Do Spin State Changes Matter in Organometallic Chemistry?

A Computational Study.

*Jose-Luis Carreon-Macedo and Jeremy N. Harvey**

School of Chemistry and Centre for Computational Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, UK. Email: jeremy.harvey@bristol.ac.uk

Suplementary Information.

Full details of the BS1, BS2, BSW1 and BSW2 basis sets used for the *ab initio* calculations.

Cobalt: the exponents of the polarization functions were optimized at the CI level for Co^+ (^3F), using the Ahlrichs-TZV (17s,10p,6d)/[6s,3p,3d] basis set as a starting point. Two bases of increasing size were developed. Where required, these basis are simply referred to as ''BS1'' and "BS2". In the first one, the most diffuse primitive within the contraction scheme was decontracted for the *s*, *p*, and *d* functions. Additionally, one diffuse *s* function ($\alpha = 0.02$) and three (uncontracted) diffuse *p* functions ($\alpha = 0.141308, 0.043402, 0.018$) were added. The final contraction was of the form (18s,13p,6d,2f,1g)/[8s,7p,4d,2f,1g] which included two f functions ($\alpha_1 = 4.147168$, $\alpha_2 = 1.063376$) and one g function ($\alpha = 2.7$). The second basis set, BS2, was constructed from the previous one. For this we added one d function ($\alpha = 0.1$) and optimized for f ($\alpha_1 = 6.82$, $\alpha_2 = 2.20$, $\alpha_3 = 0.709677$), two g ($\alpha_1 = 4.723135$, $\alpha_2 = 1.431253$) and one h function ($\alpha = 3.0$). The final segmented contraction was of the form (18s,13p,7d,3f,2g,1h)/[8s,7p,5d,3f,2g,1h].

For **tungsten** we also developed a basis set which was optimized at the CI level for WH_6. In this case we used for the metallic atom the Stuttgart/Köln group ECP which uses quasi-relativistic reference data. The corresponding basis set for this potential is a modified segmented contraction of the form (8s7p6d2f)/[6s5p4d2f], where the most diffuse d primitive in the contraction scheme was decontracted and two f functions ($\alpha_1 = 0.528205$, $\alpha_2 = 0.170389$) were included. Another set tried for this potential used three f functions ($\alpha_1 = 1.02$, $\alpha_2 = 0.3$, $\alpha_3 = 0.088235$) instead of two and one additional g function ($\alpha = 0.3$). We named these basis sets as "BSW1" and "BSW2" respectively.

Table S1. DFT and CCSD(T) computed energetics (kcal/mol) of the simplified model $^1[M(H_3)]$ M = $W(NH_2)_3NH_3$ (See Figure S1)

	DFT[a]		CCSD(T)[b]	
Model	**B3LYP**	**BP86**	**BSW1**	**BSW2**
$^3[M(H)] + H_2$	0.0	0.0	0.0	0.0
$^1[M(H)] + H_2$	24.2	23.6	24.9	24.8
$^1[M(H_3)]$	-11.4	-22.4	-15.7	-15.0

a) Basis W: LACV3P, N,H: 6-31G*, H(hydrides):6-31G**

b) Basis W: ECP60MWB + 2f (BS1) or 2f1g (BS2), N,H: cc-pVDZ, H(hydrides): cc-pVTZ

Figure S1. Symmetrized C_{3v} simplified model $^1[M(H_3)]$

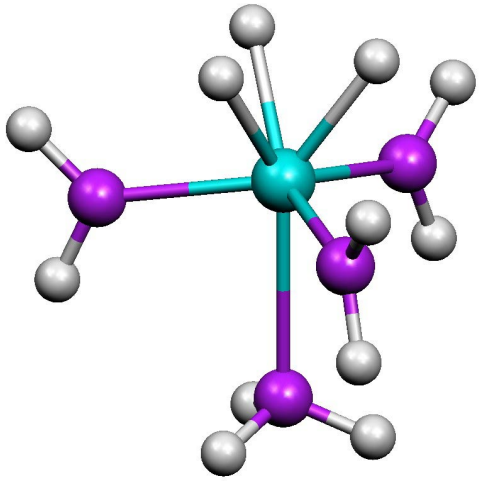

Table S2. Selected geometry parameters of $^1[CpCoCO(CH_3)H]$ for different DFT methods, bond distances (•) and angles (˚)

	B3LYP	**B3PW91**	**B3PW91***	**BPW91**	**BP86**	**PW91**
C_{Cp}-C_{Cp}	1.415	1.415	1.416	1.424	1.425	1.423
Co-C_{Cp}	2.156	2.118	2.115	2.134	2.137	2.130
Co-CO	1.734	1.717	1.711	1.714	1.715	1.710
C_{Cp}-H_{Cp}	1.082	1.082	1.084	1.088	1.090	1.088
C-O	1.151	1.152	1.156	1.169	1.170	1.168
Co-C_{CH3}	1.983	1.970	1.972	1.996	1.994	1.988
Co-H_H	1.469	1.463	1.464	1.477	1.477	1.476
C_{CO}-Co-C_{CH3}	88.7	88.1	88.3	89.1	89.3	89.1
C_{CH3}-Co-H_H	82.4	81.5	81.3	81.0	81.2	81.0
H_HCo-C_{CO}	85.1	84.3	84.5	85.6	85.8	85.7

Table S3. Some calculated and experimental bond distances (•) and angles (°) for $^{1}[W\{N_3N\}(H)_3]$

	B3LYP	**B3LYP** [a]	**BP86**	**Exp.**[c]
	2.026	1.996	2.026	2.000(5)
$W\text{-}N_{eq}$	2.027	1.996	2.027	2.003(5)
	2.033	1.996	2.032	2.013(5)
$W\text{-}N_{ax}$	2.322	2.385	2.313	2.226(4)
	115.6	117.6	115.5	114.6(2)
$N_{eq}\text{-}W\text{-}N_{eq}$	116.2	117.6	116.3	116.0(2)
	117.7	117.6	118.0	116.9(2)
	125.1		124.9	123.6(2)
W-N-Si	127.1		126.6	124.0(3)
	128.9		128.5	124.3(2)
	1.686	1.690	1.701	1.57
W-H	1.688	1.690	1.702	1.58
	1.691	1.690	1.705	1.59

a) Symmetrized C_{3v} simplified model $^{1}[M(H_3)]$ (See Figure S1)

b) X-ray crystal structure from Dobbs, D. A.; Schrock, R. R.; Davis, W. M. *Inorganica Chimica Acta* **1997**, *263*, 171-180. This is Ref. 8 (can change) in the main paper.

Table S4. Some calculated and experimental bond distances (Å) and angles (°) for $^{1}[Tp^{i\text{-}Pr,Me}Co(CO)_2]$

	B3LYP	BP86	Exp. [a]
Co-N	2.018	2.002	1.985(8)
	2.025	2.008	2.002(12)
	2.156	2.121	2.087(11)
Co-CO	1.757	1.731	1.696(19)
	1.758	1.731	1.729(15)
C-O	1.155	1.173	1.162(18)
	1.156	1.174	1.179(23)
N-Co-N	83.7	84.0	85.5(4)
	91.2	91.8	90.5(4)
	91.9	91.8	91.9(5)
C-Co-C	88.7	87.0	85.0(8)
Co-C-O	178.6	178.2	173.4(16)
	178.8	178.2	177.5(14)

a) X-ray crystal structure from Detrich, J. L.; Reinaud, O. M.; Rheingold, A. L.; Theopold, K. H. *J. Am. Chem. Soc.* **1995**, *117*, 11745-11748. This is Ref. 10 (can change) in the main paper.

Table S5 . Comparison of selected bond distances (Å) and angles (°) between calculated $^{3}[Tp^{i\text{-}Pr,Me}Co(CO)]$ and experimental $^{3}[Tp^{Np}Co(CO)]$

	$^{3}[Tp^{i\text{-}Pr,Me}Co(CO)]$	$^{3}[Tp^{Np}Co(CO)]$
	BP86	Exp. [a]
Co-N	1.551	2.055(5)
	1.551	2.055(4)
	1.559	2.010(4)
Co-CO	1.804	1.769(5)
C-O	1.156	1.145(6)
N-Co-N	109.1	90.6(2)
	109.2	91.1(2)
	110.1	93.2(2)
Co-C-O	179.1	177.8(6)

a) X-ray crystal structure from Detrich, J. L.; Konecny, R.; Vetter, W. M.; Doren, D.; Rheingold, A. L.; Theopold, K. H. *J Am Chem Soc* **1996**, *118*, 1703-1712. This is Ref. 32 (can change) in the main paper.

Table S6.
Coordinates of some species involved in the reaction CpCo(CO) + CO

^{1}[CpCo(CO)$_2$]				^{3}[CpCo(CO)$_2$]				MECP (CpCo(CO) + CO)			
Co	-0.0055	-0.1124	0.0000	Co	-0.2586	-0.2278	0.0000	Co	-0.2013	0.8380	0.0942
C	1.3987	1.4907	0.0000	C	1.2063	1.5379	0.0000	C	-1.8881	2.4386	0.0686
C	0.5459	1.5460	1.1493	C	0.3738	1.6731	1.1606	C	-1.0630	2.7147	-1.0750
C	-0.8299	1.7239	0.7078	C	-0.9789	1.7698	0.7216	C	0.2538	2.9574	-0.6048
C	-0.8299	1.7239	-0.7078	C	-0.9789	1.7698	-0.7216	C	0.2259	2.9435	0.8447
C	0.5459	1.5460	-1.1493	C	0.3738	1.6731	-1.1606	C	-1.1067	2.6773	1.2525
H	0.8715	1.4897	2.1890	H	0.7096	1.6206	2.1973	H	-1.3694	2.6371	-2.1194
H	-1.7015	1.8054	1.3573	H	-1.8576	1.8651	1.3619	H	1.1291	3.1775	-1.2202
H	-1.7015	1.8054	-1.3573	H	-1.8576	1.8651	-1.3619	H	1.0753	3.1494	1.4993
H	0.8715	1.4897	-2.1890	H	0.7096	1.6206	-2.1973	H	-1.4584	2.5762	2.2808
H	2.4816	1.3710	0.0000	H	2.2923	1.4341	0.0000	H	-2.9538	2.2040	0.0454
O	-0.2245	-2.0857	2.1144	O	0.4062	-2.0183	2.3000	O	-0.8970	-0.9178	-2.2467
C	-0.1372	-1.2936	1.2561	C	0.0957	-1.3153	1.4234	C	-0.5679	-0.2373	-1.3602
O	-0.2245	-2.0857	-2.1144	O	0.4062	-2.0183	-2.3000	O	-0.6883	-0.8984	2.5047
C	-0.1372	-1.2936	-1.2561	C	0.0957	-1.3153	-1.4234	C	-0.4447	-0.2290	1.5827

Table S7 .
Coordinates of some species involved in the reaction CpCo(CO) + CH_4

^{1}[CpCoCO(CH_3)H]

C	-1.6407	4.6372	1.9849
C	-1.5206	3.1988	1.8893
C	-0.8422	2.8875	0.6732
C	-0.5176	4.1291	0.0155
C	-1.0334	5.2022	0.8260
H	-1.8677	2.4782	2.6308
H	-0.5714	1.8902	0.3264
H	0.0176	4.2344	-0.9281
H	-0.9246	6.2667	0.6161
H	-2.1087	5.1882	2.8011
O	1.4040	3.5929	4.5527
C	0.9845	3.7998	3.4799
Co	0.4191	4.0753	1.8844
H	1.5739	3.2627	1.4501
C	1.7628	5.5349	1.6866
H	1.3564	6.4345	2.1798
H	2.7350	5.2742	2.1317
H	1.8934	5.7097	0.6063

^{1}[CpCoCO•CH_4]

Co	-2.0940	0.6522	0.4180
C	-0.0710	-0.2185	-0.2945
H	0.0785	0.4897	0.5423
H	-1.1638	-0.4328	-0.6049
H	0.4246	0.1647	-1.1982
H	0.3223	-1.2016	0.0015
O	-2.5596	-1.3634	2.4455
C	-2.3654	-0.5441	1.6221
C	-3.9038	1.4142	-0.2909
C	-2.9203	1.7384	-1.2538
C	-1.8936	2.5302	-0.5884
C	-2.2651	2.7567	0.7657
C	-3.4714	1.9928	0.9831
H	-2.9061	1.4278	-2.2994
H	-0.9785	2.8902	-1.0648
H	-1.7223	3.3439	1.5060
H	-4.0254	1.9304	1.9213
H	-4.8048	0.8213	-0.4498

TS (CpCo(CO) + CH_4)

Co	-1.9923	0.6635	0.4006
C	-0.0142	0.2963	0.8636
H	-0.1499	0.5603	1.9264
H	-0.8509	0.0814	-0.3682
H	0.7029	0.9930	0.3996
H	0.3836	-0.7299	0.8129
O	-2.8837	-1.9939	1.1117
C	-2.5203	-0.9122	0.8351
C	-3.7968	1.6293	0.5101
C	-3.3064	1.7448	-0.8468
C	-2.0624	2.4317	-0.7808
C	-1.8134	2.7896	0.6035
C	-2.8982	2.3337	1.3982
H	-3.7795	1.3374	-1.7401
H	-1.3974	2.6432	-1.6193
H	-0.9210	3.3004	0.9695
H	-3.0135	2.4485	2.4760
H	-4.7276	1.1419	0.8054

MECP (CpCo(CO) + CH_4)

Co	-1.9375	0.6292	0.5263
C	0.5031	0.1257	0.5682
H	-0.0411	0.4709	1.4779
H	-0.1514	0.0956	-0.3388
H	1.3272	0.8283	0.3696
H	0.8688	-0.8948	0.7539
O	-2.9499	-2.0473	1.1109
C	-2.4853	-0.9909	0.8862
C	-3.7856	1.6164	0.4782
C	-3.2238	1.6619	-0.8560
C	-1.9995	2.3851	-0.7775
C	-1.8061	2.7998	0.5935
C	-2.9198	2.3488	1.3675
H	-3.6575	1.2126	-1.7498
H	-1.3109	2.5743	-1.6033
H	-0.9503	3.3633	0.9723
H	-3.0841	2.5199	2.4314
H	-4.7223	1.1304	0.7570

Table S8.
Coordinates of some species involved in the reaction $Tp^{i\text{-}Pr,Me}CoCO + CO$

$^1[Tp^{i\text{-}Pr,Me}Co(CO)_2]$

Co	-0.7639	0.0871	-0.4363
C	-1.1082	1.1528	2.4763
C	-0.5953	0.7958	3.7448
C	0.2778	-0.2731	3.5300
N	0.2713	-0.5487	2.1892
N	-0.5797	0.3199	1.5437
H	-0.8215	1.2658	4.7014
C	-1.1902	-3.0875	-0.8355
C	-0.6068	-4.2758	-0.3298
C	0.3862	-3.8694	0.5660
N	0.3788	-2.5001	0.5801
N	-0.5784	-2.0198	-0.2729
H	-0.8704	-5.3031	-0.5812
N	1.9601	-0.5322	0.3518
C	3.2914	-0.2326	0.2450
C	3.4120	0.8442	-0.6373
C	2.0979	1.1795	-1.0383
N	1.2291	0.3277	-0.4369
H	4.3372	1.3321	-0.9421
B	1.2170	-1.4659	1.3542
H	2.0116	-2.0136	2.0795
C	-2.0329	2.2978	2.1380
H	-2.0998	2.3430	1.0355
C	1.1117	-1.0340	4.5178
H	0.8971	-2.1172	4.4892
H	2.1933	-0.9096	4.3286
H	0.8993	-0.6699	5.5365
C	-3.4500	2.0758	2.7108
H	-3.4241	2.0170	3.8146
H	-4.1153	2.9125	2.4303
H	-3.8947	1.1411	2.3292
C	-1.4396	3.6401	2.6237
H	-1.3401	3.6585	3.7246
H	-0.4398	3.8136	2.1889
H	-2.0971	4.4784	2.3295
C	1.3270	-4.6935	1.3951
H	2.3845	-4.4833	1.1521
H	1.1976	-4.5075	2.4769
H	1.1425	-5.7647	1.2102
C	-2.3079	-2.9362	-1.8396
H	-2.5022	-1.8522	-1.9383
C	-1.8954	-3.4757	-3.2276
H	-1.6781	-4.5589	-3.1823
H	-2.7091	-3.3228	-3.9603
H	-0.9922	-2.9629	-3.6017
C	-3.6058	-3.6099	-1.3420
H	-3.4654	-4.7000	-1.2199
H	-3.9213	-3.1973	-0.3678
H	-4.4257	-3.4535	-2.0666
C	4.3607	-0.9802	0.9853
H	5.3501	-0.5900	0.6951
H	4.2583	-0.8733	2.0804
H	4.3387	-2.0613	0.7588
C	1.6582	2.3166	-1.9295
H	0.5529	2.3390	-1.8991
C	2.1658	3.6693	-1.3807
H	3.2705	3.7124	-1.3798
H	1.7958	4.5001	-2.0088
H	1.8181	3.8349	-0.3460
C	2.1086	2.1052	-3.3919
H	3.2115	2.0713	-3.4633
H	1.7101	1.1619	-3.8019
H	1.7515	2.9347	-4.0291
O	-0.9372	0.5226	-3.3025
C	-0.8643	0.3683	-2.1416
O	-3.6299	0.5512	-0.3481
C	-2.4680	0.3851	-0.3786

$^3[Tp^{i\text{-}Pr,Me}Co(CO)_2]$

Co	-0.8368	0.1933	-0.4974
C	-1.2065	1.1038	2.6598
C	-0.6874	0.6887	3.9099
C	0.2663	-0.2925	3.6233
N	0.3025	-0.4413	2.2623
N	-0.5965	0.4109	1.6690
H	-0.9632	1.0530	4.8994
C	-1.2445	-2.9480	-0.8671
C	-0.6552	-4.1220	-0.3428
C	0.3294	-3.6951	0.5509
N	0.3191	-2.3248	0.5527
N	-0.6430	-1.8659	-0.3176
H	-0.9102	-5.1545	-0.5807
N	2.0013	-0.4224	0.4030
C	3.3510	-0.2333	0.2651
C	3.5354	0.7703	-0.6911
C	2.2380	1.1570	-1.1049
N	1.3185	0.4241	-0.4339
H	4.4900	1.1662	-1.0371
B	1.2040	-1.3373	1.3703
H	1.9676	-1.9681	2.0609
C	-2.2572	2.1533	2.3762
H	-2.3427	2.2340	1.2753
C	1.1274	-1.0860	4.5621
H	0.9520	-2.1727	4.4631
H	2.2042	-0.9125	4.3841
H	0.9028	-0.7986	5.6025
C	-3.6347	1.7377	2.9403
H	-3.5942	1.6341	4.0403
H	-4.4007	2.4972	2.6981
H	-3.9637	0.7713	2.5211
C	-1.8289	3.5359	2.9153
H	-1.7222	3.5163	4.0155
H	-0.8605	3.8480	2.4865
H	-2.5854	4.3012	2.6625
C	1.2629	-4.5197	1.3886
H	2.3226	-4.3199	1.1482
H	1.1315	-4.3273	2.4686
H	1.0685	-5.5898	1.2071
C	-2.3679	-2.8394	-1.8714
H	-2.5381	-1.7630	-2.0570
C	-1.9842	-3.5014	-3.2138
H	-1.7962	-4.5828	-3.0816
H	-2.8020	-3.3878	-3.9488
H	-1.0716	-3.0475	-3.6376
C	-3.6765	-3.4411	-1.3102
H	-3.5549	-4.5191	-1.0965
H	-3.9769	-2.9410	-0.3732
H	-4.4985	-3.3308	-2.0410
C	4.3753	-1.0097	1.0401
H	5.3868	-0.7006	0.7289
H	4.2863	-0.8419	2.1287
H	4.2833	-2.0975	0.8694
C	1.8383	2.2141	-2.1091
H	0.7326	2.2688	-2.0929
C	2.3799	3.6035	-1.7075
H	3.4853	3.6122	-1.7025
H	2.0389	4.3732	-2.4240
H	2.0340	3.8892	-0.6986
C	2.2823	1.8328	-3.5392
H	3.3834	1.7568	-3.6024
H	1.8575	0.8609	-3.8439
H	1.9513	2.5966	-4.2666
O	-0.9922	0.3451	-3.5083
C	-0.8563	0.3244	-2.3492
O	-3.8487	0.2653	-0.3220
C	-2.6823	0.3008	-0.3209

MECP ($Tp^{i\text{-}Pr,Me}CoCO + CO$)

Co	-0.8285	0.2024	-0.4641
C	-1.2078	1.1043	2.6506
C	-0.6897	0.6880	3.9002
C	0.2631	-0.2947	3.6158
N	0.3000	-0.4451	2.2556
N	-0.5976	0.4082	1.6605
H	-0.9639	1.0553	4.8887
C	-1.2418	-2.9481	-0.8646
C	-0.6546	-4.1248	-0.3425
C	0.3306	-3.7023	0.5521
N	0.3228	-2.3324	0.5553
N	-0.6389	-1.8679	-0.3110
H	-0.9117	-5.1566	-0.5824
N	1.9928	-0.4235	0.4015
C	3.3413	-0.2342	0.2619
C	3.5238	0.7693	-0.6944
C	2.2264	1.1580	-1.1058
N	1.3073	0.4248	-0.4314
H	4.4780	1.1679	-1.0376
B	1.2025	-1.3425	1.3685
H	1.9709	-1.9649	2.0611
C	-2.2571	2.1555	2.3722
H	-2.3446	2.2392	1.2719
C	1.1258	-1.0844	4.5569
H	0.9523	-2.1716	4.4613
H	2.2026	-0.9096	4.3800
H	0.8998	-0.7942	5.5962
C	-3.6331	1.7395	2.9394
H	-3.5907	1.6363	4.0394
H	-4.3988	2.4994	2.6984
H	-3.9631	0.7733	2.5207
C	-1.8267	3.5363	2.9152
H	-1.7206	3.5149	4.0155
H	-0.8584	3.8493	2.4871
H	-2.5831	4.3021	2.6636
C	1.2651	-4.5243	1.3906
H	2.3242	-4.3217	1.1498
H	1.1331	-4.3294	2.4702
H	1.0731	-5.5951	1.2113
C	-2.3651	-2.8372	-1.8693
H	-2.5356	-1.7613	-2.0551
C	-1.9824	-3.4990	-3.2123
H	-1.7950	-4.5807	-3.0809
H	-2.8006	-3.3845	-3.9466
H	-1.0701	-3.0452	-3.6366
C	-3.6743	-3.4386	-1.3092
H	-3.5536	-4.5168	-1.0961
H	-3.9751	-2.9383	-0.3725
H	-4.4954	-3.3272	-2.0408
C	4.3674	-1.0073	1.0379
H	5.3776	-0.6951	0.7256
H	4.2791	-0.8385	2.1265
H	4.2785	-2.0956	0.8685
C	1.8339	2.2172	-2.1099
H	0.7286	2.2761	-2.0970
C	2.3808	3.6045	-1.7064
H	3.4864	3.6110	-1.7015
H	2.0419	4.3756	-2.4223
H	2.0354	3.8905	-0.6975
C	2.2825	1.8350	-3.5386
H	3.3838	1.7590	-3.5995
H	1.8582	0.8632	-3.8440
H	1.9537	2.5988	-4.2670
O	-0.9956	0.3481	-3.4537
C	-0.8592	0.3524	-2.2933
O	-3.8154	0.2800	-0.3363
C	-2.6479	0.3247	-0.3214

Table S9.
Coordinates of some species involved in the reaction $[N_3N]WH + H_2$

$^1[\{N_3N\}W](H)_3$

W	0.0111	0.0298	-0.0026
H	0.9912	0.3008	1.3626
N	-0.0536	0.0674	-2.3145
N	0.8531	1.8390	-0.3843
N	1.1677	-1.5780	-0.4311
N	-1.9779	-0.1829	-0.3296
C	-1.4741	0.3241	-2.6981
H	-1.6480	0.0292	-3.7547
H	-1.6458	1.4101	-2.6050
C	0.4193	-1.2751	-2.7703
H	-0.4353	-1.9684	-2.6848
H	0.7326	-1.2322	-3.8349
C	0.8535	1.1695	-2.7564
H	1.8848	0.7777	-2.7263
H	0.6180	1.4670	-3.8003
C	1.5442	-1.7619	-1.8519
H	2.4924	-1.2294	-2.0851
H	1.7291	-2.8281	-2.0932
C	0.7404	2.3371	-1.7731
H	1.5403	3.0634	-2.0155
H	-0.2192	2.8781	-1.9286
C	-2.4063	-0.4084	-1.7301
H	-2.4381	-1.4945	-1.9668
H	-3.4338	-0.0293	-1.9103
Si	1.6529	2.8766	0.8397
Si	-3.3128	-0.1693	0.8672
Si	1.7399	-2.8207	0.7256
C	2.2217	-2.1238	2.4168
H	1.3528	-1.7031	2.9492
H	2.6626	-2.9298	3.0358
H	2.9725	-1.3199	2.3089
C	0.3872	-4.1370	0.9320
H	-0.5254	-3.6714	1.3470
H	0.1223	-4.5980	-0.0385
H	0.7091	-4.9446	1.6171
C	3.3013	-3.6554	0.0141
H	3.6983	-4.3758	0.7550
H	3.1144	-4.2152	-0.9211
H	4.0956	-2.9112	-0.1856
C	0.5376	3.1991	2.3353
H	0.3178	2.2588	2.8690
H	1.0266	3.9009	3.0386
H	-0.4254	3.6409	2.0185
C	2.0550	4.5699	0.0555
H	1.1567	5.0650	-0.3591
H	2.4685	5.2340	0.8389
H	2.8121	4.5012	-0.7485
C	3.2968	2.1172	1.4063
H	3.8256	2.7995	2.0998
H	3.1227	1.1577	1.9242
H	3.9605	1.9225	0.5427
C	-4.1002	1.5596	0.8552
H	-3.3605	2.3091	1.1923
H	-4.4385	1.8477	-0.1582
H	-4.9753	1.6082	1.5311
C	-2.7969	-0.6183	2.6288
H	-2.1301	0.1417	3.0689
H	-3.7021	-0.7056	3.2615
H	-2.2611	-1.5839	2.6489
C	-4.6184	-1.4506	0.3283
H	-5.4503	-1.4630	1.0585
H	-5.0533	-1.2388	-0.6658
H	-4.1830	-2.4676	0.3004
H	-0.1925	-0.9671	1.3650
H	-0.6935	0.6901	1.3977

TS **([N_3N]WH + H_2)**

W	0.1337	-0.1741	0.0777
H	0.5682	-0.9683	1.5001
N	0.4298	-0.2413	-2.4186
N	-1.1520	-1.5686	-0.5537
N	0.6934	1.6534	-0.4940
N	2.0588	-0.9800	-0.2154
C	1.7446	-0.9124	-2.6515
H	2.1633	-0.6013	-3.6322
H	1.5749	-2.0016	-2.6837
C	0.4354	1.1730	-2.8845
H	1.4609	1.4276	-3.2045
H	-0.2316	1.2989	-3.7593
C	-0.7028	-1.0755	-2.9012
H	-1.6012	-0.4361	-2.9471
H	-0.5008	-1.4831	-3.9161
C	0.0246	2.1109	-1.7260
H	-1.0732	2.0830	-1.5863
H	0.2982	3.1527	-1.9911
C	-0.9456	-2.1938	-1.8695
H	-1.8237	-2.7910	-2.1849
H	-0.0792	-2.8874	-1.8467
C	2.6977	-0.6133	-1.4905
H	2.9416	0.4736	-1.4871
H	3.6503	-1.1529	-1.6798
Si	-2.7556	-1.7680	0.2392
Si	3.0131	-2.1190	0.7707
Si	1.6144	2.8435	0.4844
C	0.3786	4.0619	1.2453
H	-0.3531	3.5092	1.8621
H	0.8941	4.7988	1.8904
H	-0.1801	4.6186	0.4704
C	2.5917	1.9617	1.8370
H	1.9202	1.4960	2.5789
H	3.2225	1.1636	1.4081
H	3.2456	2.6858	2.3606
C	2.8281	3.7822	-0.6406
H	3.3436	4.5730	-0.0623
H	3.6007	3.1010	-1.0437
H	2.3242	4.2729	-1.4941
C	-2.6878	-1.3993	2.0934
H	-2.5813	-0.3203	2.2919
H	-3.6177	-1.7624	2.5744
H	-1.8326	-1.9163	2.5663
C	-3.2131	-3.6126	0.0762
H	-2.4302	-4.2467	0.5330
H	-4.1598	-3.8033	0.6178
H	-3.3563	-3.9456	-0.9683
C	-4.0860	-0.7202	-0.6146
H	-5.0688	-0.8638	-0.1258
H	-3.8154	0.3484	-0.5467
H	-4.1979	-0.9887	-1.6820
C	3.0643	-3.8090	-0.1096
H	2.0459	-4.2360	-0.1773
H	3.4709	-3.7307	-1.1359
H	3.6986	-4.5251	0.4479
C	2.3411	-2.3942	2.5200
H	1.3484	-2.8772	2.5155
H	3.0438	-3.0532	3.0684
H	2.2531	-1.4458	3.0794
C	4.8103	-1.5062	0.9599
H	5.4124	-2.2672	1.4935
H	5.3044	-1.3117	-0.0101
H	4.8487	-0.5728	1.5526
H	-0.1673	0.5978	1.5672
H	-1.4660	0.6074	0.2901

Intermediate

([N_3N]WH + H_2)

W	0.0000	0.0000	0.0000
H	0.0000	0.0000	1.7189
N	0.9070	0.0000	-2.2304
N	-0.2704	-1.8557	-0.6672
N	0.0844	1.9177	-0.5592
N	2.0802	-0.0187	0.3628
C	2.3479	-0.3691	-2.0742
H	2.9167	-0.0919	-2.9882
H	2.4074	-1.4623	-1.9451
C	0.7462	1.3701	-2.8184
H	1.7328	1.8640	-2.7915
H	0.4306	1.3009	-3.8786
C	0.1267	-1.0328	-2.9601
H	-0.8644	-0.5973	-3.1646
H	0.6109	-1.3007	-3.9249
C	-0.2440	2.1899	-1.9647
H	-1.2851	1.8758	-2.1765
H	-0.1438	3.2629	-2.2309
C	-0.0355	-2.2685	-2.0623
H	-0.8683	-2.8776	-2.4726
H	0.8700	-2.9115	-2.1139
C	2.9054	0.3048	-0.8147
H	2.9346	1.4058	-0.9778
H	3.9646	-0.0131	-0.7056
Si	-1.3060	-3.0186	0.2467
Si	3.0268	-0.6077	1.7385
Si	0.5767	3.3343	0.4301
C	-0.8782	4.5530	0.3408
H	-1.7901	4.0847	0.7542
H	-0.6531	5.4581	0.9372
H	-1.1004	4.8767	-0.6926
C	0.8800	2.8829	2.2347
H	-0.0049	2.3963	2.6815
H	1.7316	2.1898	2.3314
H	1.1044	3.8020	2.8098
C	2.1252	4.1759	-0.2872
H	2.3144	5.1326	0.2374
H	3.0192	3.5382	-0.1606
H	2.0139	4.4031	-1.3643
C	-1.2924	-2.7351	2.1137
H	-1.6363	-1.7225	2.3832
H	-1.9702	-3.4737	2.5854
H	-0.2832	-2.8816	2.5372
C	-0.6005	-4.7531	-0.0871
H	0.4510	-4.8217	0.2485
H	-1.1857	-5.5055	0.4759
H	-0.6386	-5.0314	-1.1561
C	-3.0833	-2.9105	-0.4038
H	-3.7321	-3.6537	0.0983
H	-3.4872	-1.9010	-0.2071
H	-3.1410	-3.0929	-1.4931
C	3.7414	-2.3265	1.3186
H	2.9226	-3.0537	1.1621
H	4.3520	-2.3026	0.3955
H	4.3850	-2.7029	2.1371
C	2.0419	-0.7542	3.3478
H	1.2074	-1.4706	3.2626
H	2.7195	-1.1040	4.1515
H	1.6139	0.2164	3.6544
C	4.5013	0.5544	2.0888
H	5.1183	0.1470	2.9132
H	5.1621	0.6802	1.2105
H	4.1526	1.5592	2.3941
H	-1.5667	0.0976	0.7213
H	-1.4275	0.2310	-0.9675

MECP **([N_3N]WH + H_2)**

W	0.4274	0.0191	0.1485
H	0.1579	-0.0888	1.8689
N	0.6900	-0.0405	-2.2068
N	0.7767	1.9702	-0.3112
N	1.2781	-1.8077	-0.1756
N	-1.4489	-0.3250	-0.4256
C	-0.6943	0.0692	-2.7539
H	-0.7363	-0.2904	-3.8044
H	-0.9767	1.1353	-2.7410
C	1.3531	-1.3289	-2.5763
H	0.5609	-2.0599	-2.8137
H	1.9854	-1.1941	-3.4795
C	1.5383	1.1398	-2.5257
H	2.5689	0.8743	-2.2315
H	1.5288	1.3604	-3.6169
C	2.1468	-1.8471	-1.3629
H	3.0510	-1.2148	-1.2100
H	2.5196	-2.8690	-1.5896
C	1.0676	2.3505	-1.7110
H	1.8614	3.1265	-1.7764
H	0.1696	2.7978	-2.1933
C	-1.6563	-0.7083	-1.8456
H	-1.4951	-1.8012	-1.9728
H	-2.6922	-0.5036	-2.1878
Si	0.6175	3.3885	0.7602
Si	-2.9598	-0.1267	0.5159
Si	0.9550	-3.3534	0.6384
C	2.5625	-4.0963	1.3353
H	2.9785	-3.4445	2.1260
H	2.3644	-5.0900	1.7819
H	3.3386	-4.2254	0.5579
C	-0.2792	-3.1343	2.0490
H	0.0704	-2.3769	2.7719
H	-1.2559	-2.7970	1.6603
H	-0.4271	-4.0947	2.5795
C	0.2182	-4.5704	-0.6306
H	0.0380	-5.5627	-0.1745
H	-0.7507	-4.1858	-1.0019
H	0.8813	-4.7204	-1.5038
C	-0.2011	2.9799	2.4115
H	0.2921	2.1337	2.9193
H	-0.1548	3.8689	3.0705
H	-1.2636	2.7143	2.2703
C	-0.4588	4.6988	-0.1100
H	-1.4412	4.2731	-0.3900
H	-0.6440	5.5484	0.5752
H	0.0097	5.1035	-1.0262
C	2.3247	4.1517	1.1118
H	2.2081	5.0840	1.6982
H	2.9506	3.4559	1.7009
H	2.8750	4.4035	0.1861
C	-3.8227	1.4786	-0.0308
H	-3.2146	2.3608	0.2433
H	-3.9838	1.5062	-1.1251
H	-4.8111	1.5785	0.4575
C	-2.7081	-0.0879	2.3867
H	-2.0256	0.7168	2.7034
H	-3.6911	0.0686	2.8734
H	-2.2858	-1.0384	2.7555
C	-4.1167	-1.5878	0.1239
H	-5.0608	-1.4839	0.6924
H	-4.3793	-1.6496	-0.9483
H	-3.6521	-2.5478	0.4175
H	2.5472	0.2954	0.6396
H	2.1481	0.2517	1.3247