.700964	1.692888	3.013954	H	0.703648	1.638527	3.066235
C	-2.291693	-1.137704	-1.446519	C	-2.2937	-1.113154	-1.445259	C	-2.172606	-1.230446	-1.489714
C	-3.063443	-0.517037	-0.424804	C	-3.059348	-0.495355	-0.428911	C	-3.004660	-0.516852	-0.588866
H	-3.700856	0.352038	-0.541893	H	-3.692587	0.370544	-0.544547	H	-3.608578	0.351768	-0.822992
C	-2.855258	-1.248459	0.793253	C	-2.860625	-1.229718	0.779669	C	-2.904198	-1.148435	0.698045
H	-3.303544	-1.018840	1.752784	H	-3.313672	-1.006413	1.732934	H	-3.424451	-0.837161	1.596235
C	-1.594670	-2.235097	-0.855154	C	-1.609652	-2.211844	-0.860254	C	-1.557682	-2.300391	-0.761419
H	-0.896487	-2.888764	-1.366199	H	-0.923524	-2.869199	-1.371836	H	-0.854000	-3.016325	-1.169214
C	-1.964801	-2.323347	0.520795	C	-1.982338	-2.303587	0.506324	C	-2.040687	-2.275135	0.578367
H	-1.603546	-3.053428	1.233876	H	-1.637193	-3.041801	1.211688	H	-1.767692	-2.960387	1.370956
C	2.369217	-1.841313	-0.141237	C	2.349572	-1.848522	-0.142549	C	2.357631	-1.805026	-0.182001
C	2.970754	-1.016869	0.845181	C	2.956695	-1.034577	0.836906	C	2.963204	-1.020319	0.835053
H	3.123430	-1.273381	1.886197	H	3.117748	-1.295289	1.870625	H	3.107504	-1.313819	1.867554
C	3.300111	0.233164	0.229412	C	3.292336	0.206605	0.224921	C	3.313237	0.244203	0.263285
H	3.766461	1.080316	0.717619	H	3.771272	1.042844	0.709158	H	3.789643	1.067474	0.781814
C	2.343618	-1.113590	-1.377471	C	2.325859	-1.123106	-1.370994	C	2.353876	-1.036750	-1.395124
H	1.931741	-1.470180	-2.314061	H	1.917172	-1.476919	-2.304311	H	1.955316	-1.360987	-2.348673
C	2.931509	0.158819	-1.150834	C	2.921199	0.136992	-1.14637	C	2.960862	0.218243	-1.122537
H	3.046481	0.950251	-1.881712	H	3.048091	0.920664	-1.876336	H	3.102111	1.028146	-1.828002
H	1.973778	-2.838084	0.014650	H	1.955841	-2.840915	0.010505	H	1.959281	-2.805144	-0.063645
H	-2.219047	-0.818882	-2.479228	H	-2.222494	-0.796434	-2.473421	H	-2.011210	-0.999749	-2.535552
Ni	1.233949	-0.072068	0.093504	Ni	1.227401	-0.077029	0.097641	Ni	1.228996	-0.035586	0.100672
Ni	-1.034869	-0.446686	0.120739	Ni	-1.037378	-0.437841	0.121652	Ni	-1.003428	-0.453395	0.125953

Tables S48: Optimized coordinates for the **$Cp_2Ni_2(MeC_2NMe_2)$**structure**1N-Ni-2S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.132156	1.338613	0.503180	C	-0.125034	1.33464	0.498051	C	-0.094267	1.325369	0.522507
C	0.870093	1.177523	1.529231	C	0.857216	1.167489	1.531922	C	0.837254	1.107980	1.594613
N	-0.207075	2.534588	-0.154506	N	-0.188111	2.520117	-0.163477	N	-0.075135	2.522554	-0.136702
C	-0.836002	2.605812	-1.455946	C	-0.805935	2.59794	-1.465814	C	-0.602146	2.597811	-1.485936
C	0.682731	3.639021	0.149748	C	0.677363	3.634524	0.159995	C	0.903076	3.546091	0.186902
H	1.698399	3.477351	-0.248898	H	1.695851	3.494098	-0.22369	H	1.924383	3.247028	-0.101304
H	0.286648	4.555600	-0.296224	H	0.274648	4.543153	-0.283776	H	0.650886	4.465031	-0.349672
H	-0.088631	2.564018	-2.265180	H	-0.054633	2.574978	-2.264735	H	0.178734	2.382031	-2.233110
H	-1.399120	3.540939	-1.560524	H	-1.373716	3.524733	-1.566041	H	-1.004463	3.598778	-1.679905

H	-1.509773	1.753132	-1.567763	H	-1.469057	1.747227	-1.596761	H	-1.397821	1.860957	-1.603120
H	0.756152	3.788943	1.229805	H	0.734304	3.779153	1.236634	H	0.891034	3.767884	1.258053
C	0.875680	-0.057079	2.238154	C	0.856726	-0.060065	2.235791	C	0.828059	-0.157019	2.248457
H	-0.070644	-0.549672	2.463947	H	-0.082239	-0.556772	2.454983	H	-0.112686	-0.671806	2.436817
H	1.680420	1.895962	1.678902	H	1.657991	1.88422	1.69715	H	1.648253	1.804450	1.805049
H	1.693620	-0.261844	2.928206	H	1.664205	-0.264281	2.930157	H	1.624417	-0.365344	2.961266
C	-2.727294	-0.621995	-1.247771	C	-2.715436	-0.636525	-1.249377	C	-2.826371	-0.522231	-1.230497
C	-3.143373	0.095171	-0.082720	C	-3.13451	0.100006	-0.108477	C	-3.124933	0.265555	-0.079715
H	-3.610227	1.074654	-0.070697	H	-3.601466	1.073716	-0.119744	H	-3.521268	1.274764	-0.080489
C	-2.925934	-0.737353	1.077679	C	-2.930283	-0.707615	1.063138	C	-2.931520	-0.551637	1.100830
H	-3.182929	-0.483128	2.098565	H	-3.199133	-0.437519	2.071673	H	-3.118465	-0.239860	2.121215
C	-2.140051	-1.829155	-0.795622	C	-2.141323	-1.830958	-0.772579	C	-2.306022	-1.753724	-0.756608
H	-1.676563	-2.584711	-1.421956	H	-1.681911	-2.597814	-1.378678	H	-1.930190	-2.562826	-1.373469
C	-2.293704	-1.917006	0.632791	C	-2.30732	-1.892278	0.647814	C	-2.427094	-1.792967	0.677067
H	-1.948359	-2.735781	1.253694	H	-1.97922	-2.700718	1.282681	H	-2.128238	-2.618265	1.312476
C	1.529561	-2.147354	-0.612202	C	1.52738	-2.14267	-0.608129	C	1.476029	-2.205524	-0.557503
C	2.733893	-1.822928	0.078553	C	2.725053	-1.820938	0.079784	C	2.711296	-1.864245	0.072157
H	3.166918	-2.388894	0.894345	H	3.158354	-2.388248	0.888192	H	3.184081	-2.417012	0.875072
C	3.255018	-0.612208	-0.466644	C	3.245974	-0.618782	-0.463439	C	3.222672	-0.682154	-0.543701
H	4.158674	-0.109014	-0.144287	H	4.149443	-0.122069	-0.146674	H	4.146979	-0.179365	-0.285683
C	1.303482	-1.119097	-1.589246	C	1.304793	-1.120902	-1.580588	C	1.203913	-1.206379	-1.548042
H	0.470572	-1.070298	-2.280984	H	0.481365	-1.076602	-2.275276	H	0.367605	-1.196072	-2.235170
C	2.377674	-0.180044	-1.498321	C	2.374812	-0.188471	-1.489555	C	2.290819	-0.267662	-1.529279
H	2.487100	0.715700	-2.098867	H	2.490477	0.697834	-2.093693	H	2.379185	0.604693	-2.165979
H	0.898563	-3.009827	-0.435892	H	0.901969	-3.003679	-0.437346	H	0.854671	-3.062242	-0.329318
H	-2.802809	-0.284313	-2.274698	H	-2.786426	-0.322333	-2.278647	H	-2.911266	-0.213110	-2.265259
Ni	1.253512	-0.318665	0.314308	Ni	1.254885	-0.317895	0.317955	Ni	1.247182	-0.353053	0.339144
Ni	-1.115519	-0.199280	0.129794	Ni	-1.116345	-0.195758	0.124071	Ni	-1.110199	-0.153132	0.048783

Tables S49 : Optimized coordinates for the **$Cp_2Ni_2(MeC_2NMe_2)$**structure **1N-Ni-3T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.050104	1.342612	0.622585	C	0.057143	1.34392	0.613577	C	0.063901	1.349784	0.594893
C	0.996894	1.024941	1.652086	C	0.989947	1.02522	1.645275	C	0.995864	1.041575	1.646057
N	0.213527	2.500783	-0.094529	N	0.224904	2.487366	-0.110311	N	0.233609	2.500050	-0.121296
C	-0.492336	2.628729	-1.350924	C	-0.482491	2.618996	-1.361243	C	-0.427594	2.614865	-1.407172
C	1.439035	3.271859	0.005599	C	1.429546	3.282421	0.008262	C	1.429420	3.311564	0.029655
H	2.315521	2.697807	-0.343981	H	2.318153	2.736272	-0.335537	H	2.334611	2.761745	-0.277172
H	1.352713	4.175895	-0.601874	H	1.330108	4.185001	-0.589791	H	1.340576	4.206029	-0.592245
H	0.013093	2.085791	-2.169632	H	0.010472	2.068987	-2.174837	H	0.154846	2.126584	-2.205740
H	-0.570191	3.683651	-1.634115	H	-0.544934	3.66819	-1.648418	H	-0.565756	3.669822	-1.667883
H	-1.495400	2.210167	-1.240063	H	-1.487155	2.220049	-1.249911	H	-1.404600	2.132163	-1.352309
H	1.623824	3.576660	1.039900	H	1.597789	3.581757	1.041647	H	1.552098	3.637081	1.067211
C	0.845459	-0.255324	2.262729	C	0.837199	-0.243006	2.260203	C	0.852860	-0.217316	2.284766

H	-0.153798	-0.644889	2.477327	H	-0.153762	-0.637941	2.471997	H	-0.133401	-0.634309	2.491233
H	1.872746	1.637812	1.879301	H	1.85694	1.637596	1.879745	H	1.876192	1.647417	1.858246
H	1.612925	-0.608305	2.950962	H	1.59851	-0.590577	2.949888	H	1.634137	-0.547845	2.966874
C	-2.519439	-0.363116	-1.408908	C	-2.518457	-0.377374	-1.401945	C	-2.597715	-0.449551	-1.397078
C	-3.301368	0.378871	-0.475751	C	-3.296034	0.366837	-0.479505	C	-3.335142	0.358309	-0.483700
H	-3.703728	1.373682	-0.628173	H	-3.705988	1.35122	-0.642926	H	-3.750011	1.338544	-0.687648
C	-3.406228	-0.386049	0.713698	C	-3.397628	-0.383794	0.709838	C	-3.407117	-0.334374	0.755216
H	-3.922045	-0.089731	1.618992	H	-3.916767	-0.085458	1.606794	H	-3.893011	0.019560	1.656717
C	-2.181290	-1.613603	-0.810901	C	-2.178287	-1.61457	-0.796477	C	-2.237042	-1.658389	-0.731773
H	-1.599782	-2.404412	-1.270155	H	-1.601407	-2.405264	-1.248865	H	-1.679522	-2.482149	-1.160928
C	-2.714694	-1.624104	0.506031	C	-2.70772	-1.615329	0.513128	C	-2.728403	-1.583162	0.602172
H	-2.619767	-2.428995	1.225467	H	-2.616014	-2.412547	1.234234	H	-2.613402	-2.343018	1.366489
C	1.452698	-2.265345	-0.665509	C	1.451212	-2.263925	-0.657694	C	1.484044	-2.300135	-0.623756
C	2.659264	-1.968695	0.046648	C	2.651924	-1.967062	0.049079	C	2.684757	-1.967877	0.084029
H	3.074213	-2.557517	0.856074	H	3.068719	-2.5546	0.852033	H	3.110432	-2.531787	0.905470
C	3.215207	-0.773356	-0.483497	C	3.20492	-0.780754	-0.482609	C	3.222240	-0.779032	-0.478559
H	4.119724	-0.284266	-0.142614	H	4.109135	-0.29625	-0.149984	H	4.120985	-0.269471	-0.152237
C	1.258365	-1.232358	-1.628768	C	1.258332	-1.240587	-1.619206	C	1.281221	-1.301820	-1.619836
H	0.429610	-1.150139	-2.322967	H	0.43725	-1.164908	-2.31438	H	0.454272	-1.255509	-2.317541
C	2.335366	-0.300328	-1.497637	C	2.330275	-0.314082	-1.492776	C	2.342611	-0.350921	-1.514241
H	2.469470	0.597373	-2.091229	H	2.46679	0.574046	-2.090395	H	2.467494	0.529269	-2.134531
H	0.812837	-3.124551	-0.505348	H	0.818094	-3.122004	-0.500113	H	0.855393	-3.163241	-0.443208
H	-2.240902	-0.040042	-2.406281	H	-2.246707	-0.065857	-2.398931	H	-2.360583	-0.195355	-2.423956
Ni	1.202476	-0.431289	0.314976	Ni	1.20422	-0.430586	0.317916	Ni	1.190660	-0.435303	0.316217
Ni	-1.299190	-0.047278	0.365211	Ni	-1.300393	-0.038012	0.361815	Ni	-1.293498	-0.012804	0.309076

Tables S50 : Optimized coordinates for the **$Cp_2Ni_2(MeC_2NMe_2)$**structure **1N-Ni-4S**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	0.627007	1.829328	-0.382496	C	0.618458	1.831053	-0.376805	C	0.617622	1.842445	-0.349381
C	0.684675	1.187510	-1.661377	C	0.679451	1.198652	-1.650124	C	0.668847	1.242246	-1.651589
N	-0.678927	1.684770	0.295404	N	-0.681999	1.692155	0.301658	N	-0.689921	1.676403	0.316199
C	-1.609985	2.727524	-0.190894	C	-1.61602	2.726594	-0.184973	C	-1.628707	2.715786	-0.161491
C	-0.519889	1.810146	1.752812	C	-0.529147	1.810833	1.755706	C	-0.543523	1.790705	1.777709
H	-0.084905	2.786476	2.020451	H	-0.095178	2.779971	2.02845	H	-0.120180	2.769111	2.050876
H	-1.495536	1.712093	2.238119	H	-1.501792	1.715526	2.234732	H	-1.522716	1.680057	2.251732
H	-1.233226	3.734371	0.049944	H	-1.24774	3.730866	0.054066	H	-1.256672	3.720271	0.091506
H	-2.589069	2.590188	0.278446	H	-2.59003	2.586441	0.28077	H	-2.606893	2.564919	0.304613
H	-1.715845	2.629200	-1.273150	H	-1.721542	2.630275	-1.262218	H	-1.733882	2.629969	-1.244572
H	0.143386	1.012525	2.100565	H	0.125421	1.015632	2.106283	H	0.121565	0.999990	2.129264
C	0.007975	-0.062900	-1.568940	C	0.0074	-0.044024	-1.57474	C	0.001429	0.001375	-1.616061
H	0.095619	-0.767894	-2.402771	H	0.094361	-0.737857	-2.409826	H	0.099543	-0.661935	-2.477838
H	1.134286	2.777779	-0.169473	H	1.12784	2.770421	-0.15882	H	1.121142	2.785661	-0.120177
H	1.273378	1.555966	-2.502158	H	1.26042	1.576749	-2.485583	H	1.290871	1.621188	-2.461067

C	2.753915	-0.029599	1.403555	C	2.755662	-0.027171	1.389467	C	2.730325	-0.064139	1.411362
C	3.645439	0.006675	0.277154	C	3.632464	-0.007558	0.261644	C	3.644591	-0.020226	0.298001
H	4.391311	0.767687	0.084018	H	4.383447	0.739154	0.059883	H	4.404297	0.734098	0.132809
C	3.334325	-1.093258	-0.549518	C	3.305201	-1.103415	-0.549152	C	3.333425	-1.096567	-0.552676
H	3.798324	-1.336409	-1.497621	H	3.759704	-1.360044	-1.492781	H	3.805512	-1.325013	-1.500694
C	1.940158	-1.197757	1.307470	C	1.935264	-1.18278	1.310164	C	1.913331	-1.225730	1.284664
H	1.182008	-1.518207	2.012925	H	1.190337	-1.49395	2.025253	H	1.143808	-1.553646	1.972727
C	2.260246	-1.821388	0.066868	C	2.237701	-1.815393	0.080165	C	2.230780	-1.817340	0.029216
H	1.792306	-2.712225	-0.336369	H	1.76442	-2.703949	-0.307727	H	1.761738	-2.696951	-0.395922
C	-2.183163	-1.302257	1.382930	C	-2.161628	-1.304757	1.374397	C	-2.169391	-1.307269	1.381807
C	-1.705580	-2.143473	0.363020	C	-1.67658	-2.139348	0.365145	C	-1.644811	-2.151646	0.393096
H	-0.926952	-2.891642	0.452719	H	-0.897012	-2.878306	0.458964	H	-0.838370	-2.864817	0.511756
C	-2.388309	-1.776168	-0.856471	C	-2.358304	-1.785527	-0.849842	C	-2.305555	-1.824172	-0.847718
H	-2.235697	-2.241458	-1.823582	H	-2.2035	-2.253166	-1.809927	H	-2.118995	-2.304350	-1.801063
C	-3.182069	-0.436945	0.809446	C	-3.165381	-0.457607	0.80045	C	-3.188779	-0.486576	0.771585
H	-3.723268	0.334829	1.348842	H	-3.717196	0.301526	1.336204	H	-3.778759	0.263533	1.287887
C	-3.365981	-0.777193	-0.552130	C	-3.342263	-0.801778	-0.551663	C	-3.335633	-0.869365	-0.580730
H	-4.065297	-0.326472	-1.244569	H	-4.04839	-0.369714	-1.241451	H	-4.031526	-0.455561	-1.299615
H	-1.843827	-1.280296	2.412829	H	-1.828823	-1.278168	2.400784	H	-1.853698	-1.253677	2.417521
H	2.740799	0.688745	2.216392	H	2.759292	0.690554	2.195948	H	2.727187	0.628708	2.245343
Ni	-1.332804	-0.144120	-0.257728	Ni	-1.326601	-0.144032	-0.259997	Ni	-1.319538	-0.113121	-0.269087
Ni	1.558594	0.114474	-0.300914	Ni	1.548969	0.119258	-0.301562	Ni	1.543530	0.134781	-0.296457

Tables S51 : Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **1N-Co-1S**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	0.494775	1.887495	-0.216862	C	0.487485	1.880989	-0.223466	C	0.496658	1.882997	-0.225372
C	0.682199	1.397057	-1.555379	C	0.673758	1.388592	-1.551728	C	0.675818	1.389809	-1.563964
N	-0.869538	1.687560	0.299232	N	-0.87001	1.690238	0.299766	N	-0.862134	1.686570	0.300444
C	-1.849630	2.576901	-0.355237	C	-1.849797	2.576266	-0.350908	C	-1.835653	2.593351	-0.337023
C	-0.891959	1.896008	1.753147	C	-0.88996	1.893348	1.75032	C	-0.869898	1.896098	1.755355
H	-0.628733	2.936003	2.004325	H	-0.619742	2.92501	2.00422	H	-0.599502	2.934626	2.001264
H	-1.889741	1.681299	2.147375	H	-1.883982	1.68796	2.143018	H	-1.865704	1.686002	2.155946
H	-1.624534	3.633508	-0.142153	H	-1.624133	3.628147	-0.143312	H	-1.580953	3.644260	-0.132690
H	-2.856465	2.345173	0.008478	H	-2.850387	2.35016	0.015908	H	-2.838503	2.384309	0.049036
H	-1.809650	2.404939	-1.432477	H	-1.817889	2.405534	-1.423339	H	-1.825580	2.419012	-1.414245
H	-0.166642	1.217048	2.211761	H	-0.175077	1.212203	2.207974	H	-0.146892	1.215853	2.210410
C	0.010548	0.150663	-1.690443	C	0.009761	0.149254	-1.686617	C	0.003995	0.146298	-1.683969
H	0.098072	-0.416051	-2.623228	H	0.090599	-0.413347	-2.615109	H	0.083604	-0.421130	-2.613547
H	0.990306	2.795462	0.146149	H	0.983603	2.78364	0.13445	H	0.996520	2.792326	0.119481
H	1.349817	1.864289	-2.281104	H	1.32648	1.860641	-2.280223	H	1.340664	1.846317	-2.294672
C	2.583128	0.055933	1.411457	C	2.579662	0.065157	1.400798	C	2.610857	0.072155	1.393226
C	3.344302	0.251776	0.213853	C	3.335105	0.252369	0.20817	C	3.359628	0.231582	0.183545
H	3.981001	1.101298	-0.003094	H	3.972993	1.094054	-0.011451	H	3.998391	1.071149	-0.062405

C	3.103362	-0.860954	-0.647516	C	3.096352	-0.860333	-0.639999	C	3.107674	-0.902383	-0.643289
H	3.513887	-0.998495	-1.640690	H	3.510946	-1.007992	-1.624758	H	3.505786	-1.066613	-1.637247
C	1.864056	-1.166849	1.284885	C	1.865447	-1.152277	1.2843	C	1.882432	-1.147338	1.304261
H	1.185267	-1.585873	2.019030	H	1.196356	-1.567919	2.021196	H	1.213215	-1.547313	2.055210
C	2.179483	-1.730825	0.002493	C	2.179853	-1.722159	0.01314	C	2.183566	-1.744929	0.034312
H	1.776377	-2.649234	-0.408271	H	1.786076	-2.64375	-0.38506	H	1.769578	-2.668746	-0.350074
C	-1.887122	-1.384067	1.355500	C	-1.890213	-1.37036	1.351461	C	-1.966159	-1.343242	1.358703
C	-1.265355	-2.207102	0.368600	C	-1.261558	-2.1962	0.38381	C	-1.309189	-2.206795	0.437874
H	-0.432369	-2.881082	0.532613	H	-0.436573	-2.867376	0.5623	H	-0.492326	-2.879504	0.666625
C	-1.906295	-1.971079	-0.886992	C	-1.889347	-1.97606	-0.872604	C	-1.884835	-2.012086	-0.851798
H	-1.629523	-2.426465	-1.830325	H	-1.608817	-2.442599	-1.803674	H	-1.574166	-2.508350	-1.762764
C	-2.903052	-0.633116	0.688464	C	-2.897791	-0.63372	0.672517	C	-2.949369	-0.613933	0.621820
H	-3.527282	0.126580	1.150569	H	-3.530032	0.119403	1.121288	H	-3.601495	0.151173	1.029496
C	-2.939580	-0.998649	-0.691149	C	-2.921758	-1.01078	-0.69568	C	-2.922242	-1.033457	-0.738205
H	-3.616934	-0.611619	-1.442265	H	-3.596004	-0.640481	-1.45087	H	-3.556715	-0.670181	-1.536631
H	-1.633121	-1.328507	2.407883	H	-1.649988	-1.308937	2.401295	H	-1.758198	-1.249198	2.417433
H	2.541253	0.734597	2.255634	H	2.542697	0.743388	2.239011	H	2.587733	0.770039	2.221257
Co	-1.079216	-0.245189	-0.204208	Co	-1.080014	-0.248831	-0.204085	Co	-1.069827	-0.227407	-0.204419
Co	1.329313	0.121672	-0.217413	Co	1.328568	0.120908	-0.220815	Co	1.324633	0.117823	-0.221427

Tables S52 : Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **1N-Co-2T**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	0.126753	1.220913	0.507125	C	0.121999	1.218109	0.493427	C	0.195314	1.264124	0.529615
C	1.001492	0.993569	1.614843	C	0.98692	1.007138	1.602552	C	1.039932	0.998106	1.638783
N	0.064632	2.436657	-0.142215	N	0.041078	2.419014	-0.160528	N	0.225230	2.476570	-0.147019
C	-0.239499	2.433486	-1.556473	C	-0.269494	2.425345	-1.568606	C	-0.078761	2.442448	-1.564045
C	0.931443	3.516030	0.281452	C	0.82004	3.547134	0.291736	C	1.247328	3.442068	0.207529
H	1.986704	3.347507	-0.001552	H	1.882087	3.461747	0.020391	H	2.264835	3.091823	-0.043930
H	0.602597	4.450924	-0.183153	H	0.432917	4.460201	-0.15953	H	1.063968	4.377022	-0.331443
H	0.661557	2.269600	-2.173965	H	0.634764	2.359036	-2.188628	H	0.771342	2.069563	-2.161838
H	-0.686426	3.389798	-1.852224	H	-0.79493	3.342924	-1.839069	H	-0.338523	3.447258	-1.916249
H	-0.945255	1.625333	-1.767109	H	-0.901287	1.571433	-1.800658	H	-0.930828	1.781638	-1.740277
H	0.883856	3.633856	1.367251	H	0.753066	3.642504	1.373623	H	1.209973	3.657180	1.279878
C	0.838306	-0.302809	2.212532	C	0.838661	-0.277347	2.208929	C	0.848474	-0.301488	2.229607
H	-0.160625	-0.632134	2.512303	H	-0.148327	-0.621817	2.508016	H	-0.150462	-0.602442	2.554267
H	1.842460	1.648254	1.859660	H	1.806174	1.677535	1.85284	H	1.904194	1.611880	1.892410
H	1.622472	-0.666880	2.877886	H	1.622262	-0.626438	2.874224	H	1.630980	-0.675446	2.889764
C	-2.704597	-0.330194	-1.359706	C	-2.694248	-0.382191	-1.35193	C	-2.762947	-0.330659	-1.363700
C	-3.120892	0.561197	-0.333657	C	-3.109604	0.518614	-0.344856	C	-3.218313	0.599197	-0.391954
H	-3.302675	1.624228	-0.447868	H	-3.302706	1.572214	-0.477742	H	-3.443123	1.645212	-0.564981
C	-3.213819	-0.171865	0.885742	C	-3.19727	-0.191387	0.879486	C	-3.296271	-0.073057	0.862650
H	-3.518993	0.226445	1.845870	H	-3.508333	0.216598	1.828147	H	-3.620132	0.364450	1.799523
C	-2.526106	-1.611350	-0.776825	C	-2.512023	-1.646	-0.752305	C	-2.551906	-1.579115	-0.716553

H	-2.195119	-2.502820	-1.298538	H	-2.185434	-2.541632	-1.259063	H	-2.205197	-2.489986	-1.190607
C	-2.847879	-1.524632	0.614054	C	-2.829356	-1.539652	0.629581	C	-2.889276	-1.425838	0.661949
H	-2.844306	-2.341560	1.325462	H	-2.827474	-2.342993	1.348919	H	-2.855853	-2.201842	1.417578
C	1.395299	-2.150970	-0.807423	C	1.419079	-2.128541	-0.801404	C	1.267952	-2.224707	-0.782455
C	2.482317	-2.018502	0.104954	C	2.495715	-1.991615	0.110205	C	2.377789	-2.138932	0.109666
H	2.709027	-2.691427	0.922759	H	2.725943	-2.664287	0.920948	H	2.586196	-2.817347	0.927507
C	3.188353	-0.814802	-0.204707	C	3.193859	-0.791739	-0.195805	C	3.151151	-0.991459	-0.240890
H	4.048891	-0.430349	0.329915	H	4.051059	-0.408355	0.335176	H	4.047333	-0.650886	0.263194
C	1.430724	-1.012405	-1.684807	C	1.453894	-0.997391	-1.675241	C	1.350414	-1.109758	-1.680468
H	0.717499	-0.801419	-2.474405	H	0.750611	-0.794308	-2.468241	H	0.647168	-0.878850	-2.471431
C	2.545680	-0.198301	-1.320325	C	2.557305	-0.182954	-1.308706	C	2.515390	-0.355644	-1.346603
H	2.835485	0.734734	-1.789853	H	2.848021	0.742354	-1.780766	H	2.847986	0.550881	-1.837827
H	0.675076	-2.959303	-0.836152	H	0.710346	-2.939845	-0.837476	H	0.503224	-2.990785	-0.781490
H	-2.529385	-0.074563	-2.398813	H	-2.529613	-0.145173	-2.391655	H	-2.587113	-0.122337	-2.412962
Co	1.202159	-0.409325	0.246483	Co	1.214932	-0.393174	0.247467	Co	1.180954	-0.449394	0.268053
Co	-1.149593	-0.273750	0.276382	Co	-1.13936	-0.289046	0.269639	Co	-1.184665	-0.135595	0.270438

Tables S53 : Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **1N-Co-3T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.598427	1.861251	-0.300207	C	0.596095	1.852395	-0.311466	C	0.589737	1.865352	-0.312776
C	0.708404	1.299495	-1.620087	C	0.70155	1.288374	-1.620432	C	0.669348	1.306947	-1.636543
N	-0.746363	1.733916	0.299713	N	-0.737986	1.733919	0.301447	N	-0.739036	1.704660	0.310765
C	-1.677926	2.738030	-0.258085	C	-1.671713	2.73459	-0.24866	C	-1.684931	2.716177	-0.211316
C	-0.673674	1.880658	1.759569	C	-0.656696	1.874777	1.756972	C	-0.642271	1.839221	1.773211
H	-0.293869	2.877080	2.035915	H	-0.268221	2.861627	2.033952	H	-0.259038	2.834208	2.045386
H	-1.667825	1.747421	2.197037	H	-1.644523	1.752118	2.197608	H	-1.629958	1.701704	2.222048
H	-1.331501	3.759188	-0.036250	H	-1.324615	3.751403	-0.03498	H	-1.329106	3.730671	0.021854
H	-2.675963	2.597550	0.171192	H	-2.660557	2.598464	0.188525	H	-2.671561	2.566816	0.238781
H	-1.731037	2.609000	-1.342405	H	-1.737778	2.604813	-1.326788	H	-1.766208	2.608599	-1.295522
H	0.005389	1.116538	2.149666	H	0.01176	1.108566	2.14462	H	0.040418	1.076671	2.152545
C	0.073829	0.026509	-1.660416	C	0.073171	0.023543	-1.661105	C	0.050249	0.041560	-1.669950
H	0.128761	-0.593851	-2.559897	H	0.120228	-0.592266	-2.556516	H	0.120375	-0.570175	-2.570330
H	1.120246	2.785385	-0.022704	H	1.121216	2.769037	-0.039188	H	1.097421	2.798151	-0.052616
H	1.350244	1.725059	-2.394331	H	1.32743	1.718767	-2.39814	H	1.312021	1.727327	-2.410075
C	2.569615	-0.101794	1.471185	C	2.618494	-0.039255	1.428853	C	2.672678	-0.075947	1.437108
C	3.422895	0.205160	0.355973	C	3.442553	0.171057	0.281391	C	3.501204	0.180684	0.288617
H	4.040469	1.089590	0.254662	H	4.086982	1.019238	0.113342	H	4.132460	1.049137	0.144118
C	3.280920	-0.832356	-0.599671	C	3.236143	-0.908407	-0.600631	C	3.308284	-0.874335	-0.629473
H	3.766006	-0.880061	-1.567352	H	3.692219	-1.033344	-1.570132	H	3.757542	-0.956371	-1.612045
C	1.929574	-1.345458	1.209976	C	1.933764	-1.266719	1.264966	C	2.009146	-1.317656	1.235579
H	1.216878	-1.844259	1.857492	H	1.234858	-1.702397	1.962305	H	1.314140	-1.788737	1.920813
C	2.334832	-1.779771	-0.089070	C	2.284441	-1.789018	-0.009009	C	2.355907	-1.788187	-0.065688
H	2.007129	-2.682302	-0.592181	H	1.923575	-2.708928	-0.441573	H	2.002469	-2.700173	-0.531746

C	-1.770246	-1.408841	1.332207	C	-1.823512	-1.349649	1.350361	C	-1.854294	-1.376577	1.354093
C	-1.376440	-2.165699	0.203370	C	-1.37628	-2.146613	0.28262	C	-1.415168	-2.156767	0.264838
H	-0.506994	-2.808964	0.135814	H	-0.509961	-2.787881	0.28593	H	-0.543580	-2.798788	0.247848
C	-2.282347	-1.868295	-0.871654	C	-2.227568	-1.901161	-0.838439	C	-2.281065	-1.890218	-0.851829
H	-2.242237	-2.286892	-1.869816	H	-2.14179	-2.360841	-1.810105	H	-2.198711	-2.333912	-1.836222
C	-2.936969	-0.654128	0.968517	C	-2.973712	-0.625037	0.90697	C	-3.001033	-0.624856	0.922872
H	-3.476828	0.031238	1.613729	H	-3.551081	0.069223	1.49901	H	-3.569662	0.069368	1.531669
C	-3.270229	-0.966390	-0.372988	C	-3.238756	-0.99346	-0.426899	C	-3.291859	-0.984453	-0.419045
H	-4.087181	-0.538814	-0.942741	H	-4.032953	-0.606974	-1.046882	H	-4.094224	-0.584963	-1.028077
H	-1.274168	-1.387420	2.296209	H	-1.374842	-1.286069	2.329624	H	-1.389717	-1.322397	2.331564
H	2.459081	0.498069	2.367771	H	2.553274	0.613905	2.285443	H	2.610568	0.546135	2.322380
Co	-1.300574	-0.121695	-0.315463	Co	-1.302142	-0.123747	-0.315439	Co	-1.329949	-0.106334	-0.317024
Co	1.405535	0.074243	-0.240889	Co	1.407061	0.068992	-0.249715	Co	1.415949	0.078498	-0.234676

Tables S54: Optimized coordinates for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **1N-Co-4T**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	-0.169952	1.245602	0.033793	C	-0.24973	1.244634	0.037515	C	1.066895	1.150390	0.036769
C	-0.089613	0.671416	1.304174	C	-0.132431	0.694225	1.298325	C	0.198353	0.857500	1.068510
N	-0.510632	2.463689	-0.511947	N	-0.635925	2.421014	-0.538126	N	1.702400	2.218420	-0.447558
C	-0.702124	2.480477	-1.950115	C	-0.877896	2.40689	-1.962624	C	2.667133	2.084865	-1.521222
C	-1.471958	3.260779	0.228891	C	-1.498349	3.296632	0.224657	C	1.440197	3.567714	0.020771
H	-1.522134	4.268003	-0.197501	H	-1.517319	4.285852	-0.232678	H	2.336058	4.006602	0.480161
H	-2.486676	2.823620	0.203872	H	-2.531997	2.925966	0.275267	H	1.132579	4.210004	-0.815464
H	-0.649398	3.509185	-2.323287	H	-0.806526	3.418123	-2.364612	H	3.660270	2.427579	-1.200309
H	-1.675626	2.051710	-2.248584	H	-1.870303	2.007685	-2.213512	H	2.362162	2.678184	-2.394344
H	0.087834	1.888961	-2.420362	H	-0.129852	1.780736	-2.444643	H	2.725373	1.032035	-1.802796
H	-1.160594	3.343195	1.273109	H	-1.122586	3.394934	1.240432	H	0.638709	3.545886	0.760461
C	-0.277759	1.089481	2.721817	C	-0.360924	1.077781	2.711793	C	0.020591	1.470198	2.436315
H	-1.303096	1.443142	2.898506	H	-1.388254	1.417931	2.869681	H	-0.632360	2.353198	2.402165
H	-0.091566	0.263072	3.413890	H	-0.186594	0.244085	3.390894	H	-0.436188	0.753696	3.125535
H	0.403222	1.907787	2.990229	H	0.300813	1.89176	3.018891	H	0.985410	1.781692	2.858527
C	-2.108702	-1.383708	-1.461751	C	-2.118831	-1.353527	-1.427914	C	-2.751225	-0.309325	-1.555789
C	-2.953662	-0.669634	-0.571923	C	-2.920721	-0.760533	-0.426639	C	-3.019879	0.991277	-1.035097
H	-3.581931	0.176183	-0.826831	H	-3.606173	0.061281	-0.564012	H	-2.991460	1.919753	-1.593234
C	-2.818909	-1.258433	0.731339	C	-2.660829	-1.437886	0.804911	C	-3.340001	0.853135	0.346057
H	-3.324224	-0.930354	1.632177	H	-3.111858	-1.211189	1.758309	H	-3.577102	1.661423	1.028153
C	-1.438173	-2.403599	-0.716036	C	-1.346133	-2.381358	-0.818162	C	-2.911641	-1.247194	-0.489397
H	-0.712347	-3.106450	-1.108580	H	-0.624763	-3.011251	-1.314956	H	-2.777300	-2.320495	-0.558340
C	-1.901999	-2.339843	0.633315	C	-1.707198	-2.449035	0.55469	C	-3.276822	-0.526902	0.680123
H	-1.568838	-2.967353	1.451019	H	-1.28619	-3.118908	1.287736	H	-3.450335	-0.952276	1.661547
C	2.431573	-1.722958	0.043918	C	2.421959	-1.659436	0.018655	C	0.698670	-2.675834	0.594992
C	3.070181	-0.764301	0.883939	C	3.071382	-0.726572	0.866033	C	1.928506	-2.221534	1.153933
H	3.298878	-0.884716	1.935336	H	3.313112	-0.870194	1.906582	H	2.179663	-2.206487	2.207464

C	3.348274	0.388733	0.087295	C	3.352865	0.4295	0.09267	C	2.754271	-1.749242	0.090211
H	3.803198	1.307246	0.439271	H	3.823522	1.330363	0.455565	H	3.745432	-1.324947	0.193984
C	2.314558	-1.161867	-1.262517	C	2.303571	-1.07773	-1.26932	C	0.761946	-2.483447	-0.821262
H	1.841542	-1.636153	-2.114425	H	1.832522	-1.534652	-2.125309	H	-0.019562	-2.720768	-1.532398
C	2.887022	0.144315	-1.238789	C	2.883846	0.215882	-1.227051	C	2.031077	-1.908960	-1.131249
H	2.945463	0.834098	-2.071804	H	2.954317	0.910991	-2.048119	H	2.377901	-1.636275	-2.120599
H	2.058880	-2.693177	0.350576	H	2.054675	-2.631929	0.306389	H	-0.143647	-3.076188	1.145139
H	-1.955960	-1.159373	-2.511138	H	-2.069846	-1.052059	-2.462526	H	-2.496877	-0.545416	-2.582238
Co	1.272301	0.039338	0.130803	Co	1.266221	0.108727	0.142212	Co	0.971010	-0.656682	0.152559
Co	-0.959143	-0.526123	0.091940	Co	-0.915803	-0.564409	0.08602	Co	-1.235601	0.129572	-0.055245

Tables S55 : Optimized coordinates for the **$Cp_2Fe_2(MeC_2NMe_2)$**structure **1N-Fe-1T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.484812	1.947968	-0.135346	C	0.472825	1.944483	-0.146542	C	0.501460	1.929271	-0.143191
C	0.714290	1.506344	-1.482612	C	0.70149	1.495661	-1.48139	C	0.700730	1.513961	-1.507867
N	-0.899139	1.753932	0.329399	N	-0.901957	1.752801	0.329452	N	-0.878820	1.754699	0.338917
C	-1.861885	2.640747	-0.357206	C	-1.870064	2.632036	-0.351089	C	-1.837204	2.660646	-0.326693
C	-0.983475	1.953106	1.780926	C	-0.980318	1.948019	1.777548	C	-0.939728	1.950523	1.793684
H	-0.722353	2.989351	2.049521	H	-0.711294	2.975936	2.047898	H	-0.665853	2.983774	2.056775
H	-2.000208	1.746218	2.127883	H	-1.992642	1.751568	2.125168	H	-1.952958	1.750092	2.152861
H	-1.644208	3.697208	-0.139072	H	-1.656199	3.68504	-0.139181	H	-1.584598	3.709757	-0.114278
H	-2.879634	2.408858	-0.023808	H	-2.879596	2.400301	-0.01152	H	-2.850555	2.452324	0.032874
H	-1.787115	2.472972	-1.434085	H	-1.806175	2.464698	-1.423362	H	-1.798281	2.494785	-1.405336
H	-0.285568	1.265960	2.269065	H	-0.292514	1.258745	2.264146	H	-0.242207	1.257828	2.269708
C	0.052164	0.271339	-1.736242	C	0.04954	0.265664	-1.730764	C	0.052308	0.282513	-1.749826
H	0.192163	-0.227680	-2.701679	H	0.187528	-0.232323	-2.690059	H	0.146535	-0.198782	-2.725350
H	0.977161	2.841477	0.266060	H	0.963741	2.835025	0.246912	H	1.013833	2.809381	0.254725
H	1.437601	1.991503	-2.141765	H	1.411914	1.984254	-2.143638	H	1.400831	2.011339	-2.177881
C	2.131841	-0.814932	1.506823	C	2.132965	-0.818302	1.495409	C	2.079883	-0.876005	1.487129
C	2.940960	0.271088	1.073585	C	2.927741	0.273159	1.076057	C	2.881652	0.245248	1.135550
H	3.189450	1.151205	1.655087	H	3.172321	1.142697	1.665927	H	3.078816	1.108654	1.758858
C	3.322383	0.026882	-0.279736	C	3.31372	0.044295	-0.270588	C	3.329805	0.061753	-0.205597
H	3.925189	0.682624	-0.897454	H	3.915535	0.703833	-0.876403	H	3.936717	0.757507	-0.772431
C	2.016337	-1.738944	0.423570	C	2.029726	-1.72968	0.411409	C	2.052267	-1.767051	0.369057
H	1.462587	-2.670840	0.440664	H	1.49138	-2.664186	0.421394	H	1.523039	-2.710536	0.323742
C	2.753769	-1.222689	-0.682498	C	2.761418	-1.200584	-0.681972	C	2.825765	-1.191687	-0.676493
H	2.858914	-1.689207	-1.654838	H	2.878902	-1.659843	-1.65079	H	2.987431	-1.614914	-1.660247
C	-1.260333	-1.895752	1.027746	C	-1.245496	-1.896444	1.01492	C	-1.294087	-1.942763	0.995173
C	-1.229780	-2.262012	-0.355580	C	-1.23073	-2.254628	-0.363435	C	-1.293124	-2.268948	-0.393097
H	-0.472176	-2.866849	-0.841138	H	-0.486964	-2.861448	-0.855668	H	-0.564681	-2.886298	-0.903998
C	-2.378016	-1.699994	-0.996845	C	-2.379509	-1.69108	-0.985725	C	-2.436527	-1.663050	-1.002579
H	-2.640621	-1.811773	-2.041606	H	-2.657417	-1.804393	-2.021351	H	-2.716793	-1.743174	-2.045477
C	-2.402251	-1.077525	1.226577	C	-2.378117	-1.083321	1.228841	C	-2.404019	-1.087922	1.229233

H	-2.694860	-0.614935	2.163220	H	-2.661051	-0.631186	2.16748	H	-2.674555	-0.648108	2.182533
C	-3.096278	-0.960081	-0.013149	C	-3.081303	-0.95841	0.004358	C	-3.118135	-0.927486	0.004247
H	-4.000373	-0.384210	-0.180546	H	-3.9862	-0.388847	-0.147178	H	-4.013860	-0.332379	-0.134876
H	-0.538323	-2.180655	1.783928	H	-0.524351	-2.191451	1.759952	H	-0.573958	-2.273136	1.732472
H	1.664689	-0.912193	2.481250	H	1.670644	-0.930004	2.464677	H	1.574364	-1.025001	2.433705
Fe	-1.116440	-0.181257	-0.282514	Fe	-1.118277	-0.187685	-0.282588	Fe	-1.099435	-0.151556	-0.266924
Fe	1.232765	0.110494	-0.159277	Fe	1.231077	0.11333	-0.159442	Fe	1.234904	0.086170	-0.182429

Tables S56 : Optimized coordinates for the **$Cp_2Fe_2(MeC_2NMe_2)$**structure **1N-Fe-2S**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	1.611681	-0.147487	0.000000	C	1.602434	-0.158793	0.000000	C	1.580913	-0.169089	0.000000
C	-1.126483	-0.043374	0.000000	C	-1.131863	-0.042464	0.000000	C	-1.114527	-0.058247	0.000000
C	3.086468	-0.313580	0.000000	C	3.067936	-0.333383	0.000000	N	3.065497	-0.344708	0.000000
H	3.585363	0.665891	0.000000	H	3.574136	0.637113	0.000000	C	3.563981	0.634041	0.000000
H	3.441102	-0.857946	0.885597	H	3.419796	-0.876800	0.880780	C	3.402391	-0.895632	0.886154
H	3.441102	-0.857946	-0.885597	H	3.419796	-0.876800	-0.880780	H	3.402391	-0.895632	-0.886154
N	-2.472347	-0.137500	0.000000	N	-2.468646	-0.132892	0.000000	H	-2.457522	-0.143052	0.000000
C	-3.256831	-0.093732	-1.222512	C	-3.251668	-0.102221	-1.221398	H	-3.246748	-0.102473	-1.222316
H	-3.478781	0.936430	-1.539828	H	-3.459312	0.919251	-1.556560	H	-3.477242	0.928381	-1.527269
H	-2.719874	-0.599630	-2.024692	H	-2.727641	-0.627763	-2.011990	H	-2.710053	-0.601103	-2.026872
H	-4.209657	-0.609146	-1.062346	H	-4.206702	-0.598463	-1.053170	H	-4.192746	-0.630349	-1.062743
C	-3.256831	-0.093732	1.222512	C	-3.251668	-0.102221	1.221398	C	-3.246748	-0.102473	1.222316
H	-2.719874	-0.599630	2.024692	H	-2.727641	-0.627763	2.011990	H	-2.710053	-0.601103	2.026872
H	-3.478781	0.936430	1.539828	H	-3.459312	0.919251	1.556560	H	-3.477242	0.928381	1.527269
H	-4.209657	-0.609146	1.062346	H	-4.206702	-0.598463	1.053170	H	-4.192746	-0.630349	1.062743
Fe	0.278995	-0.014367	1.172627	Fe	0.273821	-0.014847	1.168956	C	0.274690	-0.026811	1.171860
Fe	0.278995	-0.014367	-1.172627	Fe	0.273821	-0.014847	-1.168956	C	0.274690	-0.026811	-1.171860
C	-0.385059	-0.774191	2.997010	C	-0.362657	-0.773744	2.993265	H	-0.371077	-0.760569	3.031915
C	-0.648340	0.628784	2.939297	C	-0.642571	0.617537	2.935245	C	-0.648392	0.640104	2.952388
H	-1.619252	1.104394	2.986042	H	-1.612454	1.080042	3.001022	H	-1.619206	1.111582	3.014194
C	0.586589	1.308811	2.743520	C	0.575140	1.309047	2.728255	C	0.578270	1.325408	2.749974
H	0.715671	2.377539	2.627661	H	0.689497	2.375247	2.618137	H	0.695710	2.392518	2.610192
C	1.023972	-0.958956	2.860416	C	1.040014	-0.939135	2.846793	C	1.036766	-0.932156	2.894960
H	1.542309	-1.910377	2.844555	H	1.569122	-1.878953	2.834368	H	1.563600	-1.878587	2.889456
C	1.622602	0.328127	2.727141	C	1.618061	0.347501	2.706130	C	1.623261	0.356573	2.731806
H	2.676086	0.527221	2.573663	H	2.663621	0.559793	2.552960	C	2.675303	0.566844	2.589520
C	-0.385059	-0.774191	-2.997010	C	-0.362657	-0.773744	-2.993265	H	-0.371077	-0.760569	-3.031915
C	-0.648340	0.628784	-2.939297	C	-0.642571	0.617537	-2.935245	C	-0.648392	0.640104	-2.952388
H	-1.619252	1.104394	-2.986042	H	-1.612454	1.080042	-3.001022	H	-1.619206	1.111582	-3.014194
C	0.586589	1.308811	-2.743520	C	0.575140	1.309047	-2.728255	C	0.578270	1.325408	-2.749974
H	0.715671	2.377539	-2.627661	H	0.689497	2.375247	-2.618137	H	0.695710	2.392518	-2.610192
C	1.023972	-0.958956	-2.860416	C	1.040014	-0.939135	-2.846793	C	1.036766	-0.932156	-2.894960
H	1.542309	-1.910377	-2.844555	H	1.569122	-1.878953	-2.834368	H	1.563600	-1.878587	-2.889456

C	1.622602	0.328127	-2.727141	C	1.618061	0.347501	-2.706130	H	1.623261	0.356573	-2.731806
H	2.676086	0.527221	-2.573663	H	2.663621	0.559793	-2.552960	H	2.675303	0.566844	-2.589520
H	-1.113540	-1.566352	3.125457	H	-1.075518	-1.569761	3.138229	Fe	-1.088502	-1.558096	3.180959
H	-1.113540	-1.566352	-3.125457	H	-1.075518	-1.569761	-3.138229	Fe	-1.088502	-1.558096	-3.180959

Tables S57 : Optimized coordinates for the **$Cp_2Fe_2(MeC_2NMe_2)$**structure **1N-Fe-3T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.088989	1.235690	0.165464	C	-0.084473	1.222554	0.168326	C	-0.742310	1.316617	0.027347
C	0.060459	0.513784	1.328780	C	0.060137	0.517164	1.331843	C	-0.172225	0.893510	1.215865
N	0.246112	2.468899	-0.313289	N	0.238528	2.439473	-0.330935	N	-1.017055	2.491522	-0.555857
C	1.431697	3.123159	0.207099	C	1.371841	3.160414	0.205794	C	-0.559060	3.762401	-0.026160
C	-0.050735	2.762117	-1.701035	C	-0.079048	2.73302	-1.708888	C	-1.777566	2.546729	-1.787358
H	-0.155765	3.843647	-1.843697	H	-0.236087	3.804842	-1.838907	H	-2.729997	3.075730	-1.642222
H	0.739325	2.401746	-2.382266	H	0.721935	2.423704	-2.393089	H	-1.210732	3.067828	-2.571674
H	1.360188	4.205497	0.052040	H	1.228786	4.234028	0.074488	H	-1.402881	4.386787	0.298533
H	2.351520	2.766789	-0.288240	H	2.30939	2.882767	-0.292984	H	0.001576	4.315989	-0.791888
H	1.520804	2.929776	1.278559	H	1.474193	2.953197	1.267612	H	0.095903	3.585971	0.828266
H	-0.989286	2.274012	-1.975128	H	-0.988981	2.206805	-1.986597	H	-1.983788	1.525063	-2.112296
C	0.477074	0.819012	2.731140	C	0.466866	0.821203	2.729861	C	-0.095231	1.545461	2.579287
H	-0.140042	1.624393	3.150908	H	-0.140552	1.631055	3.143114	H	-1.003725	2.124875	2.791566
H	0.377404	-0.049457	3.389149	H	0.352319	-0.038277	3.389405	H	0.009901	0.791172	3.365381
H	1.525253	1.149578	2.783572	H	1.512692	1.137354	2.792576	H	0.762211	2.227759	2.666293
C	-2.697999	-0.496368	-1.426955	C	-2.666032	-0.502446	-1.423212	C	-1.590152	-2.028500	-1.220674
C	-3.271350	0.414827	-0.483813	C	-3.248271	0.401715	-0.491134	C	-2.799912	-1.328367	-0.939865
H	-3.563343	1.439876	-0.679451	H	-3.541979	1.420457	-0.689916	H	-3.394734	-0.775618	-1.657778
C	-3.397905	-0.266934	0.765185	C	-3.387796	-0.27683	0.748703	C	-3.074568	-1.449753	0.445867
H	-3.802520	0.145547	1.680913	H	-3.80776	0.130564	1.654089	H	-3.907508	-0.998200	0.971319
C	-2.470747	-1.734753	-0.758032	C	-2.446138	-1.734918	-0.756291	C	-1.116837	-2.596348	0.004500
H	-2.033674	-2.624723	-1.194509	H	-2.01587	-2.623608	-1.189769	H	-0.240050	-3.220669	0.124601
C	-2.911928	-1.593395	0.582899	C	-2.90176	-1.595079	0.571425	C	-2.031677	-2.218022	1.035750
H	-2.829191	-2.348905	1.355637	H	-2.83437	-2.349676	1.340079	H	-1.951605	-2.477156	2.084557
C	2.377543	-2.329072	-0.184703	C	2.387276	-2.307722	-0.183046	C	3.080700	-1.435889	0.320215
C	2.925551	-1.442937	0.787218	C	2.938106	-1.416319	0.771265	C	3.532122	-0.083298	0.426993
H	3.079021	-1.667674	1.836840	H	3.113307	-1.63547	1.81349	H	4.054999	0.348276	1.272838
C	3.204250	-0.203910	0.154662	C	3.198518	-0.186148	0.131713	C	3.208203	0.587533	-0.789405
H	3.594332	0.681972	0.644523	H	3.590285	0.699865	0.6077	H	3.409678	1.628352	-1.015228
C	2.310230	-1.617659	-1.426938	C	2.298771	-1.607439	-1.42133	C	2.463716	-1.584652	-0.957580
H	1.972149	-2.020815	-2.374425	H	1.958547	-2.017684	-2.359257	H	2.014896	-2.490633	-1.347722
C	2.826796	-0.303604	-1.206492	C	2.805474	-0.295671	-1.215302	C	2.547372	-0.335990	-1.638544
H	2.904892	0.481737	-1.950243	H	2.870511	0.481158	-1.961457	H	2.148089	-0.121665	-2.622897
H	2.101115	-3.364321	-0.025035	H	2.129313	-3.341504	-0.016711	H	3.207410	-2.212099	1.065457
H	-2.466011	-0.285448	-2.464236	H	-2.432078	-0.29358	-2.455237	H	-1.122965	-2.126675	-2.193173
Fe	0.904790	-0.727328	-0.029163	Fe	0.908675	-0.721926	-0.01114	Fe	1.293553	-0.112742	0.294773

Fe	-1.351430	-0.124413	0.182673	Fe	-1.339988	-0.13897	0.190354	Fe	-1.096351	-0.488963	0.174443

Tables S58 : Optimized coordinates for the **$Cp_2Fe_2(MeC_2NMe_2)$**structure **1N-Fe-4T**

M06L/DZP				M06L/def2tzvpp				WB97XD/DZP			
	x	y	z		x	y	z		x	y	z
C	0.054984	-1.638227	-0.085777	C	0.054705	-1.630672	-0.09589	C	0.073196	-1.609974	-0.143557
C	0.087017	1.093764	0.000911	C	0.09028	1.094739	-0.005309	C	0.099890	1.087805	-0.026102
C	-0.019908	-3.115490	-0.187674	C	-0.025369	-3.099181	-0.200628	N	0.002507	-3.092642	-0.299091
H	-0.587048	-3.550892	0.647333	H	-0.603933	-3.534512	0.620249	C	-0.507364	-3.554548	0.556584
H	-0.537576	-3.411724	-1.110385	H	-0.529443	-3.392403	-1.126082	C	-0.574422	-3.341388	-1.199233
H	0.970560	-3.590852	-0.205682	H	0.956573	-3.580022	-0.206135	H	0.995361	-3.547161	-0.402490
N	0.078203	2.439577	-0.039099	N	0.082744	2.431404	-0.044395	H	0.096418	2.424811	-0.068018
C	1.139857	3.208921	-0.660369	C	1.137496	3.20187	-0.670416	H	1.164032	3.192114	-0.689239
H	1.731369	3.763483	0.083796	H	1.740516	3.741249	0.067387	H	1.768984	3.721296	0.060680
H	1.795730	2.536213	-1.213887	H	1.779245	2.540789	-1.243073	H	1.801362	2.523234	-1.266402
H	0.711854	3.939968	-1.359356	H	0.703561	3.941966	-1.347803	H	0.730839	3.938897	-1.367120
C	-0.999042	3.240620	0.508907	C	-0.98524	3.234993	0.511588	C	-0.987156	3.235581	0.462395
H	-1.678690	2.597627	1.068768	H	-1.648782	2.605885	1.09474	H	-1.645688	2.611466	1.064303
H	-0.595458	4.004781	1.186802	H	-0.571478	4.00809	1.164498	H	-0.575992	4.031843	1.096286
H	-1.561015	3.758185	-0.283518	H	-1.56227	3.736876	-0.272314	H	-1.567026	3.704192	-0.345587
Fe	-1.173988	-0.278761	0.076550	Fe	-1.169575	-0.273979	0.066971	C	-1.184925	-0.272520	0.075323
Fe	1.205226	-0.316657	-0.011428	Fe	1.202996	-0.315422	-0.013702	C	1.202668	-0.313642	-0.022324
C	-3.041070	0.771519	-0.439987	C	-3.043533	0.769389	-0.41377	H	-3.067110	0.757844	-0.449079
C	-3.072362	0.334348	0.924785	C	-3.05913	0.318716	0.938547	C	-3.090296	0.369304	0.932729
H	-3.152617	0.971722	1.797878	H	-3.137533	0.94281	1.81463	H	-3.174160	1.035470	1.783402
C	-2.992578	-1.085853	0.925286	C	-2.973145	-1.092637	0.921696	C	-3.014750	-1.046551	0.985643
H	-2.975546	-1.730639	1.795748	H	-2.950199	-1.745163	1.77996	H	-2.997287	-1.657430	1.880303
C	-2.988840	-0.372457	-1.272585	C	-2.994832	-0.358443	-1.255241	C	-3.015140	-0.416199	-1.237905
H	-2.909469	-0.369710	-2.352839	H	-2.936342	-0.343206	-2.332023	H	-2.953792	-0.455020	-2.318954
C	-2.908370	-1.515701	-0.435059	C	-2.902255	-1.504553	-0.437138	C	-2.932250	-1.529023	-0.357384
H	-2.823201	-2.543695	-0.766981	H	-2.82255	-2.523641	-0.780294	C	-2.861352	-2.569378	-0.650372
C	3.032262	0.180631	-0.915964	C	3.029654	0.162626	-0.90703	H	3.076977	0.159046	-0.873037
C	2.986870	0.734722	0.404305	C	2.980923	0.724714	0.400888	C	3.001425	0.726346	0.440933
H	3.023619	1.787837	0.654658	H	3.033306	1.77339	0.642983	H	3.062772	1.778417	0.686468
C	2.826423	-0.325122	1.337281	C	2.809405	-0.320774	1.336259	C	2.814695	-0.323057	1.376425
H	2.741011	-0.226205	2.411859	H	2.727929	-0.213924	2.405588	H	2.695571	-0.211345	2.446623
C	2.918090	-1.232985	-0.792875	C	2.907906	-1.24161	-0.773133	C	2.939777	-1.249416	-0.741121
H	2.900659	-1.944682	-1.609444	H	2.897632	-1.957514	-1.579468	H	2.939373	-1.967753	-1.551576
C	2.788659	-1.542886	0.595877	C	2.770551	-1.538048	0.609374	H	2.767229	-1.546649	0.647792
H	2.646836	-2.531968	1.015275	H	2.62928	-2.518827	1.034658	H	2.620750	-2.530733	1.075350
H	-3.083781	1.799671	-0.779140	H	-3.102048	1.795625	-0.738426	Fe	-3.120208	1.771649	-0.825967
H	3.151222	0.729907	-1.842723	H	3.163887	0.700356	-1.832098	Fe	3.227889	0.697661	-1.800549

Tables S59 : Optimized coordinates for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-1S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.002699	1.417775	-0.678839	C	0.001819	1.414064	-0.673911	C	0.002404	1.435482	-0.669230
C	-0.002699	1.417769	0.678842	C	-0.001817	1.414073	0.673905	C	-0.002404	1.435482	0.669230
C	0.009791	2.325555	-1.853292	C	0.006649	2.308798	-1.84802	C	0.007986	2.303645	-1.880668
H	0.893889	2.974938	-1.833365	H	0.887226	2.955463	-1.838077	H	0.894346	2.949082	-1.877654
H	-0.874786	2.974513	-1.844269	H	-0.872568	2.957352	-1.844184	H	-0.882159	2.943828	-1.888542
H	0.015734	1.776762	-2.799190	H	0.009308	1.759326	-2.788282	H	0.015157	1.705378	-2.795485
C	-0.009799	2.325536	1.853307	C	-0.006644	2.308831	1.847997	C	-0.007985	2.303644	1.880668
H	-0.893934	2.974873	1.833416	H	-0.887214	2.955505	1.838035	H	-0.894344	2.949083	1.877655
H	-0.015686	1.776730	2.799197	H	-0.009315	1.759378	2.78827	H	-0.015157	1.705377	2.795485
H	0.874743	2.974543	1.844266	H	0.87258	2.957375	1.844152	H	0.882161	2.943826	1.888543
C	-2.647275	-0.827983	-1.215284	C	-2.670338	-0.779943	-1.202852	C	-2.663477	-0.805465	-1.212734
C	-3.221274	0.080621	-0.273362	C	-3.218976	0.087812	-0.21953	C	-3.220315	0.088953	-0.247123
H	-3.800909	0.964148	-0.512890	H	-3.806268	0.971975	-0.411629	H	-3.807253	0.973640	-0.463814
C	-2.925460	-0.395947	1.046607	C	-2.895441	-0.435442	1.066797	C	-2.916461	-0.415310	1.060729
H	-3.222064	0.079566	1.973593	H	-3.176403	-0.002537	2.013649	H	-3.208992	0.039022	1.999601
C	-1.959122	-1.829222	-0.479742	C	-1.97064	-1.802169	-0.526775	C	-1.961658	-1.817044	-0.505125
H	-1.382376	-2.645322	-0.900115	H	-1.41398	-2.603017	-0.988075	H	-1.401486	-2.632248	-0.946833
C	-2.141530	-1.569544	0.921040	C	-2.118616	-1.595162	0.879292	C	-2.128464	-1.581868	0.904326
H	-1.729346	-2.155521	1.733383	H	-1.69581	-2.212631	1.655516	H	-1.714048	-2.186976	1.701153
C	1.959219	-1.829083	0.480170	C	1.970559	-1.802291	0.526463	C	1.961656	-1.817047	0.505118
C	2.647523	-0.827606	1.215249	C	2.67016	-0.780229	1.202897	C	2.663473	-0.805471	1.212735
H	2.694432	-0.743372	2.293597	H	2.7482	-0.660185	2.271278	H	2.728205	-0.704281	2.288957
C	3.221331	0.080712	0.272915	C	3.218944	0.087758	0.219868	C	3.220314	0.088951	0.247130
H	3.801022	0.964319	0.512048	H	3.806204	0.971878	0.412264	H	3.807251	0.973638	0.463829
C	2.141329	-1.569831	-0.920741	C	2.118753	-1.594959	-0.87953	C	2.128467	-1.581864	-0.904331
H	1.728964	-2.156064	-1.732816	H	1.696072	-2.212246	-1.655965	H	1.714055	-2.186967	-1.701163
C	2.925253	-0.396280	-1.046846	C	2.895597	-0.435185	-1.066635	C	2.916464	-0.415305	-1.060725
H	3.221669	0.078938	-1.974048	H	3.176699	-0.002049	-2.01334	H	3.208999	0.039033	-1.999593
H	1.382560	-2.645056	0.900920	H	1.413832	-2.603249	0.98749	H	1.401483	-2.632253	0.946819
H	-2.693963	-0.744100	-2.293663	H	-2.748539	-0.659638	-2.271193	H	-2.728213	-0.704269	-2.288955
Ni	1.147201	0.055989	0.004758	Ni	1.145131	0.058777	0.002986	Ni	1.132291	0.059364	0.005049
Ni	-1.147196	0.055985	-0.004765	Ni	-1.145134	0.058779	-0.002976	Ni	-1.132291	0.059364	-0.005049

Tables S60 : Optimized coordinates for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-2T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.070742	1.509382	-0.659567	C	-0.070902	1.507621	-0.654677	C	-0.180183	1.548019	-0.633357
C	0.070724	1.509360	0.659581	C	0.070904	1.507625	0.654675	C	0.180182	1.548014	0.633360
C	-0.126015	2.367670	-1.869199	C	-0.129379	2.359156	-1.858928	C	-0.390076	2.420505	-1.827794
H	0.777369	2.984218	-1.948254	H	0.772086	2.969414	-1.94714	H	0.485829	3.057724	-1.995096
H	-0.987326	3.044420	-1.816911	H	-0.982423	3.039138	-1.805745	H	-1.261421	3.065534	-1.664754
H	-0.216555	1.780292	-2.786307	H	-0.228413	1.777323	-2.773276	H	-0.567801	1.824588	-2.725942

C	0.125973	2.367621	1.869234	C	0.129385	2.35917	1.858919	C	0.390073	2.420491	1.827804
H	-0.777408	2.984174	1.948279	H	-0.772076	2.969434	1.947125	H	-0.485844	3.057690	1.995124
H	0.216488	1.780225	2.786333	H	0.228415	1.777344	2.773272	H	0.567821	1.824568	2.725943
H	0.987291	3.044365	1.816979	H	0.982434	3.039146	1.80573	H	1.261402	3.065540	1.664760
C	-2.683938	-0.869419	-1.164576	C	-2.696011	-0.841188	-1.155434	C	-2.726996	-0.937991	-1.104578
C	-3.320076	0.033365	-0.263620	C	-3.314957	0.0314	-0.226799	C	-3.352304	-0.037262	-0.192850
H	-3.911277	0.897881	-0.539452	H	-3.916085	0.893125	-0.469088	H	-3.989984	0.797826	-0.456838
C	-2.978097	-0.359788	1.056195	C	-2.951523	-0.391758	1.06953	C	-2.961109	-0.408428	1.124105
H	-3.272240	0.146280	1.968113	H	-3.237397	0.082992	1.995066	H	-3.250402	0.095283	2.038871
C	-1.994539	-1.860353	-0.393407	C	-1.994031	-1.842994	-0.425145	C	-1.975456	-1.886177	-0.343639
H	-1.416270	-2.687587	-0.788175	H	-1.428458	-2.658046	-0.848543	H	-1.379730	-2.695792	-0.747972
C	-2.167836	-1.537953	0.979686	C	-2.145816	-1.559792	0.950386	C	-2.114370	-1.556920	1.033993
H	-1.750730	-2.078451	1.820747	H	-1.722327	-2.122771	1.766822	H	-1.659993	-2.080977	1.865828
C	1.994712	-1.860125	0.394126	C	1.994001	-1.843034	0.425028	C	1.975438	-1.886192	0.343579
C	2.684349	-0.868771	1.164546	C	2.695943	-0.841294	1.155444	C	2.726951	-0.938040	1.104585
H	2.736555	-0.829729	2.246145	H	2.77061	-0.779736	2.229806	H	2.819810	-0.920653	2.183933
C	3.320164	0.033546	0.262907	C	3.314945	0.031373	0.226918	C	3.352296	-0.037274	0.192918
H	3.911433	0.898226	0.538078	H	3.916064	0.893074	0.469318	H	3.989968	0.797801	0.456965
C	2.167553	-1.538466	-0.979195	C	2.145863	-1.559709	-0.95047	C	2.114404	-1.556878	-1.034034
H	1.750181	-2.079423	-1.819829	H	1.722417	-2.122614	-1.766979	H	1.660057	-2.080900	-1.865908
C	2.977729	-0.360303	-1.056592	C	2.951587	-0.391672	-1.069466	C	2.961151	-0.408386	-1.124067
H	3.271561	0.145291	-1.968873	H	3.237514	0.083158	-1.994946	H	3.250480	0.095362	-2.038801
H	1.416583	-2.687154	0.789529	H	1.428402	-2.658122	0.848322	H	1.379694	-2.695822	0.747856
H	-2.735793	-0.830947	-2.246212	H	-2.770738	-0.779536	-2.229787	H	-2.819897	-0.920560	-2.183922
Ni	1.142437	0.037394	0.018200	Ni	1.141745	0.043699	0.016821	Ni	1.176311	0.071642	0.004067
Ni	-1.142424	0.037368	-0.018232	Ni	-1.141747	0.043702	-0.016815	Ni	-1.176310	0.071641	-0.004074

Tables S61 : Optimized coordinates for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-3S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.105124	1.589172	0.211148	C	0.100184	1.582938	0.216328	C	0.083128	1.535152	0.238596
C	-0.817645	1.987727	-0.802131	C	-0.805376	1.982499	-0.80036	C	-0.758953	2.018425	-0.792733
C	0.199543	2.419181	1.458050	C	0.189198	2.400712	1.464122	C	0.168854	2.329340	1.521938
H	0.422206	1.811187	2.340459	H	0.391409	1.790099	2.34321	H	0.289491	1.673520	2.389504
H	-0.713247	3.001217	1.653480	H	-0.712673	2.992322	1.651391	H	-0.710951	2.967864	1.683636
H	1.023989	3.137050	1.353976	H	1.02131	3.104934	1.378321	H	1.053681	2.978026	1.481964
C	-0.931579	1.135150	-1.936461	C	-0.914463	1.139686	-1.930601	C	-0.968554	1.180873	-1.924304
H	-0.028291	0.687931	-2.352929	H	-0.019279	0.687636	-2.344654	H	-0.124847	0.652417	-2.366363
H	-1.548693	2.784900	-0.624787	H	-1.525115	2.784611	-0.632468	H	-1.423139	2.867883	-0.611742
H	-1.764802	1.263440	-2.626286	H	-1.738505	1.271292	-2.622744	H	-1.787894	1.414073	-2.602107
C	2.556170	-1.059279	1.132296	C	2.556001	-1.053267	1.125185	C	2.661315	-1.283796	0.894192
C	3.022376	0.216938	0.735265	C	3.016789	0.215624	0.728256	C	3.015228	0.077004	0.885446
H	3.333633	1.021393	1.392617	H	3.33519	1.014002	1.381165	H	3.268703	0.687571	1.743726
C	3.057436	0.259818	-0.717454	C	3.049173	0.256695	-0.717504	C	2.967938	0.533023	-0.493242

H	3.408931	1.093299	-1.313693	H	3.404485	1.083081	-1.31252	H	3.213438	1.533261	-0.830274
C	2.216567	-1.766877	-0.061013	C	2.216455	-1.758075	-0.059744	C	2.381431	-1.672095	-0.462711
H	1.779011	-2.759893	-0.100824	H	1.785538	-2.748395	-0.097072	H	2.058216	-2.659060	-0.775729
C	2.595180	-0.987762	-1.200323	C	2.5894	-0.983867	-1.194558	C	2.662342	-0.582834	-1.326989
H	2.493005	-1.282009	-2.237490	H	2.491167	-1.280677	-2.226311	H	2.583526	-0.577661	-2.406918
C	-1.687267	-1.861683	-0.322780	C	-1.67829	-1.855868	-0.31782	C	-1.793051	-1.799395	-0.508743
C	-2.902484	-1.146730	-0.563651	C	-2.887002	-1.149569	-0.57108	C	-3.014264	-1.050152	-0.459269
H	-3.482970	-1.182092	-1.477538	H	-3.459782	-1.194695	-1.483848	H	-3.741040	-0.982398	-1.259878
C	-3.209859	-0.371413	0.591911	C	-3.206887	-0.37712	0.573118	C	-3.123831	-0.444630	0.826269
H	-4.066621	0.280077	0.711203	H	-4.066735	0.263822	0.684482	H	-3.935131	0.184458	1.170898
C	-1.228987	-1.502291	0.985292	C	-1.236365	-1.493336	0.985919	C	-1.114705	-1.621204	0.734967
H	-0.342496	-1.879744	1.480002	H	-0.361948	-1.87007	1.490478	H	-0.220926	-2.134504	1.065750
C	-2.174268	-0.575429	1.540301	C	-2.185495	-0.573157	1.525913	C	-1.937683	-0.746294	1.540163
H	-2.093243	-0.102250	2.511687	H	-2.120187	-0.104525	2.495295	H	-1.688771	-0.402539	2.537137
H	-1.195806	-2.542651	-1.006377	H	-1.184596	-2.539859	-0.988662	H	-1.443242	-2.390467	-1.345900
H	2.421279	-1.410352	2.148184	H	2.430974	-1.405287	2.136662	H	2.571074	-1.920011	1.766863
Ni	-1.274975	0.156194	-0.238047	Ni	-1.276277	0.160159	-0.238446	Ni	-1.341628	0.203416	-0.241066
Ni	1.116128	0.060212	-0.053181	Ni	1.115878	0.059424	-0.047831	Ni	1.079579	-0.015307	0.038136

Tables S62 : Optimized coordinates for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-4S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.961650	1.855372	-0.725288	C	-0.962597	1.852809	-0.720498	C	-0.985378	1.866430	-0.729047
C	-0.114373	1.486814	0.330050	C	-0.113957	1.487236	0.322926	C	-0.121529	1.489209	0.296392
C	-2.119280	2.801697	-0.523415	C	-2.116064	2.794103	-0.520494	C	-2.111668	2.852842	-0.496484
H	-1.819103	3.839498	-0.719331	H	-1.824228	3.826337	-0.732242	H	-1.794967	3.870976	-0.756889
H	-2.497412	2.751820	0.502401	H	-2.485634	2.75904	0.503532	H	-2.422190	2.847330	0.552959
H	-2.947048	2.569726	-1.202092	H	-2.946369	2.554369	-1.185288	H	-2.980613	2.603914	-1.115034
C	0.628216	1.652300	1.508632	C	0.623183	1.654782	1.494057	C	0.617490	1.713311	1.461208
H	0.312431	1.181224	2.440022	H	0.314495	1.188779	2.424508	H	0.353390	1.215903	2.392534
H	-0.567294	1.798993	-1.742981	H	-0.580474	1.794083	-1.737058	H	-0.646030	1.754210	-1.759074
H	1.248983	2.544471	1.628635	H	1.237583	2.545011	1.616759	H	1.184576	2.639790	1.557268
C	-2.509522	-1.299421	-1.038789	C	-2.501243	-1.299256	-1.034465	C	-2.451445	-1.372833	-1.055167
C	-3.110428	-0.607740	0.068949	C	-3.101542	-0.613563	0.06722	C	-3.107254	-0.641084	-0.006410
H	-3.941401	0.085782	0.000716	H	-3.933084	0.071457	-0.000299	H	-3.945148	0.033587	-0.140884
C	-2.465695	-1.019661	1.274707	C	-2.461441	-1.023477	1.266845	C	-2.532772	-1.015480	1.248874
H	-2.701554	-0.676993	2.274210	H	-2.703659	-0.689954	2.262769	H	-2.827659	-0.643170	2.221952
C	-1.438976	-2.063419	-0.524332	C	-1.435933	-2.056311	-0.522447	C	-1.394269	-2.093201	-0.459849
H	-0.757662	-2.681506	-1.097836	H	-0.757608	-2.67229	-1.091754	H	-0.678601	-2.724709	-0.972238
C	-1.400527	-1.876134	0.909094	C	-1.400593	-1.872182	0.904085	C	-1.436932	-1.859190	0.968887
H	-0.685157	-2.331894	1.583734	H	-0.691852	-2.330098	1.575931	H	-0.750429	-2.280474	1.693351
C	2.131370	-1.616866	-0.109834	C	2.125513	-1.610466	-0.098685	C	2.144251	-1.619554	-0.016308
C	2.989115	-0.884964	0.741236	C	2.977826	-0.880429	0.745121	C	3.002646	-0.834427	0.780233
H	3.275310	-1.148623	1.751110	H	3.263573	-1.14058	1.750953	H	3.296219	-1.032574	1.803417

C	3.368648	0.309460	0.039446	C	3.362551	0.301072	0.040405	C	3.374018	0.318861	0.003376
H	4.001115	1.095918	0.434548	H	3.998415	1.081688	0.428475	H	4.011586	1.125640	0.345725
C	2.008278	-0.892889	-1.356082	C	2.010984	-0.898806	-1.344189	C	2.010593	-0.968561	-1.302797
H	1.416110	-1.204708	-2.208496	H	1.427864	-1.216	-2.194262	H	1.415897	-1.333854	-2.131358
C	2.815237	0.266780	-1.276051	C	2.816767	0.251515	-1.269421	C	2.829115	0.186072	-1.307095
H	2.930691	1.023428	-2.041607	H	2.943827	0.995371	-2.039008	H	2.943166	0.890371	-2.121511
H	1.641888	-2.555165	0.124851	H	1.636668	-2.542492	0.137604	H	1.663252	-2.545366	0.274889
H	-2.802445	-1.214822	-2.077382	H	-2.796114	-1.220195	-2.067955	H	-2.693464	-1.330991	-2.109689
Ni	1.284676	0.263981	0.239914	Ni	1.285305	0.270088	0.23529	Ni	1.281107	0.283877	0.229793
Ni	-1.107173	-0.040593	-0.081358	Ni	-1.10831	-0.038898	-0.079412	Ni	-1.107899	-0.041911	-0.088732

Tables S63 : Optimized coordinates for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-5S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	1.988449	-0.744372	0.710952	C	1.984858	-0.734529	0.706291	C	2.005141	-0.780365	0.702519
C	1.988449	-0.744372	-0.710952	C	1.984858	-0.734529	-0.706291	C	2.005141	-0.780365	-0.702519
C	1.613959	0.560497	1.302715	C	1.612373	0.560457	1.301227	C	1.568011	0.509723	1.311378
H	2.387249	1.340130	1.214106	H	2.379599	1.338817	1.220114	H	2.347512	1.285769	1.281189
H	1.251702	0.505875	2.334321	H	1.248183	0.504766	2.326094	H	1.192128	0.404902	2.333012
H	2.387249	1.340130	-1.214106	H	2.379599	1.338817	-1.220114	H	2.347512	1.285769	-1.281189
C	1.613959	0.560497	-1.302715	C	1.612373	0.560457	-1.301227	C	1.568011	0.509723	-1.311378
H	1.251702	0.505875	-2.334321	H	1.248183	0.504766	-2.326094	H	1.192128	0.404902	-2.333012
H	2.429756	-1.555924	1.293452	H	2.430017	-1.541477	1.282877	H	2.439055	-1.596495	1.280308
H	2.429756	-1.555924	-1.293452	H	2.430017	-1.541477	-1.282877	H	2.439055	-1.596495	-1.280308
C	-0.190849	-3.253530	0.000000	C	-0.186914	-3.249062	0.000000	C	-0.172988	-3.230061	0.000000
C	-0.788518	-2.669629	-1.161455	C	-0.783831	-2.671053	-1.154987	C	-0.801953	-2.681298	-1.165770
H	-0.549889	-2.909438	-2.189992	H	-0.550154	-2.913894	-2.178951	H	-0.560629	-2.921195	-2.193752
C	-1.693635	-1.674332	-0.721640	C	-1.687984	-1.685664	-0.717873	C	-1.713906	-1.700586	-0.724087
H	-2.287221	-1.026328	-1.356179	H	-2.286610	-1.047843	-1.348762	H	-2.321510	-1.062802	-1.354235
C	-0.788518	-2.669629	1.161455	C	-0.783831	-2.671053	1.154987	C	-0.801953	-2.681298	1.165770
H	-0.549889	-2.909438	2.189992	H	-0.550154	-2.913894	2.178951	H	-0.560629	-2.921195	2.193752
C	-1.693635	-1.674332	0.721640	C	-1.687984	-1.685664	0.717873	C	-1.713906	-1.700586	0.724087
H	-2.287221	-1.026328	1.356179	H	-2.286610	-1.047843	1.348762	H	-2.321510	-1.062802	1.354235
C	-0.195705	3.112546	0.707803	C	-0.203138	3.109312	0.703699	C	-0.180631	3.153214	0.705076
C	-1.213734	2.203571	1.148591	C	-1.212707	2.202033	1.142124	C	-1.188579	2.227184	1.145519
H	-1.453181	1.970656	2.179455	H	-1.454539	1.973906	2.168287	H	-1.429517	2.000456	2.177277
C	-1.863618	1.681548	0.000000	C	-1.856936	1.680366	0.000000	C	-1.849958	1.713352	0.000000
H	-2.677168	0.966205	0.000000	H	-2.667781	0.970473	0.000000	H	-2.671647	1.008713	0.000000
C	-0.195705	3.112546	-0.707803	C	-0.203138	3.109312	-0.703699	C	-0.180631	3.153214	-0.705076
H	0.477767	3.669381	-1.347906	H	0.461222	3.671004	-1.340960	H	0.484594	3.717451	-1.347506
C	-1.213734	2.203571	-1.148591	C	-1.212707	2.202033	-1.142124	C	-1.188579	2.227184	-1.145519
H	-1.453181	1.970656	-2.179455	H	-1.454539	1.973906	-2.168287	H	-1.429517	2.000456	-2.177277
H	0.477767	3.669381	1.347906	H	0.461222	3.671004	1.340960	H	0.484594	3.717451	1.347506
H	0.567833	-4.027728	0.000000	H	0.569192	-4.019054	0.000000	H	0.602740	-3.987440	0.000000

Ni	0.217465	-1.187653	0.000000	Ni	0.217991	-1.189213	0.000000	Ni	0.204712	-1.169187	0.000000
Ni	0.260891	1.153558	0.000000	Ni	0.260274	1.157911	0.000000	Ni	0.282657	1.158057	0.000000

Tables S64 : Optimized coordinates for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-6T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.031878	1.596184	0.240968	C	0.026545	1.591532	0.248842	C	0.007343	1.605525	0.241007
C	-0.932113	2.036323	-0.700040	C	-0.925024	2.033843	-0.691057	C	-0.942642	2.051363	-0.704296
C	0.070762	2.257608	1.587994	C	0.064693	2.235756	1.597413	C	0.048304	2.300134	1.582882
H	0.307185	1.541405	2.383470	H	0.283536	1.513673	2.384959	H	0.260848	1.590313	2.388875
H	-0.867406	2.769129	1.852436	H	-0.863415	2.755144	1.859154	H	-0.885895	2.828856	1.821922
H	0.870716	3.009975	1.605820	H	0.87089	2.973911	1.632453	H	0.863114	3.035852	1.583351
C	-1.077930	1.239575	-1.876991	C	-1.067529	1.252792	-1.867486	C	-1.129522	1.255369	-1.873023
H	-0.188357	0.873297	-2.393270	H	-0.18556	0.88519	-2.383395	H	-0.267871	0.869487	-2.417305
H	-1.677526	2.802007	-0.452443	H	-1.660821	2.802194	-0.446598	H	-1.680013	2.818178	-0.447183
H	-1.948453	1.378645	-2.517569	H	-1.930682	1.397296	-2.508061	H	-2.016180	1.418531	-2.483612
C	2.422089	-0.789357	1.265833	C	2.421966	-0.794498	1.255659	C	2.809546	-0.377658	1.221090
C	3.225569	0.238067	0.694948	C	3.219449	0.230042	0.691653	C	3.404475	0.340248	0.145395
H	3.611902	1.106254	1.215218	H	3.612726	1.087103	1.215067	H	3.936146	1.280781	0.221776
C	3.352114	-0.027495	-0.693968	C	3.343733	-0.027385	-0.690772	C	3.140591	-0.377405	-1.056730
H	3.886105	0.582144	-1.412813	H	3.88052	0.579021	-1.403018	H	3.452933	-0.085214	-2.052622
C	2.090425	-1.720479	0.234670	C	2.089981	-1.714631	0.225975	C	2.193712	-1.546656	0.686846
H	1.493846	-2.617519	0.354968	H	1.499162	-2.609416	0.343425	H	1.651717	-2.295158	1.253301
C	2.652698	-1.245927	-0.980460	C	2.648079	-1.23784	-0.980582	C	2.397403	-1.550346	-0.722679
H	2.578415	-1.725349	-1.949122	H	2.578596	-1.714012	-1.945811	H	2.054318	-2.307236	-1.417887
C	-1.582952	-1.943084	-0.150242	C	-1.57206	-1.937487	-0.144239	C	-1.414098	-1.943223	0.058660
C	-2.749855	-1.309463	-0.679732	C	-2.73155	-1.317128	-0.684056	C	-2.515646	-1.489902	-0.724183
H	-3.158675	-1.468647	-1.670335	H	-3.132577	-1.487532	-1.670802	H	-2.740328	-1.793703	-1.739412
C	-3.307660	-0.460287	0.327074	C	-3.300985	-0.472187	0.308967	C	-3.323619	-0.619947	0.088702
H	-4.193516	0.153398	0.222461	H	-4.189914	0.12719	0.196554	H	-4.234251	-0.125328	-0.226631
C	-1.378951	-1.421988	1.159825	C	-1.384309	-1.412355	1.157601	C	-1.485350	-1.268863	1.313977
H	-0.559376	-1.667881	1.825598	H	-0.576447	-1.653337	1.830535	H	-0.774552	-1.362312	2.126336
C	-2.446753	-0.507531	1.448594	C	-2.456141	-0.509814	1.432052	C	-2.686269	-0.482083	1.338305
H	-2.556651	0.060386	2.365197	H	-2.581325	0.05341	2.343766	H	-3.014236	0.141751	2.161123
H	-0.953389	-2.657211	-0.665979	H	-0.940614	-2.65225	-0.645628	H	-0.638813	-2.628610	-0.258610
H	2.117804	-0.855493	2.304520	H	2.125025	-0.868784	2.290409	H	2.811112	-0.079527	2.262875
Ni	-1.289539	0.131231	-0.236781	Ni	-1.291934	0.135413	-0.237664	Ni	-1.304259	0.138325	-0.234178
Ni	1.254591	0.192432	-0.275326	Ni	1.254427	0.196278	-0.271365	Ni	1.239851	0.194318	-0.206965

Tables S65 : Optimized coordinates for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-1T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.123285	1.642363	-0.076084	C	0.130587	1.641571	-0.079721	C	-0.067704	1.569959	0.237544
C	0.865313	1.768873	1.126389	C	0.867742	1.768695	1.115769	C	-0.987876	2.017078	-0.733607

C	0.225838	2.689944	-1.148638	C	0.227771	2.678474	-1.154776	C	0.099888	2.325088	1.534904
H	0.090367	2.275804	-2.154928	H	0.112114	2.258895	-2.155073	H	0.335243	1.647662	2.362571
H	1.198079	3.204310	-1.124179	H	1.185616	3.208026	-1.123235	H	-0.806918	2.888527	1.796808
H	-0.546588	3.457884	-1.012375	H	-0.554891	3.432364	-1.036718	H	0.925848	3.043284	1.454171
C	0.740417	0.695383	2.060865	C	0.741901	0.711003	2.053294	C	-1.143472	1.184788	-1.889874
H	-0.254042	0.333655	2.319544	H	-0.243842	0.348191	2.316933	H	-0.262291	0.886540	-2.459014
H	1.672491	2.506568	1.211566	H	1.66621	2.507777	1.200499	H	-1.721934	2.793885	-0.499175
H	1.486075	0.600593	2.850439	H	1.485507	0.616666	2.837308	H	-2.034960	1.313789	-2.502549
C	-2.985072	-0.644336	-1.008059	C	-2.977422	-0.635555	-1.006282	C	2.572727	-0.860218	1.217842
C	-3.272835	0.351712	-0.018416	C	-3.269153	0.34227	-0.011019	C	3.181040	0.327398	0.732386
H	-3.836637	1.263753	-0.175485	H	-3.84047	1.24596	-0.156257	H	3.467078	1.185479	1.329152
C	-2.713580	-0.078845	1.220880	C	-2.712733	-0.097011	1.217052	C	3.313571	0.212209	-0.680966
H	-2.748121	0.468469	2.155389	H	-2.758619	0.432666	2.155374	H	3.742714	0.955863	-1.342019
C	-2.225490	-1.669647	-0.370209	C	-2.218227	-1.658405	-0.382474	C	2.322282	-1.715017	0.108010
H	-1.833512	-2.561059	-0.848254	H	-1.828366	-2.541256	-0.866393	H	1.871250	-2.699551	0.152331
C	-2.069514	-1.324023	1.001557	C	-2.066562	-1.329647	0.985722	C	2.786146	-1.054255	-1.071600
H	-1.505932	-1.887348	1.736733	H	-1.509331	-1.89909	1.713164	H	2.763806	-1.453609	-2.078707
C	1.509609	-1.958185	-0.083063	C	1.494866	-1.951006	-0.089204	C	-1.569497	-1.947959	-0.126866
C	2.605308	-1.391058	0.627028	C	2.582227	-1.399973	0.629576	C	-2.724758	-1.318293	-0.675652
H	2.925778	-1.668887	1.623513	H	2.893169	-1.687707	1.621118	H	-3.119041	-1.477526	-1.671499
C	3.170928	-0.347486	-0.169209	C	3.161139	-0.364084	-0.15271	C	-3.265111	-0.429204	0.305448
H	3.999835	0.289564	0.114918	H	3.993335	0.257588	0.137657	H	-4.134272	0.204374	0.178836
C	1.394994	-1.252348	-1.332912	C	1.400154	-1.245066	-1.331556	C	-1.377411	-1.419718	1.192333
H	0.656174	-1.442955	-2.103969	H	0.673858	-1.429381	-2.108319	H	-0.579098	-1.685490	1.874263
C	2.430588	-0.269469	-1.386839	C	2.438463	-0.276738	-1.370989	C	-2.430021	-0.489564	1.454256
H	2.593750	0.438651	-2.190720	H	2.620972	0.423912	-2.170651	H	-2.546124	0.094806	2.359145
H	0.869332	-2.762660	0.258004	H	0.85002	-2.75011	0.238888	H	-0.945696	-2.682600	-0.620226
H	-3.307861	-0.634856	-2.042017	H	-3.303559	-0.619431	-2.033972	H	2.320305	-1.067927	2.251204
Co	1.167276	0.032368	0.217360	Co	1.169082	0.03404	0.214743	Co	-1.282948	0.099018	-0.202239
Co	-1.176829	0.221012	-0.338765	Co	-1.178202	0.22847	-0.329796	Co	1.152032	0.109825	-0.249992

Tables S66 : Optimized coordinates for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-2T**

	M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
	x	y	z	x	y	z	x	y	z
C	0.000000	0.698330	1.357109	C	0.000000	0.693033	1.360134	C	1.394211	-0.028531	0.680894
C	0.000000	-0.698330	1.357109	C	0.000000	-0.693033	1.360134	C	1.394211	-0.028531	-0.680894
C	0.000000	1.779542	2.380212	C	0.000000	1.781081	2.364523	C	2.345926	0.184513	1.814461
H	-0.883877	1.705415	3.026782	H	-0.879325	1.718674	3.010324	H	3.026223	-0.672045	1.895947
H	0.000000	2.774827	1.926742	H	0.000000	2.767740	1.903231	H	1.813466	0.286358	2.763953
H	0.883877	1.705415	3.026782	H	0.879325	1.718674	3.010324	H	2.950267	1.085350	1.652952
C	0.000000	-1.779542	2.380212	C	0.000000	-1.781081	2.364523	C	2.345926	0.184513	-1.814461
H	-0.883877	-1.705415	3.026782	H	-0.879325	-1.718674	3.010324	H	3.026223	-0.672045	-1.895947
H	0.000000	-2.774827	1.926742	H	0.000000	-2.767740	1.903231	H	1.813466	0.286358	-2.763953
H	0.883877	-1.705415	3.026782	H	0.879325	-1.718674	3.010324	H	2.950267	1.085350	-1.652952

C	-1.155771	0.000000	0.025301	Co	-1.153333	0.000000	0.030493	C	0.135587	-1.255144	0.000000
C	1.155771	0.000000	0.025301	Co	1.153333	0.000000	0.030493	C	-0.073066	1.090360	0.000000
H	-3.132702	-0.717841	-0.055606	C	-3.122788	-0.713902	-0.062725	H	-0.100527	-3.209372	-0.718704
C	-2.433616	-1.155916	-1.211125	C	-2.422118	-1.149460	-1.207961	C	-1.207424	-2.435510	-1.157463
H	-2.232313	-2.185026	-1.481945	H	-2.227467	-2.174297	-1.480997	H	-1.469240	-2.217536	-2.185261
C	-1.978089	0.000000	-1.915824	C	-1.965081	0.000000	-1.906152	C	-1.878563	-1.937665	0.000000
H	-1.395640	0.000000	-2.829081	H	-1.386383	0.000000	-2.815720	H	-2.738799	-1.280021	0.000000
C	-3.132702	0.717841	-0.055606	C	-3.122788	0.713902	-0.062725	C	-0.100527	-3.209372	0.718704
H	-3.576793	1.353983	0.700665	H	-3.575720	1.347071	0.683866	H	0.620965	-3.708519	1.354061
C	-2.433616	1.155916	-1.211125	C	-2.422118	1.149460	-1.207961	C	-1.207424	-2.435510	1.157463
C	-2.232313	2.185026	-1.481945	H	-2.227467	2.174297	-1.480997	C	-1.469240	-2.217536	2.185261
H	3.132702	-0.717841	-0.055606	C	3.122788	-0.713902	-0.062725	H	-0.013361	3.134457	-0.716343
C	2.433616	-1.155916	-1.211125	C	2.422118	-1.149460	-1.207961	C	-1.209394	2.507051	-1.154613
H	2.232313	-2.185026	-1.481945	H	2.227467	-2.174297	-1.480997	H	-1.498706	2.340705	-2.185627
C	1.978089	0.000000	-1.915824	C	1.965081	0.000000	-1.906152	C	-1.949046	2.102060	0.000000
H	1.395640	0.000000	-2.829081	H	1.386383	0.000000	-2.815720	H	-2.914349	1.610538	0.000000
C	3.132702	0.717841	-0.055606	C	3.122788	0.713902	-0.062725	C	-0.013361	3.134457	0.716343
H	3.576793	1.353983	0.700665	H	3.575720	1.347071	0.683866	H	0.765812	3.536178	1.353152
H	2.433616	1.155916	-1.211125	C	2.422118	1.149460	-1.207961	H	-1.209394	2.507051	1.154613
H	2.232313	2.185026	-1.481945	H	2.227467	2.174297	-1.480997	H	-1.498706	2.340705	2.185627
Co	-3.576793	-1.353983	0.700665	H	-3.575720	-1.347071	0.683866	Co	0.620965	-3.708519	-1.354061
Co	3.576793	-1.353983	0.700665	H	3.575720	-1.347071	0.683866	Co	0.765812	3.536178	-1.353152

Tables S67 : Optimized coordinates for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-3T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	1.240744	2.050564	0.171711	C	1.243162	2.049583	0.16593	C	1.354542	2.058733	0.183891
C	1.043420	1.725922	-1.216314	C	1.038804	1.722649	-1.21077	C	1.083341	1.796428	-1.201240
C	0.156417	2.607568	1.061190	C	0.177048	2.599304	1.069841	C	0.314428	2.566522	1.170051
H	0.229640	3.703749	1.127483	H	0.257488	3.689516	1.148071	H	0.411928	3.653518	1.299809
H	0.211256	2.218574	2.084315	H	0.241071	2.204644	2.084776	H	0.421323	2.101409	2.156056
H	-0.845994	2.378916	0.670938	H	-0.827204	2.38304	0.694286	H	-0.708916	2.379758	0.816679
C	0.030280	0.768597	-1.484429	C	0.033637	0.771468	-1.48003	C	0.059258	0.866305	-1.482654
H	-0.127065	0.441363	-2.516918	H	-0.129134	0.4524	-2.507792	H	-0.076651	0.576189	-2.527027
H	2.229709	2.458273	0.405468	H	2.230396	2.45026	0.392886	H	2.349941	2.462502	0.383116
H	1.787351	2.000588	-1.971376	H	1.771029	2.006118	-1.966592	H	1.810874	2.081984	-1.965252
C	2.693470	-0.514064	1.182909	C	2.666948	-0.52516	1.192311	C	2.652649	-0.631752	1.213280
C	3.195454	-0.672851	-0.147150	C	3.187458	-0.669268	-0.123791	C	3.221526	-0.773681	-0.094180
H	4.061434	-0.170385	-0.561262	H	4.058773	-0.168444	-0.515645	H	4.128181	-0.297381	-0.446538
C	2.341503	-1.583213	-0.836339	C	2.352062	-1.570616	-0.83041	C	2.366681	-1.615262	-0.853113
H	2.436802	-1.889141	-1.870821	H	2.469004	-1.871049	-1.859381	H	2.498152	-1.886568	-1.893473
C	1.520453	-1.311341	1.317297	C	1.500833	-1.322132	1.299421	C	1.455300	-1.400730	1.267170
H	0.907976	-1.408098	2.205860	H	0.88091	-1.433045	2.174795	H	0.802438	-1.510802	2.124178
C	1.299028	-1.967915	0.055551	C	1.302309	-1.964305	0.035452	C	1.265007	-1.991843	-0.026758

H	0.473748	-2.630774	-0.176799	H	0.49032	-2.629042	-0.212584	H	0.439686	-2.629051	-0.319339
C	-2.802562	-0.112690	1.248423	C	-2.784938	-0.122625	1.253264	C	-2.790513	-0.108828	1.290577
C	-2.330121	-1.406386	0.851558	C	-2.331376	-1.407373	0.834096	C	-2.354017	-1.396882	0.851151
H	-1.898487	-2.155254	1.507370	H	-1.904535	-2.167425	1.471321	H	-1.897081	-2.160668	1.469927
C	-2.533443	-1.546533	-0.547026	C	-2.549738	-1.524136	-0.555829	C	-2.641157	-1.508436	-0.538079
H	-2.256184	-2.403743	-1.148964	H	-2.293803	-2.373683	-1.169012	H	-2.413077	-2.359527	-1.168992
C	-3.277594	0.546214	0.077394	C	-3.265035	0.553669	0.104354	C	-3.337243	0.572242	0.162916
H	-3.698465	1.543609	0.032667	H	-3.681481	1.548403	0.080872	H	-3.753547	1.572702	0.161853
C	-3.106973	-0.340200	-1.026667	C	-3.115581	-0.313013	-1.008288	C	-3.242888	-0.294828	-0.963143
H	-3.344166	-0.115655	-2.059770	H	-3.3686	-0.075231	-2.029617	H	-3.552036	-0.057245	-1.974005
H	-2.820702	0.283620	2.256714	H	-2.792604	0.255141	2.263498	H	-2.736015	0.274050	2.302989
H	3.108923	0.135902	1.943284	H	3.070376	0.110812	1.964205	H	3.062155	-0.037967	2.021146
Co	-1.149655	0.162954	-0.065084	Co	-1.148603	0.157266	-0.072935	Co	-1.183795	0.182143	-0.135082
Co	1.250535	0.064692	-0.163688	Co	1.252101	0.063079	-0.167339	Co	1.286431	0.077455	-0.173078

Tables S68 : Optimized coordinates for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-4S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.753097	1.993387	0.646338	C	0.742644	1.991325	0.643368	C	0.753210	2.014845	0.644232
C	1.027258	1.991368	-0.752380	C	1.020166	1.986068	-0.744812	C	1.026594	2.006030	-0.746396
C	-0.643099	1.749279	1.085254	C	-0.644731	1.748479	1.083435	C	-0.647540	1.741147	1.086969
H	-1.325741	2.597372	0.902939	H	-1.328153	2.589458	0.90663	H	-1.329075	2.592682	0.929486
H	-0.697957	1.477878	2.145938	H	-0.701294	1.474425	2.137182	H	-0.678613	1.458527	2.144430
H	-0.994486	1.424671	-1.305186	H	-0.989832	1.41774	-1.30691	H	-0.983777	1.388998	-1.309833
C	0.121300	1.109957	-1.458414	C	0.124288	1.110503	-1.452327	C	0.144550	1.106585	-1.456958
H	0.260282	0.912689	-2.521792	H	0.265366	0.915196	-2.510302	H	0.292420	0.913025	-2.517713
H	1.486404	2.442267	1.322500	H	1.471117	2.439938	1.316581	H	1.476607	2.479254	1.316422
H	1.903175	2.449428	-1.207484	H	1.887793	2.452249	-1.195273	H	1.907684	2.456307	-1.195770
C	3.174286	-0.235255	0.249317	C	3.164624	-0.231784	0.258982	C	3.182130	-0.252357	0.251378
C	2.742857	-0.916284	-0.927474	C	2.74564	-0.903196	-0.91778	C	2.755635	-0.939032	-0.920040
H	3.136147	-0.774087	-1.926979	H	3.147988	-0.759191	-1.908206	H	3.152910	-0.803488	-1.918729
C	1.659573	-1.771066	-0.565412	C	1.670066	-1.760274	-0.570052	C	1.663760	-1.780301	-0.560476
H	1.096590	-2.404130	-1.241353	H	1.12154	-2.394225	-1.248316	H	1.102311	-2.411709	-1.237667
C	2.377294	-0.690145	1.348411	C	2.366863	-0.693775	1.344012	C	2.375430	-0.693450	1.348693
H	2.450770	-0.348271	2.373411	H	2.437598	-0.365071	2.368481	H	2.449776	-0.349353	2.372518
C	1.445423	-1.640916	0.847027	C	1.447004	-1.639857	0.833715	C	1.441179	-1.642313	0.848975
H	0.695145	-2.162031	1.429815	H	0.704086	-2.170891	1.406649	H	0.692066	-2.162253	1.431358
C	-2.970674	-0.054474	0.895555	C	-2.958954	-0.063152	0.89719	C	-2.977282	-0.064460	0.900734
C	-1.991067	-1.073208	1.154236	C	-1.986449	-1.080377	1.143347	C	-2.025215	-1.108721	1.136238
H	-1.564009	-1.310931	2.121736	H	-1.56101	-1.328034	2.103019	H	-1.608851	-1.379365	2.098468
C	-1.722164	-1.748083	-0.085130	C	-1.723282	-1.741257	-0.095655	C	-1.769803	-1.761888	-0.113662
H	-1.026890	-2.567027	-0.224830	H	-1.039707	-2.561515	-0.241922	H	-1.097804	-2.595808	-0.269153
C	-3.240981	-0.054550	-0.495691	C	-3.232782	-0.05162	-0.484821	C	-3.238681	-0.019506	-0.489866
H	-3.907661	0.622399	-1.016168	H	-3.902547	0.623036	-0.994447	H	-3.889250	0.683575	-0.995600

C	-2.464587	-1.107439	-1.100577	C	-2.464087	-1.095057	-1.097137	C	-2.485769	-1.076852	-1.116341
H	-2.434018	-1.343971	-2.157581	H	-2.444489	-1.327653	-2.150461	H	-2.458676	-1.290911	-2.178120
H	-3.372317	0.638577	1.624538	H	-3.359236	0.617938	1.631094	H	-3.367982	0.617085	1.645837
H	3.951758	0.518142	0.300609	H	3.938601	0.517476	0.320244	H	3.965040	0.494810	0.302075
Co	-1.229988	0.288546	-0.112478	Co	-1.231325	0.284736	-0.11311	Co	-1.208771	0.294274	-0.107110
Co	1.183014	0.174846	-0.097391	Co	1.184144	0.174633	-0.097365	Co	1.178624	0.177217	-0.096553

Tables S69 : Optimized coordinates for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-5T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	2.012759	-1.256569	0.712597	C	2.008117	-1.258309	0.707820	C	-1.463987	1.966500	-0.804407
C	2.012759	-1.256569	-0.712597	C	2.008117	-1.258309	-0.707820	C	-1.650722	2.028633	0.604724
C	1.321028	-0.139322	1.322488	C	1.329938	-0.145214	1.318618	C	-0.254177	1.344755	-1.280404
H	1.768366	0.881535	1.127842	H	1.773260	0.869491	1.125493	H	0.716666	1.815503	-0.963632
H	1.077674	-0.234819	2.380809	H	1.084816	-0.239116	2.370964	H	-0.242789	1.091995	-2.338927
H	1.768366	0.881535	-1.127842	H	1.773260	0.869491	-1.125493	H	0.420667	1.732635	1.284285
C	1.321028	-0.139322	-1.322488	C	1.329938	-0.145214	-1.318618	C	-0.629591	1.440058	1.416035
H	1.077674	-0.234819	-2.380809	H	1.084816	-0.239116	-2.370964	H	-0.876374	1.231612	2.454607
H	2.398631	-2.100269	1.281494	H	2.396071	-2.097139	1.273064	H	-2.280782	2.223607	-1.474387
H	2.398631	-2.100269	-1.281494	H	2.396071	-2.097139	-1.273064	H	-2.618095	2.315366	1.010787
C	-0.621969	-3.174694	0.000000	C	-0.629069	-3.162788	0.000000	C	-3.119667	-0.944883	-0.058133
C	-1.061672	-2.462870	-1.157751	C	-1.064762	-2.454109	-1.151190	C	-2.372495	-1.229951	1.120360
H	-0.865595	-2.735452	-2.187506	H	-0.876979	-2.730356	-2.176539	H	-2.704832	-1.067220	2.138257
C	-1.748241	-1.293143	-0.714851	C	-1.744045	-1.288959	-0.710963	C	-1.090405	-1.738588	0.730196
H	-2.153328	-0.512861	-1.348273	H	-2.152934	-0.516005	-1.341620	H	-0.283041	-2.025393	1.390829
C	-1.061672	-2.462870	1.157751	C	-1.064762	-2.454109	1.151190	C	-2.295523	-1.241213	-1.180085
H	-0.865595	-2.735452	2.187506	H	-0.876979	-2.730356	2.176539	H	-2.557311	-1.097727	-2.220992
C	-1.748241	-1.293143	0.714851	C	-1.744045	-1.288959	0.710963	C	-1.043790	-1.743796	-0.692959
H	-2.153328	-0.512861	1.348273	H	-2.152934	-0.516005	1.341620	H	-0.192327	-2.033257	-1.295219
C	0.192719	3.255635	0.711102	C	0.197952	3.245544	0.706741	C	3.334701	0.441730	-0.632847
C	-0.945483	2.507898	1.153777	C	-0.938551	2.508239	1.147150	C	2.836556	-0.813746	-1.091148
H	-1.229089	2.327917	2.184676	H	-1.226245	2.337189	2.173041	H	2.816019	-1.156037	-2.119474
C	-1.649489	2.065689	0.000000	C	-1.641583	2.073197	0.000000	C	2.411640	-1.553901	0.053640
H	-2.558173	1.472726	0.000000	H	-2.551672	1.492981	0.000000	H	2.002756	-2.559516	0.044258
C	0.192719	3.255635	-0.711102	C	0.197952	3.245544	-0.706741	C	3.215592	0.480346	0.789370
H	0.924416	3.739756	-1.347512	H	0.925431	3.728337	-1.340635	H	3.547153	1.285903	1.434635
C	-0.945483	2.507898	-1.153777	C	-0.938551	2.508239	-1.147150	C	2.646022	-0.762811	1.214229
H	-1.229089	2.327917	-2.184676	H	-1.226245	2.337189	-2.173041	H	2.456399	-1.059841	2.239808
H	0.924416	3.739756	1.347512	H	0.925431	3.728337	1.340635	H	3.746209	1.228461	-1.255394
H	-0.038762	-4.088112	0.000000	H	-0.056163	-4.077144	0.000000	H	-4.116935	-0.523320	-0.092735
Co	0.379357	1.243012	0.000000	Co	0.371457	1.240399	0.000000	Co	1.235927	0.300827	-0.052386
Co	0.181020	-1.272706	0.000000	Co	0.181178	-1.272599	0.000000	Co	-1.346235	0.164300	0.001714

Tables S70 : Optimized coordinates for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-6S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.063965	1.450820	0.669112	C	0.062594	1.45104	0.664026	C	-0.260798	1.493193	-0.627449
C	-0.063960	1.450855	-0.669101	C	-0.062594	1.45104	-0.664026	C	0.260849	1.493209	0.627459
C	0.112888	2.390845	1.817095	C	0.112412	2.380821	1.81003	C	-0.490272	2.539250	-1.671601
H	-0.794556	3.006976	1.854076	H	-0.790985	2.994159	1.853692	H	0.455941	3.023344	-1.944248
H	0.964731	3.075390	1.715507	H	0.959034	3.065045	1.713368	H	-1.159133	3.317346	-1.281357
H	0.209885	1.874527	2.776725	H	0.211187	1.866037	2.764949	H	-0.938837	2.120673	-2.576833
C	-0.112848	2.390951	-1.817028	C	-0.112412	2.380819	-1.810031	C	0.490377	2.539304	1.671560
H	0.794629	3.007036	-1.853977	H	0.790987	2.994156	-1.853695	H	-0.455833	3.023364	1.944275
H	-0.209876	1.874696	-2.776688	H	-0.211188	1.866034	-2.764949	H	0.939036	2.120773	2.576765
H	-0.964654	3.075535	-1.715394	H	-0.959033	3.065044	-1.713369	H	1.159168	3.317421	1.281235
C	2.555566	-0.807693	1.177412	C	2.5591	-0.78355	1.169366	C	-2.616122	-0.849990	-1.081856
C	3.149177	0.136015	0.287044	C	3.141747	0.133386	0.257903	C	-3.190575	0.018398	-0.115627
H	3.665747	1.044639	0.570756	H	3.672419	1.036155	0.514865	H	-3.794954	0.893838	-0.317148
C	2.849740	-0.280635	-1.041039	C	2.825578	-0.306797	-1.050057	C	-2.751386	-0.423025	1.170926
H	3.105512	0.253857	-1.948347	H	3.079292	0.200633	-1.967666	H	-2.968756	0.064056	2.113975
C	1.943191	-1.848130	0.392754	C	1.935176	-1.830866	0.417944	C	-1.862608	-1.859508	-0.385260
H	1.413516	-2.711125	0.778682	H	1.414552	-2.682592	0.826596	H	-1.293351	-2.654755	-0.850321
C	2.131005	-1.519762	-0.976260	C	2.107121	-1.534808	-0.951522	C	-1.967405	-1.608922	1.007044
H	1.747646	-2.072899	-1.825235	H	1.721473	-2.106788	-1.780623	H	-1.490813	-2.170424	1.800222
C	-1.943201	-1.848134	-0.392720	C	-1.93518	-1.83086	-0.41796	C	1.862736	-1.859372	0.385739
C	-2.555607	-0.807728	-1.177395	C	-2.559109	-0.783535	-1.169365	C	2.616453	-0.849612	1.081768
H	-2.565579	-0.751381	-2.259589	H	-2.587596	-0.709093	-2.245285	H	2.711533	-0.761129	2.157065
C	-3.149196	0.136008	-0.287042	C	-3.141749	0.13339	-0.257887	C	3.190593	0.018450	0.115070
H	-3.665783	1.044618	-0.570771	H	-3.672422	1.036163	-0.514833	H	3.795011	0.893977	0.316103
C	-2.130974	-1.519718	0.976289	C	-2.107116	-1.53482	0.951511	C	1.967132	-1.609287	-1.006689
H	-1.747584	-2.072819	1.825273	H	-1.721462	-2.106811	1.780602	H	1.490328	-2.171084	-1.799529
C	-2.849719	-0.280595	1.041046	C	-2.82557	-0.306809	1.050066	C	2.751032	-0.423430	-1.171208
H	-3.105462	0.253929	1.948342	H	-3.079278	0.200609	1.967683	H	2.968115	0.063333	-2.114488
H	-1.413537	-2.711142	-0.778635	H	-1.414558	-2.682581	-0.826626	H	1.293611	-2.654454	0.851248
H	2.565502	-0.751307	2.259604	H	2.587581	-0.709121	2.245287	H	-2.710880	-0.761874	-2.157212
Co	-1.079719	-0.031461	-0.007738	Co	-1.078200	-0.026625	-0.006381	Co	1.104592	0.011535	-0.013138
Co	1.079708	-0.031469	0.007689	Co	1.078200	-0.026625	0.006382	Co	-1.104600	0.011563	0.013175

Tables S71 : Optimized coordinates for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-7S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.834284	2.041196	0.361154	C	0.840107	2.042318	0.34692	C	0.870681	2.049329	0.337709
C	0.832389	1.824350	-1.063800	C	0.828273	1.813477	-1.066738	C	0.830337	1.828708	-1.083035
C	-0.471256	2.195867	1.088852	C	-0.446299	2.208502	1.091277	C	-0.417378	2.216980	1.113471
H	-0.733937	3.252069	1.269670	H	-0.699702	3.262949	1.270312	H	-0.670482	3.277683	1.264298
H	-0.508071	1.687364	2.056621	H	-0.471844	1.710663	2.059216	H	-0.400666	1.732887	2.092974
H	-1.362308	1.927885	0.440079	H	-1.344599	1.933182	0.468229	H	-1.329315	1.906070	0.521138

C	-0.089038	0.814451	-1.456741	C	-0.089032	0.810734	-1.453334	C	-0.093494	0.815718	-1.450848
H	-0.129786	0.492805	-2.502449	H	-0.13651	0.491957	-2.493147	H	-0.146241	0.502998	-2.495966
H	1.666856	2.608833	0.783638	H	1.676846	2.603200	0.756044	H	1.712288	2.621519	0.730841
H	1.592894	2.248216	-1.724420	H	1.576418	2.239011	-1.732006	H	1.576686	2.242593	-1.761505
C	2.781074	-0.275739	1.104777	C	2.753402	-0.290911	1.119511	C	2.720433	-0.333692	1.169776
C	3.191252	-0.341385	-0.263159	C	3.185012	-0.335894	-0.234464	C	3.206922	-0.324729	-0.175554
H	3.952141	0.274408	-0.727879	H	3.952293	0.281962	-0.673962	H	3.983585	0.322203	-0.564942
C	2.403619	-1.338400	-0.912780	C	2.417105	-1.321209	-0.907049	C	2.481946	-1.305887	-0.914534
H	2.457241	-1.613808	-1.959050	H	2.494747	-1.585829	-1.949586	H	2.600480	-1.528509	-1.967823
C	1.730085	-1.216294	1.306101	C	1.708891	-1.232397	1.288269	C	1.678945	-1.296781	1.259583
H	1.208302	-1.405503	2.236813	H	1.178931	-1.440127	2.204128	H	1.101436	-1.532986	2.144280
C	1.494832	-1.869687	0.046834	C	1.498701	-1.866101	0.023429	C	1.526574	-1.890091	-0.039895
H	0.755626	-2.639814	-0.141558	H	0.772873	-2.6358	-0.185292	H	0.807926	-2.654007	-0.308532
C	-2.640492	-0.591117	1.239685	C	-2.619781	-0.592761	1.241956	C	-2.627370	-0.596661	1.253132
C	-1.746449	-1.564412	0.740406	C	-1.74641	-1.563097	0.724473	C	-1.795077	-1.595077	0.702441
H	-1.097868	-2.201633	1.329413	H	-1.102349	-2.212461	1.294869	H	-1.154505	-2.271531	1.253315
C	-1.822258	-1.520482	-0.698439	C	-1.843569	-1.508164	-0.705141	C	-1.913165	-1.513531	-0.727479
H	-1.238771	-2.121053	-1.387253	H	-1.281634	-2.108988	-1.403196	H	-1.378186	-2.122339	-1.445759
C	-3.306698	0.033645	0.124732	C	-3.291919	0.043508	0.147507	C	-3.303258	0.076622	0.173868
H	-4.032335	0.835629	0.192353	H	-4.009397	0.844953	0.232721	H	-3.999529	0.899899	0.281338
C	-2.827828	-0.558230	-1.069950	C	-2.840504	-0.539696	-1.052184	C	-2.891443	-0.512882	-1.045585
H	-3.120489	-0.299096	-2.079538	H	-3.150948	-0.27741	-2.050524	H	-3.206163	-0.221421	-2.039460
H	-2.774520	-0.325246	2.281909	H	-2.741164	-0.339898	2.283995	H	-2.725387	-0.356324	2.305162
H	3.172253	0.407249	1.849315	H	3.13181	0.375452	1.878572	H	3.061651	0.310474	1.970533
Co	-1.251345	0.263731	-0.077553	Co	-1.251489	0.25843	-0.078922	Co	-1.234540	0.266597	-0.075771
Co	1.177704	0.146236	-0.115176	Co	1.178539	0.143323	-0.119113	Co	1.179670	0.146834	-0.124903

Tables S72 : Optimized coordinates for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-8T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.914487	1.858051	-0.704073	C	-0.921579	1.855349	-0.699765	C	-0.919891	1.872409	-0.705523
C	-0.100656	1.407715	0.343886	C	-0.102386	1.410726	0.33419	C	-0.097199	1.417968	0.322305
C	-1.989173	2.894510	-0.502803	C	-1.992534	2.886318	-0.50045	C	-1.953710	2.958353	-0.502157
H	-1.606620	3.910333	-0.668254	H	-1.620749	3.897298	-0.687991	H	-1.544147	3.947038	-0.745946
H	-2.382829	2.852265	0.518036	H	-2.372026	2.862012	0.520752	H	-2.287172	2.975490	0.540410
H	-2.825506	2.744675	-1.194072	H	-2.834751	2.724557	-1.173829	H	-2.827930	2.790154	-1.140453
C	0.585845	1.580495	1.555311	C	0.584533	1.596506	1.532684	C	0.591719	1.646605	1.518356
H	0.260618	1.047021	2.452713	H	0.278908	1.065853	2.432321	H	0.311883	1.096676	2.419532
H	-0.521747	1.766726	-1.723914	H	-0.548634	1.753146	-1.720172	H	-0.577035	1.715840	-1.733806
H	1.137125	2.503419	1.747594	H	1.123404	2.521765	1.720602	H	1.100096	2.595600	1.684723
C	-2.585350	-1.379291	-0.944475	C	-2.571808	-1.38508	-0.938876	C	-2.556641	-1.428656	-0.966422
C	-3.125655	-0.523705	0.061118	C	-3.116006	-0.536101	0.05883	C	-3.148299	-0.552876	-0.007325
H	-3.923265	0.196340	-0.083483	H	-3.918261	0.171261	-0.08612	H	-3.952078	0.147284	-0.202645
C	-2.438514	-0.769072	1.290691	C	-2.434379	-0.775656	1.283863	C	-2.526476	-0.776841	1.263107

H	-2.611631	-0.259615	2.230765	H	-2.617536	-0.275042	2.221102	H	-2.757653	-0.261132	2.186688
C	-1.513022	-2.113647	-0.354658	C	-1.502369	-2.107873	-0.350044	C	-1.506233	-2.132958	-0.314792
H	-0.885995	-2.846749	-0.849186	H	-0.87756	-2.839297	-0.838351	H	-0.847911	-2.867113	-0.762909
C	-1.428134	-1.730905	1.030001	C	-1.423714	-1.725607	1.027405	C	-1.493620	-1.723898	1.065735
H	-0.707244	-2.109981	1.746361	H	-0.708614	-2.101711	1.743142	H	-0.803926	-2.083374	1.820580
C	2.245326	-1.594649	-0.234093	C	2.236879	-1.589846	-0.213839	C	2.240034	-1.620488	-0.192896
C	3.116499	-0.838572	0.606409	C	3.105427	-0.832001	0.613325	C	3.115741	-0.864026	0.634811
H	3.526418	-1.151905	1.558483	H	3.515947	-1.136996	1.562485	H	3.506397	-1.159850	1.600837
C	3.330924	0.425299	-0.023302	C	3.325915	0.415734	-0.028184	C	3.364933	0.380242	-0.024005
H	3.912688	1.242790	0.386061	H	3.914453	1.229102	0.367043	H	3.967756	1.190257	0.369142
C	1.950041	-0.796114	-1.392529	C	1.950356	-0.809017	-1.3772	C	1.974822	-0.843876	-1.373492
H	1.309039	-1.091703	-2.216013	H	1.315847	-1.112385	-2.195853	H	1.339899	-1.149921	-2.196854
C	2.643070	0.438666	-1.273026	C	2.645195	0.416393	-1.272926	C	2.703186	0.371922	-1.287101
H	2.599143	1.267389	-1.968730	H	2.614579	1.229196	-1.980398	H	2.697699	1.176331	-2.011712
H	1.876219	-2.596295	-0.044804	H	1.869974	-2.585192	-0.017065	H	1.847103	-2.608126	0.015988
H	-2.911101	-1.432020	-1.976081	H	-2.898255	-1.446086	-1.964835	H	-2.830772	-1.503887	-2.011867
Co	1.280086	0.128021	0.356820	Co	1.28294	0.138737	0.351483	Co	1.291188	0.153329	0.356588
Co	-1.091404	-0.098220	-0.233346	Co	-1.095456	-0.097128	-0.229887	Co	-1.108685	-0.087571	-0.223822

Tables S73 : Optimized coordinates for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-9S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.045871	1.605136	-0.163343	C	-0.044359	1.601996	-0.165462	C	-0.041529	1.570562	-0.143226
C	0.815947	1.921171	0.918759	C	0.808075	1.913407	0.914642	C	0.737163	1.851918	1.003574
C	-0.103487	2.521097	-1.355327	C	-0.111111	2.515904	-1.350979	C	-0.035769	2.534215	-1.310934
H	-0.312626	1.983165	-2.287272	H	-0.300846	1.981706	-2.282701	H	-0.184455	2.022757	-2.269385
H	0.833994	3.081322	-1.492820	H	0.810903	3.093027	-1.479391	H	0.909783	3.091771	-1.370546
H	-0.906502	3.259146	-1.228121	H	-0.925577	3.235356	-1.231493	H	-0.850377	3.260879	-1.199226
C	0.903687	0.987431	1.995896	C	0.886391	0.989429	1.988342	C	0.777569	0.855579	2.028533
H	-0.003340	0.577311	2.437437	H	-0.014808	0.581042	2.427962	H	-0.142124	0.431284	2.420127
H	1.568109	2.712581	0.811496	H	1.550273	2.707794	0.816995	H	1.477295	2.657160	0.983489
H	1.743869	1.074213	2.684887	H	1.720494	1.070485	2.677045	H	1.589079	0.916330	2.753330
C	-2.861829	-0.627026	-1.014473	C	-2.833295	-0.632023	-1.023724	C	-2.978456	-0.688306	-0.946841
C	-3.112850	0.442199	-0.115941	C	-3.110797	0.427154	-0.133954	C	-3.198739	0.403164	-0.067046
H	-3.553562	1.399986	-0.362031	H	-3.56302	1.373026	-0.38434	H	-3.702914	1.331214	-0.303575
C	-2.581132	0.052590	1.159700	C	-2.602797	0.042324	1.14219	C	-2.550186	0.076443	1.164837
H	-2.563657	0.662852	2.055580	H	-2.610589	0.645602	2.03689	H	-2.482600	0.717556	2.035451
C	-2.248372	-1.713105	-0.293751	C	-2.22894	-1.709336	-0.297784	C	-2.279130	-1.730195	-0.246884
H	-1.930048	-2.658192	-0.718671	H	-1.90373	-2.649752	-0.715126	H	-1.979297	-2.684711	-0.661633
C	-2.081722	-1.298848	1.047744	C	-2.091086	-1.297189	1.037969	C	-2.015272	-1.258858	1.059791
H	-1.605316	-1.863004	1.841543	H	-1.630699	-1.856783	1.837667	H	-1.459259	-1.777069	1.831277
C	1.497810	-1.915881	0.033306	C	1.501731	-1.904958	0.032088	C	1.586108	-1.912743	-0.068762
C	2.654156	-1.307004	0.602345	C	2.642836	-1.296378	0.613013	C	2.648113	-1.297674	0.648671
H	3.061895	-1.525522	1.581763	H	3.039261	-1.516147	1.591593	H	2.970293	-1.557696	1.649199

C	3.161772	-0.338960	-0.314141	C	3.158395	-0.334307	-0.292595	C	3.192380	-0.249202	-0.157115
H	4.023834	0.298265	-0.160087	H	4.017426	0.29702	-0.130826	H	4.000552	0.414814	0.123942
C	1.261361	-1.298323	-1.242578	C	1.285434	-1.294724	-1.24129	C	1.460396	-1.229251	-1.327793
H	0.489701	-1.567883	-1.955641	H	0.529716	-1.567245	-1.961732	H	0.757985	-1.472283	-2.116989
C	2.297274	-0.319173	-1.444986	C	2.315865	-0.319178	-1.429561	C	2.465506	-0.214015	-1.380378
H	2.387217	0.334863	-2.305038	H	2.421202	0.325192	-2.288922	H	2.615392	0.487248	-2.192465
H	0.891073	-2.689169	0.489228	H	0.897191	-2.679639	0.475752	H	0.969059	-2.732712	0.274914
H	-3.069016	-0.616879	-2.078982	H	-3.023723	-0.623983	-2.086664	H	-3.274536	-0.724724	-1.989749
Co	1.159973	0.096363	0.215262	Co	1.160864	0.098916	0.209104	Co	1.150718	0.076516	0.214666
Co	-1.100569	0.024715	-0.148318	Co	-1.104253	0.02592	-0.137255	Co	-1.144155	0.047497	-0.270471

Tables S74 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-1S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.000000	-1.354900	-0.017560	C	0.000003	-1.352796	-0.020958	C	0.000004	-1.330335	-0.029617
C	0.000001	1.354902	-0.017558	C	-0.000002	1.352797	-0.020956	C	-0.000004	1.330335	-0.029615
C	0.000003	-2.836205	-0.067634	C	0.000001	-2.825787	-0.070624	C	0.000006	-2.821667	-0.066815
H	-0.000149	-3.247658	0.951133	H	-0.000127	-3.238716	0.942751	H	-0.000132	-3.211809	0.959692
H	-0.887379	-3.235949	-0.577202	H	-0.882571	-3.226258	-0.577002	H	-0.889758	-3.212835	-0.574997
H	0.887518	-3.235967	-0.576954	H	0.882681	-3.22628	-0.576794	H	0.889895	-3.212851	-0.574768
C	-0.000003	2.836207	-0.067635	C	0.000001	2.825787	-0.07062	C	-0.000005	2.821667	-0.066811
H	-0.887512	3.235965	-0.576968	H	-0.882677	3.226281	-0.576795	H	-0.889891	3.212852	-0.574768
H	0.000129	3.247662	0.951132	H	0.000123	3.238715	0.942754	H	0.000128	3.211808	0.959696
H	0.887384	3.235953	-0.577189	H	0.882574	3.226259	-0.576994	H	0.889761	3.212836	-0.574989
Fe	-1.162878	0.000001	0.007323	Fe	-1.15917	-0.000001	0.005493	Fe	-1.160927	-0.000002	-0.005350
Fe	1.162879	0.000001	0.007311	Fe	1.15917	0.000001	0.005502	Fe	1.160927	0.000002	-0.005340
C	-2.847402	0.715456	-0.966137	C	-2.840224	0.711557	-0.957825	C	-2.879230	0.714464	-0.954965
C	-2.857093	1.154086	0.388771	C	-2.846161	1.147798	0.389219	C	-2.867007	1.153869	0.400782
H	-2.815200	2.182578	0.726269	H	-2.812691	2.171725	0.72544	H	-2.837502	2.182043	0.738965
C	-2.826248	-0.000084	1.229666	C	-2.813816	-0.00007	1.225363	C	-2.836005	-0.000096	1.238026
H	-2.790408	-0.000146	2.311954	H	-2.784204	-0.000133	2.303066	H	-2.779642	-0.000182	2.319356
C	-2.847397	-0.715330	-0.966231	C	-2.840224	-0.71144	-0.957909	C	-2.879232	-0.714308	-0.955078
H	-2.814533	-1.349053	-1.844366	H	-2.817033	-1.342619	-1.832081	H	-2.862484	-1.348242	-1.833007
C	-2.857091	-1.154141	0.388619	C	-2.846166	-1.147839	0.389085	C	-2.867018	-1.153928	0.400599
H	-2.815191	-2.182677	0.725980	H	-2.812702	-2.171806	0.725184	H	-2.837524	-2.182157	0.738618
C	2.847410	0.715334	-0.966219	C	2.840228	0.711443	-0.95789	C	2.879237	0.714310	-0.955060
C	2.857086	1.154136	0.388634	C	2.846164	1.147838	0.389104	C	2.867016	1.153927	0.400619
H	2.815188	2.182670	0.726005	H	2.812699	2.171804	0.725206	H	2.837520	2.182155	0.738640
C	2.826228	0.000073	1.229674	C	2.81381	0.000067	1.22538	C	2.836000	0.000093	1.238043
H	2.790369	0.000145	2.311962	H	2.784194	0.000127	2.303083	H	2.779632	0.000176	2.319373
C	2.847416	-0.715453	-0.966130	C	2.840229	-0.711555	-0.95781	C	2.879234	-0.714462	-0.954950
H	2.814569	-1.349287	-1.844186	H	2.817037	-1.342834	-1.83191	H	2.862484	-1.348532	-1.832781
C	2.857086	-1.154092	0.388774	C	2.846159	-1.147799	0.389233	C	2.867005	-1.153870	0.400796
H	2.815191	-2.182585	0.726268	H	2.812687	-2.171727	0.725451	H	2.837499	-2.182045	0.738976

H	-2.814547	1.349294	-1.844189	H	-2.817029	1.342838	-1.831922	H	-2.862477	1.348537	-1.832794
H	2.814576	1.349059	-1.844354	H	2.817041	1.342624	-1.832061	H	2.862491	1.348246	-1.832987

Tables S75 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-2T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.021732	1.503661	0.687301	C	-0.018254	1.506706	0.68181	C	-0.047920	1.506734	0.674264
C	0.021669	1.503666	-0.687305	C	0.018238	1.506707	-0.681811	C	-0.043756	1.511325	-0.677582
C	-0.045348	2.536692	1.759225	C	-0.038622	2.521447	1.760586	C	0.054286	2.532653	1.759087
H	-0.917927	3.193584	1.646975	H	-0.907852	3.177166	1.663235	H	-0.468316	3.455974	1.478024
H	0.844924	3.176867	1.704274	H	0.845914	3.16194	1.712881	H	1.107476	2.784942	1.934910
H	-0.082350	2.099488	2.761169	H	-0.07083	2.076876	2.754342	H	-0.363590	2.165107	2.700579
C	0.044967	2.536728	-1.759207	C	0.038591	2.521453	-1.760583	C	0.065035	2.546240	-1.753124
H	0.917343	3.193884	-1.646938	H	0.907802	3.177196	-1.663221	H	1.119881	2.793314	-1.926423
H	0.082108	2.099560	-2.761162	H	0.07082	2.076887	-2.75434	H	-0.354257	2.189674	-2.698232
H	-0.845503	3.176629	-1.704245	H	-0.845963	3.16192	-1.712883	H	-0.451727	3.470485	-1.464302
C	2.654698	-0.797010	1.197190	C	2.646561	-0.785722	1.187988	Fe	2.800295	-0.626421	1.159838
C	3.239131	0.006320	0.183204	C	3.227159	-0.002817	0.167316	Fe	3.288718	0.097997	0.041858
H	3.820702	0.905706	0.350252	H	3.819902	0.886274	0.320011	C	3.834283	1.033523	0.080158
C	2.822685	-0.489910	-1.082356	C	2.803224	-0.507248	-1.083307	C	2.837628	-0.555288	-1.133687
H	3.085128	-0.079146	-2.049494	H	3.068187	-0.115694	-2.052334	H	3.015980	-0.229034	-2.151442
C	1.909237	-1.836899	0.559068	C	1.893928	-1.821502	0.568814	C	2.094866	-1.775906	0.678291
H	1.344815	-2.614568	1.060175	H	1.335831	-2.590392	1.079493	H	1.628387	-2.537168	1.291592
C	2.009451	-1.645690	-0.849586	C	1.987806	-1.648373	-0.834466	C	2.115908	-1.731056	-0.745173
H	1.540193	-2.254833	-1.613002	H	1.518511	-2.264263	-1.58523	H	1.672889	-2.454164	-1.418940
C	-1.909311	-1.837010	-0.559070	C	-1.893909	-1.821513	-0.568809	C	-1.880093	-1.913194	-0.303590
C	-2.654678	-0.797053	-1.197185	C	-2.646551	-0.785743	-1.187988	H	-2.548188	-1.026175	-1.203940
H	-2.757735	-0.648973	-2.265161	H	-2.762513	-0.632173	-2.248977	C	-2.503531	-1.065822	-2.285524
C	-3.239043	0.006334	-0.183204	C	-3.227156	-0.002838	-0.16732	C	-3.246058	-0.059722	-0.435301
H	-3.820528	0.905775	-0.350253	H	-3.819908	0.886245	-0.320018	H	-3.819751	0.769369	-0.832192
C	-2.009487	-1.645782	0.849584	C	-1.98779	-1.648379	0.83447	C	-2.167180	-1.480121	1.022810
H	-1.540296	-2.254970	1.613006	H	-1.518489	-2.264265	1.585235	H	-1.780641	-1.925780	1.931498
C	-2.822620	-0.489926	1.082348	C	-2.803218	-0.507261	1.083306	C	-3.005244	-0.328840	0.948539
H	-3.085002	-0.079123	2.049487	H	-3.068183	-0.115703	2.052331	H	-3.392281	0.234887	1.788084
H	-1.344962	-2.614725	-1.060188	H	-1.335807	-2.590402	-1.079484	C	-1.257514	-2.754957	-0.579488
H	2.757765	-0.648937	2.265166	H	2.762523	-0.632146	2.248976	H	2.942965	-0.360971	2.200703
Fe	-1.074829	0.021429	-0.007175	Fe	-1.073199	0.027903	-0.006108	H	-1.159615	0.065619	-0.005584
Fe	1.074969	0.021612	0.007171	Fe	1.0732	0.027906	0.006105	H	1.050383	-0.056339	-0.003752

Tables S76 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-3T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.091951	1.476461	-0.331387	C	-0.087079	1.477083	-0.327196	C	0.111678	1.519171	0.328465
C	0.829514	2.094454	0.531600	C	0.835195	2.09023	0.525523	C	-0.822907	2.227136	-0.432909

C	-0.546085	1.712091	-1.721576	C	-0.548604	1.719915	-1.707552	C	0.592387	1.766876	1.729468
H	-1.283731	0.873910	-2.016912	H	-1.287375	0.892314	-2.009334	H	1.331949	0.941701	2.022757
H	0.232722	1.616633	-2.489601	H	0.222712	1.631716	-2.477013	H	-0.178744	1.688787	2.503992
H	-1.113035	2.637142	-1.872052	H	-1.108495	2.645299	-1.851243	H	1.156484	2.697466	1.842376
C	1.032508	1.429848	1.783962	C	1.045868	1.440589	1.773249	C	-1.180731	1.648607	-1.689026
H	0.152530	1.106979	2.346014	H	0.180451	1.115429	2.344426	H	-0.379167	1.269102	-2.325904
H	1.524662	2.860785	0.174354	H	1.517064	2.860435	0.16649	H	-1.444344	3.008733	0.012532
H	1.881893	1.723259	2.399761	H	1.896674	1.731808	2.378139	H	-2.055342	2.022856	-2.216622
C	-3.079577	-0.952376	-0.576149	C	-3.045451	-0.982687	-0.576382	Fe	3.052534	-1.050042	0.593331
C	-3.267988	0.282327	0.144326	C	-3.274975	0.247837	0.123336	Fe	3.348443	0.171405	-0.102637
H	-3.920777	1.096333	-0.148745	H	-3.946188	1.034339	-0.185537	C	4.025575	0.947707	0.233485
C	-2.452408	0.240455	1.307231	C	-2.484901	0.24161	1.292827	C	2.574879	0.198802	-1.292934
H	-2.341860	1.032287	2.038692	H	-2.412042	1.038148	2.016225	H	2.544711	1.005241	-2.015071
C	-2.156359	-1.747870	0.159995	C	-2.115288	-1.738801	0.178287	C	2.105875	-1.775874	-0.183447
H	-1.777294	-2.720531	-0.134110	H	-1.715394	-2.705275	-0.088781	H	1.666374	-2.731577	0.078407
C	-1.734855	-1.002540	1.301839	C	-1.735764	-0.972286	1.311367	C	1.790417	-0.998906	-1.338379
H	-1.016647	-1.327621	2.046983	H	-1.024825	-1.267901	2.067673	H	1.085187	-1.267465	-2.115322
C	1.635185	-1.882097	-0.026736	C	1.633284	-1.878382	-0.001368	C	-1.581495	-1.872684	-0.220232
C	2.630627	-1.258940	0.785343	C	2.632995	-1.245137	0.782166	H	-2.707413	-1.229231	-0.808805
H	2.891769	-1.521411	1.803190	H	2.913494	-1.496937	1.792317	C	-3.065241	-1.360556	-1.822735
C	3.234557	-0.220105	0.001186	C	3.219848	-0.2221	-0.021965	C	-3.332792	-0.421161	0.201323
H	4.014239	0.454003	0.337179	H	4.004842	0.450388	0.28855	H	-4.211280	0.197538	0.061326
C	1.634867	-1.230848	-1.303135	C	1.613294	-1.251011	-1.280342	C	-1.476570	-1.407854	1.130448
H	0.977293	-1.468773	-2.133785	H	0.949612	-1.503503	-2.094617	H	-0.736895	-1.726616	1.856879
C	2.646302	-0.234096	-1.295055	C	2.615591	-0.25627	-1.301993	C	-2.590924	-0.549342	1.391663
H	2.873478	0.449883	-2.105004	H	2.83558	0.405794	-2.125311	H	-2.786935	-0.032005	2.323739
H	0.981451	-2.696141	0.266538	H	0.991345	-2.687433	0.311523	C	-0.914900	-2.576975	-0.702962
H	-3.581598	-1.238359	-1.492667	H	-3.53325	-1.294722	-1.486378	H	3.490453	-1.371638	1.530684
Fe	1.180102	0.118333	0.265172	Fe	1.183644	0.120984	0.261171	H	-1.256450	0.210930	-0.258015
Fe	-1.271684	0.069399	-0.403191	Fe	-1.272424	0.076192	-0.402204	H	1.301521	0.093927	0.369341

Tables S77 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-4T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.942712	2.109808	0.318780	C	0.941933	2.110421	0.307472	C	0.920815	2.149605	0.289139
C	0.900662	1.821293	-1.085186	C	0.89726	1.810705	-1.08439	C	0.793175	1.884968	-1.112124
C	-0.309831	2.320817	1.125710	C	-0.297751	2.328317	1.119445	C	-0.297262	2.206565	1.197384
H	-0.539471	3.390347	1.259441	H	-0.519066	3.394861	1.257096	H	-0.516051	3.242268	1.493538
H	-0.264816	1.876154	2.125482	H	-0.252462	1.886127	2.114735	H	-0.193713	1.622922	2.117930
H	-1.267374	1.988360	0.638135	H	-1.252935	1.999554	0.638592	H	-1.275339	1.948689	0.703787
C	-0.050259	0.831123	-1.478466	C	-0.046966	0.826207	-1.474049	C	-0.088860	0.830562	-1.461724
H	-0.012541	0.475552	-2.515414	H	-0.011832	0.472473	-2.505034	H	-0.085102	0.495534	-2.501854
H	1.804806	2.673506	0.683006	H	1.803844	2.669173	0.663247	H	1.742125	2.791163	0.607524
H	1.706045	2.159406	-1.744474	H	1.693784	2.151231	-1.744637	H	1.519603	2.302427	-1.812941

Fe	2.825846	-0.376013	1.067139	C	2.81503	-0.380332	1.067388	Fe	2.746068	-0.451572	1.218295
Fe	3.139100	-0.346637	-0.330995	C	3.133212	-0.345006	-0.321506	Fe	3.336078	-0.320614	-0.082372
C	3.856084	0.312389	-0.807117	H	3.851311	0.311223	-0.788559	C	4.123812	0.371648	-0.354886
C	2.344392	-1.335324	-0.985107	C	2.347703	-1.326712	-0.97948	C	2.698897	-1.240691	-0.949872
H	2.333166	-1.546310	-2.047819	H	2.345803	-1.535542	-2.037695	H	2.891563	-1.356513	-2.009867
C	1.828610	-1.372904	1.262808	C	1.823908	-1.374505	1.252782	C	1.744641	-1.464698	1.142575
H	1.353188	-1.622582	2.205311	H	1.352422	-1.633982	2.188641	H	1.131859	-1.820530	1.962042
C	1.525764	-1.955023	-0.002769	C	1.529619	-1.948489	-0.00967	C	1.697211	-1.925921	-0.207832
H	0.791282	-2.731866	-0.183647	H	0.804417	-2.725226	-0.195401	H	1.022158	-2.677978	-0.599011
C	-2.659899	-0.576548	1.268492	C	-2.645952	-0.569752	1.266463	C	-2.714800	-0.631563	1.270534
H	-1.718569	-1.522040	0.801670	C	-1.718075	-1.514943	0.796263	H	-1.845741	-1.602990	0.718242
C	-1.036248	-2.100837	1.412456	H	-1.041668	-2.098354	1.399302	C	-1.161757	-2.236759	1.267673
C	-1.807030	-1.544552	-0.633900	C	-1.819484	-1.540599	-0.630701	C	-1.988361	-1.553533	-0.704143
H	-1.205707	-2.151306	-1.302087	H	-1.233656	-2.152631	-1.298968	H	-1.435038	-2.149256	-1.419581
C	-3.363860	-0.035705	0.148349	C	-3.35335	-0.031436	0.15786	C	-3.428926	0.000163	0.203806
H	-4.142006	0.717121	0.199042	H	-4.128422	0.717362	0.214398	H	-4.175525	0.777540	0.314039
C	-2.855919	-0.651126	-1.037094	C	-2.862046	-0.64797	-1.024131	C	-2.992028	-0.586028	-1.022001
H	-3.184541	-0.475049	-2.054000	H	-3.202773	-0.479425	-2.033201	H	-3.332525	-0.327974	-2.017196
C	-2.796011	-0.276134	2.301530	H	-2.776346	-0.273106	2.296383	C	-2.804812	-0.386339	2.322645
H	3.270476	0.246746	1.833850	H	3.258988	0.231674	1.836348	H	3.041586	0.092894	2.106955
H	-1.317422	0.351565	-0.147749	Fe	-1.319855	0.347585	-0.14933	H	-1.366271	0.337767	-0.117856
H	1.120627	0.143108	-0.030723	Fe	1.12133	0.140459	-0.030198	H	1.213260	0.183185	-0.081384

Tables S78 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-5T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	0.942712	2.109808	0.318780	C	-0.080115	1.353385	-0.039786	C	0.000002	-1.347783	-0.047063
C	0.900662	1.821293	-1.085186	C	-0.080116	-1.353384	-0.039786	C	-0.000002	1.347784	-0.047055
C	-0.309831	2.320817	1.125710	C	-0.041509	2.824932	-0.093517	C	0.000004	-2.834794	-0.075458
H	-0.539471	3.390347	1.259441	H	0.119306	3.241513	0.905694	H	-0.000089	-3.206673	0.958285
H	-0.264816	1.876154	2.125482	H	0.777062	3.189825	-0.720228	H	-0.892476	-3.230242	-0.575041
H	-1.267374	1.988360	0.638135	H	-0.970190	3.256833	-0.477140	H	0.892565	-3.230251	-0.574888
C	-0.050259	0.831123	-1.478466	C	-0.041512	-2.824932	-0.093517	C	0.000003	2.834795	-0.075444
H	-0.012541	0.475552	-2.515414	H	0.777059	-3.189825	-0.720227	H	-0.892559	3.230260	-0.574866
H	1.804806	2.673506	0.683006	H	0.119302	-3.241513	0.905693	H	0.000106	3.206670	0.958301
H	1.706045	2.159406	-1.744474	H	-0.970193	-3.256831	-0.477141	H	0.892482	3.230239	-0.575032
C	2.825846	-0.376013	1.067139	Fe	1.154236	0.000000	-0.000609	Fe	-1.157484	0.000000	-0.010073
C	3.139100	-0.346637	-0.330995	Fe	-1.198303	0.000001	0.002350	Fe	1.157484	0.000001	-0.010066
H	3.856084	0.312389	-0.807117	C	2.953133	-0.707143	-0.957512	C	-2.955363	0.710489	-0.951616
C	2.344392	-1.335324	-0.985107	C	2.973983	-1.141468	0.397813	C	-2.927944	1.148741	0.411221
H	2.333166	-1.546310	-2.047819	H	2.971717	-2.167261	0.730891	H	-2.911861	2.178772	0.745949
C	1.828610	-1.372904	1.262808	C	3.034698	0.000001	1.225038	C	-2.939768	-0.000062	1.250181
H	1.353188	-1.622582	2.205311	H	3.024237	0.000002	2.303627	H	-2.903006	-0.000119	2.332417
C	1.525764	-1.955023	-0.002769	C	2.953136	0.707138	-0.957514	C	-2.955370	-0.710383	-0.951691

H	0.791282	-2.731866	-0.183647	H	2.925040	1.348287	-1.824175	H	-2.954371	-1.350204	-1.825609
C	-2.659899	-0.576548	1.268492	C	2.973984	1.141467	0.397810	C	-2.927951	-1.148779	0.411100
C	-1.718569	-1.522040	0.801670	H	2.971720	2.167261	0.730885	H	-2.911876	-2.178845	0.745719
H	-1.036248	-2.100837	1.412456	C	-2.920375	-0.708981	-0.938456	C	2.955374	0.710381	-0.951675
C	-1.807030	-1.544552	-0.633900	C	-2.897399	-1.143759	0.412054	C	2.927950	1.148779	0.411114
H	-1.205707	-2.151306	-1.302087	H	-2.861066	-2.168484	0.745746	H	2.911876	2.178845	0.745732
C	-3.363860	-0.035705	0.148349	C	-2.864066	0.000005	1.250830	C	2.939761	0.000064	1.250198
H	-4.142006	0.717121	0.199042	H	-2.836057	0.000009	2.328217	H	2.902992	0.000124	2.332434
C	-2.855919	-0.651126	-1.037094	C	-2.920377	0.708973	-0.938462	C	2.955364	-0.710492	-0.951597
H	-3.184541	-0.475049	-2.054000	H	-2.921286	1.343251	-1.810450	H	2.954365	-1.350405	-1.825446
H	-2.796011	-0.276134	2.301530	C	-2.897401	1.143762	0.412045	C	2.927938	-1.148741	0.411241
H	3.270476	0.246746	1.833850	H	-2.861069	2.168489	0.745729	H	2.911852	-2.178771	0.745971
Fe	-1.317422	0.351565	-0.147749	H	2.925035	-1.348294	-1.824171	H	-2.954359	1.350401	-1.825466
Fe	1.120627	0.143108	-0.030723	H	-2.921283	-1.343266	-1.810439	H	2.954381	1.350199	-1.825594

Tables S79 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-6T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.361162	1.863006	0.836428	C	-0.347822	1.862444	0.829109	C	-0.533268	1.845562	0.887076
C	0.577478	2.100969	-0.269975	C	0.579984	2.095026	-0.275704	C	0.524427	2.048725	-0.129666
C	-1.770708	1.993909	0.594046	C	-1.750969	1.995443	0.601106	C	-1.897723	2.036038	0.546444
H	-2.108964	2.656755	-0.205279	H	-2.097	2.654433	-0.190358	H	-2.165651	2.666166	-0.302831
H	-2.432094	1.975138	1.459479	H	-2.404509	1.976542	1.465383	H	-2.630836	2.029703	1.349637
H	-1.005149	1.235172	-1.530378	H	-0.998971	1.236259	-1.529536	H	-0.892872	1.390890	-1.669999
C	0.128309	1.357773	-1.424340	C	0.129606	1.355707	-1.420446	C	0.181816	1.509144	-1.412017
H	0.532376	1.497189	-2.427089	H	0.53052	1.490402	-2.419822	H	0.763901	1.730286	-2.303389
H	0.015678	1.862597	1.860556	H	0.034425	1.864481	1.84541	H	-0.233105	1.766493	1.930354
H	1.383771	2.835749	-0.258691	H	1.383531	2.825181	-0.268471	H	1.372998	2.713289	0.026755
C	3.293761	0.123399	-0.339229	C	3.272705	0.087647	-0.378401	Fe	3.436212	0.237772	-0.260730
C	2.717214	-1.020020	-0.960460	C	2.675523	-1.064706	-0.942559	Fe	2.995541	-0.942693	-0.906152
H	2.799911	-1.290650	-2.005786	H	2.740035	-1.3769	-1.972386	C	3.180013	-1.211925	-1.939698
C	2.007996	-1.733786	0.041371	C	1.98348	-1.72926	0.093487	C	2.257267	-1.711691	0.043759
H	1.458561	-2.657635	-0.105590	H	1.426922	-2.648623	-0.006924	H	1.810724	-2.684103	-0.134547
C	2.967246	0.107592	1.044608	C	2.974572	0.127779	1.003669	C	2.981977	0.205649	1.088692
H	3.256744	0.851260	1.777495	H	3.290202	0.888223	1.700422	H	3.163990	0.966926	1.838730
C	2.160580	-1.034293	1.282924	C	2.166821	-0.989684	1.298775	C	2.260125	-1.005134	1.286301
H	1.746459	-1.331177	2.240303	H	1.773397	-1.247886	2.270092	H	1.820903	-1.343087	2.217692
C	-3.181431	-0.530902	0.118458	C	-3.172352	-0.529075	0.069664	C	-3.255212	-0.628840	0.126537
C	-2.328268	-0.904944	1.211903	C	-2.360692	-0.878676	1.191797	H	-2.380807	-0.995417	1.205918
H	-2.468667	-0.635077	2.251988	H	-2.537138	-0.592956	2.216836	C	-2.528424	-0.752550	2.251292
C	-1.255730	-1.688465	0.685920	C	-1.274966	-1.664862	0.721568	C	-1.290175	-1.733113	0.668197
H	-0.462921	-2.143569	1.266637	H	-0.507531	-2.106246	1.335957	H	-0.477113	-2.171172	1.232172
C	-2.621341	-1.059690	-1.071470	C	-2.574012	-1.07994	-1.082063	C	-2.683222	-1.115075	-1.076214
H	-3.003409	-0.907482	-2.074221	H	-2.922767	-0.954181	-2.095618	H	-3.082657	-0.975135	-2.073953

C	-1.427907	-1.773699	-0.733524	C	-1.399747	-1.78212	-0.692655	C	-1.461505	-1.782041	-0.752431
H	-0.769985	-2.277989	-1.431576	H	-0.728007	-2.306834	-1.353211	H	-0.792385	-2.259114	-1.459130
H	-4.066064	0.089844	0.185043	H	-4.061465	0.079794	0.094727	C	-4.175524	-0.065985	0.216070
H	3.858782	0.899191	-0.844465	H	3.834984	0.833386	-0.920368	H	3.999803	1.040728	-0.722189
Fe	-1.245168	0.190238	-0.113821	Fe	-1.242235	0.191142	-0.113137	H	-1.337105	0.220767	-0.126016
Fe	1.084735	0.214976	-0.126886	Fe	1.081873	0.21465	-0.128256	H	1.108394	0.138667	-0.195186

Tables S80 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-7S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.001090	1.773691	-0.816913	C	0.002617	1.762008	-0.812764	C	0.004182	1.783298	-0.836862
C	-0.822579	2.029193	0.375086	C	-0.816185	2.021209	0.371449	C	-0.814388	2.050096	0.349577
C	1.450493	2.000932	-0.697171	C	1.446566	1.998286	-0.698524	C	1.463486	2.023353	-0.691009
H	1.777834	2.775906	0.002255	H	1.772771	2.772937	-0.007246	H	1.756125	2.819145	-0.000922
H	1.993481	2.034803	-1.643168	H	1.986027	2.033788	-1.63998	H	2.010113	2.077212	-1.633017
H	0.908903	1.300373	1.475021	H	0.906956	1.300012	1.469649	H	0.864720	1.266391	1.501737
C	-0.236480	1.268103	1.444277	C	-0.234194	1.269273	1.435579	C	-0.275504	1.329987	1.454004
H	-0.595109	1.301192	2.472229	H	-0.588614	1.305094	2.459679	H	-0.662603	1.411398	2.466115
H	-0.442636	1.872050	-1.811172	H	-0.436096	1.855964	-1.802629	H	-0.437199	1.907784	-1.825027
H	-1.663846	2.716163	0.444032	H	-1.646906	2.712981	0.438482	H	-1.689829	2.691364	0.389598
C	-3.190988	0.165026	-0.064157	C	-3.177621	0.171256	-0.07678	Fe	-3.123325	0.202686	-0.361415
C	-2.764630	-0.695044	0.986981	C	-2.765504	-0.676856	0.979057	Fe	-2.910515	-0.463824	0.882907
H	-3.001125	-0.585433	2.038611	H	-3.011851	-0.560522	2.022636	C	-3.277679	-0.141069	1.849573
C	-1.922049	-1.695952	0.418769	C	-1.930826	-1.682784	0.428538	C	-2.077568	-1.588819	0.641579
H	-1.425117	-2.483364	0.976868	H	-1.450089	-2.468914	0.99223	H	-1.722795	-2.281495	1.395432
C	-2.604317	-0.291965	-1.278041	C	-2.591832	-0.299529	-1.276024	C	-2.433764	-0.527650	-1.372810
H	-2.710066	0.182977	-2.247310	H	-2.69277	0.161437	-2.247085	H	-2.371541	-0.252728	-2.419098
C	-1.819664	-1.456376	-0.993918	C	-1.819815	-1.458735	-0.978458	C	-1.785520	-1.634152	-0.764221
H	-1.283416	-2.057764	-1.719578	H	-1.290417	-2.071026	-1.691828	H	-1.182434	-2.376335	-1.272024
C	3.080449	-0.346560	-0.578420	C	3.057342	-0.357576	-0.598263	C	2.836931	-0.560275	-0.913263
C	2.050356	-1.114883	-1.203629	C	2.024122	-1.131816	-1.191431	H	1.709684	-1.420910	-1.033292
H	1.849236	-1.161582	-2.267483	H	1.810928	-1.199751	-2.246766	C	1.227330	-1.703522	-1.960818
C	1.331848	-1.803403	-0.179744	C	1.327174	-1.802041	-0.151439	C	1.312171	-1.823054	0.279914
H	0.525201	-2.508118	-0.328708	H	0.529909	-2.513417	-0.275907	H	0.529588	-2.523082	0.534632
C	2.986798	-0.516086	0.827192	C	2.988595	-0.50606	0.803563	C	3.146108	-0.409926	0.474253
H	3.615303	-0.048103	1.574712	H	3.631902	-0.036623	1.530345	H	3.940920	0.191670	0.896122
C	1.889779	-1.409142	1.076681	C	1.903445	-1.391717	1.082116	C	2.193346	-1.179682	1.202049
H	1.536580	-1.720685	2.053234	H	1.57319	-1.693433	2.064307	H	2.125052	-1.241819	2.282142
H	3.768637	0.314939	-1.089738	H	3.738361	0.287378	-1.129845	C	3.351982	-0.078377	-1.734475
H	-3.798750	1.054857	0.050184	H	-3.782769	1.058571	0.02386	H	-3.693530	1.111245	-0.510023
Fe	1.184288	0.233856	0.099374	Fe	1.18617	0.235813	0.099175	H	1.209186	0.268866	0.077775
Fe	-1.092852	0.134090	0.059013	Fe	-1.091318	0.132111	0.06007	H	-1.064577	0.132498	0.082671

Tables S81 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-8S**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-0.042268	1.583630	-0.234564	C	-0.040622	1.580631	-0.235345	C	-0.026767	1.564173	-0.230816
C	1.014815	2.130582	0.506465	C	1.009681	2.125553	0.502459	C	1.021650	2.161073	0.476398
C	-0.646527	1.904718	-1.549926	C	-0.65536	1.910154	-1.537037	C	-0.615401	1.902680	-1.566400
H	-1.397787	1.075684	-1.837134	H	-1.409695	1.092185	-1.827627	H	-1.375670	1.091295	-1.860846
H	0.040038	1.883353	-2.406272	H	0.020528	1.897349	-2.396024	H	0.090763	1.877164	-2.404118
H	-1.234950	2.828296	-1.563807	H	-1.236158	2.833541	-1.541589	H	-1.184360	2.836949	-1.571568
C	1.363524	1.430240	1.707096	C	1.359682	1.438165	1.698093	C	1.422824	1.501311	1.679452
H	0.559356	1.141659	2.389222	H	0.565489	1.140069	2.378341	H	0.645085	1.201573	2.384676
H	1.705008	2.852626	0.057211	H	1.688626	2.85466	0.059929	H	1.681039	2.887441	-0.005379
H	2.311746	1.654137	2.192826	H	2.303144	1.660965	2.181011	H	2.378041	1.760541	2.130713
C	-2.921130	-0.997189	-0.576547	C	-2.90969	-0.998611	-0.579508	Fe	-2.961048	-1.005201	-0.595185
C	-3.194938	0.189940	0.189908	C	-3.191728	0.174288	0.190162	Fe	-3.250222	0.201402	0.130229
H	-3.883005	0.982318	-0.082266	H	-3.887976	0.956011	-0.072978	C	-3.922499	0.990064	-0.186535
C	-2.357404	0.179578	1.345477	C	-2.362234	0.162373	1.341281	C	-2.463862	0.208536	1.316567
H	-2.306676	0.954600	2.101196	H	-2.325311	0.925224	2.103095	H	-2.432988	1.002260	2.052530
C	-1.922941	-1.734169	0.115204	C	-1.912157	-1.727575	0.105051	C	-1.996765	-1.730884	0.150409
H	-1.470556	-2.659962	-0.225092	H	-1.457771	-2.645786	-0.236499	H	-1.542002	-2.667810	-0.150560
C	-1.554801	-1.013296	1.300670	C	-1.554961	-1.017525	1.290687	C	-1.670312	-0.987688	1.331356
H	-0.823455	-1.322729	2.038802	H	-0.83203	-1.328788	2.028093	H	-0.973956	-1.286067	2.104806
C	1.478308	-1.926028	0.156185	C	1.479587	-1.915386	0.159174	C	1.482789	-1.932295	0.173482
C	2.637744	-1.259618	0.637845	C	2.629142	-1.251484	0.644268	H	2.661959	-1.300274	0.650917
H	3.100727	-1.407598	1.605354	H	3.087557	-1.40135	1.608267	C	3.123366	-1.455963	1.617635
C	3.051337	-0.324883	-0.363267	C	3.048772	-0.327105	-0.352315	C	3.102331	-0.388318	-0.359215
H	3.875603	0.374629	-0.286845	H	3.873921	0.363864	-0.276407	H	3.947747	0.284891	-0.287359
C	1.161772	-1.424945	-1.150608	C	1.17604	-1.424081	-1.145178	C	1.181370	-1.432894	-1.137907
H	0.362178	-1.769950	-1.796147	H	0.389975	-1.775441	-1.794496	H	0.389551	-1.775804	-1.792220
C	2.138219	-0.418702	-1.464258	C	2.150004	-0.42561	-1.454007	C	2.196079	-0.468106	-1.457934
H	2.177414	0.173476	-2.372279	H	2.201173	0.155018	-2.362748	H	2.250424	0.120538	-2.366214
H	0.899146	-2.661144	0.705185	H	0.902411	-2.64881	0.701967	C	0.883611	-2.646360	0.726460
H	-3.393306	-1.280783	-1.509334	H	-3.381599	-1.282361	-1.506848	H	-3.397663	-1.305061	-1.539881
Fe	1.157062	0.118798	0.205188	Fe	1.159053	0.120238	0.198823	H	1.200337	0.124601	0.224824
Fe	-1.224591	0.160519	-0.310138	Fe	-1.230561	0.163643	-0.306985	H	-1.241423	0.157063	-0.310219

Tables S82 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-9T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-2.858440	-0.173608	0.648769	C	-2.857601	-0.175783	0.642792	C	-2.861543	-0.188178	0.645828
C	-2.858439	-0.173618	-0.648770	C	-2.857602	-0.175791	-0.642790	C	-2.861546	-0.188310	-0.645686
C	-3.620599	-0.353855	1.906642	C	-3.602251	-0.359166	1.900191	C	-3.659194	-0.418176	1.886266
H	-4.686170	-0.529411	1.714274	H	-4.659759	-0.567790	1.721194	H	-4.697536	-0.690483	1.659176
H	-3.535152	0.525037	2.553970	H	-3.541920	0.526217	2.534247	H	-3.665122	0.482427	2.510367
H	-3.238922	-1.204715	2.481139	H	-3.197148	-1.185364	2.486214	H	-3.213297	-1.220646	2.484939

C	-3.620606	-0.353882	-1.906635	C	-3.602252	-0.359188	-1.900185	C	-3.659199	-0.418585	-1.886072
H	-4.686175	-0.529441	-1.714257	H	-4.659760	-0.567810	-1.721185	H	-4.697522	-0.690909	-1.658919
H	-3.535167	0.525003	-2.553974	H	-3.541923	0.526189	-2.534251	H	-3.665186	0.481905	-2.510336
H	-3.238930	-1.204747	-2.481125	H	-3.197150	-1.185392	-2.486200	H	-3.213263	-1.221137	-2.484605
C	2.582146	-1.464006	-0.713928	C	2.570740	-1.462073	-0.709795	Fe	2.603000	-1.474210	-0.713863
C	1.247111	-1.705027	-1.160707	C	1.243806	-1.704963	-1.153877	Fe	1.277890	-1.756354	-1.158275
H	0.915514	-1.747496	-2.191479	H	0.916292	-1.757111	-2.180277	C	0.945613	-1.806588	-2.187718
C	0.409032	-1.853225	0.000003	C	0.411319	-1.856474	0.000007	C	0.449319	-1.937241	-0.000209
H	-0.646943	-2.123377	0.000004	H	-0.637019	-2.132906	0.000006	H	-0.592731	-2.243875	-0.000315
C	2.582141	-1.464003	0.713946	C	2.570737	-1.462066	0.709813	C	2.602875	-1.474280	0.713866
H	3.437843	-1.273626	1.350709	H	3.423318	-1.276240	1.343841	H	3.452835	-1.262632	1.350634
C	1.247104	-1.705021	1.160716	C	1.243801	-1.704952	1.153893	C	1.277692	-1.756477	1.158020
H	0.915504	-1.747479	2.191488	H	0.916283	-1.757091	2.180292	H	0.945239	-1.806826	2.187400
C	2.115426	1.637693	-0.715457	C	2.112698	1.629959	-0.711176	C	2.100222	1.648006	-0.713317
C	2.115421	1.637696	0.715452	C	2.112696	1.629966	0.711161	H	2.100135	1.647935	0.713498
H	2.985505	1.599286	1.361536	H	2.978622	1.592084	1.354298	C	2.968117	1.595903	1.359622
C	0.745957	1.680550	1.138342	C	0.750873	1.676164	1.132045	C	0.737304	1.727670	1.144361
H	0.435678	1.730528	2.177983	H	0.443142	1.731809	2.166885	H	0.435280	1.810035	2.182315
C	0.745965	1.680542	-1.138358	C	0.750875	1.676152	-1.132063	C	0.737444	1.727769	-1.144336
H	0.435693	1.730501	-2.178001	H	0.443147	1.731787	-2.166905	H	0.435534	1.810199	-2.182317
C	-0.137555	1.970228	-0.000013	C	-0.127101	1.968474	-0.000012	C	-0.127830	2.040795	-0.000027
H	-0.931794	2.728157	-0.000020	H	-0.914572	2.726816	-0.000016	H	-0.927709	2.786723	-0.000046
H	2.985511	1.599267	-1.361540	H	2.978625	1.592070	-1.354310	C	2.968284	1.596025	-1.359338
H	3.437854	-1.273639	-1.350686	H	3.423323	-1.276252	-1.343820	H	3.453069	-1.262494	-1.350463
Fe	-1.099294	0.231454	-0.000001	Fe	-1.104162	0.246452	-0.000002	H	-1.086853	0.304822	0.000010
Fe	1.283224	-0.037863	-0.000001	Fe	1.277319	-0.040397	0.000000	H	1.270275	-0.052507	-0.000037

Tables S83 : Optimized coordinates for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-10T**

	M06L/DZP				M06L/def2tzvpp				WB97XD/DZP		
	x	y	z		x	y	z		x	y	z
C	-1.032660	1.832407	-0.726895	C	-1.037289	1.832238	-0.720924	C	-1.108408	1.878940	-0.681558
C	-0.142190	1.429063	0.268735	C	-0.142879	1.432852	0.259797	C	-0.192604	1.456283	0.268591
C	-2.087254	2.885953	-0.527158	C	-2.089563	2.878549	-0.520985	C	-2.056797	3.041379	-0.519912
H	-1.719846	3.887970	-0.784793	H	-1.735266	3.87521	-0.79748	H	-1.651893	3.954433	-0.974424
H	-2.405037	2.913573	0.520435	H	-2.392926	2.92182	0.524942	H	-2.224150	3.239528	0.543584
H	-2.971857	2.693858	-1.144276	H	-2.978442	2.676205	-1.119518	H	-3.023649	2.831398	-0.990483
C	0.481412	1.673176	1.514112	C	0.486286	1.689995	1.489783	C	0.566627	1.824051	1.387379
H	0.087015	1.203092	2.421663	H	0.113166	1.224982	2.402209	H	0.420764	1.284181	2.328178
H	-0.734878	1.637993	-1.771016	H	-0.760965	1.626531	-1.76289	H	-0.948535	1.521943	-1.716317
H	0.981313	2.629105	1.690049	H	0.975377	2.647273	1.657056	H	0.985822	2.824607	1.484145
C	-2.543716	-1.597041	-0.807094	C	-2.518556	-1.607387	-0.805487	Fe	-2.768319	-1.418456	-0.815968
C	-3.068609	-0.624934	0.089533	C	-3.060779	-0.641567	0.074882	Fe	-3.126362	-0.640003	0.322551
H	-3.910995	0.031648	-0.093927	H	-3.909945	-0.004347	-0.116823	C	-3.946466	0.065840	0.377222
C	-2.268506	-0.653893	1.282245	C	-2.278908	-0.657706	1.270806	C	-2.206378	-0.938707	1.376701

H	-2.394190	-0.013120	2.147936	H	-2.423766	-0.021125	2.130219	H	-2.206257	-0.502113	2.367677
C	-1.415477	-2.219860	-0.189424	C	-1.397968	-2.212102	-0.175858	C	-1.611734	-2.181012	-0.480587
H	-0.788060	-2.986545	-0.630208	H	-0.766164	-2.976852	-0.600862	H	-1.080114	-2.856913	-1.139726
C	-1.254750	-1.649659	1.112478	C	-1.259253	-1.638019	1.118318	C	-1.265461	-1.885256	0.872125
H	-0.493570	-1.917071	1.837476	H	-0.509579	-1.895021	1.850864	H	-0.426903	-2.302263	1.417041
C	2.333096	-1.574674	-0.206351	C	2.322096	-1.571009	-0.181363	C	2.788587	-1.278032	0.559671
C	3.211306	-0.752662	0.543632	C	3.199699	-0.74726	0.550793	H	3.424731	-0.003723	0.470430
H	3.674411	-1.015267	1.487969	H	3.665017	-0.999364	1.491567	C	4.029670	0.464462	1.237671
C	3.309662	0.513896	-0.106670	C	3.303911	0.501898	-0.114724	C	3.190900	0.521157	-0.842773
H	3.894496	1.360830	0.230486	H	3.896205	1.344635	0.204222	H	3.533783	1.481049	-1.210443
C	1.907109	-0.825804	-1.352615	C	1.903512	-0.842772	-1.334447	C	2.093096	-1.492075	-0.666831
H	1.255040	-1.193052	-2.138157	H	1.255804	-1.218635	-2.111801	H	1.507314	-2.365877	-0.925573
C	2.529867	0.456729	-1.300691	C	2.52832	0.430646	-1.301863	C	2.373603	-0.387738	-1.538799
H	2.400403	1.261449	-2.014335	H	2.410672	1.218636	-2.028613	H	1.987062	-0.260611	-2.543301
H	2.039410	-2.590260	0.034105	H	2.030233	-2.578855	0.070384	C	2.820582	-1.953477	1.406456
H	-2.902933	-1.792852	-1.811233	H	-2.86773	-1.817317	-1.805278	H	-3.268001	-1.406453	-1.777507
Fe	1.259608	0.183780	0.409486	Fe	1.263265	0.196546	0.401685	H	1.297210	0.229295	0.333159
Fe	-1.096780	-0.163300	-0.315071	Fe	-1.099937	-0.162466	-0.310938	H	-1.186361	-0.113932	-0.262018

Tables S84 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2(MeC_2NMe_2)_2$**structure **2N-Ni-1S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
18(0)	785(41)	1405(5)	18(0)	795(34)	1392(3)	42(0)	801(70)	1420(127)
29(0)	786(37)	1408(0)	27(0)	798(29)	1430(0)	43(0)	817(22)	1443(1)
58(0)	789(22)	1412(0)	60(0)	800(15)	1435(0)	60(0)	823(5)	1447(2)
60(0)	825(0)	1432(11)	62(0)	826(10)	1451(12)	66(0)	842(1)	1463(4)
61(0)	826(8)	1439(5)	65(0)	828(0)	1453(1)	67(0)	845(1)	1464(0)
69(1)	828(7)	1447(1)	74(0)	830(13)	1455(0)	75(0)	845(18)	1470(7)
76(1)	834(0)	1448(0)	77(0)	838(1)	1459(5)	82(2)	854(1)	1475(11)
81(0)	843(9)	1450(5)	80(0)	843(8)	1469(0)	86(1)	868(9)	1482(3)
103(2)	860(0)	1453(3)	106(2)	877(0)	1471(0)	109(0)	895(0)	1483(4)
138(4)	861(1)	1463(19)	141(3)	879(0)	1474(4)	139(7)	896(1)	1485(1)
152(4)	862(1)	1463(11)	156(4)	881(0)	1477(3)	149(10)	898(2)	1486(1)
193(1)	863(3)	1465(22)	191(0)	882(1)	1485(22)	192(0)	900(0)	1497(22)
197(1)	927(11)	1466(14)	192(1)	926(8)	1487(38)	197(0)	949(11)	1497(1)
202(0)	1010(84)	1469(2)	202(0)	1009(87)	1493(1)	201(0)	1018(11)	1497(40)
208(0)	1013(9)	1473(1)	210(0)	1020(7)	1496(2)	206(1)	1019(13)	1501(1)
213(1)	1015(14)	1488(2)	215(0)	1022(9)	1509(2)	217(3)	1034(0)	1517(5)
214(1)	1025(25)	1499(46)	217(2)	1033(19)	1517(38)	218(1)	1035(31)	1529(94)
262(3)	1026(3)	1682(149)	263(4)	1033(3)	1686(146)	264(9)	1036(74)	1735(219)
264(5)	1055(5)	2954(94)	266(4)	1062(5)	2981(63)	269(2)	1069(0)	3007(47)
297(5)	1058(0)	2958(86)	299(4)	1065(1)	2984(37)	286(3)	1070(7)	3007(36)
299(5)	1063(1)	2960(167)	302(4)	1071(1)	2987(141)	288(7)	1072(0)	3010(162)
321(1)	1064(2)	2961(59)	323(1)	1073(3)	2989(64)	309(0)	1074(3)	3011(4)

327(0)	1066(1)	3074(72)	329(1)	1074(1)	3094(41)	323(1)	1077(4)	3116(37)
337(4)	1067(2)	3075(98)	340(4)	1076(2)	3095(32)	338(2)	1081(0)	3117(84)
346(2)	1094(3)	3079(12)	347(2)	1109(5)	3098(18)	341(6)	1118(2)	3117(23)
352(0)	1097(3)	3080(34)	356(0)	1112(4)	3100(20)	354(1)	1121(2)	3117(6)
385(16)	1130(142)	3137(11)	387(14)	1139(159)	3156(6)	392(15)	1149(12)	3171(28)
417(10)	1142(43)	3141(16)	417(8)	1147(10)	3157(7)	425(16)	1150(2)	3172(0)
469(2)	1143(16)	3141(41)	476(1)	1148(6)	3157(18)	438(72)	1156(135)	3178(13)
475(23)	1145(3)	3141(29)	484(25)	1159(38)	3159(13)	473(4)	1169(40)	3178(15)
548(27)	1150(13)	3214(0)	552(25)	1165(8)	3225(0)	554(70)	1177(12)	3262(0)
576(39)	1244(32)	3214(0)	580(49)	1241(33)	3225(0)	568(27)	1277(0)	3262(0)
586(1)	1250(9)	3214(1)	597(1)	1249(8)	3225(0)	594(2)	1278(0)	3264(0)
598(17)	1254(0)	3215(0)	606(23)	1275(0)	3227(0)	611(32)	1285(23)	3264(0)
598(16)	1255(0)	3230(29)	609(0)	1275(0)	3240(8)	612(0)	1292(11)	3277(7)
606(4)	1279(12)	3232(27)	616(4)	1289(11)	3241(9)	621(5)	1305(10)	3277(7)
743(18)	1367(121)	3234(27)	752(19)	1370(132)	3245(10)	774(16)	1405(8)	3279(1)
757(3)	1395(0)	3235(27)	771(0)	1383(0)	3246(7)	790(1)	1411(1)	3279(13)
765(2)	1400(12)	3246(12)	779(3)	1387(11)	3255(5)	792(81)	1411(36)	3291(6)
776(40)	1401(10)	3247(16)	787(48)	1389(8)	3256(4)	795(44)	1416(5)	3291(2)

Tables S85 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2(MeC_2NMe_2)_2$**structure **2N-Ni-2T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
18(0)	773(2)	1402(2)	8(0)	785(16)	1389(18)	10(3)	803(8)	1423(141)
20(0)	780(3)	1410(2)	33(0)	795(44)	1434(1)	24(6)	808(95)	1446(2)
41(0)	783(71)	1412(1)	47(0)	795(9)	1436(1)	30(0)	809(1)	1447(3)
45(3)	828(0)	1431(16)	52(2)	828(14)	1452(14)	36(1)	853(2)	1469(17)
58(0)	828(1)	1441(10)	59(0)	831(1)	1458(0)	52(0)	854(0)	1473(0)
61(0)	832(0)	1452(1)	71(1)	833(1)	1459(0)	64(0)	857(1)	1474(0)
71(2)	834(0)	1452(0)	76(1)	837(0)	1462(6)	77(3)	857(0)	1477(10)
73(1)	837(9)	1454(7)	76(1)	838(0)	1470(0)	81(3)	863(3)	1480(1)
99(0)	851(0)	1455(0)	105(0)	870(0)	1470(0)	99(0)	890(0)	1481(0)
102(6)	855(1)	1464(0)	108(8)	874(1)	1478(7)	101(4)	894(0)	1486(4)
139(4)	857(1)	1464(1)	144(3)	876(1)	1479(0)	139(1)	898(0)	1486(0)
169(1)	860(0)	1465(10)	172(1)	877(0)	1488(12)	162(3)	899(0)	1497(1)
171(3)	918(15)	1466(53)	175(1)	916(12)	1489(53)	168(3)	934(28)	1498(41)
173(1)	1017(27)	1471(11)	183(0)	1019(70)	1495(6)	168(1)	1027(35)	1499(22)
175(1)	1017(1)	1474(4)	185(4)	1023(21)	1497(1)	173(0)	1028(1)	1502(13)
186(0)	1021(47)	1487(1)	196(0)	1025(2)	1509(1)	179(0)	1031(12)	1513(5)
187(0)	1025(9)	1503(64)	200(0)	1033(8)	1521(48)	184(1)	1032(10)	1530(100)
230(0)	1026(44)	1678(195)	234(1)	1033(18)	1684(172)	229(0)	1051(65)	1681(276)
250(8)	1055(6)	2966(42)	250(7)	1062(5)	2990(19)	260(8)	1072(0)	3016(20)
263(1)	1060(2)	2966(66)	266(1)	1067(0)	2990(59)	272(12)	1073(0)	3016(46)
269(4)	1063(2)	2968(301)	272(4)	1073(0)	2993(203)	282(2)	1074(0)	3017(201)
276(1)	1064(0)	2969(24)	279(1)	1073(1)	2994(31)	290(1)	1076(0)	3018(13)

289(5)	1066(0)	3078(63)	292(4)	1075(1)	3098(25)	293(3)	1077(6)	3117(47)
305(6)	1067(0)	3078(134)	307(5)	1077(0)	3098(71)	309(2)	1084(2)	3117(49)
305(0)	1096(1)	3081(10)	313(0)	1112(1)	3099(0)	314(6)	1118(1)	3120(0)
342(10)	1098(2)	3082(14)	346(11)	1114(2)	3100(17)	355(10)	1119(2)	3120(53)
343(6)	1124(156)	3139(2)	346(4)	1132(169)	3155(1)	357(3)	1143(167)	3171(23)
377(68)	1140(54)	3141(38)	385(11)	1148(9)	3156(18)	394(14)	1155(8)	3171(1)
388(22)	1145(12)	3145(24)	395(74)	1149(3)	3162(11)	416(19)	1155(1)	3181(11)
403(10)	1146(0)	3145(20)	406(12)	1157(47)	3162(9)	426(78)	1164(50)	3181(13)
465(5)	1151(6)	3212(2)	470(4)	1166(3)	3224(0)	478(6)	1174(5)	3260(0)
529(22)	1255(0)	3212(0)	534(21)	1252(18)	3224(0)	544(39)	1278(0)	3260(0)
585(0)	1256(1)	3213(0)	596(0)	1259(9)	3225(0)	613(0)	1279(0)	3262(0)
592(0)	1256(16)	3214(4)	603(0)	1276(0)	3226(1)	616(0)	1296(11)	3262(1)
594(1)	1262(10)	3229(5)	605(1)	1277(0)	3241(1)	620(1)	1303(11)	3276(1)
602(0)	1286(6)	3230(49)	613(0)	1294(6)	3241(16)	624(0)	1312(2)	3276(13)
745(6)	1380(129)	3236(24)	757(7)	1380(124)	3244(8)	778(24)	1411(1)	3279(5)
750(0)	1398(1)	3236(24)	763(0)	1385(1)	3245(7)	789(27)	1412(16)	3279(8)
759(22)	1399(9)	3246(20)	764(20)	1386(11)	3255(5)	789(5)	1413(0)	3290(2)
771(87)	1401(2)	3246(4)	780(79)	1388(2)	3255(2)	791(149)	1414(2)	3291(3)

Tables S86 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2(MeC_2NMe_2)_2$**structure **2N-Ni-3S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
19(0)	777(31)	1403(8)	18(0)	787(17)	1393(14)	18(0)	792(95)	1418(16)
26(0)	784(20)	1404(2)	23(0)	796(35)	1421(2)	28(0)	817(6)	1438(5)
36(0)	787(14)	1406(11)	30(0)	801(5)	1427(1)	31(1)	827(1)	1441(2)
46(0)	811(12)	1420(24)	48(0)	815(18)	1441(32)	52(1)	844(10)	1456(2)
70(0)	820(3)	1424(3)	72(0)	825(1)	1442(2)	70(0)	848(5)	1458(21)
78(1)	827(11)	1437(2)	80(1)	831(14)	1447(2)	80(1)	850(16)	1466(1)
81(1)	833(4)	1449(1)	84(1)	837(5)	1459(0)	85(1)	851(0)	1468(2)
95(1)	834(1)	1452(0)	96(1)	838(1)	1467(0)	99(1)	853(18)	1484(0)
111(2)	850(0)	1455(4)	114(1)	869(0)	1471(1)	116(3)	891(0)	1485(0)
138(0)	856(7)	1458(4)	140(0)	874(6)	1476(1)	148(0)	893(1)	1487(6)
149(1)	858(1)	1462(1)	150(1)	875(0)	1476(4)	155(0)	895(4)	1491(7)
166(0)	862(3)	1464(8)	168(0)	880(2)	1479(5)	175(0)	898(7)	1493(4)
193(0)	910(4)	1466(21)	196(0)	912(3)	1485(8)	197(1)	932(6)	1496(11)
206(0)	976(65)	1471(0)	211(0)	971(60)	1487(15)	211(0)	1009(7)	1502(13)
208(0)	1003(14)	1474(1)	219(0)	1009(11)	1495(3)	217(0)	1016(73)	1506(7)
233(4)	1017(11)	1476(11)	239(3)	1024(9)	1497(10)	242(3)	1020(15)	1509(15)
243(2)	1026(16)	1483(8)	250(2)	1032(2)	1503(7)	254(1)	1034(20)	1515(19)
257(2)	1026(6)	1660(265)	264(2)	1032(11)	1655(253)	259(6)	1035(20)	1702(359)
268(1)	1027(14)	2989(76)	270(1)	1034(15)	3012(27)	267(4)	1058(9)	3045(37)
273(3)	1051(5)	2993(91)	280(2)	1057(6)	3016(76)	270(3)	1067(2)	3047(69)
284(8)	1059(1)	2995(113)	290(9)	1067(1)	3018(73)	277(4)	1070(7)	3050(50)
300(1)	1062(5)	3009(156)	308(1)	1071(5)	3031(102)	292(6)	1071(1)	3057(97)

313(7)	1066(0)	3084(59)	318(6)	1074(0)	3104(28)	315(4)	1073(3)	3130(35)
337(5)	1068(0)	3090(5)	343(4)	1076(1)	3107(2)	334(6)	1074(3)	3133(5)
340(2)	1093(10)	3095(48)	345(1)	1105(18)	3114(18)	351(3)	1114(5)	3138(26)
371(6)	1095(1)	3102(15)	372(5)	1108(1)	3118(13)	381(5)	1118(2)	3139(15)
388(1)	1118(119)	3116(10)	395(0)	1123(107)	3132(4)	395(3)	1148(61)	3164(3)
446(1)	1138(12)	3159(10)	454(1)	1142(8)	3174(3)	463(1)	1149(5)	3198(4)
491(0)	1142(2)	3163(17)	503(0)	1149(6)	3179(7)	500(1)	1153(47)	3201(7)
511(0)	1145(9)	3173(12)	511(0)	1156(3)	3190(5)	532(2)	1170(1)	3202(13)
529(6)	1162(5)	3206(0)	537(5)	1176(6)	3217(0)	546(4)	1198(8)	3254(0)
578(2)	1211(9)	3209(2)	588(3)	1207(8)	3219(2)	603(1)	1251(9)	3258(1)
589(1)	1251(3)	3211(1)	601(3)	1251(12)	3223(1)	609(0)	1275(0)	3258(1)
600(7)	1252(0)	3215(1)	609(9)	1261(3)	3225(1)	614(1)	1277(0)	3259(0)
601(3)	1255(0)	3223(38)	612(2)	1272(0)	3233(15)	623(12)	1282(4)	3270(12)
634(37)	1258(13)	3229(34)	638(32)	1276(0)	3239(11)	670(7)	1297(23)	3272(11)
708(12)	1337(19)	3230(32)	713(13)	1336(16)	3240(12)	727(11)	1380(87)	3274(9)
722(1)	1389(4)	3236(30)	735(1)	1377(4)	3246(10)	761(0)	1404(4)	3279(8)
755(1)	1398(2)	3243(19)	770(1)	1389(14)	3251(7)	780(9)	1412(3)	3287(5)
765(72)	1402(15)	3247(18)	777(69)	1390(2)	3255(6)	784(114)	1416(3)	3289(5)

Tables S87 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2(MeC_2NMe_2)_2$**structure **2N-Ni-4S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
17(0)	781(52)	1402(0)	-31(0)	797(0)	1391(12)	20(0)	799(98)	1429(0)
28(0)	799(6)	1408(24)	-29(0)	798(2)	1399(17)	21(0)	835(6)	1429(5)
30(2)	802(0)	1412(2)	56(0)	802(50)	1423(0)	33(3)	835(0)	1446(11)
58(1)	827(0)	1414(4)	58(2)	831(0)	1424(2)	58(1)	847(0)	1447(33)
76(1)	831(2)	1440(48)	61(0)	834(0)	1447(0)	69(0)	849(3)	1464(0)
82(0)	832(1)	1443(52)	73(1)	837(3)	1449(32)	73(0)	852(6)	1464(0)
93(0)	834(0)	1446(0)	85(0)	837(2)	1458(0)	84(0)	853(0)	1485(30)
118(0)	859(32)	1448(14)	107(1)	855(49)	1458(0)	96(1)	879(64)	1486(0)
120(1)	864(2)	1453(0)	109(0)	873(2)	1464(0)	105(0)	900(0)	1487(22)
129(0)	864(0)	1454(3)	147(0)	880(0)	1465(6)	133(0)	900(0)	1488(0)
143(0)	865(0)	1465(0)	155(0)	880(0)	1469(0)	138(0)	904(0)	1491(0)
153(0)	873(41)	1466(21)	160(0)	883(0)	1470(0)	139(0)	904(3)	1491(24)
159(0)	893(4)	1467(0)	162(0)	895(0)	1480(2)	142(0)	915(5)	1497(0)
173(0)	894(5)	1468(18)	179(0)	933(8)	1484(22)	173(1)	915(4)	1498(0)
178(0)	1011(0)	1477(0)	193(1)	1022(0)	1494(0)	182(0)	1016(0)	1503(1)
196(0)	1012(20)	1478(0)	198(0)	1023(19)	1496(11)	195(0)	1018(27)	1504(28)
226(7)	1030(2)	1528(33)	210(1)	1030(8)	1520(51)	229(2)	1039(7)	1589(80)
234(0)	1032(24)	1530(124)	232(1)	1031(13)	1521(12)	241(2)	1041(28)	1593(206)
237(2)	1036(0)	3002(0)	235(4)	1058(0)	3005(60)	249(1)	1052(0)	3051(0)
265(2)	1037(12)	3002(66)	263(9)	1058(10)	3005(0)	255(1)	1052(11)	3051(37)
276(0)	1064(0)	3005(415)	279(0)	1071(0)	3011(206)	275(0)	1072(0)	3054(237)
278(1)	1067(3)	3007(91)	294(1)	1072(2)	3011(35)	278(24)	1072(7)	3055(77)

300(16)	1067(3)	3078(4)	310(17)	1073(5)	3092(0)	300(2)	1073(0)	3121(10)
307(0)	1068(1)	3079(154)	319(0)	1074(5)	3093(103)	307(0)	1075(2)	3121(83)
342(2)	1085(1)	3084(0)	344(0)	1100(0)	3094(0)	350(0)	1105(1)	3123(0)
348(0)	1086(0)	3084(0)	348(9)	1101(0)	3094(0)	351(2)	1105(0)	3123(0)
372(0)	1137(45)	3172(1)	385(1)	1125(170)	3145(1)	377(1)	1156(4)	3217(0)
391(5)	1137(28)	3172(1)	408(4)	1134(87)	3146(0)	392(4)	1156(0)	3217(0)
427(4)	1144(129)	3173(0)	498(4)	1148(10)	3147(7)	455(3)	1168(75)	3217(1)
485(2)	1145(18)	3174(4)	501(2)	1149(0)	3147(23)	498(3)	1169(20)	3217(4)
492(2)	1147(11)	3208(0)	516(3)	1151(10)	3221(0)	515(1)	1171(48)	3254(0)
538(3)	1149(11)	3208(0)	585(12)	1178(19)	3221(0)	570(3)	1174(26)	3254(0)
579(0)	1228(0)	3211(4)	598(0)	1254(0)	3225(0)	592(0)	1269(0)	3259(0)
588(3)	1237(59)	3211(0)	609(4)	1257(43)	3227(3)	602(3)	1275(54)	3259(2)
597(0)	1256(0)	3225(0)	611(1)	1274(0)	3239(0)	611(2)	1278(0)	3270(0)
601(0)	1256(0)	3225(71)	626(5)	1274(0)	3239(23)	615(0)	1278(0)	3270(24)
738(1)	1391(0)	3234(30)	711(0)	1371(171)	3241(8)	770(0)	1412(0)	3276(6)
744(1)	1393(1)	3234(25)	759(0)	1373(93)	3243(6)	777(0)	1414(1)	3276(8)
758(0)	1395(72)	3246(11)	773(1)	1386(0)	3254(7)	790(0)	1423(3)	3288(3)
776(109)	1398(22)	3247(11)	785(76)	1391(12)	3257(6)	792(173)	1425(3)	3289(3)

Tables S88 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)_2$**structure **2N-Co-1S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
-35(0)	790(0)	1410(21)	-46(0)	805(30)	1418(152)	-33(0)	828(7)	1433(0)
-27(0)	808(10)	1411(0)	-41(0)	812(4)	1418(0)	-24(0)	846(28)	1433(4)
34(2)	813(12)	1412(1)	31(2)	819(7)	1419(1)	38(2)	849(5)	1449(64)
61(0)	826(0)	1412(0)	55(0)	829(0)	1421(43)	51(0)	853(2)	1450(20)
70(0)	826(0)	1448(68)	64(0)	830(0)	1456(0)	56(1)	854(0)	1472(0)
78(0)	827(0)	1449(0)	75(0)	830(0)	1457(1)	77(0)	854(0)	1474(0)
78(0)	831(0)	1450(19)	91(0)	834(0)	1461(0)	95(0)	857(1)	1476(1)
110(0)	857(59)	1453(2)	106(0)	866(116)	1461(6)	99(0)	901(32)	1477(2)
115(0)	865(1)	1454(58)	111(0)	877(13)	1467(72)	102(0)	910(64)	1486(0)
116(0)	867(78)	1454(0)	113(0)	888(0)	1473(88)	113(0)	915(2)	1487(41)
147(0)	877(0)	1458(5)	144(0)	890(0)	1475(0)	147(0)	923(0)	1488(7)
166(0)	877(0)	1459(41)	159(0)	891(2)	1476(4)	154(0)	924(0)	1492(68)
174(2)	918(9)	1468(3)	167(1)	916(5)	1488(3)	165(1)	947(9)	1497(0)
187(2)	918(6)	1469(0)	190(2)	918(8)	1489(6)	197(3)	948(10)	1497(18)
206(0)	1012(0)	1469(6)	208(0)	1020(0)	1492(0)	211(0)	1023(0)	1502(6)
220(0)	1013(20)	1470(17)	226(2)	1021(16)	1492(16)	230(2)	1025(29)	1503(15)
224(2)	1023(4)	1551(239)	229(0)	1028(3)	1555(181)	231(0)	1031(6)	1599(327)
254(1)	1023(16)	1557(100)	263(1)	1029(11)	1557(73)	269(2)	1032(20)	1601(179)
283(0)	1043(0)	2999(0)	284(0)	1048(0)	3023(0)	292(1)	1066(0)	3044(0)
286(6)	1044(7)	2999(82)	287(6)	1048(9)	3023(55)	294(7)	1066(8)	3045(54)
307(1)	1062(1)	3003(403)	310(1)	1070(2)	3028(250)	314(0)	1070(0)	3048(248)
314(0)	1062(0)	3005(113)	317(0)	1071(0)	3029(75)	328(0)	1070(1)	3049(95)

360(3)	1064(0)	3074(6)	365(2)	1073(0)	3098(2)	376(4)	1073(0)	3112(8)
372(5)	1068(2)	3075(169)	376(6)	1076(1)	3098(94)	384(5)	1077(2)	3113(107)
387(3)	1089(0)	3081(0)	394(5)	1101(0)	3101(0)	401(5)	1110(0)	3115(0)
402(0)	1090(3)	3081(0)	405(0)	1102(3)	3101(0)	416(0)	1111(3)	3116(0)
408(0)	1138(17)	3174(7)	409(1)	1147(19)	3188(2)	431(0)	1156(11)	3213(0)
430(6)	1139(25)	3175(0)	430(6)	1147(21)	3188(0)	442(7)	1156(17)	3213(12)
442(10)	1143(27)	3175(0)	458(7)	1151(24)	3189(0)	475(13)	1167(12)	3213(4)
514(2)	1143(9)	3176(12)	520(2)	1153(22)	3189(6)	543(4)	1167(17)	3213(0)
524(10)	1160(171)	3210(0)	534(10)	1172(156)	3222(0)	550(8)	1188(136)	3263(0)
569(5)	1169(55)	3211(3)	574(4)	1179(59)	3223(2)	587(0)	1194(60)	3263(2)
592(0)	1235(0)	3213(0)	602(2)	1228(0)	3225(0)	615(0)	1275(0)	3267(1)
594(1)	1243(62)	3213(1)	602(0)	1236(56)	3227(1)	615(1)	1276(0)	3267(0)
594(2)	1251(0)	3229(32)	603(0)	1271(0)	3240(13)	616(0)	1279(0)	3279(0)
599(0)	1251(0)	3230(48)	609(0)	1271(0)	3241(0)	626(0)	1287(60)	3279(19)
698(0)	1393(0)	3230(0)	700(0)	1396(6)	3241(25)	728(0)	1422(3)	3280(15)
778(29)	1395(1)	3230(68)	789(29)	1399(0)	3242(15)	808(62)	1424(0)	3280(11)
786(29)	1401(80)	3243(17)	798(7)	1399(5)	3252(6)	824(60)	1427(5)	3293(2)
789(8)	1406(23)	3243(8)	799(0)	1400(0)	3254(4)	826(0)	1427(0)	3293(3)

Tables S89 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)_2$**structure **2N-Co-2T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
-10(0)	789(44)	1407(1)	38(0)	793(57)	1403(0)	-168(10)	821(68)	1422(4)
20(0)	790(15)	1410(1)	46(0)	800(35)	1413(17)	27(0)	828(1)	1442(2)
34(1)	796(32)	1411(1)	59(0)	818(8)	1418(3)	33(0)	829(28)	1445(4)
52(1)	811(23)	1428(17)	77(3)	820(0)	1418(0)	44(0)	851(3)	1466(27)
56(0)	824(2)	1439(5)	80(0)	827(0)	1454(3)	58(0)	853(0)	1471(2)
62(0)	825(0)	1450(5)	95(0)	829(1)	1456(0)	66(1)	854(2)	1474(1)
65(0)	830(0)	1451(2)	112(0)	833(0)	1461(33)	70(1)	855(0)	1476(1)
81(0)	832(7)	1453(0)	120(0)	836(1)	1466(34)	78(1)	875(17)	1477(9)
111(2)	861(0)	1454(2)	121(0)	883(0)	1476(2)	89(0)	894(0)	1481(1)
123(3)	862(1)	1457(1)	133(1)	883(0)	1477(2)	97(0)	902(1)	1483(5)
166(3)	864(0)	1457(2)	146(0)	884(6)	1480(0)	129(1)	906(0)	1487(0)
187(11)	867(0)	1464(18)	165(0)	885(2)	1480(4)	136(1)	908(0)	1495(11)
191(0)	933(17)	1465(62)	182(0)	896(8)	1490(0)	151(1)	962(13)	1498(16)
200(0)	998(72)	1471(4)	182(0)	900(1)	1490(5)	164(3)	1026(13)	1502(9)
203(0)	1017(7)	1474(0)	202(2)	1022(0)	1491(10)	185(1)	1028(11)	1504(20)
211(0)	1018(15)	1487(1)	220(0)	1022(11)	1492(14)	209(1)	1032(28)	1512(7)
222(1)	1022(26)	1497(48)	230(0)	1038(0)	1529(70)	217(1)	1033(7)	1524(47)
224(1)	1023(0)	1591(171)	254(1)	1041(0)	1540(8)	242(3)	1045(78)	1689(378)
264(3)	1055(6)	2951(147)	264(0)	1042(18)	3021(0)	247(0)	1073(6)	2987(38)
301(7)	1059(0)	2951(71)	297(1)	1044(12)	3021(51)	270(3)	1074(1)	2990(101)
302(2)	1063(1)	2956(170)	307(0)	1077(0)	3026(327)	279(4)	1074(5)	3034(33)
327(10)	1064(0)	2958(51)	316(1)	1077(1)	3028(7)	295(7)	1075(0)	3037(165)

334(1)	1065(0)	3071(35)	322(0)	1079(1)	3097(12)	341(10)	1076(1)	3102(59)
343(2)	1068(1)	3072(144)	332(1)	1080(2)	3097(100)	363(6)	1084(1)	3107(1)
356(5)	1096(1)	3077(25)	343(0)	1093(1)	3099(0)	376(23)	1117(2)	3108(42)
359(2)	1099(1)	3077(31)	361(3)	1093(0)	3099(0)	399(8)	1120(1)	3110(48)
372(2)	1132(152)	3136(22)	370(1)	1138(165)	3200(0)	413(7)	1152(92)	3161(10)
415(8)	1143(23)	3137(18)	389(0)	1146(19)	3200(3)	425(7)	1155(2)	3162(28)
462(19)	1143(26)	3139(22)	437(12)	1151(18)	3201(0)	481(28)	1156(72)	3178(4)
482(0)	1146(26)	3139(28)	508(1)	1152(3)	3201(6)	497(4)	1170(12)	3189(9)
507(46)	1151(18)	3212(0)	511(0)	1154(76)	3223(0)	554(29)	1174(21)	3258(0)
544(31)	1241(30)	3213(0)	556(5)	1166(10)	3223(0)	583(17)	1277(22)	3261(0)
584(0)	1249(11)	3213(0)	587(0)	1216(0)	3226(0)	616(4)	1278(0)	3265(0)
589(1)	1254(0)	3213(0)	591(2)	1221(16)	3226(1)	619(0)	1280(0)	3268(0)
592(0)	1254(0)	3229(20)	600(0)	1277(0)	3239(0)	621(1)	1297(16)	3275(5)
597(0)	1263(1)	3229(31)	605(0)	1277(0)	3239(26)	625(1)	1305(20)	3275(5)
735(11)	1357(136)	3232(5)	690(3)	1391(212)	3244(3)	783(9)	1408(93)	3280(7)
775(1)	1400(4)	3233(49)	706(0)	1399(0)	3244(9)	790(0)	1415(2)	3281(7)
777(1)	1403(3)	3244(16)	764(2)	1401(34)	3255(4)	796(50)	1416(1)	3288(2)
782(2)	1405(1)	3244(6)	771(3)	1402(0)	3255(4)	800(108)	1421(3)	3293(2)

Tables S90 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)_2$**structure **2N-Co-3S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
17(0)	800(27)	1407(2)	17(0)	809(16)	1398(1)	26(0)	829(68)	1425(2)
28(0)	804(10)	1409(0)	34(0)	813(15)	1430(1)	42(0)	844(3)	1444(2)
49(0)	810(1)	1409(2)	48(0)	820(1)	1432(1)	50(0)	848(2)	1446(3)
53(1)	815(1)	1427(14)	53(1)	821(3)	1445(0)	51(0)	851(5)	1465(1)
72(0)	818(1)	1437(1)	74(0)	822(1)	1445(0)	74(0)	853(0)	1467(0)
73(0)	824(1)	1438(0)	76(0)	827(1)	1448(19)	89(0)	856(1)	1469(14)
82(1)	824(0)	1440(9)	84(1)	828(0)	1461(9)	96(1)	857(1)	1479(14)
92(0)	842(1)	1450(6)	92(0)	838(1)	1465(1)	105(0)	883(0)	1484(4)
100(2)	858(0)	1455(1)	103(1)	874(0)	1465(0)	108(2)	909(1)	1484(0)
135(4)	861(2)	1459(1)	130(4)	877(1)	1473(3)	144(5)	910(0)	1486(3)
160(1)	863(1)	1459(1)	164(1)	880(1)	1479(0)	174(1)	912(1)	1488(0)
179(0)	864(1)	1465(16)	175(0)	881(1)	1486(16)	176(1)	914(0)	1498(7)
183(0)	943(15)	1467(70)	177(0)	944(11)	1488(65)	185(0)	976(26)	1500(13)
184(1)	1008(22)	1472(6)	186(1)	1015(17)	1494(4)	196(1)	1025(29)	1500(51)
189(0)	1009(1)	1474(0)	198(1)	1017(4)	1497(0)	208(1)	1028(1)	1501(15)
206(3)	1017(45)	1486(0)	210(4)	1018(60)	1507(0)	223(0)	1036(0)	1518(4)
211(0)	1024(6)	1502(53)	215(0)	1032(5)	1519(44)	227(4)	1037(7)	1526(86)
256(0)	1025(43)	1638(228)	261(0)	1033(23)	1637(223)	263(1)	1044(76)	1642(295)
264(5)	1055(6)	2960(45)	268(4)	1063(6)	2984(22)	287(16)	1074(0)	3003(43)
288(16)	1059(3)	2960(64)	292(13)	1066(1)	2984(56)	309(11)	1074(1)	3004(18)
316(3)	1062(0)	2962(339)	315(2)	1070(0)	2988(239)	335(2)	1075(2)	3005(242)
344(0)	1062(1)	2964(39)	348(0)	1071(1)	2989(48)	362(0)	1077(7)	3006(23)

368(0)	1064(0)	3070(44)	378(0)	1072(0)	3089(12)	396(3)	1078(0)	3109(14)
372(1)	1066(0)	3071(158)	381(1)	1075(0)	3089(73)	401(1)	1084(2)	3110(100)
394(2)	1097(2)	3075(3)	402(2)	1110(4)	3094(34)	424(5)	1119(3)	3112(41)
403(16)	1099(0)	3076(40)	414(17)	1112(1)	3094(14)	445(3)	1122(0)	3113(26)
410(0)	1130(124)	3138(2)	418(0)	1139(122)	3154(15)	447(19)	1156(49)	3168(0)
431(2)	1137(44)	3140(29)	439(2)	1144(57)	3155(0)	456(0)	1159(12)	3168(20)
463(15)	1138(23)	3142(16)	469(14)	1144(11)	3161(12)	477(11)	1161(66)	3178(16)
464(32)	1143(39)	3142(28)	477(26)	1157(47)	3161(8)	514(17)	1169(45)	3178(16)
490(6)	1154(28)	3209(4)	495(5)	1166(19)	3221(1)	529(6)	1183(42)	3266(0)
554(33)	1251(0)	3209(0)	562(33)	1249(23)	3221(0)	593(47)	1278(0)	3266(0)
573(0)	1252(19)	3212(0)	586(0)	1262(10)	3223(0)	616(0)	1280(0)	3268(0)
580(0)	1252(3)	3212(5)	594(0)	1271(0)	3223(1)	621(0)	1288(17)	3268(1)
585(7)	1263(12)	3226(8)	596(5)	1272(0)	3237(3)	621(1)	1300(7)	3280(0)
585(0)	1281(4)	3226(46)	598(0)	1291(3)	3237(16)	623(18)	1304(15)	3280(10)
766(6)	1374(131)	3234(25)	774(8)	1376(138)	3242(10)	795(5)	1411(129)	3284(5)
772(1)	1399(13)	3234(26)	786(1)	1390(3)	3242(8)	814(5)	1421(5)	3284(5)
774(7)	1400(3)	3243(5)	786(2)	1390(16)	3251(4)	820(1)	1422(4)	3294(1)
791(36)	1406(1)	3243(15)	802(32)	1395(2)	3251(2)	823(76)	1424(17)	3295(1)

Tables S91 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)_2$**structure **2N-Co-4S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
28(0)	789(29)	1405(2)	29(0)	801(28)	1395(4)	39(1)	819(33)	1425(1)
37(1)	796(13)	1406(4)	42(0)	804(14)	1415(5)	43(0)	837(7)	1434(6)
67(0)	803(11)	1407(0)	69(0)	816(2)	1430(1)	66(0)	840(10)	1443(4)
70(1)	810(1)	1417(9)	72(1)	817(3)	1440(11)	71(1)	842(9)	1459(1)
80(1)	814(11)	1425(25)	80(0)	820(19)	1441(5)	80(1)	849(11)	1463(21)
85(0)	819(3)	1435(1)	88(0)	825(2)	1446(27)	88(0)	853(1)	1464(22)
94(0)	821(8)	1442(1)	95(0)	827(8)	1449(1)	94(0)	855(5)	1468(2)
97(0)	826(5)	1450(4)	98(0)	831(6)	1461(0)	100(0)	871(5)	1480(0)
120(1)	850(1)	1452(16)	119(1)	868(1)	1467(1)	116(1)	897(1)	1482(14)
125(1)	854(3)	1455(2)	134(1)	870(3)	1473(3)	127(2)	901(7)	1488(3)
156(0)	857(1)	1461(22)	162(1)	875(1)	1476(15)	157(0)	903(1)	1489(1)
167(1)	861(2)	1462(6)	168(1)	886(1)	1482(26)	170(0)	906(1)	1493(28)
169(1)	911(4)	1465(16)	174(1)	913(6)	1486(12)	175(1)	942(12)	1498(8)
206(3)	967(107)	1467(4)	211(3)	961(99)	1488(4)	210(2)	1012(12)	1502(8)
213(1)	1002(13)	1474(10)	221(0)	1008(10)	1496(9)	218(3)	1019(105)	1507(12)
219(2)	1010(6)	1485(2)	223(2)	1017(4)	1502(1)	225(1)	1025(18)	1516(3)
252(3)	1024(19)	1491(2)	256(4)	1032(13)	1510(3)	256(4)	1036(23)	1520(16)
267(1)	1027(3)	1660(330)	268(1)	1034(4)	1656(311)	286(8)	1040(6)	1695(456)
283(4)	1029(5)	2980(59)	289(1)	1035(4)	3004(45)	298(3)	1061(6)	3032(35)
285(3)	1057(5)	2981(124)	292(6)	1064(6)	3005(51)	302(6)	1069(1)	3033(12)
304(4)	1060(3)	2985(163)	310(4)	1069(2)	3009(133)	310(4)	1072(4)	3034(117)
343(4)	1061(1)	2993(209)	354(4)	1070(1)	3016(147)	333(3)	1074(1)	3037(211)

358(7)	1064(0)	3070(100)	368(6)	1073(0)	3090(49)	374(6)	1079(0)	3105(47)
369(0)	1069(1)	3077(6)	375(1)	1078(0)	3095(6)	386(0)	1080(4)	3113(19)
389(10)	1094(4)	3083(62)	400(8)	1108(23)	3103(30)	417(8)	1117(9)	3125(39)
397(2)	1096(7)	3087(5)	403(3)	1109(3)	3105(3)	424(4)	1119(2)	3127(3)
414(3)	1108(168)	3138(20)	424(3)	1113(160)	3156(10)	437(2)	1137(201)	3174(14)
453(4)	1135(30)	3146(21)	462(4)	1140(25)	3163(10)	477(7)	1152(17)	3189(7)
475(5)	1138(22)	3151(15)	480(4)	1143(14)	3167(2)	495(8)	1156(16)	3190(12)
498(6)	1140(6)	3152(6)	507(9)	1155(10)	3168(6)	516(16)	1167(6)	3197(5)
530(13)	1159(4)	3199(11)	541(11)	1173(4)	3213(4)	561(32)	1191(6)	3252(5)
571(4)	1207(12)	3206(2)	580(13)	1202(10)	3220(1)	597(22)	1252(21)	3261(1)
580(5)	1250(0)	3209(3)	592(8)	1259(1)	3223(1)	611(29)	1276(0)	3262(2)
581(3)	1251(1)	3210(0)	594(4)	1267(15)	3224(0)	613(5)	1280(0)	3266(1)
585(1)	1254(0)	3221(26)	598(0)	1270(0)	3234(12)	616(13)	1287(4)	3273(8)
595(24)	1274(18)	3224(42)	602(16)	1274(0)	3237(15)	624(1)	1311(12)	3277(11)
755(2)	1348(46)	3228(37)	769(3)	1348(46)	3240(11)	784(5)	1396(95)	3279(9)
766(1)	1390(7)	3231(29)	779(2)	1387(2)	3241(13)	797(50)	1415(1)	3281(6)
770(10)	1397(2)	3239(8)	782(3)	1394(4)	3249(5)	809(29)	1421(6)	3289(2)
784(26)	1404(5)	3240(15)	794(19)	1394(1)	3250(4)	817(23)	1421(6)	3292(2)

Tables S92 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)_2$**structure **2N-Co-5T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
37(1)	782(62)	1412(0)	39(1)	783(62)	1414(0)	34(3)	817(102)	1432(1)
46(0)	789(38)	1412(7)	47(0)	790(37)	1414(7)	50(0)	830(2)	1433(6)
60(0)	805(8)	1414(0)	58(0)	805(8)	1415(0)	54(0)	837(81)	1449(16)
75(3)	807(0)	1417(2)	76(3)	808(0)	1418(1)	73(0)	839(2)	1449(32)
77(0)	824(0)	1440(57)	81(0)	824(0)	1439(62)	75(0)	850(0)	1470(0)
92(0)	825(1)	1449(0)	95(0)	825(2)	1449(49)	84(0)	854(3)	1473(0)
107(0)	831(1)	1450(49)	107(0)	831(1)	1450(0)	84(0)	855(2)	1483(0)
122(0)	834(1)	1450(11)	121(0)	834(2)	1451(9)	113(0)	857(2)	1489(18)
123(0)	866(0)	1455(0)	121(0)	866(0)	1455(0)	114(2)	903(3)	1490(14)
128(2)	866(0)	1456(5)	130(2)	866(0)	1455(5)	156(0)	904(1)	1490(1)
139(0)	868(8)	1467(11)	135(0)	869(8)	1467(12)	159(0)	911(2)	1491(13)
157(0)	870(1)	1468(3)	155(0)	871(1)	1467(3)	166(0)	917(1)	1493(7)
176(0)	899(11)	1468(0)	174(0)	898(10)	1468(12)	172(0)	922(5)	1496(1)
179(0)	903(2)	1468(12)	178(0)	902(2)	1468(0)	174(0)	926(6)	1497(30)
192(1)	1015(0)	1471(2)	188(1)	1016(0)	1472(1)	192(0)	1020(11)	1505(4)
215(0)	1016(14)	1471(3)	214(0)	1016(14)	1472(2)	198(1)	1030(17)	1506(20)
223(0)	1032(1)	1519(109)	223(0)	1033(0)	1518(107)	250(0)	1035(14)	1592(108)
244(2)	1034(23)	1535(16)	245(2)	1035(24)	1534(15)	262(1)	1037(21)	1594(178)
265(0)	1038(0)	2997(0)	264(0)	1037(0)	2996(0)	281(4)	1055(0)	3048(19)
293(1)	1039(13)	2997(76)	293(1)	1038(13)	2996(76)	295(0)	1055(9)	3048(52)
303(0)	1067(1)	3001(523)	303(0)	1068(1)	3000(529)	298(2)	1071(1)	3052(197)
311(1)	1068(0)	3003(15)	312(1)	1069(0)	3002(14)	318(5)	1072(1)	3053(98)
318(0)	1069(1)	3071(11)	317(0)	1069(1)	3070(12)	320(0)	1078(0)	3118(23)
324(1)	1071(2)	3072(187)	327(1)	1072(3)	3071(188)	337(1)	1078(0)	3118(56)

341(0)	1081(1)	3078(0)	341(0)	1081(1)	3077(0)	351(0)	1107(1)	3122(0)
357(3)	1082(0)	3078(0)	355(3)	1082(0)	3077(0)	380(3)	1107(1)	3122(17)
369(1)	1129(113)	3186(2)	366(1)	1129(124)	3187(1)	381(1)	1153(3)	3199(2)
387(0)	1133(12)	3186(4)	386(0)	1133(12)	3187(4)	396(0)	1155(6)	3199(6)
420(13)	1142(129)	3187(0)	418(13)	1141(121)	3188(0)	461(5)	1171(0)	3215(1)
501(1)	1147(8)	3187(12)	499(1)	1148(9)	3188(13)	502(2)	1171(3)	3215(4)
503(0)	1148(25)	3210(0)	503(0)	1149(25)	3209(0)	525(4)	1175(118)	3249(0)
545(6)	1157(11)	3210(0)	544(6)	1156(9)	3209(0)	582(8)	1180(57)	3259(3)
575(0)	1222(0)	3213(4)	576(0)	1223(0)	3212(4)	602(0)	1269(0)	3261(0)
580(2)	1227(18)	3213(0)	580(2)	1227(19)	3212(0)	608(2)	1275(39)	3266(0)
589(0)	1257(0)	3226(0)	589(0)	1257(0)	3226(0)	614(1)	1277(0)	3270(9)
594(0)	1257(0)	3227(68)	594(0)	1257(0)	3226(68)	621(2)	1283(0)	3274(4)
695(5)	1387(181)	3233(18)	686(3)	1386(185)	3232(18)	739(1)	1413(3)	3279(11)
708(0)	1392(0)	3233(29)	707(0)	1391(0)	3232(28)	780(22)	1418(0)	3280(12)
752(1)	1393(5)	3245(11)	752(0)	1392(5)	3244(12)	800(38)	1423(2)	3293(4)
759(2)	1400(8)	3245(12)	760(2)	1399(7)	3245(11)	808(42)	1426(4)	3303(3)

Tables S93 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2(MeC_2NMe_2)_2$**structure **2N-Fe-1S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
8(0)	802(7)	1422(3)	-4(0)	814(5)	1417(0)	-17(0)	830(49)	1439(0)
50(0)	804(5)	1423(0)	51(0)	815(5)	1418(29)	18(0)	832(21)	1442(0)
54(0)	809(3)	1427(11)	53(0)	821(1)	1426(0)	46(0)	850(7)	1444(61)
107(5)	810(0)	1428(0)	111(4)	822(0)	1426(0)	104(0)	851(0)	1445(3)
118(0)	822(2)	1450(25)	122(0)	830(4)	1459(0)	106(5)	852(3)	1478(8)
130(0)	823(0)	1451(0)	135(0)	832(0)	1459(0)	110(0)	852(0)	1479(0)
151(0)	840(3)	1452(63)	160(0)	843(4)	1466(5)	114(0)	860(3)	1482(1)
160(1)	841(46)	1453(21)	171(2)	844(39)	1468(1)	129(0)	860(23)	1484(1)
169(0)	867(0)	1460(1)	176(0)	887(0)	1469(64)	130(0)	913(0)	1484(115)
176(0)	868(2)	1463(8)	177(0)	887(2)	1474(17)	134(1)	913(1)	1485(0)
178(0)	872(2)	1467(0)	183(0)	892(2)	1485(0)	173(1)	920(7)	1488(6)
190(0)	873(5)	1467(12)	188(0)	893(7)	1485(6)	181(3)	921(1)	1489(49)
192(0)	919(0)	1475(0)	194(1)	916(0)	1493(8)	186(0)	947(1)	1499(0)
204(0)	922(8)	1477(2)	201(0)	919(7)	1494(13)	190(0)	950(9)	1502(3)
204(1)	1018(0)	1478(5)	212(0)	1026(0)	1496(0)	194(0)	1032(0)	1504(0)
211(3)	1018(12)	1479(12)	222(2)	1026(9)	1497(6)	213(0)	1032(13)	1506(9)
229(3)	1041(1)	1521(246)	224(2)	1049(0)	1533(161)	220(4)	1050(1)	1551(336)
268(0)	1042(23)	1524(3)	264(0)	1049(17)	1535(1)	240(0)	1051(29)	1559(9)
308(0)	1056(0)	2991(0)	307(0)	1058(0)	3016(0)	294(2)	1072(0)	3035(0)
339(1)	1057(13)	2991(97)	338(0)	1059(15)	3016(67)	332(1)	1073(11)	3035(67)
345(1)	1075(0)	2997(483)	349(0)	1085(0)	3022(314)	340(2)	1085(0)	3039(358)
349(0)	1076(0)	2998(4)	350(0)	1086(4)	3024(2)	343(0)	1086(8)	3041(2)
388(11)	1077(4)	3073(74)	393(13)	1086(0)	3097(49)	394(6)	1088(2)	3109(54)
395(5)	1078(1)	3074(163)	406(5)	1088(1)	3098(91)	403(6)	1089(2)	3109(122)
426(0)	1091(2)	3079(0)	434(15)	1100(2)	3098(0)	430(19)	1107(0)	3110(0)

427(4)	1091(0)	3079(0)	435(0)	1100(0)	3098(0)	438(0)	1109(0)	3110(0)
440(22)	1124(147)	3204(1)	449(0)	1134(174)	3217(0)	451(0)	1148(196)	3241(0)
441(0)	1128(11)	3204(8)	453(10)	1139(14)	3217(0)	464(19)	1154(7)	3241(0)
490(0)	1147(3)	3204(0)	494(0)	1153(38)	3217(4)	502(0)	1164(27)	3241(8)
556(0)	1148(46)	3205(14)	560(0)	1153(1)	3217(8)	566(0)	1165(2)	3241(14)
574(6)	1157(170)	3212(0)	581(7)	1167(151)	3225(7)	586(6)	1175(205)	3267(0)
585(0)	1163(0)	3212(13)	599(0)	1172(1)	3225(0)	607(0)	1183(3)	3267(5)
586(0)	1245(0)	3224(4)	600(0)	1237(0)	3235(1)	610(0)	1280(0)	3277(0)
587(1)	1249(53)	3224(9)	600(0)	1240(46)	3235(1)	611(1)	1284(53)	3277(1)
588(7)	1260(0)	3232(9)	601(9)	1280(0)	3242(14)	612(0)	1285(0)	3282(1)
592(10)	1260(0)	3232(32)	605(8)	1280(0)	3242(3)	638(26)	1286(0)	3282(8)
723(0)	1389(469)	3244(0)	725(0)	1388(549)	3257(0)	762(40)	1418(522)	3296(0)
777(41)	1401(7)	3244(44)	776(40)	1402(8)	3257(20)	772(0)	1434(0)	3296(14)
783(0)	1404(0)	3253(13)	798(0)	1411(3)	3264(4)	820(18)	1434(3)	3304(3)
787(8)	1404(1)	3253(14)	801(3)	1413(2)	3264(5)	821(0)	1439(1)	3304(2)

Tables S94 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2(MeC_2NMe_2)_2$**structure **2N-Fe-2T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
38(0)	783(0)	1410(1)	39(1)	794(0)	1411(161)	21(0)	823(3)	1437(1)
42(0)	791(11)	1413(25)	43(0)	796(82)	1415(17)	33(0)	829(37)	1438(7)
51(0)	794(100)	1418(8)	50(0)	807(30)	1422(0)	56(0)	832(1)	1440(250)
82(3)	802(4)	1420(0)	84(2)	815(4)	1422(0)	79(0)	844(8)	1445(4)
103(0)	819(3)	1447(53)	102(0)	824(2)	1454(0)	82(2)	850(10)	1473(0)
113(0)	821(0)	1448(72)	111(0)	826(0)	1460(4)	101(3)	850(0)	1477(1)
126(0)	830(15)	1453(43)	129(0)	832(13)	1466(97)	114(1)	851(0)	1481(3)
136(0)	836(1)	1456(13)	135(0)	837(1)	1468(24)	127(0)	855(1)	1483(55)
144(0)	859(2)	1460(0)	142(0)	872(3)	1471(1)	157(2)	903(1)	1485(3)
146(0)	862(1)	1460(6)	152(1)	879(1)	1473(12)	157(1)	911(0)	1490(1)
156(2)	864(4)	1464(5)	158(1)	880(4)	1481(0)	169(0)	913(1)	1493(34)
160(0)	870(1)	1466(6)	164(0)	886(0)	1481(4)	184(0)	919(5)	1496(4)
178(0)	918(2)	1471(2)	177(0)	915(2)	1490(4)	187(0)	946(2)	1499(14)
202(3)	919(13)	1472(1)	203(2)	917(10)	1491(13)	188(1)	948(11)	1499(38)
209(0)	1013(6)	1473(9)	211(0)	1019(5)	1494(1)	200(0)	1022(6)	1505(7)
215(0)	1017(10)	1474(10)	221(0)	1023(8)	1495(12)	205(1)	1025(16)	1506(15)
223(3)	1033(12)	1531(272)	233(2)	1039(8)	1540(186)	244(0)	1043(15)	1565(465)
235(0)	1038(13)	1536(12)	236(0)	1044(10)	1542(6)	249(8)	1048(18)	1566(3)
273(7)	1048(0)	2991(63)	273(7)	1052(0)	3015(33)	283(4)	1072(1)	3032(6)
299(0)	1049(9)	2991(79)	302(0)	1053(12)	3015(55)	289(2)	1073(12)	3032(65)
312(0)	1070(1)	2997(472)	315(0)	1078(2)	3022(312)	298(2)	1077(0)	3035(357)
325(0)	1070(2)	2998(5)	328(0)	1079(1)	3023(4)	308(5)	1080(4)	3036(1)
331(0)	1073(4)	3064(31)	335(0)	1082(3)	3089(19)	330(1)	1081(5)	3093(0)
360(3)	1075(2)	3065(179)	367(2)	1083(2)	3089(87)	353(4)	1085(1)	3093(85)
364(3)	1088(2)	3073(2)	369(4)	1099(3)	3094(4)	360(8)	1109(1)	3104(20)

382(6)	1089(0)	3073(9)	384(7)	1099(0)	3094(16)	383(9)	1110(2)	3104(29)
411(5)	1130(114)	3195(1)	418(7)	1142(149)	3208(0)	413(7)	1158(107)	3203(6)
431(10)	1134(16)	3195(9)	445(4)	1146(25)	3208(5)	457(1)	1158(9)	3203(10)
444(4)	1144(8)	3204(1)	448(6)	1148(9)	3216(0)	471(0)	1159(2)	3207(5)
511(4)	1144(26)	3205(8)	521(2)	1149(13)	3216(4)	513(0)	1160(9)	3207(8)
522(1)	1153(205)	3211(1)	532(2)	1164(174)	3225(1)	552(9)	1171(308)	3258(1)
541(6)	1162(7)	3214(1)	548(6)	1172(8)	3227(0)	571(16)	1182(3)	3266(0)
589(0)	1237(0)	3215(2)	600(0)	1229(0)	3228(0)	606(1)	1279(0)	3267(0)
589(0)	1241(55)	3219(1)	600(0)	1233(48)	3231(0)	608(0)	1280(0)	3267(0)
592(2)	1257(0)	3229(33)	602(1)	1277(0)	3242(16)	610(0)	1283(69)	3275(4)
593(1)	1258(0)	3231(32)	605(1)	1277(0)	3243(12)	618(1)	1284(0)	3281(12)
691(0)	1395(266)	3233(29)	693(0)	1396(144)	3245(10)	690(0)	1421(5)	3282(8)
746(16)	1398(4)	3235(20)	755(20)	1397(0)	3246(4)	777(65)	1425(3)	3283(9)
763(10)	1399(1)	3244(12)	778(20)	1403(105)	3255(4)	797(80)	1428(50)	3293(3)
778(55)	1404(11)	3249(8)	786(27)	1407(2)	3259(2)	807(171)	1431(0)	3294(3)

Tables S95 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2(MeC_2NMe_2)_2$**structure **2N-Fe-3S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
38(0)	783(0)	1410(1)	32(0)	807(0)	1417(158)	22(0)	825(23)	1437(0)
42(0)	791(11)	1413(25)	40(0)	808(4)	1417(150)	31(0)	827(0)	1438(5)
51(0)	794(100)	1418(8)	48(1)	809(13)	1422(0)	52(2)	828(8)	1451(83)
82(3)	802(4)	1420(0)	66(0)	823(40)	1424(1)	70(0)	838(30)	1452(59)
103(0)	819(3)	1447(53)	67(1)	827(0)	1454(0)	70(0)	850(0)	1472(0)
113(0)	821(0)	1448(72)	73(0)	827(0)	1454(2)	74(1)	851(0)	1472(0)
126(0)	830(15)	1453(43)	75(0)	827(0)	1455(19)	75(1)	852(1)	1482(0)
136(0)	836(1)	1456(13)	87(0)	827(4)	1461(111)	88(0)	852(0)	1483(2)
144(0)	859(2)	1460(0)	100(1)	878(4)	1469(0)	100(1)	902(5)	1483(29)
146(0)	862(1)	1460(6)	110(1)	879(1)	1470(0)	107(2)	902(0)	1484(1)
156(2)	864(4)	1464(5)	138(0)	881(0)	1471(3)	113(1)	903(0)	1487(5)
160(0)	870(1)	1466(6)	159(0)	886(0)	1474(6)	149(2)	912(0)	1491(122)
178(0)	918(2)	1471(2)	165(1)	936(9)	1484(6)	149(0)	958(9)	1499(16)
202(3)	919(13)	1472(1)	187(0)	942(13)	1487(3)	202(0)	962(12)	1502(0)
209(0)	1013(6)	1473(9)	195(0)	1022(0)	1495(0)	205(0)	1027(0)	1502(0)
215(0)	1017(10)	1474(10)	210(4)	1022(16)	1496(13)	214(5)	1028(29)	1503(18)
223(3)	1033(12)	1531(272)	225(3)	1035(2)	1540(88)	215(7)	1035(2)	1586(312)
235(0)	1038(13)	1536(12)	252(3)	1035(7)	1541(90)	244(2)	1036(18)	1587(256)
273(7)	1048(0)	2991(63)	287(0)	1066(0)	3002(0)	290(1)	1075(0)	3031(0)
299(0)	1049(9)	2991(79)	288(0)	1066(8)	3002(85)	298(0)	1075(0)	3031(73)
312(0)	1070(1)	2997(472)	296(1)	1074(2)	3007(203)	302(1)	1076(1)	3034(214)
325(0)	1070(2)	2998(5)	302(1)	1075(0)	3009(112)	308(0)	1078(0)	3035(122)
331(0)	1073(4)	3064(31)	384(3)	1076(0)	3078(13)	387(15)	1078(7)	3098(20)
360(3)	1075(2)	3065(179)	385(13)	1079(0)	3079(98)	388(12)	1079(0)	3099(107)
364(3)	1088(2)	3073(2)	393(9)	1104(4)	3083(0)	394(6)	1113(0)	3103(0)

382(6)	1089(0)	3073(9)	441(6)	1104(0)	3083(1)	435(0)	1114(4)	3103(0)
411(5)	1130(114)	3195(1)	442(0)	1145(64)	3147(0)	453(0)	1155(19)	3182(0)
431(10)	1134(16)	3195(9)	450(0)	1147(27)	3148(13)	455(10)	1155(19)	3182(15)
444(4)	1144(8)	3204(1)	509(7)	1147(19)	3148(10)	522(1)	1163(33)	3182(14)
511(4)	1144(26)	3205(8)	520(7)	1149(10)	3148(8)	540(3)	1163(15)	3182(4)
522(1)	1153(205)	3211(1)	537(0)	1173(102)	3214(4)	542(10)	1191(114)	3255(0)
541(6)	1162(7)	3214(1)	585(6)	1187(98)	3214(1)	583(5)	1201(100)	3255(3)
589(0)	1237(0)	3215(2)	600(3)	1251(0)	3221(0)	609(5)	1279(0)	3265(0)
589(0)	1241(55)	3219(1)	603(0)	1255(47)	3222(0)	614(0)	1280(0)	3265(1)
592(2)	1257(0)	3229(33)	607(0)	1275(0)	3234(16)	616(0)	1291(0)	3275(8)
593(1)	1258(0)	3231(32)	608(0)	1275(0)	3235(10)	617(0)	1294(41)	3275(10)
691(0)	1395(266)	3233(29)	655(0)	1399(6)	3238(25)	678(0)	1424(0)	3278(0)
746(16)	1398(4)	3235(20)	779(8)	1399(0)	3238(0)	802(23)	1424(9)	3278(17)
763(10)	1399(1)	3244(12)	802(20)	1401(9)	3248(3)	815(77)	1426(10)	3291(2)
778(55)	1404(11)	3249(8)	803(7)	1402(23)	3248(6)	820(20)	1427(1)	3291(2)

Tables S96 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $\mathbf{Cp_2Fe_2(MeC_2NMe_2)_2}$structure **2N-Fe-4T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
26(1)	787(32)	1409(2)	28(1)	801(10)	1403(4)	20(0)	816(17)	1428(1)
40(0)	795(11)	1411(3)	40(0)	803(9)	1420(3)	33(1)	818(30)	1432(7)
44(0)	799(15)	1415(6)	46(1)	810(15)	1429(1)	62(1)	828(64)	1445(4)
59(0)	803(2)	1423(25)	67(0)	812(3)	1444(31)	69(0)	844(3)	1461(14)
70(0)	809(1)	1427(12)	72(0)	814(1)	1448(1)	76(0)	845(4)	1468(22)
75(1)	817(6)	1440(0)	77(0)	823(1)	1448(12)	79(1)	851(0)	1469(5)
82(1)	818(3)	1445(2)	84(1)	825(7)	1451(1)	87(2)	851(2)	1475(0)
90(2)	824(1)	1447(0)	94(2)	829(4)	1455(0)	104(1)	853(8)	1479(0)
100(0)	846(0)	1450(3)	104(0)	863(0)	1468(2)	112(0)	894(2)	1486(3)
127(0)	852(1)	1455(2)	130(0)	869(0)	1471(3)	121(1)	899(1)	1486(9)
155(1)	859(2)	1463(3)	156(1)	883(1)	1477(1)	144(0)	913(3)	1487(11)
158(0)	866(1)	1463(17)	161(0)	883(2)	1484(2)	156(1)	918(2)	1492(10)
165(0)	916(3)	1464(22)	167(0)	917(5)	1486(29)	176(1)	937(2)	1498(2)
208(2)	979(100)	1471(6)	213(2)	976(95)	1492(5)	196(0)	1015(68)	1507(31)
217(0)	1009(12)	1477(10)	221(1)	1015(9)	1500(9)	206(1)	1021(30)	1510(15)
225(5)	1013(10)	1484(5)	235(4)	1020(7)	1504(5)	218(1)	1031(19)	1520(4)
237(0)	1019(9)	1498(6)	239(1)	1028(8)	1518(6)	232(1)	1036(14)	1524(5)
259(2)	1025(12)	1689(321)	265(2)	1032(8)	1685(311)	238(4)	1039(18)	1711(440)
281(0)	1034(5)	2983(63)	290(2)	1041(5)	3007(41)	261(0)	1056(5)	3031(75)
286(5)	1055(3)	2987(74)	292(4)	1062(3)	3010(42)	286(1)	1073(3)	3037(112)
293(2)	1062(1)	2988(282)	300(1)	1070(1)	3012(162)	295(2)	1075(2)	3043(62)
305(5)	1063(0)	2992(163)	312(5)	1073(2)	3014(148)	304(0)	1080(1)	3051(105)
350(1)	1065(3)	3060(106)	355(1)	1075(1)	3078(51)	346(1)	1082(10)	3093(41)
369(2)	1066(1)	3067(3)	377(1)	1077(1)	3084(10)	363(3)	1087(1)	3119(28)
387(6)	1094(43)	3085(61)	396(9)	1104(123)	3105(31)	371(7)	1116(4)	3131(35)

391(7)	1098(2)	3090(2)	399(5)	1111(3)	3107(1)	386(1)	1123(5)	3134(17)
422(4)	1106(143)	3141(14)	432(4)	1114(66)	3157(7)	416(13)	1137(114)	3156(23)
457(1)	1136(32)	3141(25)	462(0)	1140(22)	3159(11)	466(2)	1151(13)	3187(5)
478(6)	1137(19)	3151(14)	486(10)	1142(19)	3169(5)	483(0)	1153(6)	3187(10)
484(22)	1142(4)	3172(11)	493(18)	1157(6)	3191(5)	525(22)	1159(3)	3189(18)
510(4)	1159(5)	3201(5)	521(5)	1173(4)	3213(2)	549(9)	1193(3)	3257(3)
542(1)	1216(16)	3204(1)	546(1)	1211(14)	3216(1)	569(1)	1249(14)	3264(1)
576(1)	1250(0)	3204(2)	590(0)	1256(11)	3218(0)	606(0)	1279(0)	3266(0)
579(1)	1255(0)	3210(5)	592(1)	1270(5)	3223(2)	607(0)	1288(0)	3270(0)
581(0)	1260(2)	3220(44)	596(0)	1271(0)	3232(20)	613(1)	1291(7)	3278(8)
596(0)	1267(16)	3224(39)	608(0)	1275(0)	3236(11)	616(1)	1326(16)	3279(14)
735(1)	1362(64)	3225(37)	747(1)	1364(62)	3237(16)	784(4)	1403(46)	3283(11)
758(12)	1382(2)	3228(20)	768(11)	1371(2)	3238(7)	788(12)	1409(7)	3285(5)
775(13)	1396(4)	3235(7)	785(9)	1398(3)	3246(5)	803(44)	1421(2)	3294(2)
781(22)	1405(2)	3240(10)	793(33)	1399(2)	3250(4)	810(58)	1426(3)	3297(2)

Tables S97 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2(MeC_2NMe_2)_2$**structure **2N-Fe-5S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
35(1)	795(5)	1405(1)	47(1)	803(6)	1404(3)	32(1)	830(25)	1426(3)
51(0)	798(11)	1406(1)	51(0)	809(6)	1419(3)	41(0)	835(26)	1435(4)
61(0)	805(12)	1415(4)	61(0)	815(4)	1430(0)	60(0)	842(12)	1442(3)
75(1)	812(3)	1420(18)	74(1)	821(3)	1443(25)	67(1)	846(5)	1463(31)
82(0)	816(4)	1426(19)	80(0)	826(1)	1446(2)	73(0)	851(1)	1464(3)
87(0)	821(4)	1439(1)	94(0)	829(5)	1446(4)	84(1)	854(12)	1465(5)
98(1)	825(8)	1440(1)	95(1)	831(6)	1448(12)	94(0)	856(11)	1466(4)
105(0)	828(13)	1444(1)	105(1)	835(17)	1451(1)	102(0)	858(11)	1469(1)
123(0)	855(1)	1448(0)	119(0)	874(1)	1455(0)	122(2)	898(1)	1477(0)
134(4)	857(3)	1450(3)	139(3)	877(4)	1475(1)	131(6)	903(5)	1487(2)
164(1)	862(1)	1455(15)	161(2)	882(1)	1478(12)	157(0)	912(0)	1488(12)
170(1)	863(2)	1462(20)	174(1)	884(2)	1485(40)	168(1)	916(4)	1494(33)
175(1)	919(2)	1465(11)	179(1)	921(4)	1487(2)	184(4)	946(2)	1500(3)
210(1)	973(109)	1467(23)	214(1)	971(101)	1490(6)	207(3)	1018(83)	1502(6)
227(1)	1012(12)	1477(12)	235(1)	1018(9)	1497(11)	221(1)	1024(27)	1508(24)
235(3)	1013(6)	1486(2)	240(3)	1021(6)	1506(2)	236(2)	1026(14)	1520(5)
237(1)	1015(20)	1496(1)	246(2)	1022(13)	1514(0)	244(1)	1029(22)	1522(5)
263(1)	1020(0)	1672(352)	278(1)	1027(1)	1671(336)	283(1)	1033(6)	1702(515)
280(3)	1033(4)	2976(75)	289(3)	1040(4)	2998(54)	298(1)	1063(5)	3025(43)
296(2)	1056(4)	2978(144)	302(2)	1063(5)	3005(77)	306(1)	1070(3)	3030(103)
304(2)	1059(0)	2986(108)	307(2)	1069(1)	3012(77)	321(1)	1072(0)	3031(126)
383(5)	1061(3)	2989(224)	391(5)	1070(2)	3014(167)	408(7)	1074(0)	3041(88)
394(4)	1063(0)	3068(101)	406(4)	1072(0)	3089(45)	414(2)	1077(7)	3100(48)
413(1)	1070(2)	3076(16)	424(1)	1077(1)	3096(17)	428(4)	1084(1)	3118(34)
418(15)	1093(9)	3081(56)	428(15)	1108(23)	3101(22)	439(11)	1117(6)	3124(34)

436(11)	1098(7)	3086(6)	446(10)	1112(17)	3105(9)	456(7)	1120(3)	3126(12)
468(8)	1111(145)	3140(19)	477(4)	1119(122)	3158(9)	477(9)	1140(129)	3179(9)
475(5)	1133(47)	3142(16)	481(8)	1138(40)	3161(8)	500(5)	1152(25)	3180(10)
487(5)	1135(22)	3144(21)	493(5)	1141(18)	3163(9)	513(4)	1153(15)	3182(21)
502(3)	1140(9)	3150(17)	510(3)	1154(11)	3166(7)	524(7)	1164(6)	3187(9)
527(6)	1161(7)	3194(9)	541(7)	1177(7)	3206(5)	573(0)	1195(6)	3256(2)
572(2)	1211(12)	3199(6)	575(4)	1206(10)	3215(2)	591(16)	1252(15)	3258(1)
575(5)	1247(0)	3201(8)	587(3)	1264(1)	3215(2)	613(0)	1275(0)	3259(1)
579(1)	1251(0)	3205(4)	594(0)	1267(0)	3219(1)	616(1)	1279(0)	3264(0)
583(0)	1255(1)	3215(31)	597(0)	1269(14)	3226(16)	618(3)	1292(4)	3272(13)
584(0)	1277(17)	3218(43)	597(0)	1271(0)	3232(18)	625(0)	1318(16)	3273(8)
762(12)	1360(53)	3227(33)	772(11)	1361(54)	3236(10)	798(11)	1405(51)	3277(9)
768(0)	1391(5)	3228(19)	781(1)	1391(8)	3241(10)	815(14)	1417(7)	3280(3)
784(4)	1401(9)	3234(8)	793(4)	1394(1)	3244(4)	820(5)	1419(3)	3287(2)
787(7)	1403(2)	3237(12)	801(7)	1396(2)	3248(4)	821(36)	1424(4)	3292(0)

Tables S98 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2(MeC_2NMe_2)$**structure **1N-Ni-1S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
23(0)	784(38)	1400(18)	24(0)	796(21)	1390(3)	29(0)	803(8)	1409(27)
32(0)	785(33)	1403(3)	31(0)	796(38)	1393(6)	35(0)	816(14)	1412(5)
60(0)	792(10)	1406(5)	63(0)	806(4)	1397(4)	49(1)	824(3)	1415(6)
66(1)	824(6)	1411(0)	70(0)	827(10)	1435(0)	60(0)	835(23)	1443(2)
68(0)	825(9)	1434(2)	73(0)	828(8)	1454(2)	68(1)	840(2)	1463(3)
73(0)	828(11)	1448(1)	79(0)	831(13)	1455(1)	71(0)	845(22)	1467(3)
95(1)	833(1)	1449(1)	97(0)	837(1)	1455(2)	99(1)	852(2)	1468(0)
123(1)	844(11)	1452(8)	126(0)	847(13)	1470(0)	126(2)	858(11)	1476(10)
141(4)	859(1)	1455(8)	145(3)	878(0)	1471(0)	142(3)	893(0)	1482(1)
167(1)	862(0)	1464(0)	171(1)	879(1)	1473(8)	155(1)	898(1)	1484(5)
188(0)	862(1)	1465(29)	189(0)	879(0)	1479(6)	186(0)	901(1)	1485(1)
197(0)	868(3)	1466(0)	194(0)	887(2)	1487(22)	199(0)	902(2)	1493(13)
203(0)	960(31)	1469(5)	213(0)	960(31)	1490(9)	208(0)	975(25)	1497(16)
214(0)	1005(21)	1474(1)	216(0)	1020(17)	1498(3)	211(1)	1018(18)	1501(6)
239(0)	1015(9)	1492(12)	244(1)	1022(11)	1514(8)	236(0)	1021(18)	1517(22)
261(6)	1016(8)	1684(100)	263(6)	1024(4)	1688(102)	262(7)	1023(4)	1740(131)
288(4)	1026(27)	2958(55)	289(2)	1034(22)	2985(46)	283(5)	1034(23)	3006(52)
318(1)	1028(2)	2962(161)	322(1)	1035(1)	2990(113)	298(3)	1035(12)	3010(75)
326(2)	1056(6)	3004(79)	330(3)	1066(7)	3024(49)	306(2)	1069(7)	3053(41)
334(1)	1060(18)	3074(84)	336(3)	1071(3)	3095(36)	319(3)	1070(7)	3116(60)
343(10)	1064(5)	3079(22)	343(7)	1073(3)	3098(13)	329(3)	1073(1)	3118(12)
362(11)	1065(2)	3085(33)	366(9)	1076(2)	3100(22)	351(18)	1074(1)	3129(17)
400(6)	1067(0)	3119(29)	401(6)	1076(1)	3131(13)	396(7)	1076(0)	3160(14)
438(0)	1069(7)	3139(24)	445(0)	1081(22)	3155(12)	436(1)	1078(24)	3171(13)
487(4)	1097(4)	3141(29)	501(4)	1114(4)	3160(12)	472(15)	1119(4)	3175(18)

522(3)	1136(102)	3212(1)	526(2)	1147(28)	3224(1)	522(1)	1149(7)	3262(1)
567(28)	1144(12)	3214(3)	570(29)	1148(35)	3225(1)	550(24)	1150(5)	3265(0)
587(1)	1145(3)	3216(0)	597(2)	1150(75)	3227(0)	585(2)	1160(110)	3266(0)
594(7)	1155(29)	3219(1)	604(7)	1167(11)	3228(0)	602(15)	1175(13)	3268(0)
601(1)	1255(0)	3229(28)	611(1)	1258(23)	3239(9)	611(1)	1278(0)	3276(8)
605(5)	1256(0)	3234(25)	615(4)	1275(0)	3243(8)	615(9)	1279(0)	3281(6)
635(8)	1259(24)	3237(24)	644(7)	1276(0)	3245(8)	652(8)	1293(24)	3282(2)
754(1)	1338(81)	3238(24)	768(1)	1346(90)	3247(6)	784(2)	1370(76)	3282(7)
767(2)	1376(13)	3249(13)	779(2)	1383(1)	3256(5)	793(103)	1402(9)	3293(4)
778(45)	1396(2)	3249(16)	789(50)	1387(17)	3257(5)	803(63)	1405(19)	3294(4)

Tables S99 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2(MeC_2NMe_2)$**structure **1N-Ni-2S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
26(0)	783(5)	1383(5)	25(0)	795(51)	1378(27)	27(0)	815(56)	1401(7)
41(0)	784(55)	1396(4)	41(0)	797(10)	1384(3)	39(0)	826(8)	1408(3)
64(1)	799(18)	1403(14)	57(1)	810(15)	1391(14)	51(3)	841(2)	1412(12)
66(0)	816(0)	1408(17)	64(0)	820(0)	1396(18)	66(0)	844(11)	1421(27)
81(0)	823(3)	1409(4)	83(0)	828(6)	1429(79)	77(1)	849(7)	1446(2)
88(0)	829(0)	1419(85)	91(0)	832(0)	1431(43)	84(0)	850(5)	1453(138)
120(1)	830(1)	1435(4)	121(1)	834(1)	1441(3)	116(5)	853(8)	1456(4)
124(5)	852(1)	1446(45)	124(5)	868(1)	1457(1)	122(6)	896(4)	1464(2)
169(0)	857(1)	1450(4)	168(0)	875(2)	1464(30)	154(1)	899(3)	1480(3)
177(1)	863(9)	1460(1)	179(1)	877(6)	1467(4)	189(1)	907(5)	1484(24)
186(7)	868(0)	1462(3)	188(6)	886(0)	1480(0)	200(9)	908(7)	1492(21)
200(4)	878(1)	1467(27)	202(5)	890(1)	1481(2)	210(2)	912(1)	1497(11)
209(1)	893(1)	1476(4)	213(1)	896(1)	1487(35)	219(1)	918(1)	1501(4)
245(2)	913(4)	1477(30)	250(2)	933(4)	1493(25)	252(0)	962(5)	1504(14)
253(1)	983(25)	1491(13)	261(0)	989(25)	1504(5)	256(2)	1005(14)	1525(17)
290(1)	1001(11)	1524(133)	297(1)	1007(9)	1533(86)	297(3)	1010(17)	1547(194)
302(3)	1017(9)	2974(50)	307(3)	1024(7)	2999(34)	307(5)	1021(12)	3014(36)
319(2)	1025(15)	2979(164)	323(2)	1032(11)	3004(112)	326(5)	1031(13)	3019(91)
341(1)	1029(11)	3068(72)	343(1)	1036(9)	3087(37)	350(5)	1040(17)	3110(45)
347(4)	1058(3)	3090(43)	349(4)	1066(4)	3108(22)	360(2)	1069(2)	3123(34)
353(1)	1062(9)	3098(32)	358(0)	1070(8)	3115(18)	364(3)	1072(5)	3149(17)
392(2)	1063(4)	3114(45)	391(1)	1072(5)	3129(28)	408(9)	1073(1)	3167(16)
447(6)	1067(1)	3144(21)	452(5)	1075(1)	3159(10)	463(12)	1074(2)	3187(19)
473(8)	1068(2)	3154(3)	468(8)	1077(1)	3167(1)	487(15)	1080(9)	3192(4)
538(25)	1098(7)	3198(17)	547(25)	1107(7)	3212(8)	569(52)	1117(4)	3242(8)
575(15)	1127(98)	3201(1)	583(14)	1131(95)	3214(1)	580(13)	1148(35)	3253(2)
583(1)	1139(10)	3205(9)	587(0)	1143(7)	3217(3)	595(2)	1149(67)	3258(2)
585(3)	1141(19)	3216(1)	596(3)	1145(3)	3227(0)	607(8)	1152(20)	3263(0)
590(0)	1142(9)	3221(24)	601(0)	1154(28)	3231(9)	612(3)	1164(4)	3270(3)
599(2)	1192(9)	3221(6)	607(2)	1196(12)	3232(3)	618(3)	1223(9)	3270(6)

607(1)	1216(6)	3230(28)	614(1)	1225(8)	3242(9)	626(2)	1233(14)	3277(5)
712(1)	1253(0)	3235(18)	726(1)	1274(0)	3245(5)	759(3)	1277(0)	3281(4)
732(2)	1256(0)	3237(23)	740(2)	1277(0)	3247(6)	764(6)	1279(0)	3284(4)
758(57)	1298(31)	3242(14)	771(55)	1292(27)	3251(6)	786(104)	1337(22)	3288(3)
769(14)	1370(33)	3249(14)	782(10)	1370(24)	3258(4)	794(49)	1395(31)	3296(3)

Tables S100 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2(MeC_2NMe_2)$**structure **1N-Ni-3T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
23(0)	773(51)	1399(10)	22(0)	784(59)	1387(3)	30(0)	804(9)	1411(1)
45(1)	781(12)	1400(2)	49(1)	795(60)	1388(2)	46(0)	809(106)	1411(12)
49(1)	783(89)	1401(1)	55(0)	798(30)	1388(1)	61(2)	815(4)	1413(1)
60(0)	827(4)	1402(2)	66(0)	832(2)	1389(1)	62(0)	850(1)	1415(1)
71(0)	829(1)	1408(0)	79(0)	833(1)	1429(28)	79(0)	852(9)	1441(27)
84(0)	831(3)	1420(53)	86(0)	834(4)	1435(69)	80(1)	855(0)	1450(126)
107(1)	832(1)	1445(49)	110(1)	837(1)	1458(1)	108(4)	856(2)	1471(1)
136(6)	852(2)	1452(0)	139(5)	871(1)	1460(3)	131(5)	891(1)	1474(2)
140(1)	856(0)	1455(1)	143(1)	873(1)	1467(28)	142(2)	896(1)	1480(5)
153(1)	857(1)	1460(11)	153(0)	874(3)	1469(2)	150(0)	897(0)	1482(9)
167(1)	863(2)	1463(1)	171(1)	879(1)	1471(1)	169(5)	902(2)	1483(20)
179(3)	865(1)	1465(0)	180(3)	882(1)	1482(7)	193(3)	903(2)	1493(14)
214(1)	884(3)	1470(2)	214(1)	885(2)	1490(2)	211(1)	908(2)	1497(4)
245(4)	903(3)	1477(14)	246(4)	923(3)	1499(14)	257(3)	946(3)	1508(15)
251(1)	981(15)	1496(28)	254(0)	986(16)	1512(7)	273(10)	1001(17)	1530(61)
266(2)	1016(24)	1512(109)	269(2)	1022(19)	1521(84)	276(1)	1026(29)	1544(141)
270(4)	1020(4)	2956(58)	274(2)	1027(3)	2982(46)	282(2)	1029(7)	3013(33)
279(3)	1026(10)	2965(95)	283(2)	1033(8)	2993(66)	286(4)	1032(10)	3018(78)
294(4)	1027(12)	3072(21)	297(4)	1034(9)	3093(9)	291(9)	1034(16)	3118(42)
325(3)	1058(9)	3080(82)	328(2)	1067(10)	3101(36)	317(4)	1072(2)	3123(38)
357(0)	1065(1)	3086(41)	360(1)	1074(1)	3104(25)	358(0)	1073(1)	3139(7)
365(3)	1066(0)	3119(43)	364(3)	1074(0)	3133(29)	388(7)	1074(0)	3170(18)
440(8)	1066(0)	3143(24)	438(8)	1075(0)	3160(10)	432(16)	1077(1)	3189(16)
449(6)	1069(1)	3156(7)	455(5)	1078(0)	3169(4)	454(1)	1077(7)	3191(7)
511(18)	1093(4)	3178(38)	516(17)	1109(3)	3194(19)	532(34)	1116(3)	3235(12)
548(1)	1126(81)	3208(1)	553(1)	1134(75)	3222(0)	545(5)	1147(92)	3256(0)
588(4)	1137(3)	3210(2)	593(4)	1147(7)	3224(1)	599(4)	1153(4)	3259(0)
590(2)	1145(6)	3214(1)	599(2)	1149(3)	3225(0)	609(2)	1156(6)	3260(1)
591(1)	1146(3)	3217(0)	602(1)	1151(8)	3228(1)	611(5)	1163(4)	3266(1)
597(1)	1207(7)	3228(29)	607(1)	1209(8)	3239(7)	623(0)	1221(20)	3272(6)
601(0)	1216(7)	3230(18)	613(0)	1222(9)	3242(7)	624(1)	1239(14)	3277(6)
714(7)	1255(0)	3233(28)	722(9)	1276(0)	3244(7)	739(21)	1278(0)	3278(5)
745(1)	1258(0)	3235(23)	759(1)	1279(0)	3245(7)	785(1)	1280(0)	3281(7)
753(1)	1307(25)	3245(4)	766(3)	1304(22)	3254(2)	790(83)	1338(19)	3288(2)
763(30)	1361(55)	3247(17)	773(18)	1364(71)	3256(4)	792(55)	1398(40)	3292(3)

Tables S101 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2(MeC_2NMe_2)$**structure **1N-Ni-4S**;

M06L/DZP	M06L/def2tzvpp	WB97XD/DZP

25(0)	801(4)	1360(7)	26(0)	810(3)	1371(7)	32(0)	837(3)	1405(2)
47(0)	808(1)	1387(4)	46(0)	816(2)	1376(2)	44(0)	841(3)	1407(2)
56(0)	812(12)	1396(3)	63(0)	825(8)	1384(0)	60(0)	846(2)	1410(3)
87(0)	823(3)	1397(2)	89(0)	828(4)	1395(9)	90(0)	851(9)	1419(13)
104(0)	828(6)	1407(10)	105(0)	833(14)	1401(17)	105(0)	851(10)	1427(19)
128(1)	830(2)	1412(16)	129(1)	834(2)	1420(3)	132(1)	857(7)	1439(5)
141(0)	831(2)	1416(4)	143(0)	836(1)	1427(3)	151(0)	857(1)	1456(3)
166(1)	857(4)	1435(2)	167(1)	865(1)	1441(2)	172(0)	898(4)	1459(1)
196(2)	860(1)	1437(5)	197(2)	877(3)	1449(1)	208(2)	901(1)	1460(3)
220(1)	863(4)	1442(0)	221(1)	879(1)	1451(2)	233(0)	902(4)	1475(5)
241(1)	869(3)	1452(0)	243(2)	881(2)	1475(0)	249(0)	906(2)	1488(1)
243(1)	876(7)	1459(7)	246(0)	890(5)	1479(1)	259(2)	920(8)	1492(7)
266(3)	887(19)	1470(9)	269(2)	900(20)	1482(6)	265(0)	938(21)	1497(3)
275(0)	934(26)	1475(2)	280(0)	947(37)	1487(0)	276(4)	980(7)	1507(13)
286(0)	967(46)	1476(12)	290(0)	963(30)	1491(9)	287(2)	1007(35)	1508(1)
297(2)	1000(14)	1482(2)	301(2)	1007(10)	1497(11)	300(3)	1012(35)	1513(17)
309(8)	1013(8)	2985(44)	311(8)	1019(6)	3008(27)	319(3)	1016(13)	3035(40)
323(2)	1023(7)	2986(175)	326(2)	1027(7)	3012(112)	330(4)	1039(20)	3039(87)
350(7)	1031(16)	3073(47)	351(6)	1037(13)	3095(29)	361(6)	1042(22)	3140(25)
397(0)	1031(17)	3092(35)	398(0)	1038(14)	3117(19)	416(0)	1052(8)	3142(12)
412(7)	1045(10)	3099(33)	415(7)	1056(8)	3119(12)	430(5)	1068(3)	3145(23)
436(1)	1060(0)	3103(15)	436(1)	1069(0)	3123(12)	458(1)	1071(3)	3164(17)
466(2)	1062(1)	3140(46)	461(2)	1071(1)	3152(23)	492(3)	1072(5)	3192(7)
533(10)	1066(1)	3148(12)	534(10)	1074(1)	3165(5)	545(11)	1075(2)	3195(9)
559(1)	1069(0)	3156(16)	559(1)	1077(1)	3173(7)	585(3)	1078(4)	3203(18)
565(2)	1094(2)	3195(9)	573(1)	1108(3)	3210(4)	587(7)	1118(6)	3248(3)
584(3)	1102(7)	3207(5)	595(2)	1115(5)	3220(2)	601(2)	1125(2)	3257(2)
596(1)	1141(9)	3213(1)	604(2)	1145(7)	3224(0)	615(6)	1151(2)	3262(1)
602(7)	1144(6)	3215(4)	609(6)	1147(4)	3226(1)	622(4)	1155(3)	3262(0)
605(1)	1186(3)	3221(29)	614(0)	1190(9)	3233(10)	632(1)	1222(4)	3269(8)
710(6)	1194(11)	3230(25)	714(6)	1199(2)	3239(9)	741(5)	1233(13)	3273(7)
714(0)	1223(33)	3234(21)	728(0)	1235(32)	3245(6)	761(1)	1272(14)	3279(6)
731(1)	1251(1)	3237(17)	747(0)	1258(1)	3247(6)	768(1)	1278(0)	3282(5)
760(69)	1253(0)	3247(12)	772(63)	1274(0)	3255(7)	784(117)	1279(0)	3290(3)
773(76)	1257(0)	3248(20)	787(75)	1277(0)	3255(3)	794(129)	1291(1)	3291(2)

Tables S102 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **1N-Co-1S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
21(0)	797(29)	1362(4)	20(0)	811(22)	1373(4)	32(0)	832(13)	1399(4)
57(0)	815(17)	1392(4)	62(0)	823(8)	1393(1)	67(0)	849(11)	1423(1)
87(0)	824(6)	1405(1)	89(0)	828(2)	1395(0)	97(0)	854(6)	1425(1)

97(0)	825(5)	1406(0)	97(0)	830(6)	1397(0)	108(0)	855(0)	1426(0)
128(1)	826(7)	1409(0)	130(1)	831(3)	1399(0)	139(2)	857(2)	1426(0)
146(1)	829(8)	1409(0)	146(1)	836(17)	1416(3)	156(1)	859(17)	1434(8)
176(1)	836(5)	1414(1)	177(1)	847(10)	1423(1)	190(1)	869(9)	1445(3)
199(1)	858(5)	1431(3)	202(1)	861(6)	1445(2)	210(1)	895(3)	1469(1)
222(0)	861(1)	1442(0)	223(0)	880(0)	1449(0)	232(0)	907(1)	1471(2)
230(1)	864(2)	1446(0)	232(1)	884(2)	1454(1)	240(1)	913(1)	1471(2)
247(2)	872(1)	1451(0)	251(2)	890(2)	1460(0)	256(2)	920(3)	1480(1)
260(0)	875(3)	1454(0)	269(0)	892(1)	1461(1)	269(2)	921(2)	1481(1)
283(0)	888(17)	1455(2)	292(0)	900(18)	1475(1)	298(0)	932(23)	1488(1)
329(0)	923(14)	1459(7)	333(0)	937(16)	1480(6)	337(3)	963(9)	1491(9)
338(1)	974(44)	1470(7)	343(1)	970(38)	1490(5)	359(2)	1013(48)	1506(10)
375(9)	1013(11)	1475(10)	383(7)	1020(7)	1496(9)	397(8)	1027(19)	1511(13)
386(1)	1015(7)	2986(81)	395(1)	1022(5)	3010(39)	401(5)	1028(12)	3032(37)
397(6)	1019(10)	2989(156)	404(5)	1026(6)	3015(113)	410(1)	1034(14)	3037(109)
410(1)	1022(14)	3071(50)	415(2)	1028(14)	3092(33)	426(4)	1041(7)	3135(34)
412(7)	1025(5)	3093(43)	421(7)	1033(4)	3117(11)	433(6)	1051(10)	3136(7)
427(1)	1045(4)	3096(39)	431(1)	1056(3)	3118(25)	451(2)	1067(4)	3138(23)
456(12)	1060(1)	3099(11)	457(12)	1070(1)	3120(14)	496(14)	1072(1)	3159(24)
486(0)	1064(0)	3130(72)	481(0)	1074(0)	3145(40)	510(3)	1076(1)	3187(11)
543(23)	1065(0)	3144(19)	545(23)	1075(1)	3162(9)	566(28)	1078(0)	3192(9)
577(2)	1068(1)	3158(14)	586(4)	1077(0)	3173(6)	603(6)	1082(1)	3204(25)
578(4)	1091(2)	3190(14)	589(4)	1105(2)	3206(6)	608(3)	1115(3)	3251(5)
583(1)	1104(4)	3210(1)	595(1)	1118(4)	3222(0)	617(1)	1124(3)	3265(0)
590(0)	1139(29)	3211(4)	601(0)	1144(24)	3224(0)	621(1)	1156(19)	3268(1)
605(1)	1141(12)	3213(0)	612(0)	1145(9)	3225(0)	632(1)	1158(8)	3268(1)
615(2)	1186(2)	3224(24)	621(2)	1195(3)	3235(9)	640(3)	1220(3)	3276(6)
728(8)	1201(14)	3227(35)	732(8)	1201(8)	3240(12)	756(9)	1239(14)	3280(8)
752(0)	1226(13)	3229(35)	765(0)	1237(15)	3240(13)	797(5)	1263(10)	3283(7)
777(12)	1250(0)	3231(19)	789(15)	1262(0)	3242(7)	812(52)	1277(0)	3283(7)
782(7)	1254(0)	3241(5)	798(3)	1270(0)	3251(4)	822(37)	1282(0)	3293(2)
790(17)	1256(0)	3242(19)	804(15)	1274(0)	3251(5)	826(36)	1295(0)	3294(1)

Tables S103 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **1N-Co-2T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
29(0)	781(90)	1399(7)	31(0)	796(9)	1385(6)	23(0)	816(41)	1415(0)
35(0)	799(29)	1402(1)	32(0)	811(19)	1392(2)	31(0)	828(45)	1417(3)
44(0)	807(7)	1405(4)	48(0)	821(8)	1393(3)	52(0)	839(11)	1419(2)
60(1)	824(6)	1409(2)	51(1)	827(6)	1399(1)	62(0)	851(6)	1422(0)
79(0)	827(6)	1411(1)	83(0)	830(8)	1429(3)	74(1)	852(4)	1444(2)
97(0)	830(0)	1426(27)	97(0)	834(0)	1438(60)	93(1)	854(1)	1462(54)
121(2)	832(1)	1444(1)	121(2)	835(1)	1451(1)	117(2)	856(1)	1469(2)
138(1)	855(1)	1450(23)	140(1)	869(1)	1460(0)	142(0)	890(8)	1474(0)

144(4)	860(3)	1454(1)	151(5)	872(3)	1461(0)	159(7)	899(3)	1478(1)
177(1)	861(2)	1456(0)	187(1)	876(2)	1468(8)	183(1)	904(1)	1480(1)
194(1)	866(2)	1460(63)	196(0)	886(1)	1472(29)	197(7)	910(6)	1485(9)
201(2)	873(1)	1464(0)	209(1)	890(1)	1477(36)	210(2)	914(3)	1493(48)
219(3)	892(3)	1468(5)	218(3)	895(3)	1487(4)	236(1)	915(2)	1499(4)
253(1)	915(3)	1474(5)	255(2)	931(4)	1494(3)	260(1)	955(2)	1505(10)
270(4)	982(32)	1487(6)	272(3)	987(34)	1502(6)	265(6)	1003(27)	1518(7)
283(1)	1013(6)	1522(117)	282(1)	1021(5)	1531(93)	277(4)	1026(10)	1538(128)
303(8)	1018(13)	2949(81)	304(8)	1024(11)	2979(54)	302(1)	1030(10)	2989(58)
332(4)	1023(13)	2958(137)	334(2)	1031(12)	2986(111)	344(3)	1031(26)	2999(81)
336(0)	1025(15)	3067(85)	335(1)	1031(10)	3084(37)	349(13)	1033(16)	3109(47)
366(3)	1060(5)	3068(23)	366(2)	1071(5)	3090(16)	380(7)	1072(1)	3112(12)
394(4)	1063(5)	3078(43)	400(4)	1073(5)	3095(27)	399(24)	1074(1)	3113(40)
396(6)	1066(0)	3105(47)	404(5)	1074(1)	3120(31)	407(7)	1075(0)	3160(19)
443(5)	1067(0)	3138(23)	447(6)	1076(0)	3153(10)	452(5)	1078(0)	3175(8)
470(8)	1069(2)	3150(6)	472(8)	1077(2)	3163(3)	479(14)	1079(7)	3181(21)
559(34)	1097(8)	3160(38)	561(32)	1107(10)	3178(19)	573(2)	1116(4)	3203(24)
584(1)	1120(89)	3206(1)	595(1)	1123(87)	3218(0)	580(17)	1140(96)	3257(0)
586(7)	1138(35)	3209(2)	596(11)	1143(16)	3222(1)	607(14)	1154(12)	3262(0)
594(1)	1140(14)	3213(3)	604(1)	1148(2)	3223(1)	615(2)	1156(1)	3264(1)
602(1)	1144(4)	3217(3)	611(4)	1152(32)	3227(1)	617(0)	1162(18)	3270(0)
607(12)	1192(6)	3229(29)	616(8)	1199(5)	3238(6)	620(1)	1205(7)	3275(3)
618(0)	1211(4)	3229(24)	623(0)	1213(7)	3240(12)	624(0)	1237(8)	3276(4)
732(2)	1252(0)	3230(13)	739(3)	1272(0)	3240(5)	740(6)	1277(0)	3280(6)
753(4)	1257(0)	3234(24)	762(4)	1276(0)	3243(7)	798(29)	1281(0)	3283(5)
767(1)	1293(38)	3245(11)	777(1)	1289(34)	3253(3)	800(45)	1328(24)	3289(2)
779(4)	1355(52)	3246(12)	788(79)	1361(55)	3254(3)	807(79)	1370(53)	3295(2)

Tables S104 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **1N-Co-3T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
20(0)	792(54)	1357(4)	17(0)	804(39)	1370(3)	36(0)	824(5)	1403(2)
45(0)	803(29)	1394(4)	50(0)	810(23)	1385(3)	54(0)	841(15)	1413(1)
71(0)	814(11)	1397(4)	70(0)	820(5)	1391(1)	71(0)	842(6)	1414(2)
91(0)	824(2)	1403(1)	92(0)	827(3)	1395(2)	92(0)	848(2)	1420(7)
112(0)	825(3)	1405(2)	114(0)	829(5)	1396(5)	115(0)	849(3)	1422(8)
127(0)	827(7)	1408(4)	128(0)	833(14)	1418(2)	134(0)	854(8)	1438(6)
158(1)	832(3)	1415(0)	159(1)	836(2)	1424(2)	162(1)	856(3)	1456(4)
173(0)	852(1)	1431(4)	175(0)	855(2)	1447(3)	173(0)	888(2)	1465(2)
179(2)	857(2)	1446(0)	180(2)	871(2)	1452(1)	194(1)	899(4)	1467(0)
218(2)	859(2)	1448(1)	219(1)	878(1)	1453(0)	227(1)	900(0)	1472(7)
237(1)	865(0)	1453(1)	238(1)	881(1)	1469(0)	248(2)	907(2)	1488(1)

265(0)	868(2)	1461(7)	272(0)	882(3)	1474(0)	261(0)	910(1)	1490(0)
276(1)	880(16)	1463(1)	279(1)	893(18)	1477(1)	277(0)	931(29)	1493(7)
286(0)	921(22)	1469(1)	289(0)	936(24)	1483(6)	289(0)	975(3)	1494(2)
298(1)	965(41)	1470(7)	305(1)	962(31)	1491(7)	303(2)	1005(43)	1506(13)
322(5)	1011(19)	1478(12)	323(4)	1017(13)	1498(10)	312(2)	1019(34)	1515(14)
341(3)	1014(3)	2987(86)	346(3)	1021(4)	3010(40)	316(3)	1021(3)	3038(26)
356(3)	1024(12)	2989(124)	361(2)	1028(10)	3014(92)	360(4)	1036(15)	3040(94)
377(2)	1025(10)	3064(54)	379(1)	1033(8)	3088(35)	376(1)	1038(20)	3136(14)
385(1)	1027(13)	3094(42)	383(1)	1035(11)	3115(14)	394(2)	1051(9)	3137(28)
417(1)	1036(7)	3097(7)	423(1)	1047(5)	3117(12)	432(1)	1064(9)	3143(19)
461(5)	1062(0)	3101(32)	459(5)	1071(0)	3122(22)	450(3)	1071(0)	3170(15)
474(2)	1064(0)	3124(69)	468(3)	1072(1)	3139(34)	494(1)	1073(1)	3180(11)
533(14)	1065(1)	3143(17)	536(12)	1074(0)	3160(4)	532(11)	1074(0)	3192(10)
562(5)	1067(1)	3143(14)	562(6)	1077(1)	3161(10)	571(8)	1079(0)	3193(29)
576(4)	1092(1)	3202(4)	583(4)	1105(1)	3216(1)	587(14)	1117(4)	3253(2)
584(1)	1102(4)	3206(1)	590(5)	1116(4)	3218(1)	599(3)	1122(3)	3257(1)
585(3)	1141(18)	3211(4)	594(1)	1145(13)	3223(1)	603(1)	1151(6)	3261(0)
596(4)	1143(8)	3214(2)	606(5)	1146(6)	3227(1)	613(3)	1152(3)	3266(1)
600(2)	1185(1)	3226(47)	610(1)	1192(3)	3237(10)	618(3)	1220(5)	3274(10)
717(5)	1199(16)	3226(10)	721(5)	1201(10)	3238(9)	740(6)	1234(14)	3274(4)
753(1)	1215(21)	3228(31)	765(6)	1226(21)	3239(11)	789(4)	1261(10)	3276(9)
765(2)	1252(1)	3231(24)	776(3)	1258(1)	3242(7)	794(38)	1277(0)	3280(5)
780(32)	1252(0)	3242(13)	790(25)	1273(0)	3251(5)	806(67)	1280(0)	3288(2)
788(11)	1255(0)	3244(11)	799(20)	1276(0)	3255(3)	814(104)	1288(0)	3293(1)

Tables S105 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2(MeC_2NMe_2)$**structure **1N-Co-4T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
19(0)	789(49)	1405(5)	24(0)	796(38)	1394(4)	17(0)	820(57)	1418(1)
33(0)	793(4)	1407(7)	33(0)	803(22)	1395(2)	29(0)	826(22)	1420(1)
40(0)	796(29)	1409(1)	49(0)	808(8)	1398(5)	30(0)	828(11)	1421(7)
49(0)	811(33)	1410(0)	62(0)	816(34)	1435(0)	49(0)	851(3)	1442(3)
63(0)	823(1)	1433(6)	67(1)	824(1)	1454(3)	65(2)	852(3)	1462(26)
66(0)	826(6)	1450(0)	82(0)	828(10)	1454(4)	75(0)	854(1)	1470(2)
75(1)	831(0)	1453(3)	84(0)	833(0)	1460(0)	82(0)	855(0)	1474(1)
130(2)	835(4)	1453(3)	139(1)	837(6)	1466(0)	98(1)	895(0)	1477(2)
141(2)	861(0)	1458(14)	141(2)	879(1)	1467(0)	109(1)	899(5)	1478(5)
157(1)	864(1)	1460(1)	166(1)	880(1)	1476(6)	135(0)	902(5)	1481(0)
193(1)	865(1)	1462(1)	190(2)	881(0)	1481(13)	139(0)	907(0)	1488(3)
198(1)	868(1)	1465(30)	199(0)	885(0)	1487(25)	166(0)	908(0)	1497(9)
208(0)	955(23)	1469(5)	210(0)	956(23)	1491(8)	176(2)	984(17)	1500(3)
209(0)	996(9)	1475(2)	222(2)	1013(10)	1500(4)	191(1)	1025(10)	1504(17)

230(4)	1015(9)	1486(4)	230(2)	1021(5)	1512(2)	213(2)	1027(19)	1517(7)
245(1)	1020(10)	1596(138)	251(0)	1027(8)	1615(139)	238(2)	1029(11)	1695(401)
284(2)	1025(25)	2951(73)	287(1)	1032(19)	2980(50)	254(3)	1032(24)	3038(80)
297(13)	1027(1)	2956(137)	296(11)	1033(1)	2985(113)	278(1)	1032(3)	3039(28)
341(4)	1053(15)	3003(82)	342(2)	1067(5)	3023(53)	292(2)	1073(0)	3044(154)
350(1)	1056(11)	3072(83)	352(4)	1072(7)	3090(37)	328(22)	1074(0)	3102(43)
352(1)	1065(1)	3079(30)	370(0)	1073(2)	3096(15)	384(4)	1075(1)	3107(9)
371(2)	1065(2)	3083(34)	374(0)	1074(10)	3099(24)	391(6)	1077(1)	3108(26)
401(7)	1067(0)	3117(30)	397(7)	1075(1)	3128(15)	398(13)	1078(4)	3146(18)
444(3)	1069(2)	3139(24)	448(2)	1079(5)	3152(12)	450(6)	1087(20)	3189(8)
471(3)	1097(3)	3141(25)	481(4)	1113(5)	3158(12)	467(2)	1119(2)	3197(8)
483(10)	1137(97)	3211(0)	498(5)	1145(23)	3222(0)	538(0)	1153(18)	3259(0)
521(21)	1143(16)	3214(1)	511(13)	1148(57)	3223(0)	551(32)	1155(0)	3260(0)
586(1)	1145(8)	3215(1)	594(1)	1149(72)	3224(0)	611(0)	1169(9)	3264(1)
588(1)	1159(40)	3218(1)	598(1)	1169(16)	3227(0)	615(3)	1171(129)	3268(1)
595(1)	1255(0)	3229(25)	605(0)	1260(22)	3238(8)	619(0)	1277(0)	3274(5)
595(1)	1257(0)	3232(25)	606(2)	1274(0)	3241(8)	625(0)	1280(0)	3277(4)
631(7)	1258(21)	3232(25)	641(6)	1276(0)	3241(7)	694(14)	1305(21)	3280(6)
772(1)	1325(68)	3238(23)	785(3)	1337(79)	3247(7)	788(3)	1388(24)	3281(7)
780(1)	1376(11)	3244(11)	786(2)	1387(0)	3251(3)	798(99)	1404(21)	3289(2)
782(2)	1400(1)	3249(13)	790(4)	1393(6)	3256(4)	801(57)	1413(2)	3293(2)

Tables S106 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2(MeC_2NMe_2)$**structure **1N-Fe-1T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
33(0)	799(14)	1357(4)	30(0)	811(14)	1370(3)	45(0)	832(2)	1401(13)
67(0)	807(32)	1390(5)	65(0)	817(18)	1390(0)	71(0)	837(24)	1420(0)
84(0)	815(1)	1403(0)	84(0)	819(0)	1396(0)	89(0)	847(6)	1429(5)
104(0)	821(12)	1407(0)	103(0)	824(19)	1405(1)	108(1)	851(2)	1431(4)
130(1)	823(1)	1416(0)	128(1)	825(1)	1407(0)	134(2)	852(1)	1434(8)
134(1)	824(0)	1417(1)	135(1)	826(0)	1415(3)	142(1)	854(0)	1435(0)
149(3)	836(12)	1419(0)	149(3)	844(12)	1429(1)	191(1)	862(33)	1450(6)
186(1)	851(2)	1435(2)	187(1)	854(3)	1447(2)	193(2)	883(2)	1468(3)
206(0)	858(2)	1449(0)	206(0)	875(3)	1455(0)	223(3)	898(2)	1472(1)
219(1)	865(3)	1451(2)	221(1)	881(2)	1458(2)	229(0)	908(0)	1472(1)
230(0)	867(1)	1451(1)	235(0)	884(0)	1464(0)	248(3)	912(2)	1481(2)
249(0)	876(1)	1457(0)	260(0)	890(3)	1466(0)	257(1)	915(2)	1484(1)
269(0)	881(9)	1458(7)	276(0)	895(12)	1475(1)	284(0)	928(28)	1488(2)
300(2)	914(19)	1461(1)	305(2)	928(17)	1480(6)	324(2)	963(12)	1492(9)
322(9)	971(41)	1468(7)	325(8)	968(33)	1489(6)	335(3)	1009(56)	1505(12)
356(9)	1016(9)	1475(10)	364(9)	1022(6)	1496(9)	367(9)	1027(26)	1514(14)
369(2)	1019(5)	2985(103)	372(4)	1026(7)	3009(55)	379(10)	1030(9)	3034(52)

376(10)	1022(7)	2992(122)	385(9)	1027(6)	3016(89)	406(1)	1037(18)	3040(80)
389(2)	1025(18)	3068(43)	394(2)	1033(14)	3090(28)	412(2)	1039(4)	3133(20)
406(1)	1031(5)	3081(54)	411(0)	1036(3)	3104(35)	447(2)	1051(11)	3134(27)
418(2)	1039(4)	3095(40)	419(2)	1050(2)	3115(11)	461(6)	1064(4)	3139(17)
460(11)	1065(1)	3097(4)	462(11)	1073(0)	3117(11)	492(5)	1074(1)	3160(21)
486(1)	1066(0)	3117(78)	481(1)	1075(0)	3131(45)	507(1)	1076(0)	3184(7)
537(17)	1068(1)	3142(19)	538(18)	1076(1)	3161(9)	546(59)	1077(2)	3186(12)
580(1)	1072(1)	3151(13)	591(2)	1080(1)	3166(6)	594(6)	1083(1)	3193(32)
585(3)	1091(1)	3202(3)	591(3)	1105(1)	3214(1)	609(6)	1116(1)	3253(1)
589(2)	1104(5)	3203(2)	600(2)	1118(4)	3216(1)	615(0)	1124(3)	3262(0)
597(0)	1141(20)	3210(0)	607(0)	1145(16)	3222(0)	620(1)	1153(8)	3265(0)
600(0)	1144(14)	3211(1)	609(0)	1148(11)	3223(0)	624(1)	1158(12)	3265(3)
612(1)	1185(7)	3221(32)	618(1)	1194(6)	3232(13)	629(3)	1222(2)	3273(7)
729(8)	1200(19)	3223(40)	733(7)	1201(13)	3235(11)	749(4)	1237(15)	3277(8)
759(3)	1222(9)	3228(31)	778(1)	1231(12)	3238(12)	797(11)	1267(22)	3281(9)
783(9)	1254(0)	3232(24)	795(17)	1261(1)	3244(9)	806(97)	1278(0)	3283(6)
785(15)	1255(1)	3238(11)	797(6)	1274(0)	3248(6)	826(20)	1282(0)	3291(2)
798(17)	1258(0)	3241(13)	807(14)	1278(0)	3251(4)	828(61)	1292(1)	3294(1)

Tables S107 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2(MeC_2NMe_2)$**structure **1N-Fe-2S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
18(0)	806(17)	1403(0)	15(0)	818(8)	1408(2)	-29(0)	839(38)	1434(1)
55(0)	807(2)	1419(3)	57(0)	820(1)	1410(9)	50(0)	840(3)	1437(31)
73(0)	818(4)	1421(1)	79(0)	827(1)	1415(0)	69(0)	854(4)	1439(0)
84(0)	820(6)	1426(1)	84(0)	829(6)	1415(11)	70(0)	854(0)	1443(0)
110(4)	827(1)	1427(0)	116(4)	833(2)	1428(0)	115(5)	859(8)	1445(60)
140(0)	828(3)	1442(0)	155(0)	837(2)	1461(0)	147(0)	859(19)	1468(1)
148(0)	839(34)	1452(46)	159(2)	843(33)	1461(0)	162(0)	861(3)	1478(0)
154(2)	839(2)	1453(0)	163(0)	845(3)	1462(0)	167(2)	862(8)	1478(0)
168(0)	870(2)	1454(26)	183(0)	889(2)	1464(1)	184(0)	918(2)	1483(8)
178(0)	870(1)	1454(3)	195(0)	890(1)	1465(0)	199(2)	919(1)	1485(0)
194(2)	881(16)	1456(3)	205(1)	903(13)	1475(44)	213(0)	932(13)	1492(49)
201(1)	882(5)	1459(2)	212(1)	904(4)	1483(5)	224(1)	933(3)	1495(7)
208(0)	920(4)	1467(4)	214(0)	917(3)	1483(5)	225(1)	946(3)	1496(8)
231(0)	971(3)	1475(1)	243(0)	989(3)	1499(4)	258(1)	997(6)	1515(0)
276(0)	1021(14)	1477(1)	284(0)	1028(11)	1500(0)	289(0)	1033(0)	1520(8)
320(0)	1021(0)	1519(150)	328(0)	1028(0)	1530(106)	337(1)	1033(18)	1555(235)
333(0)	1033(21)	2990(55)	342(0)	1041(16)	3012(45)	352(1)	1048(10)	3040(37)
366(2)	1033(0)	2993(99)	378(2)	1041(0)	3017(40)	378(4)	1049(27)	3043(47)
381(6)	1041(46)	2997(176)	390(7)	1054(37)	3023(126)	407(1)	1053(31)	3046(124)
389(12)	1052(7)	3080(22)	399(11)	1057(15)	3094(11)	408(13)	1072(7)	3122(14)

408(5)	1070(0)	3083(27)	421(5)	1080(0)	3097(16)	421(4)	1082(0)	3127(0)
433(3)	1070(1)	3088(118)	443(3)	1080(2)	3112(0)	443(0)	1083(1)	3130(82)
441(0)	1076(1)	3091(0)	451(0)	1086(2)	3114(64)	470(3)	1093(0)	3131(18)
496(5)	1076(3)	3179(10)	503(5)	1087(2)	3192(6)	520(7)	1094(4)	3227(10)
551(0)	1092(1)	3180(9)	558(0)	1104(1)	3193(4)	575(0)	1113(1)	3228(6)
565(14)	1125(50)	3215(0)	576(12)	1137(57)	3226(1)	598(8)	1152(67)	3267(0)
584(5)	1148(39)	3215(4)	593(6)	1153(32)	3226(0)	615(16)	1164(20)	3267(2)
588(0)	1148(1)	3222(0)	601(0)	1153(0)	3233(0)	616(0)	1164(1)	3275(0)
590(2)	1163(68)	3222(8)	604(1)	1175(58)	3233(3)	620(1)	1189(64)	3275(2)
592(0)	1244(42)	3233(2)	606(0)	1244(46)	3243(1)	623(3)	1265(37)	3282(0)
594(0)	1257(25)	3234(44)	608(0)	1253(30)	3243(14)	627(1)	1287(1)	3282(8)
644(30)	1258(0)	3240(3)	647(32)	1278(0)	3250(2)	658(40)	1287(0)	3291(1)
765(41)	1258(9)	3240(39)	766(42)	1278(0)	3250(13)	789(60)	1293(36)	3292(8)
796(0)	1362(4)	3253(16)	811(0)	1381(0)	3265(4)	830(56)	1388(8)	3307(3)
798(11)	1393(200)	3254(11)	814(10)	1395(246)	3265(5)	831(0)	1432(139)	3307(4)

Tables S108 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2(MeC_2NMe_2)$**structure **1N-Fe-3T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
21(0)	776(39)	1403(1)	23(0)	787(23)	1395(2)	24(0)	812(35)	1416(1)
41(0)	786(13)	1409(2)	43(0)	795(13)	1401(2)	27(0)	817(78)	1417(2)
56(0)	797(29)	1411(0)	57(0)	807(20)	1402(1)	34(0)	824(3)	1425(0)
58(0)	824(3)	1415(1)	61(0)	827(2)	1434(0)	46(0)	849(2)	1441(3)
67(2)	828(4)	1432(3)	69(1)	831(5)	1453(4)	54(1)	849(0)	1462(26)
75(0)	830(1)	1454(3)	80(0)	834(0)	1460(1)	70(0)	855(0)	1472(0)
89(2)	835(0)	1454(3)	95(2)	838(0)	1463(1)	78(0)	857(0)	1475(1)
108(0)	852(3)	1458(2)	110(0)	858(7)	1466(1)	91(0)	889(2)	1479(4)
136(1)	857(4)	1459(2)	141(1)	865(2)	1470(0)	101(1)	896(3)	1480(0)
145(0)	858(2)	1462(4)	144(0)	873(0)	1476(6)	131(0)	898(2)	1482(2)
169(0)	866(1)	1464(29)	173(0)	885(1)	1480(3)	142(0)	902(0)	1489(7)
179(0)	874(2)	1465(1)	178(0)	890(2)	1486(30)	157(3)	914(0)	1497(6)
186(0)	964(22)	1474(6)	185(0)	966(21)	1495(2)	171(0)	979(12)	1502(4)
192(1)	1002(9)	1476(4)	197(1)	1020(10)	1498(6)	177(2)	1025(22)	1506(19)
232(0)	1018(11)	1491(6)	237(0)	1025(14)	1512(5)	226(2)	1026(16)	1516(8)
243(4)	1019(19)	1640(149)	248(3)	1025(8)	1643(155)	228(0)	1031(24)	1670(348)
259(1)	1023(13)	2964(90)	262(0)	1030(11)	2991(49)	242(2)	1032(2)	3033(76)
270(7)	1024(10)	2970(117)	273(6)	1031(4)	2996(104)	253(1)	1033(9)	3035(36)
286(2)	1057(5)	2996(89)	289(3)	1068(6)	3018(60)	281(5)	1073(0)	3039(160)
312(4)	1062(18)	3070(94)	316(4)	1073(0)	3089(48)	308(11)	1074(2)	3094(48)
340(9)	1065(1)	3074(30)	339(8)	1074(1)	3091(24)	341(22)	1076(0)	3100(1)
344(1)	1066(1)	3077(30)	351(1)	1078(0)	3093(12)	370(10)	1078(0)	3104(36)
374(2)	1070(0)	3113(30)	377(1)	1080(16)	3125(15)	374(2)	1079(4)	3140(20)
414(34)	1071(0)	3143(21)	422(28)	1081(1)	3161(9)	448(4)	1084(18)	3184(9)
439(4)	1097(2)	3148(19)	445(4)	1111(2)	3166(8)	457(9)	1119(2)	3195(9)

477(12)	1136(84)	3207(1)	488(11)	1145(8)	3220(0)	529(14)	1150(1)	3259(0)
525(21)	1142(8)	3214(0)	529(20)	1146(24)	3223(0)	563(14)	1154(11)	3261(1)
592(0)	1143(10)	3214(2)	602(0)	1149(86)	3225(0)	612(3)	1164(108)	3261(0)
593(1)	1158(31)	3216(1)	604(1)	1168(18)	3226(1)	621(0)	1168(29)	3264(0)
599(0)	1256(0)	3229(22)	609(0)	1260(21)	3239(5)	623(0)	1278(0)	3274(4)
611(1)	1256(0)	3231(12)	621(1)	1276(0)	3239(9)	626(1)	1280(0)	3276(3)
651(7)	1264(22)	3231(33)	658(6)	1276(0)	3242(6)	689(16)	1307(21)	3277(6)
751(1)	1343(59)	3236(23)	761(1)	1351(61)	3244(8)	783(0)	1384(42)	3279(6)
758(0)	1376(6)	3245(8)	766(1)	1380(0)	3254(4)	786(1)	1402(7)	3288(1)
774(75)	1395(0)	3247(12)	784(83)	1390(1)	3254(2)	791(176)	1409(0)	3290(3)

Tables S109 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2(MeC_2NMe_2)$**structure **1N-Fe-4T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
39(0)	786(135)	1402(100)	40(0)	797(21)	1398(2)	36(0)	822(2)	1424(1)
48(0)	793(2)	1409(2)	50(0)	804(4)	1404(17)	49(0)	826(39)	1430(0)
61(0)	796(12)	1411(6)	66(0)	810(13)	1407(30)	66(0)	834(6)	1431(33)
75(0)	814(4)	1417(1)	77(0)	825(3)	1415(135)	70(0)	850(5)	1436(8)
88(3)	829(2)	1420(3)	91(2)	833(1)	1425(2)	91(2)	851(8)	1443(81)
112(0)	830(5)	1443(4)	122(0)	834(12)	1456(0)	112(0)	853(2)	1471(4)
120(1)	833(11)	1447(5)	132(1)	836(5)	1463(0)	127(0)	857(4)	1473(0)
135(1)	839(0)	1449(1)	141(1)	841(0)	1464(4)	143(1)	857(2)	1475(1)
146(2)	862(0)	1452(35)	150(2)	878(0)	1468(2)	146(1)	902(1)	1475(9)
151(0)	865(2)	1458(4)	159(0)	884(2)	1470(10)	156(2)	913(1)	1481(13)
184(0)	877(7)	1460(30)	191(1)	896(6)	1472(29)	181(1)	921(5)	1488(31)
197(1)	880(3)	1462(7)	198(1)	899(2)	1475(5)	197(2)	924(5)	1488(1)
207(0)	926(8)	1465(13)	213(0)	925(6)	1484(18)	213(0)	947(5)	1491(15)
226(2)	967(2)	1469(3)	230(2)	984(1)	1488(14)	227(3)	981(2)	1497(25)
249(1)	1015(7)	1476(4)	257(1)	1023(5)	1497(5)	251(1)	1025(13)	1507(6)
284(2)	1019(10)	1538(164)	287(3)	1025(8)	1544(116)	283(2)	1026(10)	1573(291)
286(4)	1029(59)	2984(58)	292(2)	1039(20)	3008(40)	295(6)	1043(24)	3037(32)
310(1)	1031(18)	2988(252)	316(1)	1039(4)	3008(59)	320(5)	1045(15)	3039(75)
325(4)	1034(24)	2990(74)	329(3)	1047(66)	3014(148)	340(7)	1049(82)	3041(123)
342(4)	1054(4)	3054(81)	352(3)	1059(6)	3077(44)	347(5)	1071(5)	3103(51)
355(2)	1068(1)	3062(17)	363(2)	1078(0)	3083(10)	354(4)	1078(0)	3108(11)
394(4)	1070(0)	3074(24)	401(4)	1079(2)	3087(11)	407(4)	1080(3)	3118(11)
409(5)	1070(2)	3079(32)	419(5)	1080(1)	3094(19)	412(5)	1082(2)	3126(25)
458(3)	1075(1)	3172(10)	463(3)	1082(1)	3186(4)	474(2)	1083(2)	3209(7)
512(2)	1090(1)	3175(9)	517(2)	1102(1)	3189(4)	524(1)	1108(1)	3218(6)
523(6)	1133(3)	3214(1)	536(5)	1147(4)	3227(0)	538(6)	1157(3)	3261(0)
553(9)	1145(22)	3216(0)	559(9)	1150(15)	3229(0)	561(14)	1158(10)	3265(0)
590(1)	1147(10)	3218(5)	602(1)	1151(7)	3230(0)	608(3)	1159(1)	3267(0)

593(0)	1158(166)	3218(1)	605(0)	1167(174)	3231(1)	610(0)	1178(181)	3271(1)
598(0)	1236(29)	3233(22)	610(0)	1231(30)	3245(9)	620(1)	1255(37)	3277(4)
599(0)	1240(42)	3234(25)	610(0)	1236(38)	3245(5)	622(0)	1279(44)	3282(7)
631(18)	1255(0)	3236(26)	635(19)	1276(0)	3246(10)	642(21)	1283(0)	3283(5)
750(5)	1260(0)	3237(20)	759(13)	1279(0)	3248(7)	770(58)	1283(1)	3285(7)
765(40)	1359(3)	3249(16)	769(38)	1380(0)	3258(5)	794(16)	1387(7)	3293(3)
782(2)	1400(19)	3249(7)	795(99)	1395(3)	3259(3)	809(187)	1420(2)	3298(4)

Tables S110 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-1S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
19(0)	784(16)	1373(0)	10(0)	790(51)	1388(0)	32(0)	798(16)	1399(0)
26(0)	790(16)	1396(1)	11(0)	799(37)	1389(33)	41(0)	805(76)	1405(2)
62(0)	790(16)	1401(0)	66(0)	801(8)	1394(1)	62(0)	822(15)	1410(0)
77(1)	801(32)	1402(36)	78(1)	812(26)	1395(0)	78(1)	830(8)	1411(51)
86(0)	825(1)	1407(1)	88(0)	827(2)	1397(0)	91(0)	839(3)	1417(2)
92(0)	827(19)	1446(3)	95(0)	830(24)	1452(3)	96(2)	844(33)	1462(6)
124(0)	833(0)	1447(1)	134(0)	836(0)	1453(1)	130(0)	849(0)	1464(2)
131(0)	837(0)	1450(6)	143(0)	841(1)	1471(5)	135(0)	854(1)	1474(8)
144(0)	862(0)	1453(8)	150(0)	879(0)	1473(8)	147(0)	898(0)	1476(10)
184(0)	863(1)	1467(0)	189(0)	880(0)	1473(1)	185(1)	900(1)	1487(0)
191(0)	865(2)	1468(0)	196(0)	883(2)	1474(0)	188(0)	902(1)	1487(1)
215(0)	867(1)	1469(0)	215(0)	887(0)	1489(0)	209(0)	904(1)	1492(0)
293(1)	995(0)	1470(4)	298(1)	1013(0)	1490(4)	273(2)	1012(0)	1494(7)
316(0)	1007(37)	1686(4)	320(0)	1018(16)	1690(5)	297(0)	1017(20)	1750(14)
329(0)	1013(14)	3013(60)	329(16)	1019(11)	3031(56)	304(18)	1019(18)	3059(44)
329(15)	1014(1)	3013(95)	333(0)	1025(17)	3031(37)	313(0)	1022(5)	3059(28)
339(1)	1028(28)	3097(53)	345(1)	1035(22)	3109(24)	323(3)	1036(35)	3138(25)
362(1)	1029(0)	3098(0)	366(1)	1036(0)	3110(0)	344(3)	1036(0)	3138(0)
386(9)	1051(40)	3120(35)	388(9)	1067(34)	3132(19)	369(12)	1061(38)	3164(16)
460(0)	1062(4)	3121(16)	479(0)	1071(1)	3132(5)	441(0)	1069(1)	3164(8)
517(0)	1065(10)	3216(2)	520(1)	1073(11)	3226(0)	514(1)	1072(15)	3265(0)
539(8)	1067(0)	3216(1)	545(9)	1075(0)	3228(1)	523(1)	1074(0)	3265(0)
570(9)	1068(8)	3218(1)	585(8)	1078(6)	3228(0)	566(9)	1076(5)	3268(0)
588(3)	1069(3)	3219(0)	598(6)	1086(13)	3228(0)	589(10)	1083(11)	3268(0)
592(5)	1144(13)	3233(21)	602(4)	1148(10)	3242(6)	601(14)	1148(8)	3279(6)
600(0)	1145(2)	3233(29)	610(0)	1148(1)	3242(9)	609(0)	1149(1)	3280(7)
600(0)	1177(14)	3240(2)	611(0)	1179(14)	3248(0)	614(0)	1180(7)	3283(0)
762(0)	1256(0)	3240(44)	774(0)	1275(0)	3248(12)	780(3)	1278(0)	3283(9)
764(3)	1256(0)	3250(25)	776(3)	1276(0)	3257(8)	795(76)	1279(0)	3294(6)
780(52)	1373(0)	3250(3)	789(0)	1383(1)	3258(1)	795(0)	1398(1)	3294(2)

Tables S111 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in

parentheses in km/mol) for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-2T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
17(0)	777(5)	1374(1)	11(0)	782(85)	1384(7)	13(0)	799(10)	1400(0)
24(0)	779(1)	1396(0)	19(0)	789(0)	1387(1)	24(0)	810(28)	1411(0)
47(0)	781(2)	1397(7)	44(0)	791(3)	1389(3)	55(0)	811(72)	1411(0)
58(1)	791(71)	1401(1)	59(1)	797(76)	1395(0)	59(0)	812(2)	1412(0)
64(0)	827(0)	1404(3)	64(0)	830(1)	1398(1)	65(0)	853(0)	1413(2)
65(0)	829(0)	1450(7)	67(0)	832(0)	1458(0)	68(0)	854(2)	1472(1)
79(0)	834(0)	1452(1)	80(0)	837(1)	1458(1)	74(0)	856(0)	1472(0)
84(0)	835(0)	1452(0)	84(0)	838(0)	1470(6)	87(0)	856(1)	1474(11)
115(0)	857(0)	1453(6)	118(0)	873(0)	1470(0)	128(0)	898(0)	1476(7)
150(0)	858(1)	1466(0)	155(0)	874(1)	1471(0)	152(7)	899(1)	1479(1)
167(1)	860(1)	1467(0)	170(1)	876(1)	1472(7)	155(0)	901(0)	1480(0)
183(0)	861(0)	1468(0)	185(0)	877(0)	1489(0)	182(1)	902(0)	1493(1)
254(4)	986(5)	1470(6)	256(5)	1001(4)	1490(5)	252(21)	1009(30)	1495(8)
274(1)	986(0)	1780(20)	279(2)	1004(0)	1781(19)	281(1)	1015(0)	1813(41)
277(2)	1016(26)	3018(88)	279(1)	1023(21)	3035(51)	283(1)	1026(34)	3063(44)
300(4)	1017(1)	3018(59)	303(4)	1023(1)	3035(35)	296(7)	1026(3)	3063(24)
305(1)	1027(9)	3103(42)	306(2)	1033(8)	3113(18)	302(8)	1031(14)	3142(23)
317(1)	1027(15)	3104(0)	322(0)	1033(12)	3115(0)	315(0)	1032(17)	3143(0)
324(4)	1043(48)	3130(26)	324(4)	1059(43)	3141(13)	323(1)	1054(46)	3172(11)
384(2)	1061(18)	3130(17)	390(3)	1072(1)	3141(5)	377(6)	1072(0)	3172(8)
387(4)	1063(3)	3215(0)	404(2)	1072(0)	3226(0)	427(0)	1073(0)	3263(0)
469(2)	1064(0)	3216(1)	469(3)	1075(0)	3226(0)	511(3)	1074(0)	3263(0)
559(12)	1067(0)	3217(1)	573(11)	1076(0)	3226(0)	585(14)	1075(0)	3264(0)
588(0)	1068(0)	3217(0)	597(0)	1080(22)	3226(0)	615(0)	1083(16)	3264(0)
589(0)	1145(9)	3232(43)	600(0)	1146(6)	3242(2)	619(1)	1147(15)	3278(3)
601(2)	1145(1)	3232(11)	610(2)	1148(7)	3242(14)	621(2)	1152(3)	3278(8)
602(0)	1146(8)	3236(24)	612(0)	1149(0)	3245(8)	625(1)	1153(0)	3281(7)
749(5)	1256(0)	3237(20)	760(2)	1276(0)	3245(5)	788(1)	1278(0)	3281(3)
752(0)	1257(0)	3249(1)	763(0)	1277(0)	3256(1)	793(4)	1279(0)	3292(1)
774(89)	1372(0)	3249(24)	780(0)	1383(0)	3256(7)	797(159)	1397(2)	3292(4)

Tables S112 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-3S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
18(0)	791(59)	1257(0)	13(0)	802(58)	1276(0)	21(0)	812(79)	1291(7)
44(0)	800(9)	1374(4)	40(0)	811(5)	1378(10)	36(0)	838(5)	1396(4)
68(0)	805(9)	1389(16)	70(0)	814(3)	1384(17)	70(1)	840(6)	1401(6)
75(0)	813(0)	1395(13)	76(0)	820(4)	1385(3)	73(0)	846(8)	1405(3)
94(0)	825(3)	1397(1)	98(0)	829(4)	1391(0)	89(1)	851(2)	1409(2)
105(0)	831(1)	1403(1)	107(0)	834(0)	1396(2)	110(0)	853(9)	1421(34)
162(1)	832(1)	1421(18)	164(1)	835(3)	1430(18)	163(0)	853(5)	1454(3)

177(3)	854(1)	1440(4)	178(3)	871(1)	1445(2)	173(1)	899(1)	1459(13)
181(1)	864(1)	1450(3)	186(0)	881(1)	1455(2)	181(1)	905(2)	1462(7)
211(5)	868(6)	1454(6)	213(5)	884(4)	1469(1)	219(4)	909(10)	1479(10)
245(1)	877(1)	1463(0)	250(0)	894(1)	1474(7)	250(0)	920(2)	1481(1)
257(0)	892(2)	1470(2)	266(0)	904(3)	1477(1)	268(1)	928(8)	1494(1)
293(3)	909(3)	1472(1)	297(3)	917(4)	1490(6)	299(2)	938(2)	1501(4)
315(3)	936(2)	1488(17)	321(3)	953(2)	1493(7)	320(9)	982(1)	1527(12)
333(2)	997(14)	2994(77)	336(2)	1002(9)	3016(46)	340(3)	1006(14)	3039(45)
339(2)	999(10)	3074(65)	341(2)	1014(11)	3092(34)	345(3)	1013(12)	3114(24)
364(6)	1015(6)	3080(21)	364(6)	1022(8)	3096(17)	378(10)	1029(25)	3143(20)
393(1)	1018(11)	3100(35)	393(1)	1031(7)	3116(16)	404(3)	1032(15)	3148(16)
451(16)	1027(13)	3115(22)	447(13)	1033(9)	3132(11)	450(21)	1038(11)	3152(22)
489(10)	1031(13)	3199(8)	493(11)	1039(11)	3212(4)	524(14)	1040(18)	3244(8)
545(6)	1059(1)	3200(15)	545(6)	1067(1)	3213(6)	552(1)	1068(1)	3253(2)
574(3)	1061(2)	3211(5)	582(3)	1069(2)	3221(2)	580(2)	1069(5)	3263(0)
581(1)	1067(2)	3222(0)	587(1)	1075(1)	3230(0)	597(2)	1072(4)	3268(0)
583(1)	1069(0)	3225(14)	594(1)	1077(0)	3235(2)	610(0)	1074(0)	3271(2)
591(1)	1137(10)	3226(11)	602(0)	1141(8)	3235(8)	613(3)	1146(2)	3272(6)
600(1)	1142(5)	3235(28)	609(1)	1145(4)	3245(8)	617(3)	1149(3)	3280(5)
710(2)	1152(10)	3240(15)	724(1)	1149(10)	3248(3)	759(2)	1157(6)	3282(2)
729(1)	1207(7)	3243(19)	736(1)	1218(7)	3251(3)	765(2)	1227(10)	3288(1)
759(53)	1253(0)	3245(10)	773(51)	1262(15)	3253(5)	786(106)	1276(0)	3290(3)
774(10)	1256(16)	3254(12)	786(9)	1273(0)	3261(3)	799(19)	1277(0)	3297(4)

Tables S113 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-4S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
22(0)	782(38)	1319(8)	18(0)	794(31)	1336(9)	32(0)	802(66)	1336(5)
52(0)	805(28)	1385(5)	55(0)	815(45)	1380(15)	52(0)	824(56)	1402(21)
62(0)	808(16)	1392(19)	63(0)	819(12)	1385(0)	65(0)	838(20)	1406(2)
74(0)	815(12)	1397(0)	76(0)	824(4)	1391(42)	80(0)	843(6)	1410(14)
93(0)	822(3)	1403(33)	96(0)	828(6)	1395(5)	96(0)	844(6)	1418(37)
111(2)	826(3)	1405(7)	112(2)	829(6)	1407(2)	106(2)	851(18)	1421(10)
153(0)	832(9)	1433(4)	154(1)	836(9)	1446(19)	149(2)	852(9)	1459(38)
178(1)	838(0)	1441(27)	181(1)	843(2)	1448(1)	171(0)	857(2)	1461(5)
191(0)	859(34)	1444(0)	199(1)	863(51)	1449(3)	181(2)	881(64)	1463(1)
207(1)	863(17)	1467(3)	208(1)	878(0)	1481(0)	204(1)	902(3)	1489(3)
239(0)	866(2)	1475(4)	242(0)	885(0)	1482(0)	246(6)	902(5)	1496(0)
282(5)	870(1)	1476(0)	285(7)	888(4)	1488(3)	271(1)	907(1)	1498(5)
289(1)	874(6)	1477(1)	293(2)	892(3)	1499(4)	276(1)	913(3)	1499(1)
294(6)	878(4)	1629(15)	297(4)	895(3)	1627(14)	283(11)	913(5)	1678(27)
329(3)	1004(13)	3015(87)	328(3)	1010(10)	3035(55)	309(1)	1010(15)	3057(47)
344(0)	1006(4)	3069(46)	345(0)	1012(3)	3085(22)	322(2)	1011(5)	3134(17)
359(5)	1012(10)	3098(13)	360(4)	1023(8)	3113(9)	345(12)	1026(13)	3135(8)

364(1)	1024(12)	3101(19)	367(1)	1038(14)	3117(6)	353(8)	1042(29)	3158(11)
435(1)	1034(25)	3131(39)	433(1)	1041(17)	3147(18)	416(2)	1044(3)	3177(10)
461(2)	1037(3)	3160(15)	463(2)	1044(2)	3173(8)	467(6)	1048(15)	3229(5)
516(10)	1050(11)	3215(3)	520(11)	1064(9)	3224(1)	518(8)	1064(10)	3263(1)
588(3)	1064(0)	3217(2)	597(4)	1072(0)	3228(1)	590(23)	1071(1)	3266(0)
589(4)	1065(14)	3217(1)	599(5)	1073(14)	3228(1)	598(3)	1072(12)	3267(1)
591(7)	1066(0)	3220(1)	601(6)	1075(2)	3229(0)	605(10)	1074(6)	3267(0)
594(4)	1070(4)	3231(24)	603(3)	1079(3)	3241(8)	607(4)	1076(5)	3277(6)
696(8)	1110(9)	3232(24)	700(4)	1110(8)	3242(7)	702(16)	1123(16)	3279(8)
701(3)	1143(8)	3243(19)	705(7)	1146(6)	3251(5)	725(12)	1150(5)	3286(3)
744(3)	1144(4)	3244(18)	756(2)	1147(3)	3252(4)	778(6)	1152(1)	3286(3)
752(5)	1256(0)	3251(12)	765(5)	1276(0)	3259(4)	785(18)	1279(0)	3294(2)
776(53)	1259(0)	3253(14)	787(46)	1279(0)	3260(4)	794(70)	1281(0)	3295(4)

Tables S114 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Ni_2C_2Me_2$**structure **0N-Ni-5S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
-17(0)	784(5)	1257(0)	-18(0)	797(35)	1277(0)	28(0)	806(101)	1279(0)
77(0)	787(46)	1262(0)	75(0)	798(4)	1281(0)	62(0)	831(5)	1284(0)
98(0)	800(49)	1333(2)	97(0)	810(37)	1349(2)	99(0)	837(7)	1358(4)
106(0)	817(3)	1399(0)	102(0)	828(5)	1387(0)	99(0)	840(0)	1407(1)
119(1)	828(0)	1405(8)	118(0)	831(0)	1393(7)	123(0)	850(12)	1418(0)
133(1)	831(2)	1407(0)	132(1)	834(2)	1395(0)	137(1)	850(0)	1418(18)
183(0)	834(0)	1409(2)	183(0)	836(0)	1396(3)	187(0)	854(15)	1423(5)
200(15)	838(4)	1444(0)	200(14)	842(4)	1448(8)	205(20)	860(0)	1461(15)
212(10)	866(0)	1444(4)	213(11)	882(0)	1453(4)	209(16)	904(0)	1467(0)
257(2)	868(2)	1447(6)	258(3)	886(1)	1461(0)	251(1)	907(0)	1472(3)
289(1)	870(0)	1457(1)	292(1)	886(0)	1463(0)	263(4)	908(0)	1473(1)
295(1)	876(2)	1468(5)	299(1)	893(1)	1477(2)	289(1)	912(4)	1498(2)
319(1)	895(4)	1472(0)	328(1)	911(4)	1479(0)	300(0)	940(6)	1500(1)
341(1)	964(3)	1474(0)	339(1)	969(4)	1481(1)	315(2)	979(6)	1514(2)
363(2)	980(2)	2995(104)	363(2)	988(1)	3017(68)	369(9)	994(4)	3041(54)
375(4)	1011(8)	2999(37)	376(4)	1017(6)	3019(23)	391(1)	1012(10)	3042(22)
483(0)	1018(14)	3102(14)	479(0)	1024(11)	3121(3)	464(9)	1022(16)	3145(25)
495(4)	1031(5)	3105(13)	485(3)	1038(4)	3125(9)	500(0)	1042(10)	3146(3)
534(0)	1036(7)	3115(50)	528(18)	1043(8)	3131(31)	539(0)	1045(14)	3178(10)
535(18)	1037(8)	3132(68)	534(0)	1044(6)	3145(37)	567(2)	1061(2)	3197(33)
577(1)	1038(4)	3217(1)	588(1)	1049(2)	3226(1)	567(27)	1067(0)	3263(1)
582(0)	1055(4)	3218(1)	592(0)	1067(3)	3228(0)	596(1)	1074(0)	3264(0)
594(1)	1067(0)	3218(0)	604(1)	1075(0)	3230(0)	600(1)	1075(0)	3265(0)
595(0)	1068(0)	3219(0)	604(0)	1076(0)	3230(0)	606(4)	1078(8)	3270(0)
668(2)	1074(1)	3232(27)	677(2)	1082(6)	3242(7)	674(3)	1081(1)	3277(6)
686(15)	1075(6)	3234(23)	693(15)	1083(0)	3244(6)	697(19)	1087(5)	3279(6)
728(1)	1139(8)	3240(28)	734(1)	1147(10)	3249(6)	759(0)	1152(6)	3284(8)

758(1)	1142(16)	3241(20)	770(2)	1149(7)	3250(5)	783(2)	1157(4)	3286(3)
774(9)	1145(6)	3250(5)	785(6)	1150(7)	3258(3)	791(28)	1161(5)	3294(3)
784(55)	1151(1)	3252(14)	793(71)	1154(0)	3260(3)	801(98)	1162(3)	3296(1)

Tables S115 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $\mathbf{Cp_2Ni_2C_2Me_2}$structure **0N-Ni-6T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
20(0)	779(50)	1265(8)	18(0)	788(53)	1277(0)	20(0)	810(5)	1292(1)
43(0)	788(88)	1377(4)	39(0)	795(79)	1385(1)	47(0)	812(100)	1402(7)
66(0)	803(6)	1399(2)	59(0)	818(7)	1387(0)	58(0)	841(8)	1410(2)
77(0)	829(3)	1400(1)	76(0)	832(2)	1388(1)	69(0)	849(3)	1412(0)
96(0)	830(0)	1402(5)	96(0)	833(1)	1389(7)	88(1)	851(7)	1412(1)
111(0)	833(3)	1403(3)	114(0)	835(2)	1398(3)	107(1)	857(1)	1414(9)
143(0)	835(1)	1436(10)	144(0)	838(1)	1444(11)	140(1)	858(0)	1460(5)
165(1)	858(1)	1448(1)	164(0)	872(1)	1453(1)	149(1)	900(0)	1464(6)
171(1)	861(2)	1455(0)	171(1)	874(1)	1460(0)	162(4)	901(0)	1477(0)
202(3)	866(1)	1457(9)	205(3)	885(1)	1471(0)	208(4)	907(5)	1480(1)
250(0)	875(2)	1466(1)	252(0)	893(1)	1475(0)	256(0)	911(1)	1481(15)
258(2)	890(4)	1469(0)	259(3)	903(4)	1476(9)	283(6)	923(5)	1494(3)
274(2)	906(2)	1470(1)	279(2)	914(3)	1489(2)	284(0)	932(6)	1496(2)
280(2)	937(3)	1493(10)	282(1)	953(2)	1502(7)	287(3)	980(1)	1527(14)
297(4)	1007(10)	2986(90)	299(3)	1021(10)	3009(60)	293(2)	1019(13)	3033(53)
322(2)	1015(5)	3064(74)	324(2)	1023(7)	3081(44)	327(7)	1029(20)	3111(22)
342(2)	1016(20)	3073(26)	345(2)	1024(15)	3089(17)	347(8)	1030(20)	3132(30)
378(2)	1019(7)	3093(24)	380(2)	1030(2)	3111(9)	387(3)	1033(8)	3142(17)
418(15)	1028(16)	3101(24)	419(14)	1035(11)	3119(12)	413(32)	1037(9)	3146(15)
463(0)	1029(8)	3188(27)	464(1)	1036(7)	3203(13)	487(1)	1039(9)	3235(8)
513(2)	1066(0)	3212(1)	513(2)	1073(1)	3225(0)	531(1)	1072(1)	3260(0)
570(2)	1066(0)	3216(1)	574(3)	1074(0)	3227(0)	577(4)	1074(1)	3263(1)
584(4)	1067(1)	3218(1)	594(4)	1075(1)	3228(1)	597(3)	1075(0)	3266(0)
590(0)	1069(1)	3222(1)	600(0)	1077(0)	3231(0)	612(7)	1076(0)	3269(0)
597(2)	1145(6)	3232(30)	607(2)	1145(6)	3242(6)	619(1)	1152(3)	3275(4)
602(0)	1145(4)	3234(10)	612(1)	1148(3)	3243(5)	621(1)	1155(2)	3279(3)
719(1)	1151(5)	3236(27)	726(2)	1150(3)	3244(7)	745(2)	1163(6)	3280(5)
750(1)	1202(7)	3242(18)	762(0)	1214(7)	3251(4)	786(1)	1223(10)	3286(3)
757(4)	1256(0)	3249(7)	767(1)	1273(5)	3256(2)	796(53)	1279(0)	3291(2)
769(25)	1258(0)	3252(13)	778(23)	1276(0)	3260(3)	796(74)	1281(0)	3296(3)

Tables S116 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $\mathbf{Cp_2Co_2C_2Me_2}$structure **0N-Co-1T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
44(0)	795(16)	1263(20)	40(0)	802(15)	1278(0)	26(0)	816(36)	1288(7)
57(0)	807(24)	1377(2)	57(0)	813(24)	1386(0)	37(0)	830(53)	1405(4)

66(0)	817(13)	1400(2)	64(0)	824(4)	1390(4)	54(0)	845(10)	1414(0)
91(0)	823(0)	1400(2)	91(0)	827(3)	1395(5)	65(0)	853(3)	1418(1)
106(0)	828(3)	1409(5)	104(0)	830(2)	1398(2)	95(0)	853(4)	1419(2)
120(1)	828(11)	1411(2)	120(1)	831(13)	1400(1)	122(1)	854(1)	1422(2)
161(0)	832(1)	1441(6)	161(0)	834(1)	1451(0)	133(1)	856(0)	1468(2)
171(0)	859(3)	1444(2)	175(0)	872(3)	1451(6)	164(1)	900(3)	1476(3)
196(0)	864(3)	1455(1)	195(1)	878(3)	1462(1)	185(4)	903(8)	1478(0)
218(3)	874(0)	1457(0)	219(2)	888(0)	1462(0)	217(4)	908(2)	1478(2)
246(0)	877(1)	1460(5)	248(0)	893(1)	1468(0)	259(0)	915(0)	1481(1)
287(3)	883(1)	1462(0)	288(4)	898(2)	1480(7)	267(1)	918(0)	1485(7)
297(3)	902(1)	1468(1)	300(2)	911(2)	1488(2)	292(2)	930(4)	1499(8)
322(1)	939(3)	1488(8)	324(1)	954(2)	1493(6)	309(10)	980(2)	1521(10)
354(3)	996(17)	2991(89)	357(2)	1011(17)	3014(54)	353(5)	1024(6)	3037(49)
376(1)	1013(6)	3063(73)	379(0)	1020(4)	3082(45)	374(3)	1026(11)	3112(23)
389(1)	1020(14)	3077(28)	396(1)	1026(10)	3093(15)	396(8)	1030(16)	3130(17)
406(6)	1023(8)	3095(26)	413(6)	1031(12)	3115(12)	413(9)	1032(31)	3137(25)
452(8)	1025(13)	3108(48)	452(7)	1032(5)	3128(25)	445(30)	1033(4)	3139(22)
515(18)	1026(7)	3203(15)	518(18)	1040(6)	3220(1)	524(1)	1046(8)	3218(17)
547(3)	1063(1)	3208(3)	548(3)	1072(1)	3220(8)	544(5)	1073(1)	3260(0)
583(8)	1066(0)	3210(2)	594(11)	1073(0)	3222(0)	589(7)	1075(0)	3263(0)
590(1)	1068(0)	3216(0)	601(5)	1076(0)	3225(0)	609(7)	1075(0)	3266(0)
592(0)	1072(1)	3220(1)	602(0)	1081(1)	3228(0)	618(0)	1079(0)	3270(0)
598(12)	1138(15)	3229(21)	606(7)	1140(13)	3238(6)	622(0)	1153(10)	3276(3)
603(2)	1141(16)	3232(18)	613(0)	1144(14)	3240(6)	624(1)	1155(0)	3277(3)
731(4)	1144(2)	3235(20)	738(4)	1147(2)	3244(5)	726(8)	1163(10)	3282(5)
762(6)	1202(5)	3236(22)	768(5)	1214(5)	3244(6)	798(29)	1211(7)	3283(4)
774(1)	1253(0)	3246(10)	782(2)	1272(18)	3254(3)	805(70)	1278(0)	3290(1)
786(62)	1258(0)	3247(11)	792(57)	1272(1)	3255(3)	811(56)	1281(0)	3295(2)

Tables S117 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-2T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
-19(0)	782(10)	1374(0)	-24(0)	794(0)	1394(19)	19(0)	806(44)	1399(1)
-10(0)	792(48)	1402(0)	-17(0)	803(36)	1395(0)	28(0)	819(2)	1409(0)
40(1)	794(2)	1406(21)	29(0)	803(21)	1395(0)	41(3)	820(69)	1416(28)
53(0)	797(44)	1407(0)	48(0)	806(23)	1396(0)	56(0)	838(5)	1417(2)
66(1)	824(10)	1408(0)	57(0)	826(14)	1397(0)	77(2)	846(0)	1419(0)
66(0)	825(0)	1451(7)	66(1)	826(0)	1457(0)	86(1)	846(29)	1468(1)
87(0)	830(0)	1451(0)	85(0)	831(0)	1458(1)	90(0)	851(0)	1469(1)
95(0)	833(1)	1452(1)	96(0)	835(2)	1470(0)	105(0)	853(3)	1475(11)
143(0)	862(1)	1454(5)	145(0)	879(1)	1470(0)	135(11)	897(2)	1477(8)
189(1)	865(0)	1464(0)	191(1)	883(0)	1472(6)	156(6)	899(0)	1482(0)
205(0)	866(0)	1464(0)	209(0)	883(0)	1474(6)	183(4)	910(0)	1486(1)
210(0)	868(0)	1465(0)	211(0)	884(0)	1486(0)	185(0)	913(1)	1490(1)

255(13)	990(17)	1467(5)	254(13)	1005(16)	1488(5)	273(16)	1005(15)	1493(8)
312(3)	997(0)	1547(1)	317(2)	1014(0)	1553(1)	286(2)	1015(1)	1654(7)
323(0)	1016(2)	3008(106)	325(0)	1022(1)	3029(62)	319(3)	1022(7)	3056(52)
339(0)	1017(16)	3010(48)	342(0)	1023(13)	3030(30)	326(0)	1023(19)	3057(25)
359(0)	1027(0)	3090(53)	362(0)	1034(0)	3105(24)	345(1)	1031(14)	3133(27)
381(2)	1027(24)	3092(0)	387(2)	1034(18)	3107(0)	362(0)	1038(16)	3134(0)
409(10)	1032(28)	3119(40)	411(8)	1047(25)	3133(20)	392(9)	1052(31)	3160(17)
450(0)	1061(6)	3120(12)	467(0)	1074(5)	3133(4)	404(3)	1072(1)	3160(9)
484(0)	1066(5)	3218(0)	484(1)	1075(2)	3225(1)	435(8)	1073(8)	3261(0)
520(10)	1067(0)	3218(1)	517(11)	1075(0)	3225(0)	508(0)	1074(0)	3261(0)
575(6)	1068(0)	3221(0)	586(5)	1076(0)	3229(0)	580(9)	1076(1)	3268(0)
587(7)	1068(0)	3221(0)	596(7)	1080(5)	3229(0)	600(1)	1083(6)	3272(0)
588(1)	1144(21)	3235(33)	597(1)	1148(16)	3243(7)	602(15)	1150(9)	3276(6)
595(0)	1145(4)	3235(20)	604(0)	1149(3)	3243(8)	615(5)	1152(5)	3276(6)
596(0)	1194(22)	3239(0)	605(0)	1193(24)	3245(12)	616(0)	1191(14)	3283(5)
773(2)	1256(0)	3239(45)	771(4)	1276(0)	3245(0)	783(4)	1278(0)	3286(3)
778(2)	1256(0)	3250(15)	790(1)	1276(0)	3256(3)	801(63)	1281(0)	3289(4)
781(0)	1373(0)	3250(6)	790(13)	1389(0)	3257(3)	803(1)	1398(2)	3297(1)

Tables S118 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-3T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
33(0)	805(36)	1258(0)	33(0)	816(21)	1277(0)	24(0)	828(57)	1288(12)
47(0)	807(12)	1379(2)	49(0)	820(16)	1386(4)	43(0)	840(8)	1401(11)
61(0)	824(1)	1400(4)	61(0)	827(2)	1393(7)	60(0)	850(8)	1415(0)
68(0)	829(4)	1405(6)	68(0)	832(8)	1394(1)	68(0)	852(3)	1417(1)
99(0)	830(3)	1407(4)	98(0)	833(0)	1400(1)	93(1)	854(1)	1418(2)
115(1)	833(8)	1412(0)	114(1)	835(7)	1402(3)	112(0)	857(0)	1420(1)
124(3)	842(13)	1414(3)	126(2)	848(15)	1429(3)	120(3)	858(4)	1439(2)
175(0)	859(2)	1443(4)	176(0)	873(2)	1450(3)	165(3)	890(13)	1467(2)
219(0)	864(1)	1448(2)	221(1)	880(1)	1455(2)	209(1)	901(1)	1475(2)
229(2)	870(1)	1453(4)	230(1)	886(8)	1462(2)	217(0)	907(0)	1478(1)
267(0)	875(1)	1457(0)	269(1)	890(4)	1463(0)	258(1)	913(1)	1480(2)
283(3)	886(14)	1457(2)	286(2)	893(2)	1470(1)	276(1)	915(1)	1481(2)
293(3)	903(3)	1465(0)	293(4)	913(2)	1474(3)	282(6)	930(3)	1482(3)
324(3)	954(6)	1490(6)	326(4)	967(7)	1506(6)	323(5)	1002(3)	1514(14)
346(8)	1015(7)	2983(68)	349(7)	1023(5)	3003(45)	352(15)	1024(12)	3032(29)
375(2)	1019(13)	3060(37)	382(1)	1025(10)	3075(28)	371(5)	1030(18)	3099(43)
397(4)	1025(20)	3074(11)	404(3)	1032(18)	3090(12)	389(7)	1033(28)	3132(10)
424(11)	1027(3)	3090(68)	426(11)	1034(2)	3107(33)	426(9)	1035(4)	3137(14)
451(4)	1040(2)	3099(70)	451(4)	1050(1)	3116(43)	467(15)	1058(10)	3152(48)
551(24)	1046(17)	3106(54)	559(24)	1061(14)	3127(24)	536(9)	1064(12)	3165(37)
571(1)	1066(0)	3209(2)	573(1)	1075(1)	3220(0)	576(10)	1074(1)	3259(0)
586(4)	1067(1)	3217(0)	597(4)	1075(1)	3226(0)	608(2)	1075(0)	3263(0)

593(1)	1068(0)	3218(0)	602(1)	1077(0)	3227(0)	616(0)	1076(1)	3268(0)
594(0)	1070(1)	3218(0)	606(0)	1078(1)	3229(0)	621(2)	1079(0)	3269(0)
604(0)	1075(3)	3230(21)	614(0)	1087(3)	3240(5)	625(0)	1099(4)	3276(3)
702(5)	1141(16)	3233(23)	707(5)	1145(13)	3243(8)	711(4)	1153(9)	3277(3)
754(4)	1145(4)	3235(22)	763(3)	1148(2)	3244(5)	798(26)	1155(1)	3282(5)
774(3)	1193(4)	3237(23)	783(1)	1204(4)	3245(6)	803(64)	1207(4)	3283(4)
783(75)	1242(17)	3247(5)	790(75)	1252(16)	3254(3)	810(57)	1278(0)	3290(1)
788(6)	1255(0)	3247(16)	799(7)	1275(0)	3255(3)	814(45)	1281(0)	3294(2)

Tables S119 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-4S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
39(0)	803(17)	1253(0)	35(0)	813(30)	1272(0)	44(0)	836(5)	1279(0)
75(0)	807(18)	1257(0)	73(0)	817(11)	1276(0)	77(0)	838(31)	1283(0)
110(0)	812(24)	1359(5)	108(0)	821(15)	1372(4)	122(0)	847(22)	1384(8)
121(0)	822(11)	1403(2)	122(0)	825(17)	1392(2)	130(0)	851(12)	1421(2)
140(1)	827(0)	1408(0)	141(1)	829(0)	1396(0)	147(1)	856(1)	1425(0)
153(2)	828(3)	1411(1)	153(1)	832(6)	1400(0)	159(2)	856(11)	1427(0)
201(3)	831(5)	1413(3)	203(2)	837(6)	1404(3)	206(2)	860(1)	1427(4)
217(1)	851(0)	1438(7)	218(2)	860(0)	1444(9)	226(5)	880(3)	1468(4)
263(5)	861(0)	1444(0)	264(4)	879(0)	1449(0)	265(10)	908(0)	1469(0)
322(0)	868(0)	1447(1)	326(0)	886(0)	1454(1)	321(2)	916(0)	1472(2)
351(2)	871(1)	1458(0)	355(3)	890(1)	1464(0)	357(8)	920(2)	1482(2)
369(5)	877(0)	1460(1)	368(5)	894(0)	1474(0)	372(2)	925(0)	1489(2)
372(7)	881(2)	1472(1)	381(7)	899(3)	1477(1)	399(7)	933(4)	1496(3)
391(9)	960(6)	1607(13)	398(7)	966(6)	1604(12)	402(10)	973(9)	1624(54)
402(7)	985(4)	2327(2)	409(6)	991(4)	2328(1)	411(4)	997(6)	2296(1)
424(2)	1010(14)	2973(100)	427(2)	1015(10)	2994(73)	452(3)	1020(18)	3015(77)
459(12)	1016(6)	3082(28)	458(12)	1023(5)	3103(17)	477(12)	1029(8)	3122(23)
509(1)	1029(6)	3100(60)	507(1)	1034(5)	3116(35)	533(4)	1041(2)	3164(28)
537(5)	1029(9)	3140(23)	538(4)	1036(7)	3160(10)	571(7)	1043(16)	3200(9)
559(10)	1043(4)	3168(46)	562(13)	1055(3)	3182(23)	588(15)	1075(0)	3228(15)
581(1)	1066(1)	3213(1)	591(1)	1074(1)	3224(0)	604(1)	1077(0)	3265(0)
584(2)	1066(0)	3214(2)	596(4)	1075(0)	3225(0)	613(10)	1078(1)	3267(0)
586(7)	1067(0)	3216(0)	598(5)	1075(0)	3227(0)	617(8)	1084(1)	3271(0)
593(3)	1072(3)	3217(0)	603(3)	1079(3)	3228(0)	626(1)	1087(6)	3272(0)
669(3)	1084(3)	3229(28)	679(3)	1096(3)	3240(7)	708(2)	1108(2)	3280(4)
724(16)	1119(2)	3231(31)	731(18)	1129(2)	3241(11)	756(24)	1134(2)	3283(6)
777(5)	1141(23)	3234(27)	795(6)	1146(19)	3243(7)	812(27)	1157(15)	3284(6)
783(4)	1143(14)	3237(26)	796(3)	1147(10)	3245(8)	822(14)	1160(11)	3288(5)
795(24)	1152(4)	3244(5)	809(10)	1161(4)	3254(4)	829(66)	1172(3)	3297(4)
800(12)	1222(10)	3247(10)	810(5)	1229(11)	3255(2)	834(14)	1242(25)	3299(1)

Tables S120 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-5T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
-19(0)	801(48)	1252(0)	-20(0)	811(49)	1272(0)	23(0)	845(10)	1272(0)
61(0)	807(17)	1255(0)	66(0)	816(2)	1276(0)	45(1)	846(40)	1281(0)
89(4)	815(2)	1359(0)	87(6)	817(29)	1374(0)	53(0)	848(1)	1398(2)
105(0)	816(16)	1396(0)	105(0)	822(2)	1384(0)	77(0)	856(5)	1406(1)
107(9)	821(0)	1399(21)	107(11)	825(0)	1386(19)	86(0)	856(2)	1410(0)
135(0)	827(4)	1407(1)	130(0)	833(9)	1394(2)	97(0)	859(22)	1425(0)
161(1)	834(1)	1408(0)	158(0)	836(1)	1397(0)	158(2)	874(5)	1427(1)
172(23)	847(5)	1442(5)	168(26)	864(0)	1452(2)	180(1)	876(2)	1467(0)
212(29)	848(0)	1450(0)	212(25)	869(4)	1457(0)	198(8)	880(1)	1469(0)
256(1)	865(1)	1451(0)	261(0)	876(0)	1457(2)	252(0)	920(5)	1471(4)
284(11)	866(1)	1453(0)	281(14)	884(1)	1458(3)	284(1)	934(1)	1473(2)
299(1)	874(1)	1457(2)	306(1)	891(1)	1459(0)	309(0)	936(0)	1482(3)
329(4)	885(0)	1458(2)	329(3)	901(0)	1464(2)	325(1)	949(2)	1491(5)
364(2)	970(2)	1460(0)	366(8)	977(2)	1465(0)	384(4)	978(6)	1522(8)
365(8)	1013(19)	2673(3)	367(2)	1020(15)	2703(1)	407(3)	998(8)	2751(19)
388(20)	1020(10)	2694(7)	395(16)	1027(10)	2720(3)	414(4)	1020(27)	3049(0)
423(4)	1020(10)	3142(24)	417(4)	1027(6)	3160(5)	465(9)	1022(23)	3201(4)
482(11)	1025(11)	3144(3)	474(7)	1032(8)	3164(4)	494(6)	1031(6)	3210(1)
520(5)	1026(0)	3160(34)	521(28)	1033(2)	3174(20)	522(11)	1040(10)	3221(13)
525(20)	1056(9)	3175(49)	524(4)	1063(6)	3185(22)	544(19)	1062(4)	3232(16)
572(34)	1059(13)	3201(2)	582(38)	1065(19)	3216(1)	619(1)	1067(0)	3237(3)
578(0)	1063(0)	3208(0)	589(0)	1072(0)	3218(0)	622(1)	1069(1)	3248(0)
591(1)	1065(1)	3217(3)	604(2)	1074(1)	3225(2)	624(0)	1078(1)	3259(14)
594(0)	1067(2)	3221(0)	606(0)	1075(2)	3231(0)	631(2)	1082(3)	3264(13)
694(3)	1100(6)	3223(31)	696(4)	1091(4)	3235(12)	710(3)	1086(4)	3271(0)
746(0)	1106(2)	3225(36)	757(0)	1101(1)	3235(13)	759(5)	1137(14)	3276(4)
748(8)	1141(17)	3235(25)	765(7)	1144(14)	3243(5)	776(21)	1145(2)	3279(1)
771(57)	1143(2)	3237(20)	775(13)	1148(12)	3246(5)	780(120)	1160(6)	3289(1)
774(4)	1144(14)	3239(11)	781(38)	1155(2)	3248(4)	813(1)	1193(11)	3294(0)
788(2)	1172(7)	3248(10)	797(2)	1184(6)	3256(2)	839(8)	1225(16)	3305(1)

Tables S121 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-6S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
20(0)	800(13)	1372(0)	20(0)	806(1)	1390(11)	17(0)	829(57)	1394(2)
26(0)	804(2)	1400(0)	25(0)	811(6)	1392(0)	26(0)	846(0)	1420(9)
61(0)	809(3)	1400(11)	60(0)	820(2)	1394(0)	61(0)	848(3)	1421(0)
69(1)	816(2)	1409(1)	69(1)	821(0)	1396(0)	70(0)	850(0)	1422(1)
76(0)	818(0)	1413(1)	76(0)	823(23)	1401(0)	79(2)	854(4)	1424(1)
90(0)	819(22)	1442(0)	91(0)	824(8)	1449(0)	83(0)	855(4)	1465(4)

100(2)	827(0)	1443(1)	101(2)	829(0)	1449(1)	90(0)	856(2)	1465(0)
105(0)	831(4)	1452(5)	107(0)	833(6)	1467(0)	110(2)	857(1)	1475(11)
130(0)	862(1)	1455(9)	131(0)	880(1)	1467(0)	147(0)	912(0)	1477(8)
150(0)	863(1)	1461(0)	155(0)	881(1)	1472(4)	191(1)	914(0)	1485(1)
201(0)	866(0)	1461(0)	205(1)	882(0)	1474(10)	201(0)	916(1)	1486(0)
226(0)	868(1)	1470(0)	229(0)	884(1)	1491(0)	221(0)	918(2)	1493(0)
306(0)	984(1)	1472(6)	313(0)	999(1)	1492(6)	305(2)	1000(5)	1496(10)
337(0)	990(0)	1719(2)	342(0)	1007(0)	1723(3)	355(3)	1013(3)	1646(0)
344(1)	1011(20)	3009(101)	354(0)	1017(15)	3029(60)	372(1)	1023(24)	3050(60)
358(3)	1012(2)	3010(62)	366(2)	1018(1)	3029(38)	393(6)	1023(3)	3051(23)
388(3)	1026(12)	3092(49)	397(2)	1033(9)	3106(22)	418(6)	1038(12)	3123(31)
399(5)	1026(7)	3094(0)	406(5)	1034(6)	3107(0)	445(0)	1039(9)	3126(0)
421(0)	1051(42)	3115(43)	430(0)	1066(35)	3129(25)	447(13)	1059(26)	3155(31)
438(2)	1063(1)	3115(15)	441(2)	1071(1)	3129(5)	452(1)	1073(0)	3155(4)
438(7)	1063(1)	3213(0)	445(7)	1071(3)	3223(0)	488(1)	1074(0)	3268(0)
500(2)	1065(0)	3214(1)	501(2)	1074(0)	3223(0)	585(1)	1075(1)	3268(0)
575(0)	1068(1)	3215(1)	586(0)	1076(1)	3224(0)	610(0)	1077(0)	3269(0)
578(0)	1072(12)	3215(0)	588(0)	1092(14)	3224(0)	614(0)	1097(4)	3270(1)
586(6)	1140(35)	3229(47)	598(4)	1145(29)	3238(16)	617(1)	1157(23)	3281(2)
589(0)	1141(3)	3230(11)	601(0)	1146(2)	3238(2)	621(0)	1158(4)	3281(7)
597(6)	1176(18)	3234(29)	610(6)	1176(19)	3242(11)	659(3)	1214(19)	3286(3)
775(2)	1254(0)	3235(17)	787(1)	1273(0)	3242(4)	810(6)	1278(0)	3286(5)
778(0)	1254(0)	3245(1)	792(0)	1274(0)	3252(0)	817(0)	1279(0)	3296(1)
793(39)	1372(0)	3245(21)	803(34)	1390(0)	3252(7)	822(76)	1394(1)	3296(1)

Tables S122 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-7S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
35(0)	805(24)	1257(0)	28(0)	814(18)	1274(0)	37(0)	842(14)	1282(0)
76(0)	814(1)	1334(2)	67(0)	817(2)	1357(3)	71(0)	844(3)	1358(3)
104(0)	819(3)	1389(2)	97(0)	824(3)	1383(2)	112(0)	850(5)	1414(2)
111(0)	824(5)	1393(2)	110(0)	827(3)	1394(5)	119(0)	853(1)	1415(10)
142(1)	827(4)	1407(4)	140(1)	833(5)	1399(0)	142(1)	857(7)	1425(1)
154(4)	832(6)	1411(2)	153(4)	839(3)	1404(3)	158(4)	859(8)	1426(1)
194(1)	845(12)	1414(2)	195(1)	853(14)	1405(1)	191(2)	880(16)	1429(4)
207(1)	864(2)	1423(6)	201(1)	878(2)	1433(6)	203(1)	909(5)	1453(6)
228(1)	868(0)	1435(1)	229(1)	886(0)	1440(1)	235(1)	911(6)	1461(1)
277(1)	870(3)	1448(1)	278(1)	888(2)	1454(2)	283(3)	915(1)	1471(4)
335(0)	872(1)	1450(4)	340(0)	889(2)	1461(2)	347(2)	916(1)	1474(6)
357(7)	884(2)	1458(0)	364(5)	895(2)	1462(1)	356(4)	920(4)	1483(1)
371(1)	902(7)	1472(1)	378(1)	909(7)	1476(1)	379(1)	925(2)	1495(2)
382(3)	941(7)	1653(13)	390(3)	951(8)	1645(13)	394(4)	978(9)	1645(15)
404(2)	1004(12)	2654(3)	409(2)	1010(9)	2680(2)	419(1)	1017(17)	2694(5)
434(2)	1016(6)	2988(96)	436(2)	1021(6)	3001(63)	428(2)	1027(9)	3044(58)

448(6)	1018(2)	3089(13)	450(4)	1028(1)	3109(5)	432(8)	1036(2)	3153(10)
466(6)	1027(14)	3105(28)	466(8)	1032(7)	3121(9)	472(16)	1040(15)	3155(4)
495(7)	1030(2)	3108(60)	489(7)	1038(4)	3126(45)	506(5)	1043(7)	3163(37)
556(23)	1051(9)	3120(79)	563(22)	1063(8)	3136(43)	571(35)	1067(8)	3187(39)
573(6)	1061(2)	3211(2)	581(7)	1071(0)	3222(0)	592(13)	1074(1)	3264(0)
584(5)	1064(0)	3212(0)	594(4)	1073(0)	3224(0)	609(2)	1075(1)	3267(0)
590(1)	1065(1)	3214(2)	601(1)	1075(1)	3224(0)	614(0)	1077(0)	3270(0)
595(1)	1067(0)	3215(1)	605(1)	1076(1)	3226(0)	619(5)	1082(1)	3270(0)
607(2)	1072(3)	3227(27)	613(2)	1077(3)	3237(8)	628(2)	1084(5)	3277(5)
723(3)	1137(20)	3229(32)	728(3)	1142(16)	3239(12)	745(2)	1153(14)	3281(8)
767(1)	1142(16)	3233(28)	782(0)	1146(13)	3242(9)	810(7)	1158(11)	3284(6)
782(2)	1158(3)	3237(22)	794(2)	1169(3)	3247(7)	819(36)	1172(4)	3288(4)
794(12)	1234(18)	3244(7)	802(13)	1247(17)	3252(3)	823(25)	1269(13)	3295(2)
801(37)	1252(0)	3246(13)	812(31)	1271(0)	3254(3)	829(62)	1278(0)	3297(1)

Tables S123 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-8T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
36(0)	790(55)	1315(9)	34(0)	798(42)	1331(10)	25(0)	809(79)	1334(14)
47(0)	796(19)	1386(5)	47(0)	804(21)	1386(33)	37(0)	817(49)	1409(54)
70(0)	799(14)	1398(29)	67(0)	808(17)	1389(11)	58(0)	839(9)	1411(8)
72(0)	812(17)	1401(12)	71(0)	820(12)	1391(6)	79(1)	845(6)	1414(6)
94(0)	820(2)	1404(9)	93(0)	822(1)	1394(1)	94(0)	847(4)	1417(3)
113(1)	823(1)	1407(1)	111(1)	825(4)	1407(4)	106(0)	851(2)	1420(8)
160(0)	827(2)	1424(3)	161(0)	829(1)	1439(2)	157(2)	851(2)	1452(6)
176(0)	830(0)	1444(5)	177(0)	831(0)	1450(5)	162(0)	856(6)	1463(9)
187(1)	844(17)	1447(2)	187(1)	861(19)	1452(2)	183(1)	876(52)	1465(2)
211(1)	866(5)	1461(0)	211(1)	872(41)	1467(0)	206(1)	883(25)	1483(0)
257(1)	866(19)	1462(0)	258(1)	879(3)	1468(0)	264(2)	909(7)	1486(1)
281(5)	870(15)	1468(2)	281(4)	883(4)	1489(2)	296(7)	910(2)	1489(3)
322(1)	876(11)	1474(5)	325(1)	889(3)	1495(5)	319(3)	914(3)	1498(6)
334(0)	880(3)	1632(22)	334(0)	892(2)	1631(23)	323(2)	916(2)	1672(57)
353(5)	1008(13)	3014(96)	353(5)	1018(12)	3034(64)	334(7)	1019(6)	3056(54)
358(2)	1013(7)	3066(29)	362(2)	1018(2)	3083(13)	350(4)	1021(14)	3119(11)
374(2)	1016(11)	3069(7)	377(2)	1022(12)	3086(3)	361(3)	1023(20)	3123(2)
383(6)	1021(3)	3096(28)	388(6)	1031(9)	3111(13)	387(10)	1035(23)	3132(18)
412(2)	1026(29)	3125(35)	411(2)	1036(6)	3142(16)	405(1)	1037(5)	3159(20)
455(1)	1030(6)	3153(25)	456(1)	1037(17)	3167(14)	463(0)	1041(29)	3215(11)
493(7)	1046(13)	3209(3)	499(6)	1062(11)	3220(1)	491(3)	1063(10)	3263(0)
587(2)	1064(4)	3209(1)	597(3)	1073(5)	3221(1)	605(12)	1073(6)	3264(1)
589(2)	1066(3)	3215(1)	597(2)	1073(3)	3223(1)	606(1)	1073(2)	3264(0)
593(7)	1067(1)	3217(0)	602(7)	1075(1)	3226(0)	614(0)	1074(2)	3266(0)
596(0)	1068(1)	3227(25)	606(0)	1076(1)	3236(8)	618(36)	1074(1)	3276(6)
640(31)	1120(12)	3227(21)	644(33)	1122(11)	3237(7)	647(32)	1133(19)	3277(6)

685(2)	1140(18)	3236(20)	689(2)	1143(14)	3244(5)	694(4)	1151(2)	3281(3)
760(11)	1141(4)	3238(19)	766(14)	1145(4)	3246(5)	770(67)	1152(5)	3283(3)
766(2)	1254(0)	3245(10)	774(1)	1273(0)	3253(3)	796(6)	1278(0)	3292(1)
772(29)	1257(0)	3248(12)	778(31)	1276(0)	3255(3)	798(48)	1279(0)	3293(2)

Tables S124 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Co_2C_2Me_2$**structure **0N-Co-9S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
39(0)	799(13)	1260(12)	37(0)	806(4)	1272(0)	30(0)	829(21)	1289(16)
56(0)	803(10)	1376(2)	52(0)	814(3)	1381(3)	50(0)	838(17)	1401(3)
64(0)	811(18)	1391(3)	64(0)	818(14)	1382(1)	72(0)	847(2)	1411(2)
83(0)	814(5)	1391(1)	83(0)	820(16)	1396(4)	76(1)	850(7)	1418(2)
94(1)	819(2)	1408(5)	98(1)	827(1)	1399(2)	117(1)	854(2)	1423(2)
114(0)	824(2)	1411(0)	117(0)	831(5)	1400(1)	128(0)	856(7)	1424(1)
162(3)	829(4)	1432(1)	159(2)	831(4)	1438(1)	163(4)	859(2)	1458(2)
181(0)	863(2)	1442(4)	182(0)	879(2)	1450(1)	181(1)	905(7)	1466(2)
204(2)	866(2)	1443(2)	205(2)	883(1)	1452(3)	203(1)	913(3)	1473(8)
218(5)	868(0)	1454(0)	222(4)	886(1)	1460(0)	226(6)	917(0)	1478(2)
243(1)	874(3)	1458(6)	246(0)	890(3)	1474(1)	254(1)	919(0)	1485(6)
318(1)	882(3)	1468(2)	322(1)	896(2)	1479(8)	334(1)	920(2)	1492(1)
357(3)	906(1)	1470(1)	366(3)	915(2)	1491(2)	363(2)	928(3)	1494(0)
365(3)	937(2)	1492(9)	371(3)	951(1)	1497(7)	373(2)	975(0)	1522(14)
375(2)	1000(10)	2987(93)	382(1)	1008(9)	3011(59)	387(1)	1016(17)	3034(48)
387(2)	1003(13)	3061(75)	391(2)	1015(10)	3079(46)	403(1)	1020(14)	3113(21)
406(3)	1014(7)	3074(28)	412(4)	1021(6)	3091(17)	428(3)	1024(10)	3124(19)
448(3)	1017(6)	3096(29)	451(3)	1025(4)	3115(15)	433(13)	1032(11)	3134(34)
465(13)	1024(10)	3109(49)	466(13)	1035(10)	3129(26)	478(9)	1042(2)	3159(33)
521(10)	1027(9)	3198(23)	525(10)	1040(4)	3216(11)	542(14)	1044(20)	3251(9)
554(3)	1061(1)	3208(1)	556(3)	1069(0)	3216(1)	577(7)	1071(1)	3257(1)
568(3)	1063(1)	3208(1)	578(3)	1071(1)	3220(0)	593(15)	1073(1)	3260(1)
579(1)	1065(1)	3212(2)	588(1)	1073(1)	3221(1)	601(8)	1076(0)	3269(1)
586(6)	1068(0)	3218(2)	595(9)	1077(0)	3227(0)	608(9)	1078(2)	3269(0)
593(4)	1136(10)	3223(23)	599(1)	1138(11)	3232(6)	617(0)	1151(8)	3276(2)
598(2)	1136(28)	3228(15)	609(1)	1141(19)	3237(6)	626(1)	1153(17)	3279(4)
709(13)	1143(8)	3232(20)	719(13)	1143(10)	3240(5)	747(5)	1155(9)	3284(5)
768(1)	1203(7)	3235(19)	780(0)	1214(7)	3244(7)	798(4)	1215(9)	3286(2)
779(7)	1251(0)	3244(11)	793(7)	1269(10)	3251(3)	815(58)	1276(0)	3295(1)
791(29)	1253(0)	3246(16)	802(25)	1271(0)	3254(4)	821(36)	1280(0)	3295(2)

Tables S125 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-1S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
22(0)	816(41)	1360(0)	20(0)	826(4)	1379(0)	-15(0)	846(1)	1386(0)

46(0)	818(8)	1360(12)	53(0)	828(28)	1379(5)	36(0)	847(1)	1387(28)
66(1)	819(0)	1417(0)	67(1)	828(0)	1406(0)	55(1)	854(4)	1431(1)
105(0)	821(0)	1418(0)	100(0)	831(0)	1406(0)	99(0)	855(0)	1432(0)
105(1)	831(1)	1419(3)	100(0)	836(3)	1407(2)	104(1)	858(7)	1434(0)
117(3)	833(0)	1420(0)	119(2)	837(0)	1408(0)	120(3)	858(0)	1435(0)
119(1)	836(27)	1438(0)	120(2)	841(29)	1457(0)	129(2)	859(24)	1463(0)
157(0)	838(0)	1439(0)	165(0)	843(0)	1457(1)	170(0)	860(0)	1464(2)
166(0)	878(2)	1448(9)	169(0)	897(1)	1459(3)	188(0)	924(1)	1474(9)
197(0)	878(0)	1451(1)	206(0)	897(0)	1461(0)	218(0)	924(0)	1476(0)
215(0)	881(16)	1453(0)	218(0)	899(13)	1462(0)	223(0)	929(11)	1478(3)
287(0)	882(2)	1455(0)	293(0)	901(2)	1462(0)	290(0)	930(1)	1478(0)
335(0)	959(0)	1455(0)	346(0)	974(1)	1474(0)	347(0)	975(1)	1481(2)
380(5)	977(7)	1457(2)	387(6)	992(6)	1475(8)	393(14)	1001(14)	1484(6)
387(12)	1014(0)	2992(132)	396(11)	1029(0)	3012(79)	397(0)	1033(0)	3042(56)
392(8)	1024(16)	2992(1)	402(7)	1031(12)	3012(1)	398(9)	1035(19)	3043(0)
430(0)	1025(0)	3080(0)	439(0)	1032(0)	3094(0)	447(0)	1035(0)	3123(21)
447(0)	1025(0)	3080(58)	457(0)	1032(13)	3094(32)	452(0)	1036(22)	3123(5)
475(0)	1025(18)	3082(3)	479(0)	1035(0)	3095(5)	489(0)	1037(0)	3130(0)
529(11)	1045(100)	3082(39)	539(11)	1059(91)	3095(16)	563(14)	1061(106)	3130(38)
565(0)	1070(0)	3217(0)	569(0)	1079(0)	3227(0)	583(0)	1080(0)	3269(0)
590(7)	1070(0)	3217(0)	596(5)	1079(0)	3228(0)	605(7)	1080(0)	3269(0)
594(2)	1071(0)	3219(0)	603(0)	1080(0)	3229(0)	616(5)	1081(1)	3270(0)
594(0)	1072(13)	3219(1)	606(2)	1082(17)	3229(0)	619(0)	1082(18)	3271(0)
596(0)	1145(28)	3235(0)	609(0)	1150(22)	3244(0)	619(0)	1160(13)	3283(0)
597(0)	1145(0)	3235(51)	609(0)	1150(0)	3244(14)	619(0)	1160(0)	3283(8)
601(0)	1244(79)	3235(0)	610(0)	1247(86)	3245(0)	640(0)	1263(69)	3284(0)
670(88)	1251(0)	3236(49)	673(97)	1251(0)	3245(17)	657(126)	1271(0)	3284(11)
811(0)	1256(0)	3247(17)	823(0)	1275(0)	3255(6)	840(121)	1281(0)	3295(3)
813(1)	1256(0)	3247(1)	824(2)	1275(0)	3255(0)	843(0)	1281(0)	3295(0)

Tables S126 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-2T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
28(0)	797(48)	1374(0)	28(0)	808(37)	1394(0)	35(0)	826(3)	1398(4)
36(0)	800(11)	1404(1)	39(0)	809(0)	1395(0)	39(0)	828(19)	1416(2)
69(0)	800(5)	1408(0)	54(0)	813(3)	1396(0)	45(0)	831(4)	1418(8)
69(2)	816(28)	1413(0)	77(2)	820(0)	1402(0)	54(0)	834(26)	1420(1)
72(2)	818(13)	1414(2)	80(3)	828(1)	1402(2)	63(1)	843(1)	1427(2)
79(0)	826(2)	1454(6)	81(0)	828(44)	1464(0)	77(0)	846(4)	1474(4)
82(2)	829(5)	1456(7)	83(0)	831(5)	1464(1)	86(0)	848(5)	1475(5)
91(0)	831(0)	1459(0)	93(0)	834(0)	1466(0)	94(2)	850(3)	1476(2)
150(0)	863(0)	1459(0)	150(0)	877(0)	1467(0)	156(1)	901(0)	1476(8)
166(0)	871(1)	1461(0)	174(0)	889(2)	1474(5)	170(0)	911(0)	1483(1)
181(1)	874(2)	1461(0)	185(1)	893(0)	1476(7)	186(0)	914(1)	1486(1)

221(0)	874(0)	1468(0)	226(0)	895(1)	1489(0)	191(2)	916(0)	1492(2)
281(1)	984(1)	1471(8)	290(1)	998(1)	1491(7)	290(2)	1001(2)	1496(13)
316(2)	991(0)	1595(0)	323(1)	1007(0)	1604(0)	304(1)	1018(3)	1676(7)
332(3)	1022(0)	3006(118)	342(2)	1028(0)	3026(71)	335(1)	1026(14)	3050(60)
364(7)	1022(21)	3008(51)	371(6)	1029(16)	3027(32)	367(1)	1030(15)	3051(23)
374(5)	1025(3)	3086(52)	382(5)	1032(12)	3101(24)	369(1)	1035(9)	3125(29)
375(0)	1026(18)	3089(0)	391(0)	1032(2)	3103(0)	381(4)	1037(15)	3127(1)
402(0)	1041(28)	3117(48)	409(1)	1056(27)	3131(26)	410(5)	1060(30)	3154(21)
410(4)	1063(1)	3118(11)	416(3)	1072(0)	3131(4)	422(12)	1073(2)	3154(10)
431(1)	1069(1)	3215(0)	432(1)	1078(0)	3223(0)	435(6)	1076(1)	3263(0)
487(0)	1070(7)	3216(1)	488(1)	1079(1)	3223(0)	490(0)	1077(0)	3265(0)
584(0)	1070(0)	3216(0)	594(0)	1079(1)	3225(0)	599(5)	1078(1)	3265(0)
586(1)	1072(1)	3217(0)	597(1)	1090(6)	3227(0)	602(2)	1088(3)	3267(0)
588(4)	1144(24)	3232(32)	602(3)	1148(20)	3240(6)	606(1)	1153(7)	3278(4)
593(0)	1145(3)	3233(16)	604(0)	1149(3)	3241(9)	607(3)	1155(6)	3279(4)
599(3)	1185(23)	3236(0)	612(3)	1185(25)	3244(0)	612(4)	1194(19)	3280(5)
784(1)	1257(0)	3236(48)	794(3)	1277(0)	3244(15)	804(9)	1281(0)	3284(5)
792(1)	1258(0)	3246(3)	803(1)	1278(0)	3253(5)	811(92)	1281(0)	3291(2)
796(0)	1373(0)	3247(18)	805(6)	1392(0)	3253(3)	820(37)	1397(3)	3294(1)

Tables S127 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-3T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
26(0)	798(27)	1297(19)	27(0)	806(21)	1308(18)	40(0)	825(62)	1321(8)
37(0)	802(7)	1336(2)	42(0)	812(6)	1349(3)	52(0)	832(9)	1383(12)
72(0)	813(6)	1397(1)	71(0)	819(2)	1386(1)	64(0)	837(10)	1414(2)
94(1)	816(10)	1403(0)	92(0)	821(0)	1391(0)	82(1)	845(1)	1417(2)
111(0)	819(3)	1409(2)	108(0)	823(1)	1399(2)	98(0)	847(2)	1418(1)
128(1)	821(4)	1414(5)	126(1)	826(7)	1403(4)	118(1)	847(2)	1424(3)
185(1)	823(4)	1428(3)	182(1)	826(12)	1445(3)	164(0)	850(4)	1444(7)
197(1)	861(1)	1444(0)	197(0)	872(7)	1450(1)	186(1)	880(20)	1462(1)
229(1)	861(6)	1449(0)	231(1)	876(1)	1453(0)	221(2)	896(1)	1467(0)
278(2)	864(1)	1454(1)	277(4)	879(1)	1462(0)	253(1)	901(1)	1480(0)
292(1)	869(0)	1457(2)	291(1)	885(0)	1463(1)	293(2)	907(1)	1485(12)
350(6)	872(0)	1459(10)	353(6)	886(0)	1472(8)	322(4)	911(1)	1492(0)
360(12)	887(1)	1522(9)	364(12)	894(1)	1516(8)	344(11)	914(1)	1550(19)
373(1)	912(4)	1609(14)	376(1)	919(2)	1619(15)	367(6)	951(3)	1560(37)
385(2)	981(7)	2501(8)	390(1)	994(7)	2509(5)	378(0)	1007(2)	2591(4)
412(5)	1010(12)	3025(76)	413(4)	1017(10)	3041(46)	387(5)	1019(26)	3080(40)
417(3)	1015(12)	3083(46)	422(4)	1021(8)	3098(32)	416(3)	1023(7)	3134(11)
447(5)	1021(11)	3087(44)	449(5)	1029(9)	3109(17)	440(3)	1032(13)	3144(29)
459(8)	1024(12)	3099(22)	457(7)	1031(10)	3111(10)	446(19)	1034(10)	3152(10)
502(27)	1028(1)	3184(30)	507(27)	1036(1)	3203(15)	503(1)	1036(12)	3236(19)
564(21)	1062(0)	3198(2)	571(25)	1070(0)	3209(1)	548(11)	1071(1)	3254(0)

577(3)	1063(0)	3207(1)	590(2)	1072(1)	3218(0)	592(1)	1073(1)	3259(0)
589(1)	1066(1)	3210(2)	598(1)	1074(1)	3220(1)	603(4)	1075(1)	3262(0)
593(2)	1068(1)	3212(0)	604(2)	1077(1)	3221(1)	610(0)	1078(1)	3264(1)
600(1)	1107(4)	3220(20)	611(1)	1115(3)	3230(8)	617(3)	1121(5)	3272(3)
624(2)	1134(20)	3224(26)	625(3)	1139(15)	3234(9)	621(1)	1149(5)	3276(6)
694(6)	1140(13)	3228(25)	702(6)	1144(10)	3237(8)	698(22)	1152(10)	3277(5)
778(8)	1190(10)	3230(24)	785(1)	1199(10)	3239(7)	801(27)	1209(16)	3278(3)
778(1)	1252(0)	3239(15)	787(8)	1272(0)	3247(6)	811(78)	1278(0)	3288(3)
791(21)	1254(0)	3239(15)	800(18)	1273(0)	3248(4)	819(11)	1279(0)	3291(1)

Tables S128 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $\mathbf{Cp_2Fe_2C_2Me_2}$structure **0N-Fe-4T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
31(0)	801(10)	1259(0)	30(0)	809(9)	1278(0)	41(0)	827(57)	1281(0)
77(0)	811(23)	1354(3)	77(0)	820(8)	1374(4)	48(0)	837(7)	1372(10)
99(0)	817(7)	1384(1)	99(0)	822(4)	1385(1)	85(1)	846(2)	1415(2)
108(0)	821(1)	1397(1)	108(0)	824(5)	1392(0)	92(0)	847(3)	1417(2)
114(1)	824(6)	1405(0)	114(1)	827(8)	1399(1)	112(1)	848(1)	1418(1)
145(2)	827(3)	1413(1)	145(2)	829(10)	1403(1)	131(1)	852(1)	1423(2)
163(1)	853(16)	1421(4)	170(1)	862(15)	1409(4)	142(1)	868(8)	1425(2)
174(1)	860(2)	1429(7)	172(1)	875(1)	1441(7)	171(0)	894(2)	1454(9)
202(0)	865(1)	1438(0)	203(0)	882(1)	1445(0)	182(4)	898(2)	1466(0)
235(0)	870(0)	1454(0)	237(0)	886(0)	1460(1)	233(1)	909(2)	1474(1)
311(1)	880(1)	1461(0)	315(1)	889(1)	1466(0)	308(2)	911(9)	1484(0)
341(2)	882(1)	1464(7)	346(2)	899(0)	1469(0)	322(3)	912(1)	1485(1)
357(1)	904(7)	1465(1)	362(2)	909(7)	1471(5)	339(3)	917(1)	1488(19)
363(2)	935(2)	1593(12)	366(1)	950(1)	1595(11)	359(1)	989(1)	1613(17)
375(1)	1008(11)	2771(11)	381(1)	1015(10)	2785(8)	384(1)	1020(5)	2762(13)
397(9)	1012(12)	3001(92)	405(9)	1024(6)	3013(58)	393(5)	1024(20)	3062(41)
413(3)	1021(6)	3067(28)	416(2)	1027(5)	3090(14)	408(2)	1027(15)	3131(10)
457(11)	1026(18)	3091(65)	459(13)	1032(13)	3108(45)	450(9)	1036(6)	3143(9)
478(5)	1030(1)	3094(29)	473(5)	1036(1)	3110(15)	466(10)	1037(21)	3163(34)
539(25)	1046(12)	3116(75)	549(25)	1056(13)	3134(40)	531(17)	1055(14)	3185(35)
576(2)	1062(3)	3206(2)	584(2)	1071(1)	3218(1)	589(6)	1073(0)	3261(1)
589(2)	1063(0)	3209(1)	599(2)	1072(1)	3218(0)	606(3)	1074(0)	3261(0)
594(0)	1066(0)	3209(3)	603(1)	1074(0)	3222(0)	613(0)	1076(1)	3262(0)
597(0)	1068(1)	3212(0)	607(0)	1077(1)	3222(0)	615(0)	1079(0)	3268(0)
609(0)	1075(2)	3224(22)	615(0)	1083(1)	3233(9)	619(5)	1083(5)	3276(7)
724(3)	1137(20)	3225(36)	729(3)	1141(16)	3235(9)	740(2)	1152(10)	3277(4)
764(3)	1145(13)	3232(23)	779(1)	1148(10)	3241(9)	795(19)	1154(5)	3277(5)
786(7)	1167(3)	3234(28)	797(10)	1178(3)	3244(8)	806(73)	1173(4)	3284(3)
789(20)	1236(14)	3240(5)	798(13)	1246(13)	3249(5)	820(16)	1274(10)	3289(3)
798(21)	1253(0)	3242(13)	807(20)	1272(0)	3251(3)	822(40)	1280(0)	3295(1)

Tables S129 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $Cp_2Fe_2C_2Me_2$structure **0N-Fe-5T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
24(0)	792(2)	1359(0)	29(0)	801(2)	1379(0)	14(0)	819(0)	1382(30)
44(0)	796(1)	1359(7)	47(0)	809(0)	1379(2)	34(0)	820(247)	1382(1)
52(0)	809(18)	1406(1)	52(0)	821(14)	1393(1)	48(0)	844(0)	1421(3)
90(0)	819(4)	1409(0)	94(1)	826(2)	1396(0)	88(0)	846(8)	1423(0)
94(1)	833(0)	1417(0)	99(1)	835(0)	1405(0)	95(0)	852(0)	1423(0)
100(0)	834(0)	1417(2)	104(0)	837(11)	1405(2)	111(4)	853(0)	1424(0)
103(0)	835(11)	1438(0)	109(0)	839(2)	1457(0)	114(1)	853(0)	1457(0)
135(3)	839(4)	1440(1)	139(3)	841(4)	1458(0)	118(0)	856(0)	1459(0)
153(0)	861(0)	1449(11)	154(0)	877(0)	1458(1)	161(0)	910(0)	1471(0)
189(0)	874(1)	1449(1)	194(0)	891(0)	1462(1)	202(2)	910(0)	1471(4)
202(1)	878(1)	1451(0)	203(1)	895(1)	1464(3)	211(0)	917(6)	1475(15)
260(1)	884(13)	1457(1)	265(1)	899(9)	1469(0)	270(0)	919(0)	1476(2)
281(1)	958(1)	1460(1)	285(1)	974(1)	1471(5)	312(3)	961(1)	1483(0)
318(1)	970(5)	1466(0)	326(1)	987(4)	1472(3)	330(0)	973(8)	1485(0)
329(8)	1009(0)	2990(130)	331(7)	1024(0)	3009(79)	346(21)	1025(0)	3042(39)
337(2)	1020(15)	2991(1)	345(2)	1026(13)	3010(1)	349(7)	1026(22)	3043(0)
369(5)	1021(3)	3077(2)	380(5)	1029(0)	3091(3)	350(11)	1031(0)	3123(8)
394(4)	1028(12)	3078(54)	402(4)	1034(10)	3091(21)	397(0)	1037(0)	3123(16)
457(2)	1029(15)	3080(0)	460(2)	1036(11)	3093(0)	463(0)	1038(32)	3135(0)
493(6)	1045(113)	3080(47)	503(5)	1058(103)	3094(29)	482(9)	1074(19)	3135(38)
532(0)	1070(0)	3218(0)	536(0)	1078(0)	3229(0)	567(0)	1077(0)	3267(0)
552(3)	1071(0)	3219(0)	557(2)	1079(0)	3229(0)	583(4)	1078(0)	3267(0)
595(0)	1071(13)	3219(0)	604(1)	1080(0)	3230(0)	599(0)	1079(1)	3268(0)
595(0)	1071(0)	3220(1)	606(0)	1080(17)	3230(0)	612(1)	1102(312)	3268(0)
597(0)	1145(11)	3234(24)	609(0)	1149(2)	3245(8)	615(0)	1154(0)	3280(0)
601(0)	1146(6)	3236(24)	611(0)	1150(11)	3246(7)	617(0)	1154(5)	3280(11)
605(0)	1236(70)	3238(16)	612(0)	1236(74)	3246(3)	621(0)	1248(64)	3283(0)
681(80)	1245(3)	3239(27)	684(87)	1244(3)	3247(8)	752(234)	1259(0)	3283(5)
761(1)	1257(0)	3249(12)	772(1)	1276(0)	3257(4)	808(8)	1280(0)	3294(0)
787(112)	1258(0)	3250(6)	796(104)	1277(0)	3258(2)	809(2)	1280(0)	3294(4)

Tables S130 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $Cp_2Fe_2C_2Me_2$structure **0N-Fe-6T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
22(0)	797(4)	1253(0)	24(0)	806(6)	1273(0)	26(0)	820(30)	1278(0)
61(0)	803(26)	1261(0)	67(0)	813(18)	1279(0)	48(0)	826(40)	1281(0)
90(0)	809(9)	1345(5)	88(0)	817(3)	1355(5)	78(0)	841(11)	1377(8)
102(0)	817(16)	1383(4)	97(0)	826(4)	1390(3)	79(0)	846(0)	1415(0)
112(1)	820(2)	1407(7)	106(1)	827(8)	1394(6)	109(0)	848(3)	1416(12)
140(3)	823(3)	1409(0)	141(3)	830(5)	1398(0)	117(1)	849(6)	1420(6)

164(3)	828(0)	1414(1)	165(3)	832(2)	1401(1)	143(0)	852(1)	1422(0)
191(0)	829(4)	1415(0)	193(0)	836(3)	1405(0)	163(1)	859(16)	1425(0)
238(4)	842(9)	1442(0)	239(4)	853(11)	1450(1)	185(0)	881(16)	1465(1)
295(2)	863(1)	1455(1)	300(2)	876(1)	1461(1)	269(9)	892(4)	1475(1)
303(2)	866(3)	1459(0)	306(3)	883(4)	1464(0)	279(17)	894(1)	1482(0)
316(6)	869(3)	1471(0)	319(5)	888(1)	1476(0)	290(9)	900(1)	1486(0)
345(3)	877(1)	1473(1)	345(4)	894(0)	1486(1)	321(1)	911(1)	1522(7)
356(0)	897(4)	1599(8)	357(0)	903(5)	1600(7)	356(4)	918(1)	1560(17)
404(16)	918(4)	2547(3)	414(13)	938(3)	2550(3)	372(6)	935(16)	2916(7)
430(14)	972(11)	3082(55)	435(15)	979(11)	3104(30)	405(3)	955(2)	3136(16)
448(13)	1014(11)	3119(9)	449(13)	1022(10)	3137(4)	443(7)	1022(15)	3185(11)
500(4)	1018(9)	3128(44)	499(4)	1024(6)	3146(23)	454(7)	1028(22)	3197(9)
517(3)	1024(9)	3147(40)	520(3)	1032(8)	3163(18)	468(7)	1030(2)	3218(8)
567(2)	1027(3)	3180(27)	572(1)	1039(3)	3199(14)	566(8)	1035(24)	3237(15)
583(1)	1035(9)	3205(2)	592(1)	1041(6)	3218(0)	604(5)	1036(8)	3251(0)
588(0)	1057(1)	3209(1)	600(0)	1069(0)	3219(0)	607(4)	1069(2)	3256(0)
592(1)	1064(1)	3214(1)	603(1)	1074(1)	3223(0)	615(1)	1073(0)	3260(1)
595(1)	1069(0)	3217(1)	607(1)	1077(0)	3227(1)	617(0)	1076(1)	3267(1)
637(5)	1070(1)	3221(29)	643(5)	1078(1)	3233(8)	624(1)	1076(1)	3268(6)
753(15)	1072(2)	3229(27)	762(15)	1080(1)	3239(8)	715(6)	1077(1)	3273(6)
759(3)	1140(18)	3233(22)	769(3)	1145(15)	3243(6)	771(18)	1152(7)	3274(5)
774(3)	1148(6)	3239(27)	782(0)	1152(4)	3247(9)	787(20)	1154(1)	3284(4)
784(50)	1166(10)	3243(7)	791(49)	1176(10)	3251(4)	793(112)	1175(16)	3287(3)
793(2)	1193(11)	3246(11)	801(6)	1201(10)	3254(4)	803(12)	1228(22)	3296(1)

Tables S131 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-7S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
28(0)	806(6)	1252(0)	17(0)	815(4)	1272(0)	25(0)	842(11)	1278(0)
78(0)	816(11)	1256(0)	76(0)	824(5)	1276(0)	66(0)	847(4)	1282(0)
125(0)	819(6)	1336(7)	124(0)	824(5)	1345(3)	123(0)	849(16)	1355(10)
136(1)	822(6)	1348(5)	136(1)	829(4)	1353(8)	135(1)	851(3)	1391(10)
156(1)	826(3)	1398(1)	157(2)	830(1)	1388(1)	160(8)	855(4)	1426(3)
161(8)	827(24)	1409(1)	162(8)	835(5)	1398(1)	164(2)	857(21)	1427(1)
211(3)	828(6)	1421(2)	209(3)	837(26)	1410(2)	210(8)	861(2)	1433(1)
237(1)	837(11)	1426(1)	240(1)	845(9)	1414(1)	241(1)	870(11)	1437(1)
263(1)	838(4)	1445(1)	268(1)	850(6)	1452(1)	267(2)	898(1)	1471(3)
321(1)	865(1)	1451(0)	328(2)	879(1)	1457(1)	336(1)	914(0)	1475(2)
354(1)	877(1)	1455(0)	356(1)	894(1)	1460(0)	358(1)	921(1)	1477(0)
379(16)	879(2)	1459(1)	386(15)	899(2)	1465(0)	386(4)	924(1)	1484(1)
389(9)	892(5)	1461(0)	398(10)	910(4)	1476(1)	412(7)	926(5)	1491(0)
405(9)	918(4)	1577(4)	414(8)	923(4)	1585(4)	422(7)	931(3)	1644(14)
438(4)	962(5)	2540(3)	444(4)	969(7)	2536(5)	440(18)	971(11)	2577(3)
454(3)	975(7)	3063(77)	459(3)	993(5)	3085(46)	459(1)	1018(3)	3106(53)

492(6)	1015(16)	3111(17)	497(6)	1022(12)	3130(7)	478(10)	1027(14)	3179(5)
516(5)	1017(5)	3148(21)	517(5)	1024(4)	3165(10)	505(5)	1033(15)	3195(24)
537(4)	1025(7)	3156(40)	538(3)	1031(5)	3176(25)	564(7)	1033(9)	3216(6)
575(1)	1026(3)	3164(43)	583(1)	1033(3)	3180(17)	597(1)	1042(6)	3233(15)
588(0)	1051(5)	3197(3)	600(0)	1063(5)	3210(1)	615(1)	1058(7)	3263(0)
589(1)	1055(1)	3206(6)	600(1)	1067(1)	3217(2)	617(3)	1073(3)	3263(1)
591(3)	1064(1)	3214(3)	604(3)	1073(1)	3224(1)	622(1)	1077(1)	3264(0)
596(1)	1069(1)	3219(2)	610(1)	1077(2)	3228(1)	623(0)	1079(1)	3270(0)
669(9)	1070(1)	3220(28)	677(11)	1078(0)	3231(11)	678(13)	1079(0)	3277(6)
748(6)	1071(2)	3224(29)	755(6)	1080(1)	3234(11)	764(10)	1083(3)	3280(8)
776(0)	1134(5)	3231(22)	786(0)	1140(5)	3239(7)	806(5)	1136(7)	3281(4)
794(4)	1141(27)	3238(20)	806(5)	1146(23)	3246(6)	818(9)	1158(13)	3291(1)
799(4)	1144(13)	3244(19)	807(4)	1148(10)	3250(5)	826(27)	1161(9)	3292(3)
804(3)	1163(13)	3258(9)	813(2)	1176(12)	3269(5)	840(53)	1191(21)	3308(3)

Tables S132 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-8S**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
58(0)	802(15)	1296(17)	59(0)	811(8)	1308(15)	49(0)	835(36)	1320(11)
66(0)	806(11)	1332(4)	74(0)	813(6)	1346(4)	74(0)	842(17)	1369(9)
86(1)	810(7)	1398(3)	89(1)	818(2)	1388(3)	82(1)	848(4)	1413(8)
95(0)	815(2)	1400(0)	95(1)	823(2)	1390(0)	94(0)	851(1)	1415(0)
120(0)	819(13)	1409(0)	119(0)	826(3)	1400(0)	115(1)	854(15)	1425(0)
137(5)	821(5)	1415(0)	138(4)	828(15)	1405(0)	135(6)	855(4)	1431(0)
201(0)	827(13)	1432(3)	200(0)	837(18)	1442(0)	198(0)	858(12)	1453(5)
225(0)	857(2)	1436(0)	225(0)	869(5)	1446(1)	214(0)	886(12)	1462(0)
244(2)	860(2)	1438(0)	245(2)	877(1)	1449(2)	250(1)	906(0)	1464(0)
301(4)	861(0)	1450(0)	303(4)	878(0)	1455(0)	303(3)	911(0)	1474(1)
322(2)	864(1)	1451(1)	325(2)	881(1)	1457(0)	324(10)	914(1)	1477(0)
384(9)	867(3)	1457(10)	390(9)	887(2)	1472(8)	385(4)	915(1)	1487(10)
400(0)	890(0)	1525(2)	402(1)	896(1)	1519(2)	397(7)	918(1)	1546(26)
408(1)	912(5)	1623(17)	412(1)	921(3)	1632(16)	404(8)	957(6)	1606(24)
414(5)	980(3)	2503(6)	422(4)	992(3)	2511(3)	416(5)	1006(3)	2557(2)
426(5)	1007(13)	3023(81)	432(7)	1014(10)	3040(49)	444(1)	1021(22)	3078(46)
458(4)	1012(3)	3078(66)	461(4)	1020(3)	3092(40)	458(3)	1026(7)	3132(13)
482(5)	1019(9)	3089(25)	489(5)	1026(7)	3109(9)	486(9)	1030(9)	3147(30)
492(9)	1020(8)	3098(23)	491(9)	1028(5)	3110(11)	499(11)	1031(11)	3152(11)
509(21)	1030(1)	3190(48)	515(18)	1039(1)	3209(28)	530(8)	1043(4)	3234(37)
563(18)	1059(1)	3202(7)	571(20)	1070(0)	3214(3)	582(13)	1071(1)	3259(2)
577(1)	1062(1)	3203(1)	591(0)	1071(0)	3216(1)	610(1)	1073(0)	3261(1)
585(0)	1064(1)	3206(10)	598(0)	1073(1)	3218(3)	615(0)	1075(1)	3263(3)
591(0)	1067(1)	3210(2)	603(0)	1078(1)	3219(1)	618(0)	1080(3)	3264(2)
598(4)	1110(4)	3221(24)	609(3)	1118(3)	3232(8)	626(2)	1129(4)	3277(5)
623(1)	1132(32)	3223(22)	623(1)	1137(25)	3233(9)	631(1)	1150(19)	3277(3)

686(42)	1135(16)	3228(19)	695(44)	1140(14)	3238(9)	703(72)	1152(10)	3281(3)
771(11)	1193(10)	3229(17)	790(9)	1204(10)	3239(3)	818(16)	1211(16)	3281(1)
790(2)	1248(0)	3237(11)	803(3)	1268(0)	3245(4)	828(3)	1275(0)	3291(1)
795(2)	1251(0)	3242(18)	810(3)	1271(0)	3250(5)	830(39)	1278(0)	3292(2)

Tables S133 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-9T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
26(0)	799(20)	1379(0)	24(0)	807(20)	1385(6)	-20(0)	829(8)	1398(2)
29(0)	805(0)	1383(15)	30(0)	810(0)	1388(0)	30(0)	834(52)	1403(10)
40(0)	814(2)	1393(5)	38(0)	820(2)	1401(1)	43(0)	839(0)	1405(17)
53(0)	820(7)	1397(0)	54(0)	826(2)	1405(0)	52(1)	847(16)	1419(0)
57(0)	823(4)	1411(0)	55(0)	829(0)	1406(17)	73(0)	853(5)	1428(1)
58(0)	827(1)	1413(0)	62(0)	830(4)	1413(0)	87(0)	857(1)	1435(1)
93(0)	828(5)	1428(0)	95(0)	836(4)	1432(0)	105(1)	858(3)	1450(0)
104(2)	839(30)	1439(0)	101(1)	847(31)	1445(0)	129(0)	862(23)	1465(1)
131(1)	864(1)	1440(0)	130(1)	874(1)	1447(0)	132(1)	898(0)	1467(1)
164(0)	865(0)	1461(1)	163(1)	881(0)	1480(0)	168(0)	917(0)	1483(1)
166(1)	873(1)	1464(15)	165(1)	887(1)	1482(14)	169(1)	921(1)	1485(20)
232(6)	876(0)	1467(13)	236(6)	891(0)	1486(1)	229(7)	922(0)	1487(13)
251(16)	956(5)	1468(3)	253(16)	960(4)	1487(12)	250(18)	968(8)	1488(3)
264(6)	990(3)	1891(46)	268(6)	996(3)	1902(45)	266(5)	1000(3)	1919(62)
325(10)	1006(8)	3016(140)	328(9)	1014(6)	3031(95)	314(4)	1024(11)	3051(89)
349(0)	1013(4)	3016(83)	353(0)	1020(3)	3032(56)	327(1)	1026(8)	3051(46)
397(0)	1019(0)	3040(55)	413(2)	1039(0)	3051(38)	403(1)	1027(0)	3130(13)
411(2)	1021(0)	3104(41)	420(0)	1039(0)	3113(22)	415(0)	1043(0)	3133(38)
445(23)	1040(59)	3106(15)	448(24)	1053(54)	3114(6)	452(4)	1055(8)	3134(8)
470(18)	1040(8)	3113(42)	476(16)	1056(1)	3121(16)	475(18)	1055(77)	3140(27)
495(6)	1047(2)	3113(1)	494(5)	1058(8)	3121(0)	480(14)	1060(3)	3140(0)
534(40)	1055(3)	3159(5)	535(40)	1065(1)	3172(3)	521(36)	1069(2)	3241(0)
586(0)	1056(1)	3189(11)	599(0)	1066(1)	3203(5)	574(15)	1070(2)	3255(0)
594(10)	1066(0)	3192(8)	600(5)	1076(0)	3205(3)	618(2)	1078(0)	3259(1)
595(7)	1098(23)	3208(35)	603(9)	1102(19)	3220(13)	619(1)	1108(17)	3268(0)
598(0)	1132(21)	3213(0)	607(2)	1137(17)	3223(0)	620(0)	1135(9)	3269(7)
610(1)	1152(7)	3221(11)	621(1)	1148(8)	3231(4)	621(9)	1151(13)	3276(2)
768(7)	1236(0)	3223(39)	772(7)	1255(0)	3234(17)	796(4)	1263(1)	3281(9)
782(3)	1243(0)	3229(30)	779(4)	1263(0)	3239(11)	798(5)	1274(0)	3283(4)
784(0)	1310(1)	3239(20)	792(0)	1307(1)	3247(7)	817(0)	1332(2)	3291(3)

Tables S134 : Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in

parentheses in km/mol) for the **$Cp_2Fe_2C_2Me_2$**structure **0N-Fe-10T**;

M06L/DZP			M06L/def2tzvpp			WB97XD/DZP		
29(0)	789(18)	1313(11)	29(0)	798(15)	1330(11)	26(0)	817(5)	1341(12)
48(0)	792(10)	1387(4)	47(0)	802(7)	1387(4)	42(0)	823(15)	1411(3)
61(0)	801(16)	1399(5)	62(0)	809(11)	1389(1)	49(0)	828(57)	1415(9)
75(0)	808(25)	1401(1)	84(0)	816(8)	1397(0)	65(0)	838(15)	1416(8)
92(0)	813(1)	1407(0)	88(0)	819(6)	1397(1)	84(0)	845(2)	1420(9)
104(1)	818(3)	1410(1)	103(1)	821(5)	1408(4)	91(1)	847(2)	1424(1)
155(0)	820(3)	1426(3)	147(0)	824(11)	1439(2)	142(1)	847(3)	1451(8)
164(0)	830(11)	1441(0)	164(0)	832(11)	1448(0)	157(2)	850(1)	1464(2)
176(2)	844(11)	1449(3)	177(2)	857(10)	1455(3)	168(1)	854(14)	1472(2)
211(1)	861(1)	1451(0)	212(1)	874(2)	1457(0)	189(1)	884(53)	1475(0)
256(1)	862(2)	1462(1)	257(0)	879(3)	1467(0)	242(2)	898(5)	1487(5)
282(5)	869(1)	1465(2)	285(5)	882(1)	1487(3)	277(14)	911(3)	1496(0)
314(5)	871(2)	1475(5)	320(5)	887(9)	1493(5)	305(0)	913(1)	1498(5)
329(2)	887(54)	1621(19)	331(1)	890(48)	1621(20)	318(4)	915(2)	1675(77)
342(2)	1009(6)	3004(44)	345(2)	1017(4)	3021(30)	330(26)	1019(12)	3004(29)
350(4)	1012(4)	3014(87)	356(5)	1021(12)	3034(60)	332(6)	1023(10)	3057(51)
373(3)	1013(23)	3051(34)	380(3)	1023(2)	3070(17)	366(10)	1029(8)	3109(2)
393(4)	1017(9)	3095(29)	399(4)	1026(17)	3110(14)	393(4)	1032(18)	3131(18)
425(7)	1021(13)	3124(34)	432(7)	1028(10)	3141(16)	414(10)	1038(19)	3159(17)
448(3)	1025(6)	3133(30)	452(3)	1032(3)	3149(17)	456(2)	1045(24)	3210(13)
494(3)	1044(12)	3205(0)	502(4)	1059(11)	3216(0)	494(5)	1064(11)	3260(0)
580(0)	1062(1)	3206(1)	593(0)	1071(1)	3218(0)	578(91)	1072(1)	3261(0)
586(1)	1064(0)	3209(0)	595(1)	1073(0)	3219(0)	603(0)	1074(2)	3262(0)
588(0)	1065(2)	3214(4)	600(1)	1074(1)	3223(1)	604(0)	1076(1)	3266(0)
597(4)	1069(2)	3223(21)	606(4)	1080(2)	3233(7)	611(1)	1078(2)	3276(5)
646(20)	1123(12)	3225(21)	648(20)	1127(11)	3235(7)	620(5)	1143(25)	3277(7)
664(20)	1135(20)	3229(18)	674(18)	1140(16)	3238(6)	677(8)	1152(5)	3278(6)
729(36)	1140(8)	3231(22)	736(41)	1144(6)	3240(7)	692(52)	1154(6)	3279(2)
770(7)	1251(0)	3237(11)	777(10)	1271(0)	3245(3)	799(2)	1279(0)	3289(2)
784(22)	1256(0)	3245(14)	794(16)	1276(0)	3252(4)	806(106)	1280(0)	3291(1)