

## Electronic supplementary information (ESI)

### **Metalloradical complex Co-C•Ph<sub>3</sub> catalyzes the CO<sub>2</sub> reduction in gas phase: a theoretical study**

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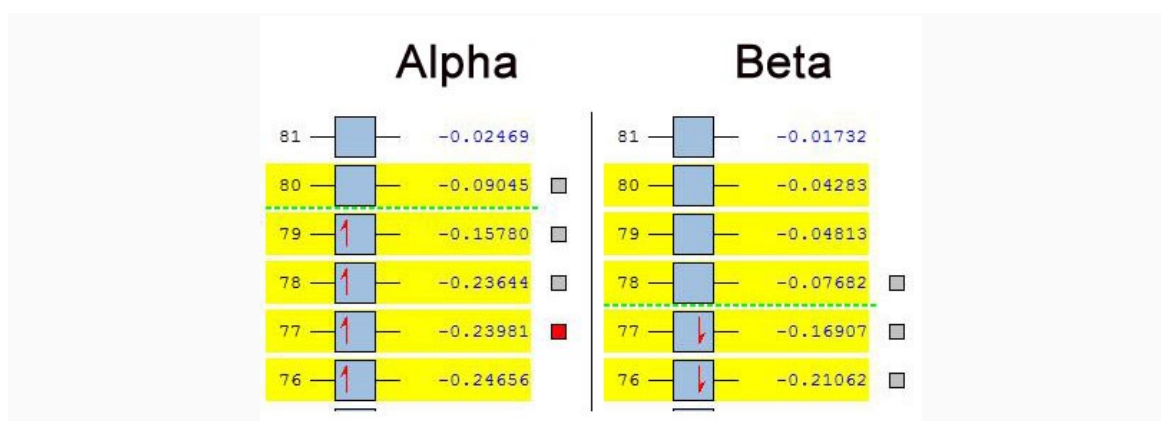


Fig. S1 Partial molecular orbital energy levels of the metalloradical Co-C•Ph<sub>3</sub> ( $\alpha$  orbital and it corresponding  $\beta$  orbital).

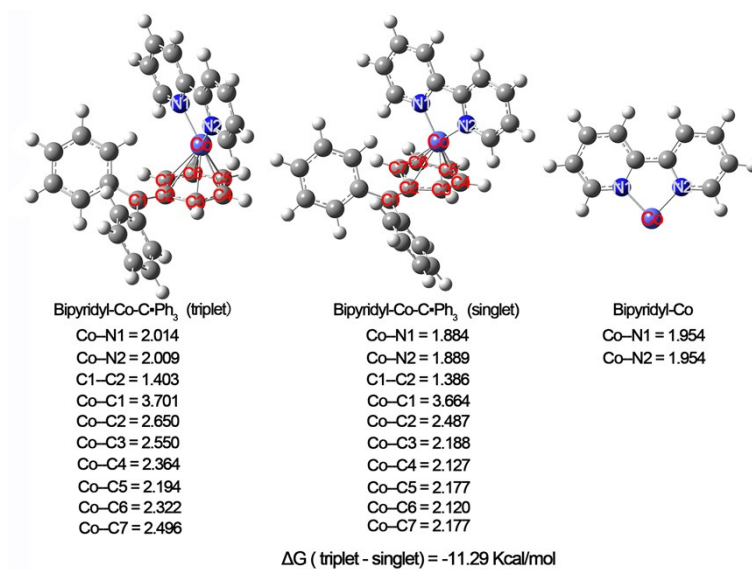


Fig. S2 The optimized geometry of the metalloradical Co-C\*Ph coordinated by a bipyridyl group, including singlet and triplet structures. The bond distances are given in Å.

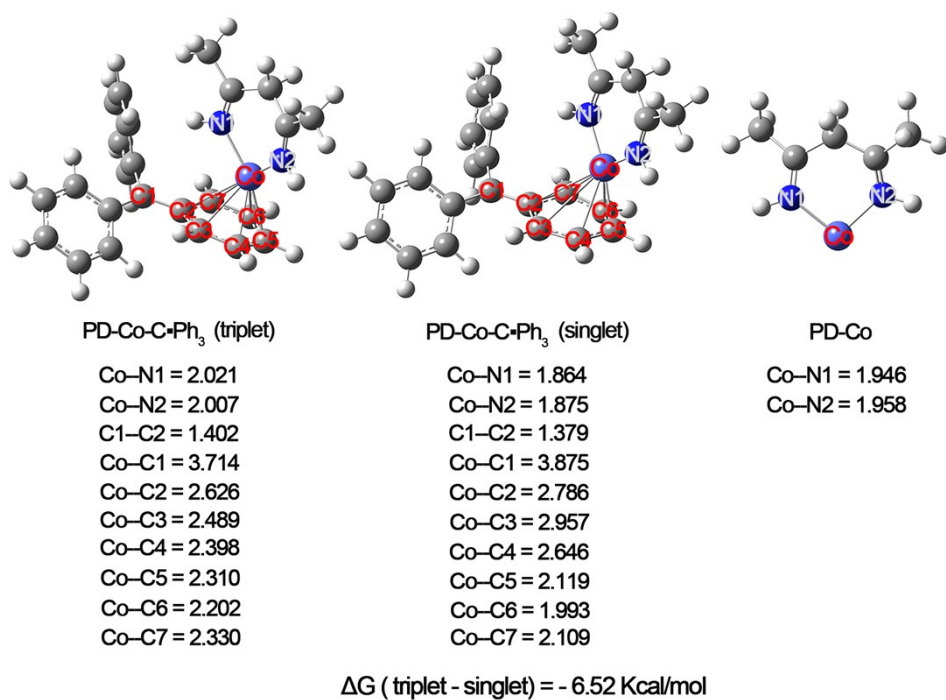


Fig. S3 The optimized geometry of the metalloradical Co-C•Ph coordinated by a pentane-2,4-diimine (PD), including singlet and triplet structures. The bond distances are given in Å.

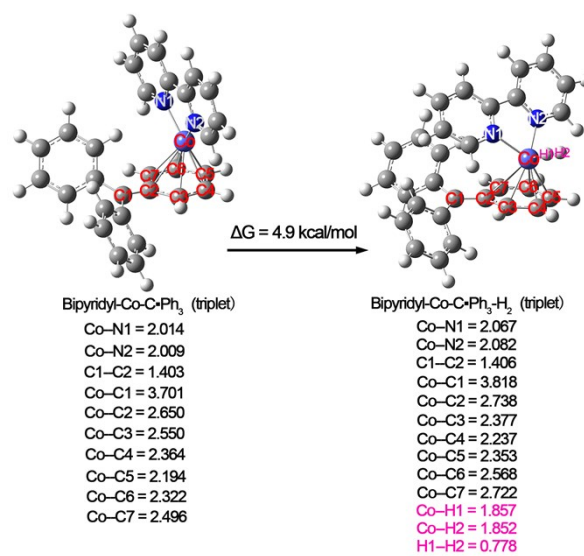


Fig. S4 The formation of Bipryridyl-Co-C•Ph<sub>3</sub>-H<sub>2</sub> with the triplet characters. The bond distances are given in Å.

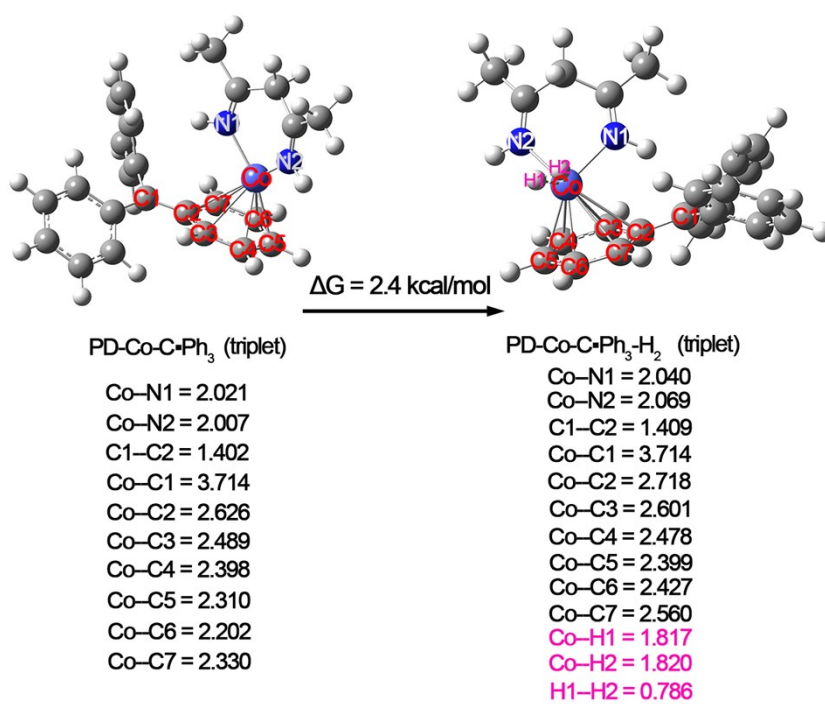
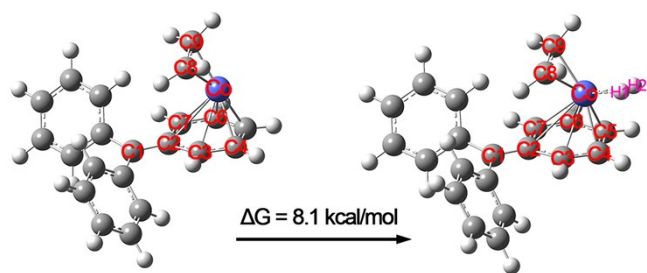


Fig. S5 The formation of PD-Co-C•Ph<sub>3</sub>-H<sub>2</sub> with the triplet characters. The bond distances are given in Å.



Ethylene-Co-C•Ph<sub>3</sub> (triplet)

C1-C2 = 1.386  
 Co-C1 = 3.868  
 Co-C2 = 2.738  
 Co-C3 = 2.426  
 Co-C4 = 2.206  
 Co-C5 = 2.123  
 Co-C6 = 2.306  
 Co-C7 = 2.557  
 Co-C8 = 2.041  
 Co-C9 = 2.042

Ethylene-Co-C•Ph<sub>3</sub>-H<sub>2</sub> (triplet)

C1-C2 = 1.385  
 Co-C1 = 3.933  
 Co-C2 = 2.828  
 Co-C3 = 2.415  
 Co-C4 = 2.187  
 Co-C5 = 2.141  
 Co-C6 = 2.465  
 Co-C7 = 2.767  
 Co-C8 = 2.096  
 Co-C9 = 2.068  
 Co-H1 = 2.043  
 Co-H2 = 2.023  
 H1-H2 = 0.759

Fig. S6 The formation of Ethylene-Co-C•Ph<sub>3</sub>-H<sub>2</sub> with the triplet characters. The bond distances are given in Å.

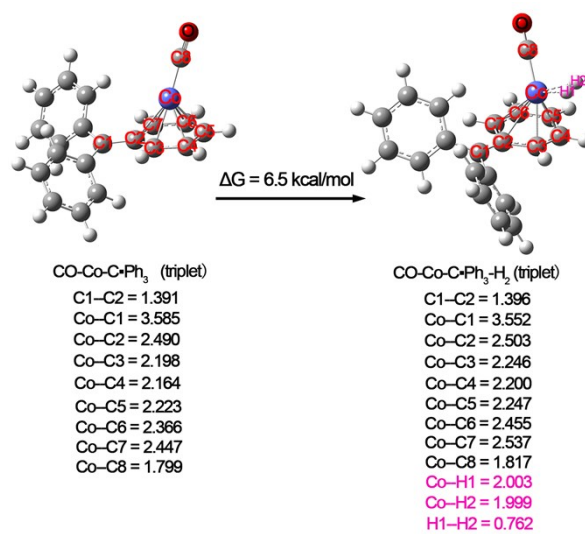


Fig. S7 The formation of CO-Co-C•Ph<sub>3</sub>-H<sub>2</sub> with the triplet characters. The bond distances are given in Å.



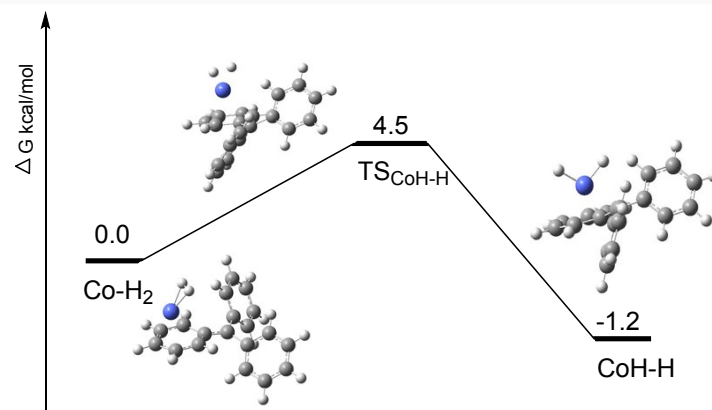


Fig. S8 The profile of splitting H<sub>2</sub> by the metalloradical Co-C•Ph<sub>3</sub>.

## Atomic coordinates of intermediates and key transition states

### Co-CO<sub>2</sub> triplet

6	0.903280	-0.006231	-0.429524
6	-0.402368	-0.455754	-0.857069
6	-1.225031	0.328792	-1.725918
6	-0.965345	-1.691079	-0.381891
6	-2.492731	-0.107057	-2.131971
1	-0.856523	1.287570	-2.065660
6	-2.226720	-2.136903	-0.815965
1	-0.409548	-2.279902	0.333807
6	-3.005367	-1.341513	-1.681293
1	-3.092948	0.525119	-2.775376
1	-2.625612	-3.065043	-0.425072
1	-4.000825	-1.658110	-1.966555
6	1.217914	1.420992	-0.355882
6	2.487566	1.891263	-0.749319
6	0.286423	2.365389	0.120014
6	2.803534	3.241974	-0.684326
1	3.218906	1.183903	-1.122589
6	0.608874	3.714487	0.192123
1	-0.683951	2.033084	0.468182
6	1.866467	4.162033	-0.213041
1	3.783108	3.579915	-1.006106
1	-0.120445	4.417110	0.581075
1	2.115722	5.216188	-0.156540
6	1.929538	-0.980825	-0.074924
6	2.046813	-2.210971	-0.755545
6	2.848162	-0.714247	0.961416
6	3.032392	-3.127474	-0.414745
1	1.372916	-2.430069	-1.576008
6	3.825754	-1.637816	1.306378
1	2.767860	0.216358	1.510172
6	3.925604	-2.848958	0.620829
1	3.111405	-4.059890	-0.964050
1	4.507953	-1.416682	2.120445
1	4.691571	-3.568206	0.889845
27	-2.355406	-0.203509	0.182812
6	-2.375552	0.101720	2.067614
8	-1.942256	-0.233545	3.129227
8	-3.147602	0.946852	1.525365

### Co-H<sub>2</sub> triplet

6	0.613403	-0.020477	-0.231300
---	----------	-----------	-----------

6	-0.753877	-0.138907	-0.435695
6	-1.609303	0.963601	-0.847189
6	-1.496677	-1.366039	-0.160975
6	-2.939519	0.782475	-1.209510
1	-1.177102	1.947677	-0.966212
6	-2.825288	-1.545919	-0.533416
1	-0.975396	-2.192270	0.303705
6	-3.601254	-0.475824	-1.070478
1	-3.497076	1.636297	-1.581190
1	-3.294837	-2.508462	-0.355879
1	-4.611289	-0.628163	-1.426580
6	1.285197	1.296170	-0.177118
6	2.485858	1.514534	-0.875033
6	0.787575	2.354156	0.602503
6	3.143768	2.738061	-0.815981
1	2.899366	0.707591	-1.470187
6	1.443835	3.580101	0.663428
1	-0.115925	2.202272	1.183441
6	2.625149	3.781559	-0.048767
1	4.064319	2.879953	-1.373528
1	1.039340	4.376246	1.281043
1	3.138942	4.735943	-0.000822
6	1.472913	-1.203644	-0.031020
6	1.339030	-2.364041	-0.815528
6	2.494075	-1.192261	0.937056
6	2.165432	-3.466535	-0.624325
1	0.591388	-2.385206	-1.600916
6	3.321612	-2.293203	1.128559
1	2.632435	-0.303975	1.543572
6	3.160751	-3.440906	0.352290
1	2.043645	-4.343437	-1.252825
1	4.095471	-2.256542	1.889076
1	3.808552	-4.298802	0.498864
27	-3.118862	0.089260	0.882037
1	-2.443956	0.108846	2.396761
1	-2.664676	0.894608	2.271653

**TS<sub>a1</sub>**

6	-	-0.041329	0.290710
	1.30804		
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6	0.02934	-0.285013	0.754532
	4		
6	0.72719	0.659269	1.569083

	6		
6	0.75419	-1.470219	0.391363
	8		
6	2.03258	0.434978	2.003502
	6		
1	0.22787	1.578087	1.846987
	9		
6	2.04718	-1.721397	0.863329
	7		
1	0.28618	-2.186374	-0.270923
	5		
6	2.71786	-0.748594	1.641433
	3		
1	2.53452	1.182902	2.605186
	7		
1	2.56881	-2.623221	0.568625
	4		
1	3.73790	-0.917300	1.956659
	5		
6	-	1.327795	0.159182
	1.81502		
	6		
6	-	1.639730	0.527949
	3.13836		
	8		
6	-	2.364849	-0.352577
	1.01079		
	9		
6	-	2.934187	0.408728
	3.62791		
	8		
1	-	0.857012	0.925916
	3.77391		
	2		
6	-	3.656606	-0.479386
	1.50685		
	4		
1	-	2.144862	-0.680086
	0.00134		
	8		
6	-	3.950284	-0.095188
	2.81523		
	9		
1	-	3.153287	0.713878

	4.64580		
	5		
1	-	4.434811	-0.891011
	0.87278		
	9		
1	-	4.959804	-0.192620
	3.19980		
	9		
6	-	-1.153818	-0.059305
	2.18976		
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6	-	-2.363108	0.666005
	2.17893		
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6	-	-1.040104	-1.130408
	3.09956		
	7		
6	-	-3.408693	0.330173
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	6		
1	-	-2.465502	1.518498
	1.51698		
	6		
6	-	-2.090878	-1.469418
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1	-	-0.122116	-1.705578
	3.12464		
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6	-	-3.281334	-0.742341
	3.91240		
	0		
1	-	-4.323101	0.913970
	3.01150		
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1	-	-1.983801	-2.308486
	4.62125		
	7		
1	-	-4.099617	-1.005810
	4.57368		
	3		
27	2.32940	0.088404	-0.314808
	2		
1	2.20371	1.420310	-1.362762

	0		
1	3.19394	1.335852	-1.566436
	3		
6	4.28334	-0.081993	-0.870075
	2		
8	5.01828	-0.966300	-0.521002
	3		
8	4.42675	0.928388	-1.650237
	6		

**HCo-COOH**

6	1.16882	0.027964	0.354873
	8		
6	-	-0.201737	0.790005
	0.11946		
	7		
6	-	-1.495026	1.251948
	0.59858		
	0		
6	-	0.772247	0.647561
	1.20258		
	5		
6	-	-1.635740	1.852719
	1.83330		
	7		
1	0.05493	-2.354818	1.191114
	0		
6	-	0.705654	1.442286
	2.38353		
	2		
1	-	1.677183	0.085880
	1.01850		
	3		
6	-	-0.527175	1.984193
	2.73972		
	9		
1	-	-2.612733	2.208047
	2.14081		
	9		
1	-	1.539085	1.453855
	3.07341		
	0		

1	-	-0.662172	2.481705
	3.69221		
	6		
6	2.09411	-1.082832	0.043753
	6		
6	3.41334	-1.070786	0.521974
	7		
6	1.68953	-2.144464	-0.780016
	0		
6	4.29005	-2.104937	0.213955
	3		
1	3.74337	-0.245536	1.143330
	3		
6	2.57213	-3.172534	-1.098414
	3		
1	0.68544	-2.142014	-1.190085
	0		
6	3.87264	-3.160593	-0.597066
	5		
1	5.30230	-2.087045	0.604132
	2		
1	2.24667	-3.978474	-1.747953
	5		
1	4.55964	-3.963248	-0.843288
	3		
6	1.66597	1.395703	0.131136
	0		
6	1.34466	2.446698	1.008134
	1		
6	2.50024	1.679443	-0.964440
	1		
6	1.81885	3.734380	0.785352
	7		
1	0.74190	2.239548	1.884998
	6		
6	2.96585	2.968752	-1.191117
	3		
1	2.76592	0.881606	-1.648112
	9		
6	2.62709	4.002668	-0.318300
	8		
1	1.56556	4.528189	1.480166
	8		
1	3.59323	3.169258	-2.053209

	6			
1	2.99598	5.007624	-0.493089	
	7			
27	-	-0.655666	-0.136404	
	2.40676			
	2			
1	-	-1.062112	-1.449125	
	1.78636			
	9			
1	-	-1.241801	-2.147682	
	3.88979			
	1			
6	-	0.395346	-1.215831	
	3.50886			
	5			
8	-	1.584106	-1.185300	
	3.67365			
	8			
8	-	-0.371306	-2.049919	
	4.30228			
	2			
<b>TS<sub>a2</sub></b>				
6	1.19222	-0.001332	-0.319582	
	7			
6	-	-0.297298	-0.786741	
	0.10469			
	1			
6	-	0.681647	-1.449963	
	0.94456			
	9			
6	-	-1.582545	-0.567624	
	0.74507			
	0			
6	-	0.371975	-1.937322	
	2.21183			
	9			
1	-	1.678523	-1.604769	
	0.55525			
	4			
6	-	-1.883377	-1.050147	
	2.02057			
	2			
1	-	-2.330522	0.008201	



	0.21734		
	0		
6	-	-0.897917	-1.703740
	2.80289		
	5		
1	-	1.144021	-2.445137
	2.78026		
	5		
1	-	-2.853376	-0.832440
	2.45240		
	4		
1	-	-1.123678	-2.053970
	3.80128		
	0		
6	1.65769	1.390421	-0.174148
	7		
6	2.93642	1.762028	-0.626639
	4		
6	0.87057	2.378150	0.443788
	5		
6	3.39678	3.066540	-0.489936
	6		
1	3.56538	1.014075	-1.096360
	5		
6	1.33174	3.682908	0.583337
	7		
1	-	2.107051	0.840822
	0.10181		
	4		
6	2.59615	4.036242	0.113601
	0		
1	4.38359	3.328721	-0.857591
	4		
1	0.70867	4.422511	1.076020
	3		
1	2.95720	5.053076	0.225176
	8		
6	2.13970	-1.067688	0.035146
	7		
6	2.26174	-2.239716	-0.735522
	1		
6	2.99049	-0.926749	1.147871
	8		
6	3.17697	-3.230377	-0.398979

	3		
1	1.64922	-2.356564	-1.622685
	5		
6	3.90175	-1.919732	1.486536
	2		
1	2.92132	-0.029613	1.752465
	8		
6	3.99988	-3.079019	0.716874
	5		
1	3.25848	-4.118363	-1.017648
	2		
1	4.53622	-1.790936	2.357447
	5		
1	4.71368	-3.852373	0.979704
	5		
27	-	-0.147673	0.250312
	2.21833		
	1		
1	-	1.021486	1.179177
	2.89503		
	5		
1	-	1.162972	-0.023026
	4.78713		
	4		
6	-	0.127402	1.260928
	3.82092		
	7		
8	-	-0.624805	2.211025
	3.81327		
	0		
8	-	0.614774	0.748013
	4.98683		
	3		
TSCoH-H			
6	0.58109	-0.023602	-0.240051
	8		
6	-	-0.293387	-0.468207
	0.79225		
	0		
6	-	0.679536	-1.049785
	1.68638		
	4		
6	-	-1.534792	-0.056521

	1.41329		
	3		
6	-	0.394790	-1.304712
	3.02867		
	9		
1	-	1.645022	-1.334053
	1.29082		
	7		
6	-	-1.820352	-0.319986
	2.75369		
	1		
1	-	-2.264352	0.469866
	0.81365		
	8		
6	-	-0.848077	-0.919171
	3.59175		
	6		
1	-	1.148659	-1.770531
	3.65233		
	2		
1	-	-2.768235	0.000634
	3.16974		
	0		
1	-	-1.055197	-1.093885
	4.63988		
	4		
6	1.09484	1.354078	-0.190674
	7		
6	2.31813	1.683506	-0.804116
	2		
6	0.41053	2.373903	0.496773
	3		
6	2.82397	2.976785	-0.749279
	5		
1	2.86631	0.912167	-1.333216
	6		
6	0.92016	3.666180	0.554529
	8		
1	-	2.138462	1.009851
	0.51474		
	7		
6	2.12737	3.977155	-0.070998
	0		
1	3.76402	3.206861	-1.240429

	0		
1	0.37915	4.430790	1.102809
	3		
1	2.52436	4.985722	-0.024721
	7		
6	1.54145	-1.116234	-0.042832
	0		
6	1.47957	-2.302764	-0.799344
	9		
6	2.58367	-0.995377	0.896666
	4		
6	2.40625	-3.322250	-0.616690
	5		
1	0.70962	-2.407550	-1.555713
	6		
6	3.50586	-2.017948	1.082861
	5		
1	2.65528	-0.090915	1.489640
	7		
6	3.42336	-3.188680	0.328760
	2		
1	2.34305	-4.219848	-1.223588
	3		
1	4.29147	-1.903147	1.822764
	2		
1	4.14635	-3.984718	0.471534
	6		
27	-	0.043151	0.907603
	2.81098		
	5		
1	-	0.046089	2.406457
	2.60300		
	0		
1	-	1.160297	1.933976
	2.80039		
	2		
<b>TS<sub>b1</sub></b>			
6	-	-0.000602	0.294631
	1.37350		
	0		
6	-	-0.023524	0.686078
	0.05527		
	6		

6	0.63871 5	1.125773	1.236370
6	0.81973 1	-1.190288	0.496627
6	1.89354 5	1.023332	1.785268
1	0.12961 3	2.079518	1.272384
6	2.00042 0	-1.354282	1.246995
1	0.42587 8	-2.040361	-0.042409
6	2.60422 3	-0.224121	1.821160
1	2.36974 3	1.906486	2.195335
1	2.52262 5	-2.304564	1.237924
1	3.55422 0	-0.297995	2.333658
6	- 2.10938 6	1.269144	0.105330
6	- 3.40697 7	1.427909	0.616183
6	- 1.55476 0	2.321541	-0.639668
6	- 4.11203 5	2.609550	0.416941
1	- 3.85721 6	0.615198	1.175699
6	- 2.26388 2	3.501379	-0.846594
1	- 0.57021 1	2.198927	-1.078143
6	- 3.54276 3	3.652908	-0.313762

1	-	2.717729	0.831027
	5.10921		
	6		
1	-	4.298645	-1.434529
	1.82093		
	0		
1	-	4.572620	-0.473352
	4.09553		
	1		
6	-	-1.241368	-0.028326
	2.10686		
	7		
6	-	-2.377751	0.794279
	2.02792		
	6		
6	-	-1.303316	-1.160565
	2.93619		
	8		
6	-	-3.537369	0.484706
	2.73063		
	6		
1	-	-2.335514	1.696950
	1.42806		
	7		
6	-	-2.464699	-1.473621
	3.63407		
	1		
1	-	-0.432070	-1.799889
	3.02300		
	9		
6	-	-3.588334	-0.654217
	3.53360		
	7		
1	-	-4.398896	1.141073
	2.66259		
	6		
1	-	-2.493309	-2.360491
	4.25864		
	1		
1	-	-4.491979	-0.895377
	4.08318		
	8		
27	2.50054	-0.051911	-0.375132
	7		

6	4.91315	0.271279	-0.889440
	0		
8	5.70319	1.110155	-1.113652
	1		
8	4.59079	-0.863882	-0.638597
	3		
1	3.43452	1.082107	-0.986046
	8		
1	1.80685	0.298462	-1.690353
	9		

### HCo-OCHO

6	-1.061072	-0.011784	0.311792
6	0.153987	-0.597946	0.556853
6	1.371795	0.083635	0.983209
6	0.501611	-1.956559	0.134820
6	2.375832	-0.619352	1.730869
1	1.406804	1.162264	1.000734
6	1.595014	-2.635043	0.655492
1	-0.140018	-2.465814	-0.571583
6	2.500448	-1.988614	1.567942
1	3.134284	-0.058008	2.263634
1	1.796616	-3.649399	0.330632
1	3.323658	-2.537216	2.008482
6	-1.267888	1.451473	0.391911
6	-2.379553	1.967592	1.076345
6	-0.399727	2.343008	-0.256677
6	-2.600195	3.338603	1.139534
1	-3.066850	1.284848	1.564539
6	-0.630029	3.715126	-0.199007
1	0.452053	1.974967	-0.816762
6	-1.724539	4.218104	0.501404
1	-3.456919	3.722128	1.684049
1	0.051987	4.386206	-0.709865
1	-1.899606	5.288061	0.545859
6	-2.224170	-0.824279	-0.097830
6	-2.525532	-2.045310	0.527696
6	-3.075958	-0.373920	-1.120531
6	-3.623968	-2.800979	0.129499
1	-1.909517	-2.384033	1.353450
6	-4.167352	-1.133780	-1.524168
1	-2.866069	0.573661	-1.602937
6	-4.446093	-2.350957	-0.901954
1	-3.846475	-3.735235	0.634536

1	-4.804235	-0.775412	-2.326057
1	-5.303652	-2.938478	-1.212166
27	2.434186	-0.966198	-0.391378
6	3.720281	1.396180	-1.223455
8	2.725765	2.098501	-1.260331
8	3.816928	0.162712	-0.820322
1	4.705793	1.787374	-1.537606
1	1.800232	-0.689470	-1.698964

**TS<sub>b2</sub>**

6	1.115893	0.027938	-0.359724
6	-0.063126	-0.633061	-0.731374
6	-1.150037	0.022777	-1.436801
6	-0.348479	-2.009251	-0.350846
6	-2.316762	-0.632441	-1.787830
1	-1.040979	1.063819	-1.708563
6	-1.510947	-2.679765	-0.743035
1	0.381064	-2.543106	0.243175
6	-2.556911	-1.989523	-1.410575
1	-3.099057	-0.076168	-2.290300
1	-1.652030	-3.713157	-0.445547
1	-3.463560	-2.497480	-1.708254
6	1.208618	1.500907	-0.361507
6	2.353940	2.144366	-0.863435
6	0.189104	2.309888	0.171035
6	2.463838	3.530242	-0.854432
1	3.159494	1.542164	-1.268818
6	0.297258	3.696283	0.180418
1	-0.690100	1.840859	0.598818
6	1.434848	4.315944	-0.335167
1	3.354878	4.000359	-1.258170
1	-0.504362	4.294233	0.602166
1	1.521121	5.397297	-0.326964
6	2.309997	-0.717666	0.072138
6	2.731111	-1.886692	-0.588908
6	3.095716	-0.258515	1.145778
6	3.869636	-2.574522	-0.183901
1	2.169868	-2.238839	-1.447455
6	4.232697	-0.947334	1.552295
1	2.800533	0.647117	1.663714
6	4.626217	-2.111705	0.892434
1	4.177128	-3.466594	-0.720462
1	4.813984	-0.575397	2.390038
1	5.516039	-2.646392	1.207384



27	-2.205779	-1.059797	0.463936
6	-3.799521	1.221573	1.393586
8	-4.143126	1.551088	0.292468
8	-3.282176	0.027394	1.739814
1	-3.874706	1.863137	2.284396
1	-3.709401	-0.881828	0.999435

**TS<sub>CH3-H</sub>**

6	0.719602	-0.030439	-0.352370
6	-0.614928	-0.262590	-0.690597
6	-1.504592	0.772151	-1.198392
6	-1.279468	-1.540548	-0.459160
6	-2.820276	0.510290	-1.587279
1	-1.108554	1.765367	-1.359481
6	-2.598843	-1.774261	-0.802791
1	-0.720928	-2.330263	0.025359
6	-3.422811	-0.744915	-1.344982
1	-3.411859	1.317740	-2.005065
1	-3.039538	-2.737750	-0.570856
1	-4.452005	-0.935110	-1.615208
6	1.275277	1.335764	-0.255086
6	2.520352	1.638728	-0.834045
6	0.620704	2.361154	0.448708
6	3.071935	2.911117	-0.734945
1	3.053062	0.860088	-1.368781
6	1.171026	3.635046	0.550266
1	-0.321727	2.147519	0.941439
6	2.399239	3.919489	-0.044771
1	4.030440	3.118303	-1.200199
1	0.646503	4.403817	1.109105
1	2.830631	4.911693	0.035150
6	1.648692	-1.139167	-0.066294
6	1.688031	-2.301722	-0.857595
6	2.564781	-1.046903	0.997856
6	2.582878	-3.331166	-0.584966
1	1.024839	-2.381640	-1.712059
6	3.458355	-2.075849	1.271970
1	2.565987	-0.154665	1.614214
6	3.471727	-3.227224	0.484447
1	2.597160	-4.211667	-1.219755
1	4.146541	-1.980593	2.105978
1	4.171489	-4.028789	0.696071
27	-2.734753	0.094472	0.572605
1	-3.942391	-0.048294	1.448664

6	-2.707098	0.009306	2.548112
1	-3.226235	0.753940	3.150693
1	-1.629030	0.246037	2.545958
1	-2.843568	-0.976042	2.989911

**TS1<sub>CoH-O</sub>**

6	0.719602	-0.030439	-0.352370
6	-0.614928	-0.262590	-0.690597
6	-1.504592	0.772151	-1.198392
6	-1.279468	-1.540548	-0.459160
6	-2.820276	0.510290	-1.587279
1	-1.108554	1.765367	-1.359481
6	-2.598843	-1.774261	-0.802791
1	-0.720928	-2.330263	0.025359
6	-3.422811	-0.744915	-1.344982
1	-3.411859	1.317740	-2.005065
1	-3.039538	-2.737750	-0.570856
1	-4.452005	-0.935110	-1.615208
6	1.275277	1.335764	-0.255086
6	2.520352	1.638728	-0.834045
6	0.620704	2.361154	0.448708
6	3.071935	2.911117	-0.734945
1	3.053062	0.860088	-1.368781
6	1.171026	3.635046	0.550266
1	-0.321727	2.147519	0.941439
6	2.399239	3.919489	-0.044771
1	4.030440	3.118303	-1.200199
1	0.646503	4.403817	1.109105
1	2.830631	4.911693	0.035150
6	1.648692	-1.139167	-0.066294
6	1.688031	-2.301722	-0.857595
6	2.564781	-1.046903	0.997856
6	2.582878	-3.331166	-0.584966
1	1.024839	-2.381640	-1.712059
6	3.458355	-2.075849	1.271970
1	2.565987	-0.154665	1.614214
6	3.471727	-3.227224	0.484447
1	2.597160	-4.211667	-1.219755
1	4.146541	-1.980593	2.105978
1	4.171489	-4.028789	0.696071
27	-2.734753	0.094472	0.572605
1	-3.942391	-0.048294	1.448664
6	-2.707098	0.009306	2.548112
1	-3.226235	0.753940	3.150693

1	-1.629030	0.246037	2.545958
1	-2.843568	-0.976042	2.989911

**Co-COOH**

6	1.245359	-0.019413	-0.332717
6	0.029399	-0.658640	-0.792327
6	-0.884954	-0.008367	-1.660204
6	-0.333376	-1.976982	-0.346034
6	-2.093832	-0.621374	-2.035017
1	-0.674120	0.997699	-1.996030
6	-1.500002	-2.608820	-0.776096
1	0.305869	-2.478027	0.367724
6	-2.411525	-1.926823	-1.613816
1	-2.795660	-0.071131	-2.649520
1	-1.740616	-3.598230	-0.405518
1	-3.346301	-2.386375	-1.906924
6	1.330022	1.434361	-0.221113
6	2.534017	2.104894	-0.526899
6	0.230471	2.211108	0.198787
6	2.628474	3.486180	-0.428267
1	3.388707	1.530297	-0.864304
6	0.333165	3.592089	0.300801
1	-0.701948	1.734436	0.468681
6	1.528738	4.238850	-0.012369
1	3.560555	3.979860	-0.683132
1	-0.526548	4.161496	0.637350
1	1.605147	5.317995	0.068622
6	2.404580	-0.834785	0.018382
6	2.723762	-2.008438	-0.696126
6	3.250352	-0.466185	1.085075
6	3.832740	-2.773511	-0.360546
1	2.107277	-2.301461	-1.538450
6	4.352692	-1.239382	1.424462
1	3.018165	0.423790	1.657563
6	4.652452	-2.396137	0.703950
1	4.065694	-3.663000	-0.936651
1	4.978306	-0.942716	2.259767
1	5.516338	-2.996437	0.968044
27	-2.162621	-0.705305	0.243609
6	-1.826038	-0.571925	2.168186
1	-2.602425	-1.161926	2.668190
1	-1.849180	0.437143	2.583228
1	-0.847331	-1.017897	2.374499
6	-3.515356	0.591216	0.491409

8	-3.114631	1.905005	0.348975
8	-4.681937	0.343931	0.708818
1	-3.907338	2.458665	0.472982

**TS1<sub>CoH-C</sub>**

6	-1.567751	-0.083800	0.243087
6	-0.336835	-0.741998	0.584456
6	0.626624	-0.118711	1.417433
6	-0.023703	-2.041138	0.092174
6	1.809063	-0.759962	1.765268
1	0.413943	0.860154	1.827763
6	1.166263	-2.662705	0.403474
1	-0.721392	-2.531144	-0.574784
6	2.114356	-2.031464	1.240602
1	2.494773	-0.281381	2.455790
1	1.391456	-3.638003	-0.012895
1	2.996571	-2.567418	1.569953
6	-1.630216	1.377226	0.191874
6	-2.769307	2.074761	0.639776
6	-0.555137	2.124360	-0.327497
6	-2.819054	3.461912	0.587562
1	-3.605973	1.518411	1.046573
6	-0.611628	3.510689	-0.386918
1	0.313801	1.606782	-0.713997
6	-1.741641	4.186487	0.074726
1	-3.698575	3.981853	0.952936
1	0.228116	4.057354	-0.800848
1	-1.784877	5.269650	0.032258
6	-2.766959	-0.856662	-0.073360
6	-3.067902	-2.056967	0.602411
6	-3.672978	-0.411778	-1.057612
6	-4.216096	-2.778756	0.303604
1	-2.404392	-2.404924	1.385601
6	-4.814860	-1.141473	-1.361237
1	-3.459147	0.503979	-1.595722
6	-5.094342	-2.328034	-0.682501
1	-4.433357	-3.691558	0.848505
1	-5.488288	-0.786573	-2.134351
1	-5.989414	-2.894068	-0.917010
27	3.155734	-0.680460	-0.413789
1	2.335478	0.486227	-1.289408
6	4.366023	-2.052536	-1.180699
1	3.778546	-2.840634	-1.666239
1	4.996587	-2.516202	-0.412157

1	5.022652	-1.601855	-1.932969
6	3.197927	1.920579	-0.431031
8	2.707631	2.841917	-0.955931
8	3.917620	1.340767	0.329098

### Co-HCOO

6	-1.365572	0.022781	0.316461
6	-0.132875	-0.586568	0.759958
6	0.773706	0.106405	1.636459
6	0.263966	-1.872360	0.332697
6	1.941747	-0.475587	2.102968
1	0.516662	1.106131	1.961029
6	1.508263	-2.416695	0.712252
1	-0.354810	-2.414102	-0.370437
6	2.352177	-1.741887	1.618529
1	2.586129	0.077311	2.775182
1	1.805833	-3.379865	0.317004
1	3.284600	-2.184017	1.943113
6	-1.487775	1.478435	0.231763
6	-0.424002	2.282102	-0.227138
6	-2.692513	2.115308	0.594102
6	-0.565466	3.661948	-0.312406
1	0.505207	1.829330	-0.552285
6	-2.823127	3.495502	0.516235
1	-3.519894	1.515430	0.955321
6	-1.760187	4.277255	0.061634
1	0.260999	4.257092	-0.686282
1	-3.754754	3.964695	0.815126
1	-1.864505	5.355052	-0.004335
6	-2.504331	-0.809780	-0.059605
6	-2.799878	-2.012089	0.616848
6	-3.359849	-0.423682	-1.112793
6	-3.892873	-2.788712	0.255462
1	-2.179389	-2.317691	1.451532
6	-4.445415	-1.208164	-1.478294
1	-3.149091	0.490622	-1.654399
6	-4.720207	-2.394484	-0.796815
1	-4.107727	-3.700523	0.803007
1	-5.077990	-0.896804	-2.302956
1	-5.571395	-3.003883	-1.080614
27	2.343375	-0.606161	-0.233737
1	4.165425	2.386796	-0.995934
6	3.027432	-1.609127	-1.749452
1	3.833285	-2.257064	-1.391199

1	3.412808	-0.910971	-2.492632
1	2.228397	-2.215058	-2.188040
6	3.747382	1.420566	-0.669274
8	4.382798	0.679454	0.091613
8	2.583128	1.129351	-1.122434

**TS<sub>2</sub><sub>CoH-O</sub>**

6	1.252744	-0.055227	-0.344915
6	0.051246	-0.606431	-0.820773
6	-0.944855	0.168508	-1.540558
6	-0.322472	-1.984070	-0.572629
6	-2.076926	-0.421452	-2.113333
1	-0.755658	1.215773	-1.727340
6	-1.491165	-2.540514	-1.064191
1	0.322471	-2.590543	0.049058
6	-2.408952	-1.767612	-1.834090
1	-2.742796	0.188662	-2.713151
1	-1.732937	-3.569919	-0.823187
1	-3.307935	-2.214811	-2.237986
6	1.496711	1.398724	-0.309645
6	2.744264	1.911285	-0.712624
6	0.531103	2.309394	0.154393
6	3.006723	3.275429	-0.675244
1	3.507383	1.225843	-1.064186
6	0.798093	3.674337	0.195995
1	-0.430794	1.960363	0.508280
6	2.033647	4.166618	-0.221405
1	3.973056	3.645546	-1.002939
1	0.035361	4.350264	0.568547
1	2.239680	5.231425	-0.188148
6	2.348705	-0.919327	0.131210
6	2.747980	-2.069805	-0.572643
6	3.060982	-0.587426	1.298088
6	3.796232	-2.863755	-0.119784
1	2.243911	-2.324221	-1.498514
6	4.104929	-1.383985	1.754320
1	2.781948	0.304984	1.847056
6	4.477653	-2.529058	1.049948
1	4.091887	-3.739137	-0.689379
1	4.630246	-1.110880	2.663900
1	5.295756	-3.147639	1.403453
27	-2.398277	-0.611333	0.005572
6	-2.426127	-0.393814	2.076463
1	-3.089847	-0.002585	2.842719

1	-1.392976	-0.165730	2.326742
1	-2.602434	-1.478669	2.043991
6	-3.075155	0.894916	0.901216
8	-4.444008	0.613346	0.777545
8	-2.673591	2.030496	1.035810
1	-4.895306	1.461151	0.636850

**TS2<sub>CoH-C</sub>**

6	0.985714	-0.062195	-0.548953
6	-0.271927	-0.413772	-1.093873
6	-1.087066	0.514701	-1.834466
6	-0.893121	-1.694376	-0.845695
6	-2.288109	0.127706	-2.445721
1	-0.733161	1.525926	-1.978746
6	-2.099971	-2.072387	-1.450247
1	-0.403755	-2.395398	-0.184331
6	-2.806329	-1.181040	-2.293104
1	-2.835659	0.855357	-3.034172
1	-2.506874	-3.056901	-1.247088
1	-3.728965	-1.477048	-2.775065
6	1.386669	1.350208	-0.410990
6	0.522175	2.311146	0.141863
6	2.672709	1.768919	-0.797142
6	0.919549	3.635886	0.285161
1	-0.453331	2.001498	0.495921
6	3.068324	3.094302	-0.658127
1	3.358520	1.041206	-1.216822
6	2.192729	4.036962	-0.118781
1	0.239143	4.354118	0.731364
1	4.062278	3.394413	-0.974384
1	2.502551	5.070614	-0.006394
6	1.927612	-1.080071	-0.084450
6	2.092401	-2.314934	-0.747634
6	2.731049	-0.846330	1.052729
6	3.005418	-3.259741	-0.298760
1	1.522742	-2.509926	-1.649014
6	3.642873	-1.794522	1.501093
1	2.630524	0.093766	1.582647
6	3.786997	-3.007974	0.830454
1	3.122183	-4.191910	-0.842495
1	4.241855	-1.585821	2.381771
1	4.501394	-3.746378	1.178407
27	-2.662774	-0.280285	-0.324942
1	-3.246624	1.863959	2.859219

6	-0.538601	-0.905107	2.548627
6	2.158667	0.333621	0.397836
6	1.283699	-0.134591	1.389161
6	1.031015	-1.545477	1.623130
6	0.508097	0.759321	2.228391
6	0.100323	-1.995001	2.545035
1	1.559553	-2.270960	1.019068
6	-0.408861	0.302072	3.162589
1	0.668520	1.824886	2.128458
6	-0.700600	-1.084927	3.292777
1	-0.064900	-3.061864	2.655839
1	-0.944054	1.019131	3.776698
1	-1.398676	-1.439661	4.039810
6	3.168733	-0.538929	-0.217605
1	-1.431023	-1.493953	2.403021
1	0.057943	-0.634704	1.695203
1	-0.101020	-0.854387	3.532944
6	-2.594391	1.137739	2.343445
8	-3.102580	0.600801	1.313801
8	-1.469991	0.945905	2.842422

Bipyridyl-Co-C•Ph<sub>3</sub> (triplet)



6	3.430754	-0.472183	-1.600325	
6	3.932284	-1.448559	0.540024	
6	4.388771	-1.284468	-2.194951	
1	2.864578	0.224638	-2.208081	
6	4.890339	-2.261883	-0.054794	
1	3.784834	-1.492655	1.613685	
6	5.124101	-2.189192	-1.428214	
1	4.560183	-1.215403	-3.264801	
1	5.470057	-2.944389	0.559256	
1	5.873948	-2.821213	-1.892290	
6	2.064441	1.715338	-0.110093	
6	0.825808	2.296979	-0.439969	
6	3.221438	2.483261	-0.336119	
6	0.745333	3.587293	-0.952505	
1	-0.080116	1.715602	-0.319603	Bipyrid
6	3.142329	3.774312	-0.846283	yl-Co-
1	4.189642	2.053437	-0.103531	C•Ph <sub>3</sub> -
6	1.903620	4.337632	-1.155601	H <sub>2</sub>
1	-0.225573	3.999872	-1.209320	(triplet)
1	4.051919	4.346510	-1.000929	
1	1.843455	5.344009	-1.556784	
27	-1.315920	-0.626404	1.237560	
6	-1.599945	-2.938960	-0.687351	
6	-2.141471	-3.619639	-1.755964	
6	-3.129884	-2.977991	-2.527611	
6	-3.503226	-1.691808	-2.198723	
6	-2.902368	-1.039138	-1.106919	
7	-1.962446	-1.686425	-0.342026	
1	-3.587495	-3.483288	-3.370588	
1	-0.839050	-3.391297	-0.060987	
1	-1.808990	-4.624775	-1.984780	
1	-4.256006	-1.182168	-2.786932	
6	-2.632494	2.060230	0.761192	
6	-3.462252	2.951630	0.117962	
6	-4.200482	2.498176	-0.993435	
6	-4.054619	1.188892	-1.402537	
6	-3.178258	0.327957	-0.717742	
7	-2.480657	0.774941	0.378486	
1	-4.869372	3.167005	-1.523047	
1	-2.046283	2.361106	1.622323	
1	-3.540049	3.972895	0.470491	
1	-4.606337	0.828078	-2.261438	
6	1.875504	-0.203124	0.720840	
6	0.838719	-1.113902	0.993308	

6	0.665287	-2.359097	0.265607
6	-0.205575	-0.861674	1.957464
6	-0.329069	-3.290292	0.583890
1	1.373277	-2.615855	-0.510412
6	-1.205581	-1.778309	2.240413
1	-0.181357	0.060040	2.522282
6	-1.305056	-3.021693	1.572126
1	-0.354132	-4.232780	0.045501
1	-1.941768	-1.522952	2.997130
1	-2.049200	-3.757783	1.847957
6	3.081342	-0.612951	-0.018445
6	3.716534	0.266818	-0.920917
6	3.681282	-1.878023	0.151431
6	4.856193	-0.101044	-1.625994
1	3.307617	1.262062	-1.051075
6	4.817576	-2.250971	-0.558430
1	3.258780	-2.566114	0.874851
6	5.414349	-1.369177	-1.459632
1	5.312576	0.606414	-2.312463
1	5.252664	-3.232002	-0.391275
1	6.303379	-1.658590	-2.010014
6	1.819509	1.193915	1.188801
6	0.643963	1.967371	1.119459
6	2.969280	1.838254	1.689776
6	0.613360	3.294662	1.531783
1	-0.256134	1.519730	0.719646
6	2.942985	3.166514	2.098594
1	3.894928	1.277521	1.756867
6	1.763596	3.909430	2.025908
1	-0.313058	3.857035	1.453873
1	3.848620	3.623942	2.485981
1	1.742759	4.945636	2.347286
27	-1.520027	-1.617257	-0.303681
6	0.230056	0.262406	-1.908507
6	0.642613	1.510673	-2.356498
6	-0.248616	2.574470	-2.291203
6	-1.527427	2.351183	-1.788881
6	-1.876363	1.072731	-1.360585
7	-1.002803	0.038409	-1.427236
1	0.049059	3.567674	-2.606702
1	0.895822	-0.588935	-1.934591
1	1.650688	1.637753	-2.728945
1	-2.225673	3.173543	-1.700463
6	-4.369106	-0.805806	0.501163

6	-5.492527	0.006544	0.546632
6	-5.444396	1.240402	-0.101662
6	-4.275670	1.613423	-0.750497
6	-3.176454	0.750474	-0.740262
7	-3.237927	-0.454531	-0.125417
1	-6.305028	1.899835	-0.103027
1	-4.353522	-1.777225	0.982509
1	-6.380871	-0.322507	1.072270
1	-4.222003	2.562660	-1.267715
1	-1.847736	-2.577416	-1.859131
1	-2.431697	-2.802122	-1.396463

PD-Co-C•Ph<sub>3</sub> (triplet)

27	1.916053	-0.460959	-0.818191
6	4.150812	-0.277426	1.162314
6	3.781224	1.158279	1.471064
6	2.354966	1.636193	1.286997
6	1.966971	2.829243	2.118322
1	1.917906	2.556793	3.178180
1	2.711876	3.626921	2.030499
1	0.996975	3.225511	1.816505
1	4.088745	1.380024	2.498112
6	5.320364	-0.811334	1.943674
1	5.624179	-1.798875	1.591850
1	6.181613	-0.138791	1.869349
1	5.070324	-0.886645	3.007537
7	3.522645	-0.961434	0.276884
7	1.568135	1.065148	0.460529
1	3.900754	-1.902403	0.176816
1	0.640256	1.486480	0.417515
1	4.425316	1.805955	0.854658
6	-1.767981	-0.275245	-0.383569
6	-0.673775	-0.802748	-1.084600
6	-0.002957	-2.042575	-0.718185
6	0.027370	-0.075094	-2.126472
6	1.035456	-2.596469	-1.463190
1	-0.333758	-2.566581	0.167258
6	1.090854	-0.631005	-2.852233
1	-0.305273	0.918550	-2.396028
6	1.597227	-1.926771	-2.574837
1	1.455451	-3.546139	-1.142509
1	1.519320	-0.052562	-3.665262
1	2.385219	-2.367413	-3.171545

6	-2.629531	-1.047245	0.509932
6	-3.403684	-0.437185	1.527244
6	-2.823280	-2.442822	0.349911
6	-4.249114	-1.170564	2.352228
1	-3.354291	0.634835	1.667827
6	-3.666382	-3.172206	1.176888
1	-2.338982	-2.952331	-0.473496
6	-4.381708	-2.549908	2.201635
1	-4.815929	-0.652505	3.120968
1	-3.784715	-4.238275	1.003092
1	-5.041123	-3.120589	2.847014
6	-2.055920	1.181063	-0.532440
6	-1.714900	2.092097	0.481783
6	-2.654556	1.703540	-1.687492
6	-1.949636	3.459994	0.347859
1	-1.286386	1.707382	1.402972
6	-2.880589	3.070762	-1.835033
1	-2.944498	1.017311	-2.476265
6	-2.527671	3.957368	-0.818396
1	-1.687690	4.137486	1.155877
1	-3.344259	3.445015	-2.742690
1	-2.711284	5.021097	-0.929385

PD-Co-C•Ph<sub>3</sub>-H<sub>2</sub> (triplet)

27	-1.995822	1.110918	0.311383
6	-3.941476	-0.766703	-1.036735
6	-3.065321	-0.628189	-2.271002
6	-1.585587	-0.799262	-1.967850
6	-0.848231	-1.904635	-2.665989
1	-1.333541	-2.868358	-2.476422
1	-0.860131	-1.753133	-3.750915
1	0.186379	-1.969063	-2.327696
1	-3.385023	-1.335163	-3.037835
6	-5.068213	-1.756418	-1.113201
1	-5.660999	-1.773435	-0.196736
1	-5.730903	-1.520813	-1.952480
1	-4.678742	-2.763890	-1.294932
7	-3.679484	-0.048739	-0.010890
7	-1.063083	-0.009263	-1.116092
1	-4.317956	-0.220910	0.764458
1	-0.072886	-0.187079	-0.915932

1	-3.214954	0.379705	-2.676554
6	1.575402	0.146959	0.646514
6	0.459825	0.618249	1.366118
6	-0.527987	-0.259403	1.964862
6	0.110099	2.018775	1.449332
6	-1.671714	0.208690	2.597074
1	-0.388558	-1.329202	1.893672
6	-1.043735	2.472555	2.081005
1	0.787048	2.751611	1.032813
6	-1.980397	1.587166	2.662987
1	-2.362066	-0.515303	3.021519
1	-1.226870	3.542393	2.119023
1	-2.854482	1.951603	3.187275
6	2.000323	-1.261350	0.701415
6	2.469754	-1.914535	-0.460327
6	1.983599	-2.026101	1.886292
6	2.865020	-3.246783	-0.445028
1	2.538912	-1.349719	-1.384642
6	2.372793	-3.361401	1.901873
1	1.686457	-1.549637	2.813648
6	2.811408	-3.989215	0.735724
1	3.218820	-3.710450	-1.361600
1	2.353893	-3.911058	2.838616
1	3.120988	-5.028981	0.749983
6	2.389921	1.040933	-0.206442
6	1.826611	1.963427	-1.110498
6	3.796841	0.959409	-0.182730
6	2.618575	2.763969	-1.928501
1	0.748163	2.046695	-1.181992
6	4.590124	1.753602	-1.002383
1	4.265158	0.254720	0.495811
6	4.008595	2.667454	-1.882434
1	2.145031	3.459102	-2.616081
1	5.671246	1.665790	-0.948173
1	4.627119	3.290875	-2.519754
1	-2.826468	2.604548	-0.305391
1	-2.227829	2.527239	-0.808615

CO-Co-C•Ph<sub>3</sub> (triplet)

6	1.801368	-0.029191	0.375022
6	0.496974	-0.364107	0.726232
6	-0.075094	-1.692136	0.503545

6	-0.468295	0.593902	1.251343
6	-1.350366	-2.059492	0.956023
1	0.540627	-2.444863	0.030286
6	-1.742825	0.231129	1.648809
1	-0.161441	1.623730	1.373901
6	-2.239400	-1.097649	1.484849
1	-1.689110	-3.079024	0.803734
1	-2.404867	0.996444	2.039468
1	-3.234332	-1.367650	1.810578
6	2.812332	-1.063593	0.083616
6	3.702988	-0.909234	-0.994236
6	2.952604	-2.212865	0.882785
6	4.670077	-1.868311	-1.273944
1	3.626112	-0.024713	-1.616805
6	3.920244	-3.172430	0.604313
1	2.308151	-2.336313	1.746416
6	4.783309	-3.008678	-0.478893
1	5.337489	-1.726720	-2.118172
1	4.011842	-4.043941	1.245022
1	5.539988	-3.755473	-0.694937
6	2.238652	1.377508	0.250304
6	1.488950	2.330503	-0.460219
6	3.459307	1.794632	0.808914
6	1.925435	3.646004	-0.585160
1	0.563904	2.025903	-0.938386
6	3.897696	3.108185	0.684473
1	4.063270	1.072824	1.347727
6	3.131354	4.044176	-0.010188
1	1.329640	4.358392	-1.147224
1	4.840295	3.404469	1.133732
1	3.474159	5.068672	-0.109556
6	-2.822578	0.329176	-1.574659
8	-3.622896	0.881999	-2.178895
27	-1.614316	-0.556530	-0.578956

CO-Co-C•Ph<sub>3</sub>-H<sub>2</sub> (triplet)

6	-0.765457	0.033860	-0.384353
6	0.450409	-0.330300	-0.967088
6	1.075624	-1.631203	-0.757667
6	1.246331	0.576539	-1.783198
6	2.287840	-1.993020	-1.352570
1	0.561623	-2.360060	-0.146188

6	2.461837	0.221003	-2.326405
1	0.856440	1.566199	-1.980134
6	3.060299	-1.051391	-2.067805
1	2.684420	-2.987074	-1.173920
1	3.008350	0.951760	-2.913158
1	4.005315	-1.324773	-2.516732
6	-1.676889	-0.972578	0.191325
6	-2.324380	-0.732810	1.417287
6	-1.963779	-2.181629	-0.468488
6	-3.196936	-1.665154	1.967114
1	-2.132772	0.198257	1.939172
6	-2.837587	-3.114583	0.080127
1	-1.511949	-2.374455	-1.435541
6	-3.457382	-2.864518	1.304184
1	-3.675001	-1.456412	2.919048
1	-3.047978	-4.033782	-0.457725
1	-4.141024	-3.590622	1.731249
6	-1.190997	1.444876	-0.291918
6	-0.317708	2.461025	0.134638
6	-2.515989	1.810326	-0.589796
6	-0.740279	3.782705	0.234233
1	0.698321	2.202059	0.412892
6	-2.940342	3.130510	-0.489935
1	-3.212837	1.042293	-0.906866
6	-2.054007	4.127169	-0.081309
1	-0.045463	4.544004	0.574989
1	-3.966653	3.384243	-0.735914
1	-2.385156	5.157190	-0.001508
6	3.867063	0.964350	0.586356
8	4.603622	1.793767	0.869698
27	2.739550	-0.353912	0.044069
1	2.906736	-1.648658	1.562907
1	3.615495	-1.656273	1.282428

Ethylene-Co-C•Ph<sub>3</sub> (triplet)

6	2.051969	0.430166	0.394756
6	1.170019	0.003742	1.375847
6	0.857850	-1.404457	1.607132
6	0.384290	0.908000	2.199112
6	0.053843	-1.841239	2.654635
1	1.307534	-2.145413	0.960165
6	-0.448571	0.467702	3.212786
1	0.488808	1.973903	2.048019

6	-0.662121	-0.923465	3.471515
1	-0.086040	-2.907878	2.800483
1	-0.975174	1.203741	3.811847
1	-1.247004	-1.257027	4.318334
6	2.984062	-0.500872	-0.272158
6	3.192741	-0.432331	-1.661851
6	3.723157	-1.458637	0.445680
6	4.074918	-1.294006	-2.304340
1	2.650946	0.310041	-2.237872
6	4.604623	-2.322922	-0.195784
1	3.618565	-1.504292	1.524390
6	4.784313	-2.249621	-1.576704
1	4.208002	-1.221500	-3.379334
1	5.167272	-3.045430	0.387522
1	5.474700	-2.920364	-2.077254
6	2.094011	1.837597	-0.059455
6	0.928452	2.546083	-0.397313
6	3.323092	2.501365	-0.216203
6	0.983653	3.862409	-0.845617
1	-0.031680	2.046775	-0.323618
6	3.382119	3.816213	-0.664958
1	4.238717	1.970731	0.021350
6	2.212119	4.507897	-0.979185
1	0.066052	4.380854	-1.106539
1	4.345637	4.305650	-0.767561
1	2.258079	5.533294	-1.330651
27	-1.467375	-0.718366	1.517477
6	-1.628230	-0.855336	-0.512506
6	-2.523696	0.094485	-0.029345
1	-3.573681	-0.159773	0.099076
1	-2.309812	1.156330	-0.099821
1	-0.676479	-0.567711	-0.947965
1	-1.967538	-1.859925	-0.755212

Ethylene-Co-C•Ph<sub>3</sub>-H<sub>2</sub> (triplet)

6	-0.804296	0.011567	-0.423812
6	0.507455	-0.175516	-0.827695
6	1.224457	-1.437022	-0.636133
6	1.327672	0.879892	-1.395509
6	2.509295	-1.655265	-1.126741
1	0.701240	-2.264141	-0.176982
6	2.637886	0.685851	-1.767165



1	0.885222	1.854801	-1.549457
6	3.297755	-0.581664	-1.618732
1	2.942819	-2.647310	-1.046614
1	3.193335	1.518813	-2.186859
1	4.276009	-0.753279	-2.049068
6	-1.669643	-1.126371	-0.044462
6	-2.467002	-1.062669	1.112108
6	-1.759841	-2.289033	-0.829343
6	-3.293492	-2.118867	1.479992
1	-2.432601	-0.168032	1.724764
6	-2.585030	-3.347929	-0.462576
1	-1.188464	-2.347797	-1.749655
6	-3.355139	-3.271839	0.697279
1	-3.891567	-2.043063	2.382872
1	-2.639502	-4.229507	-1.093980
1	-4.001887	-4.095110	0.982105
6	-1.420172	1.353645	-0.328923
6	-0.770504	2.436046	0.289080
6	-2.721232	1.574205	-0.814568
6	-1.377732	3.683440	0.394668
1	0.217476	2.288946	0.710828
6	-3.331517	2.819251	-0.709884
1	-3.252677	0.751007	-1.279472
6	-2.662456	3.884969	-0.107894
1	-0.852188	4.496941	0.885485
1	-4.333865	2.960077	-1.102266
1	-3.138875	4.856113	-0.024285
27	3.014292	-0.259273	0.478744
6	1.877818	0.064189	2.210387
6	2.787613	1.094341	2.025747
1	3.703370	1.136079	2.610197
1	2.479812	2.031968	1.572762
1	0.847860	0.155145	1.880146
1	2.065642	-0.720931	2.935904
1	4.422186	-1.543112	1.159367
1	3.822584	-1.803087	1.545759