Supporting Information

Cleavage of Carbon Monoxide Promoted by a Dinuclear Tantalum Tetrahydride Complex

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X-ray Crystallographic Analyses

Suitable single crystals were selected in a glovebox, coated in Fomblin oil and mounted on a glass fiber. X-ray data were collected on a Bruker X8 Apex II (compound **4**) or on a Rigaku/ADSC CCD (compound **1**) diffractometer with graphite-monochromated Mo K_α radiation (λ = 0.71073 Å) at a temperature of –100 ± 1°C. Data were collected and integrated using the Bruker SAINT software package.[1] Absorption corrections were performed using the multiscan technique (SADABS).[2] The structures were solved by direct methods and refined using all reflections with the SHELX-97 program package.[3] All non-hydrogen atoms were refined anisotropically (except for **1**, see below). For disordered solvent molecules in **7** (Et_2O or pentane) no satisfactory model was obtained. For further refinement, the contributions of these Q-peaks were subtracted from the reflection data using the SQUEEZE[4] routine in the PLATON program package.[5] The bridging hydride and H17 in **4** were located in the electron density map and refined isotropically. The bridging hydrides in **7** were not located in the electron density map and modeled using the XHydex program.[6] All other hydrogen atoms were placed in calculated positions and assigned to an isotropic displacement parameter. Due to these non-refined hydrides and several meaningless Q-peaks close to the Tantalum atoms, an atypical ratio between the highest peak (4.172 $e^-/Å^3$) and the deepest hole (–1.544 $e^-/Å^3$) in the residual electron density is observed. Refinement of **1** is incomplete due to low data completeness to θ (85.8%) and disordered N-Ph rings (approx. 20% of the main residue is disordered). Some carbon atoms of these N-Ph moieties could not be modeled anisotropically. The structure of **1** establishes the atom connectivity, but great care should be taken when interpreting bond distances and angles. All structures were solved and refined using the WinGX (version 1.80.05) software package.[7]

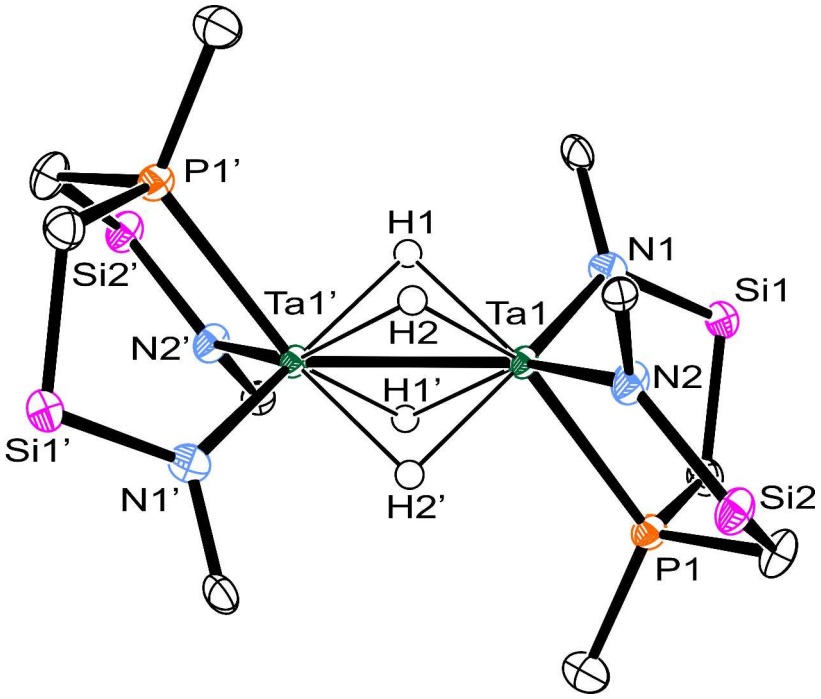

Figure S1. ORTEP plot (30% thermal ellipsoids) of the molecular structure of **1** (*refinement incomplete*). Silyl-methyl and ligand N,P-phenyl-ring carbons (except ipso positions) have been omitted for clarity. Selected bond lengths (Å, rounded to two decimal places) and angles (deg, rounded to integer values): Ta1-Ta1' 2.57; Ta1-N1 2.08; Ta1-N2 2.09; Ta1-P1 2.56; Ta-H ranging from 1.87 to 1.92; N1-Ta1-N2 113; H-Ta-H (*cis*) 61 to 64; H-Ta-H (*trans*) 91 to 94; P1-Ta1-Ta1'-P1' 180; H1-H1'-H2'-H2 0.

Table S1. Crystal data and refinement details for **1** and **4**.

compound	**1**	**4**
empirical formula	$C_{48}H_{66}N_4P_2Si_4Ta_2$	$C_{48}H_{62}N_4OP_2Si_4Ta_2$
formula weight	1235.25	1247.22
crystal size [mm]	0.50 × 0.50 × 0.30	0.22 × 0.20 × 0.12
crystal system	triclinic	monoclinic
space group	*P*–1 (No. 2)	$P2_1/n$ (No. 14)
a [Å]	11.1762(10)	11.708(3)
b [Å]	13.7750(7)	18.122(2)
c [Å]	18.7857(10)	23.792(3)
α [°]	86.1540(10)	90
β [°]	87.253(2)	95.309(3)
γ [°]	66.044(2)	90
V [Å^3]	2636.3(3)	5026(3)
$\rho_{calcd.}$ [g cm^{-3}]	1.556	1.648
Z	2	4
F(000)	1228	2472

μ [mm^{-1}]	4.334 (Mo-K_α)	4.549 (Mo-K_α)
T_{min}/T_{max}	0.646 / 1.000	0.579 / 0.593
hkl range	–10 - 14, –14- 17, ±32	–13 - 11, ±21, ±28
θ range [°]	3.24 - 27.16	1.41 - 25.27
measured refl.	10064	34274
unique refl.	10064	8944
Refined parameters	507	566
completeness to θ [%]	85.8	98.0
goodness-of-fit	1.105	1.146
*R*1, *wR*2 ($I>2\sigma(I)$)	0.0262, 0.0679	0.0248, 0.0650
*R*1, *wR*2 (all data)	0.0317, 0.0731	0.0329, 0.0754
res. el. dens. [e Å^{-3}]	2.323 / –1.734	1.369 / –1.385

References

[1] SAINT. Version 7.03A. Bruker AXS Inc., Madison, Wisconsin, USA (1997-2003).

[2] SADABS. Bruker Nonius area detector scaling and absorption correction - V2.10, Bruker AXS Inc., Madison, Wisconsin, USA (2003).

[3] G. M. Sheldrick, *Acta Cryst.* **2008**, *A64*, 112-122.

[4] P. v. d. Sluis, A. L. Spek, *Acta Cryst.* **1990**, *A46*, 194-201.

[5] A. L. Spek, *J. Appl. Cryst.* **2003**, *36*, 7-13.

[6] A. G. Orpen, *Dalton Trans.* **1980**, 2509-2516.

[7] L. J. Farrugia, *J. Appl. Cryst.* **1999**, *32*, 837-838.

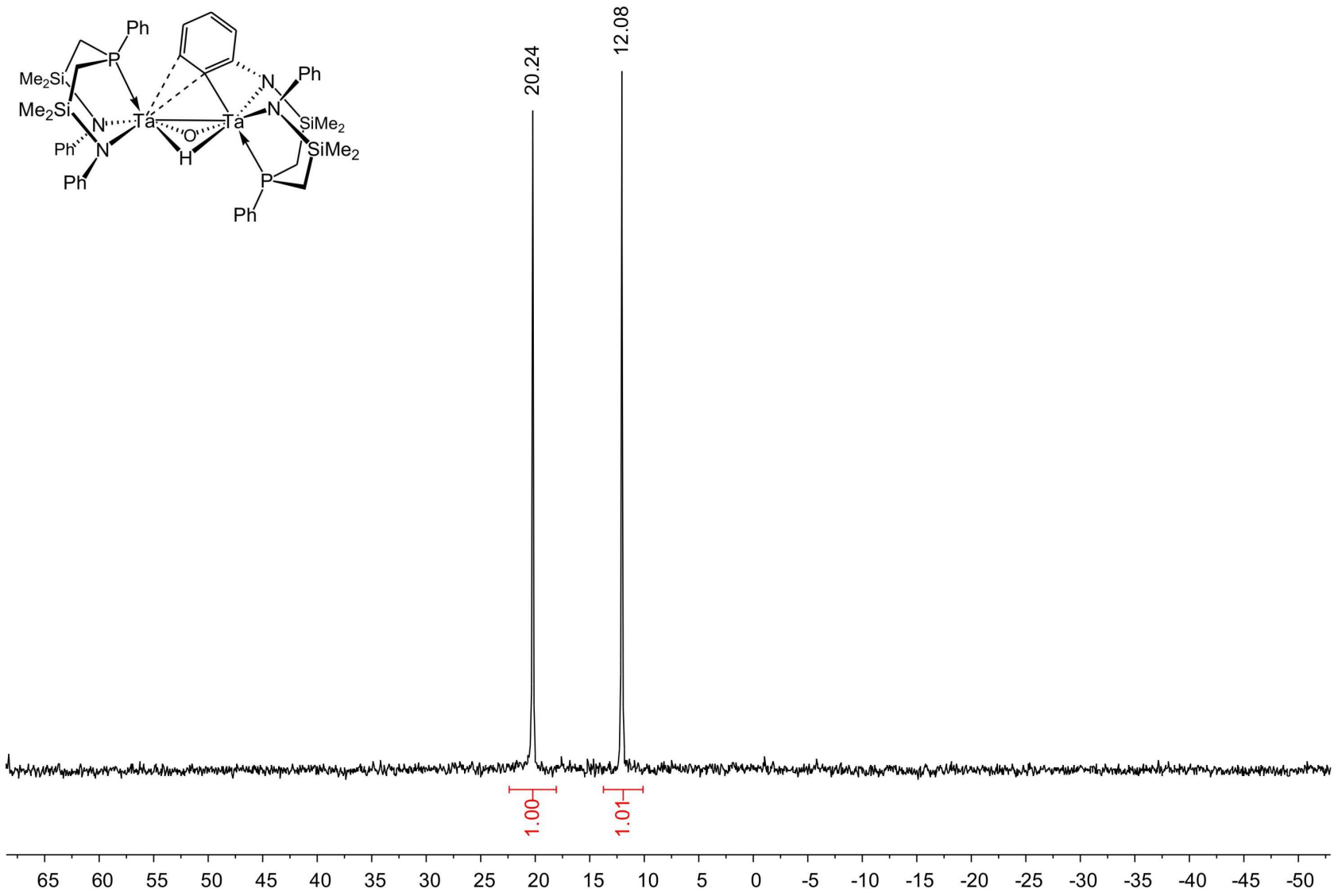

Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum (161.9 MHz, RT) of **4** in C_6D_6.

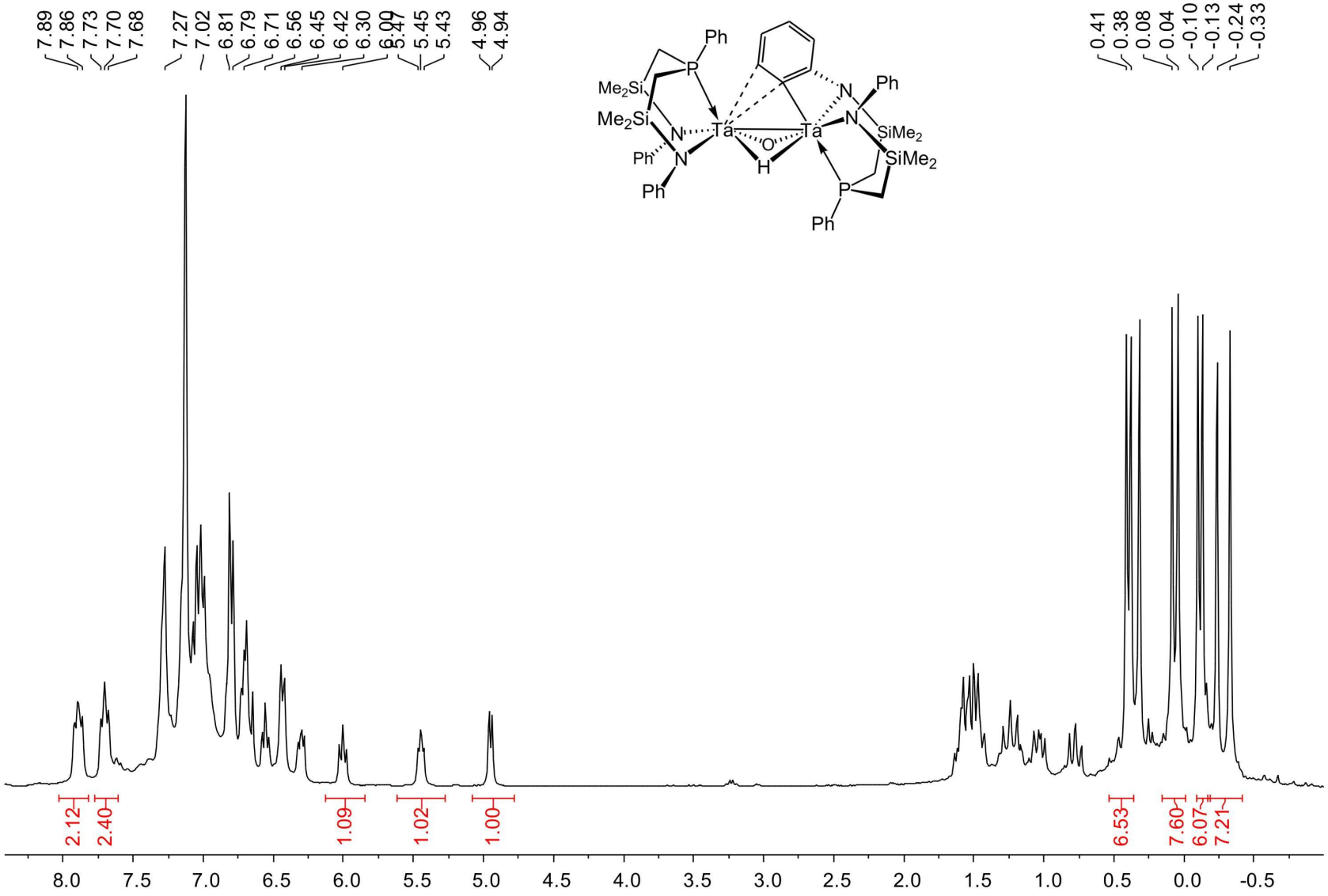

Figure S3. ^{1}H NMR spectrum (400MHz, RT) of **4** in C_6D_6.

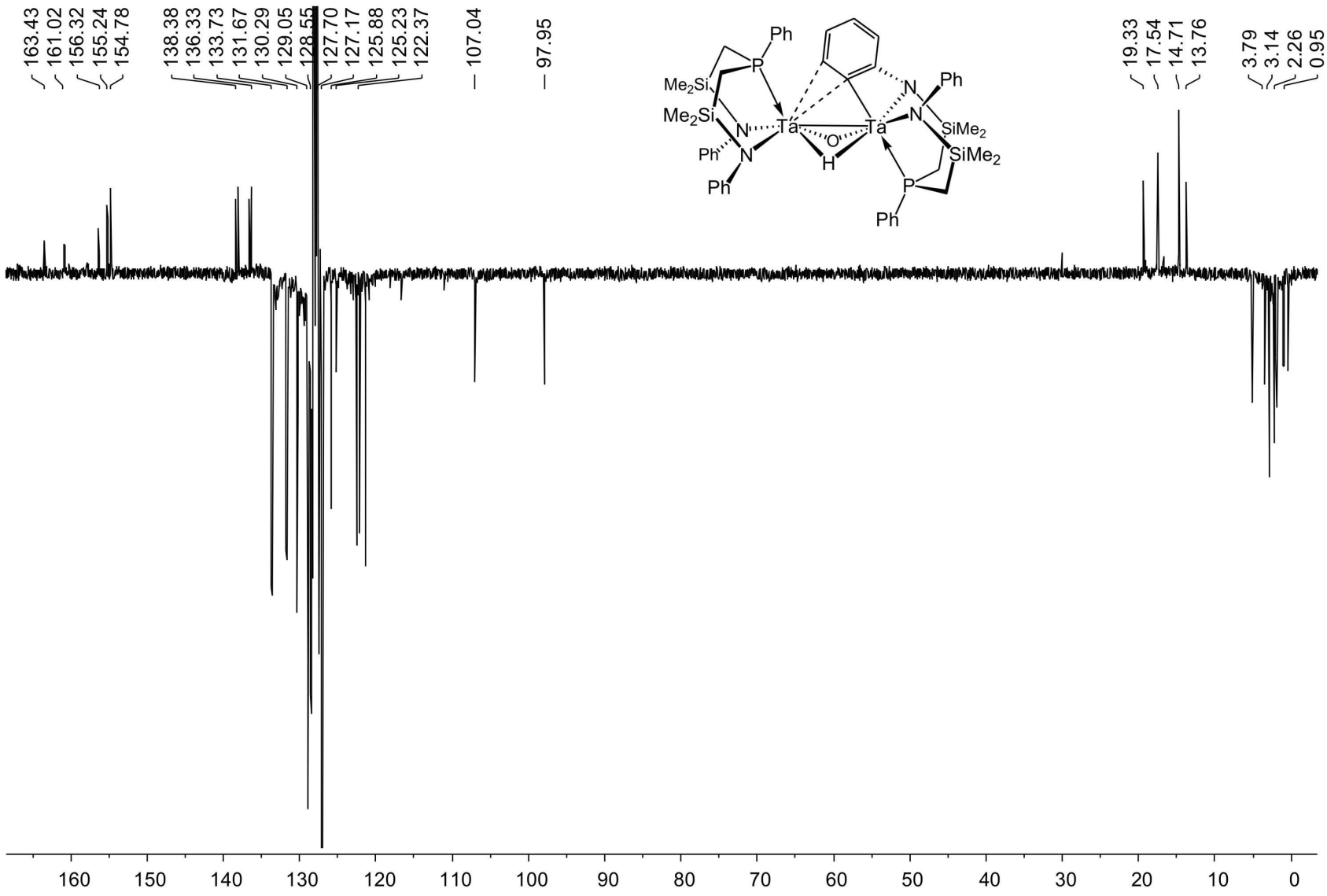

Figure S4. ^{13}C APT spectrum (100MHz, RT) of **4** in C_6D_6.

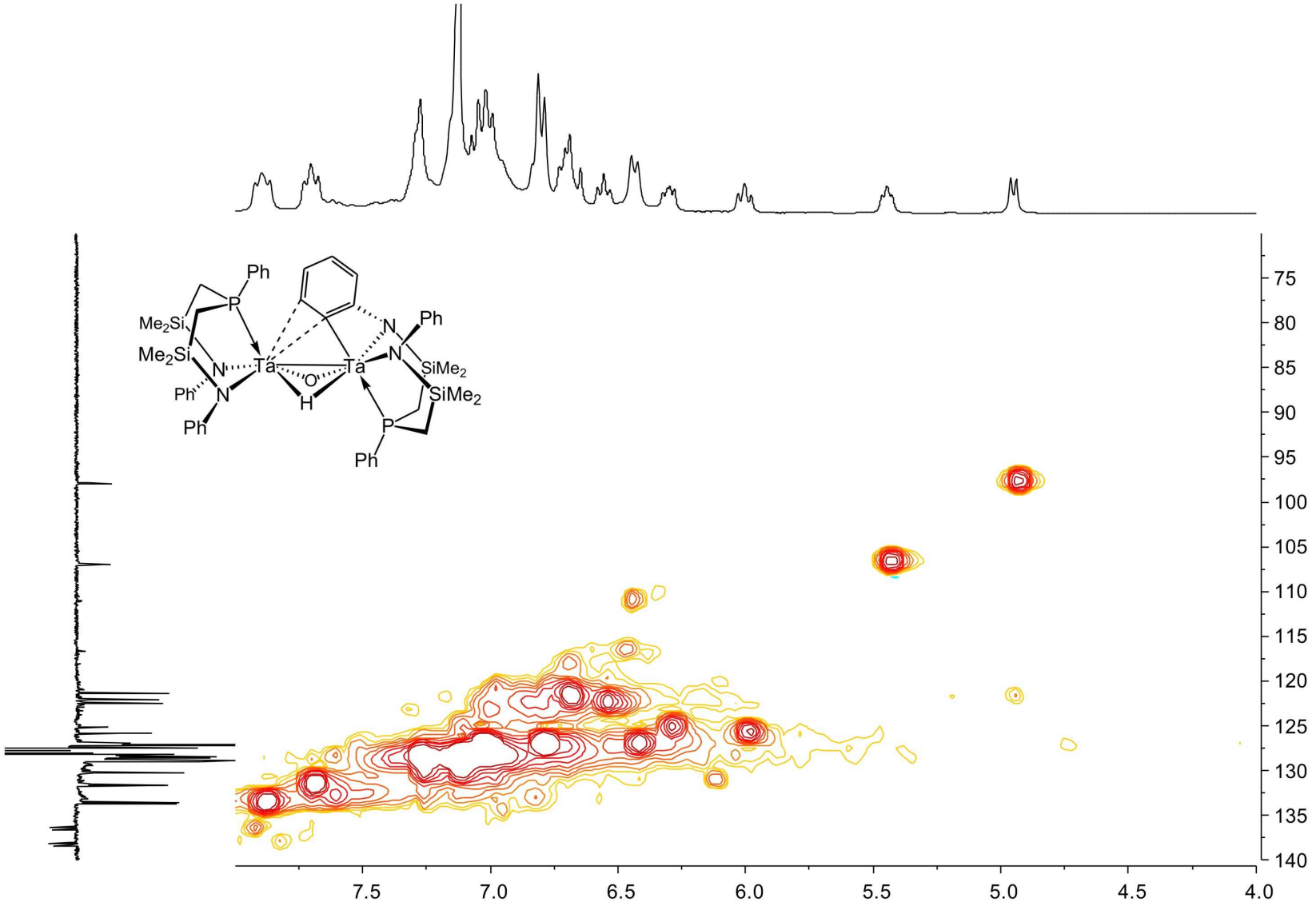

Figure S5. HSQC spectrum (RT, external ^{1}H and ^{13}C APT traces) of **4** in C_6D_6.

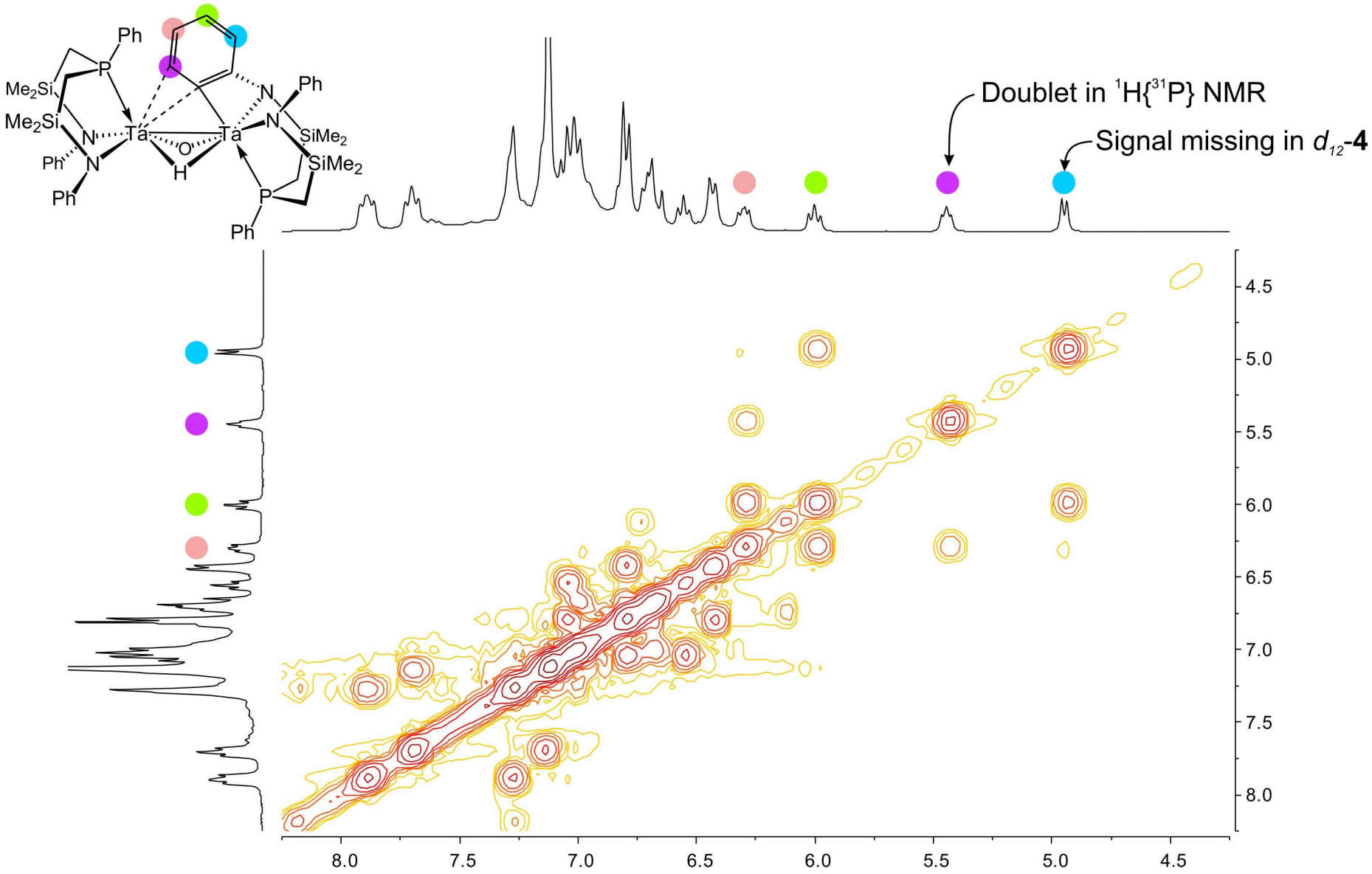

Figure S6. $^{1}H,^{1}H$-COSY spectrum (400MHz, RT) of **4** in C_6D_6.

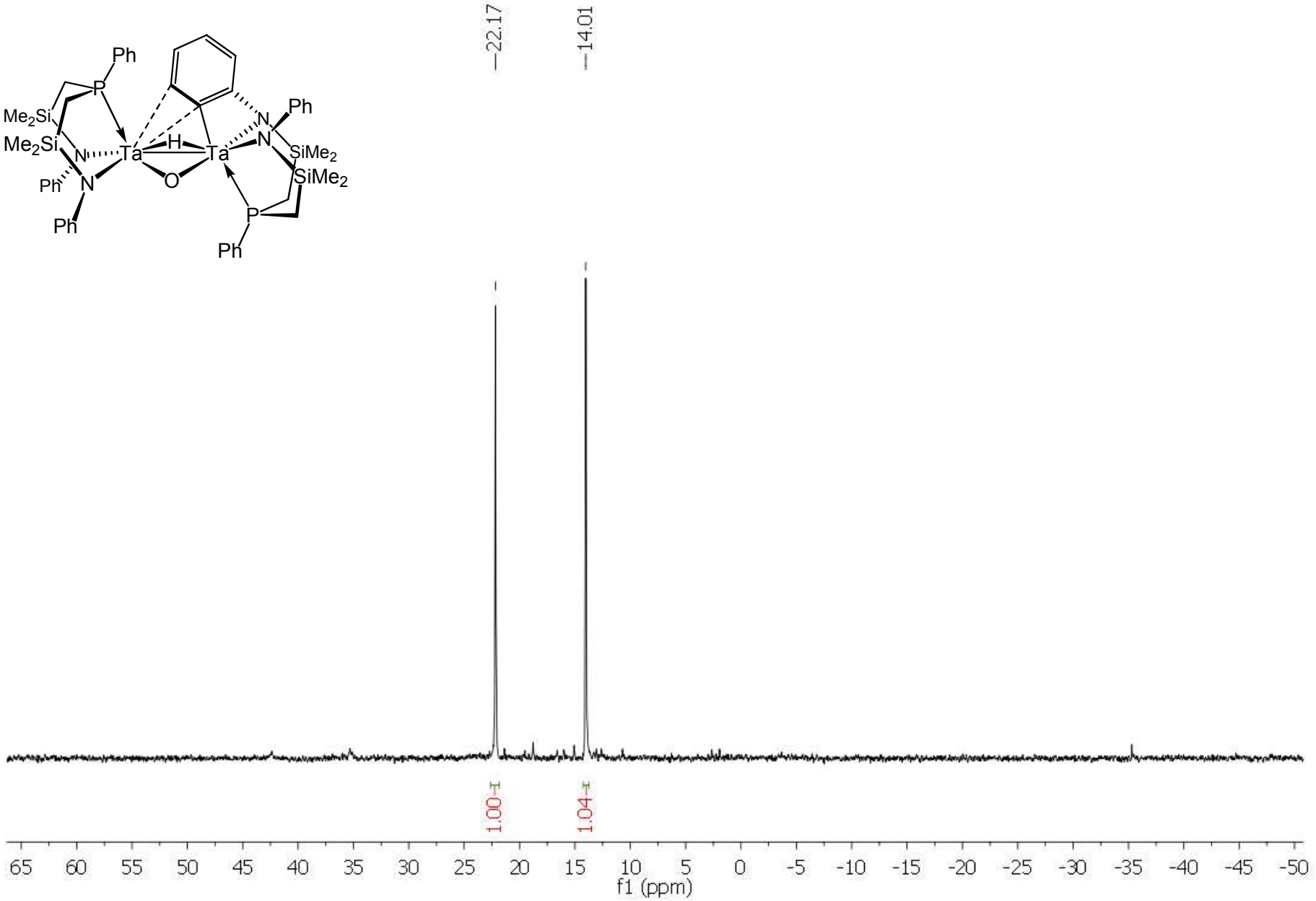

Figure S7. $^{31}P\{^{1}H\}$ spectrum (162 MHz, RT) of ^{13}C-**4** in C_6D_6

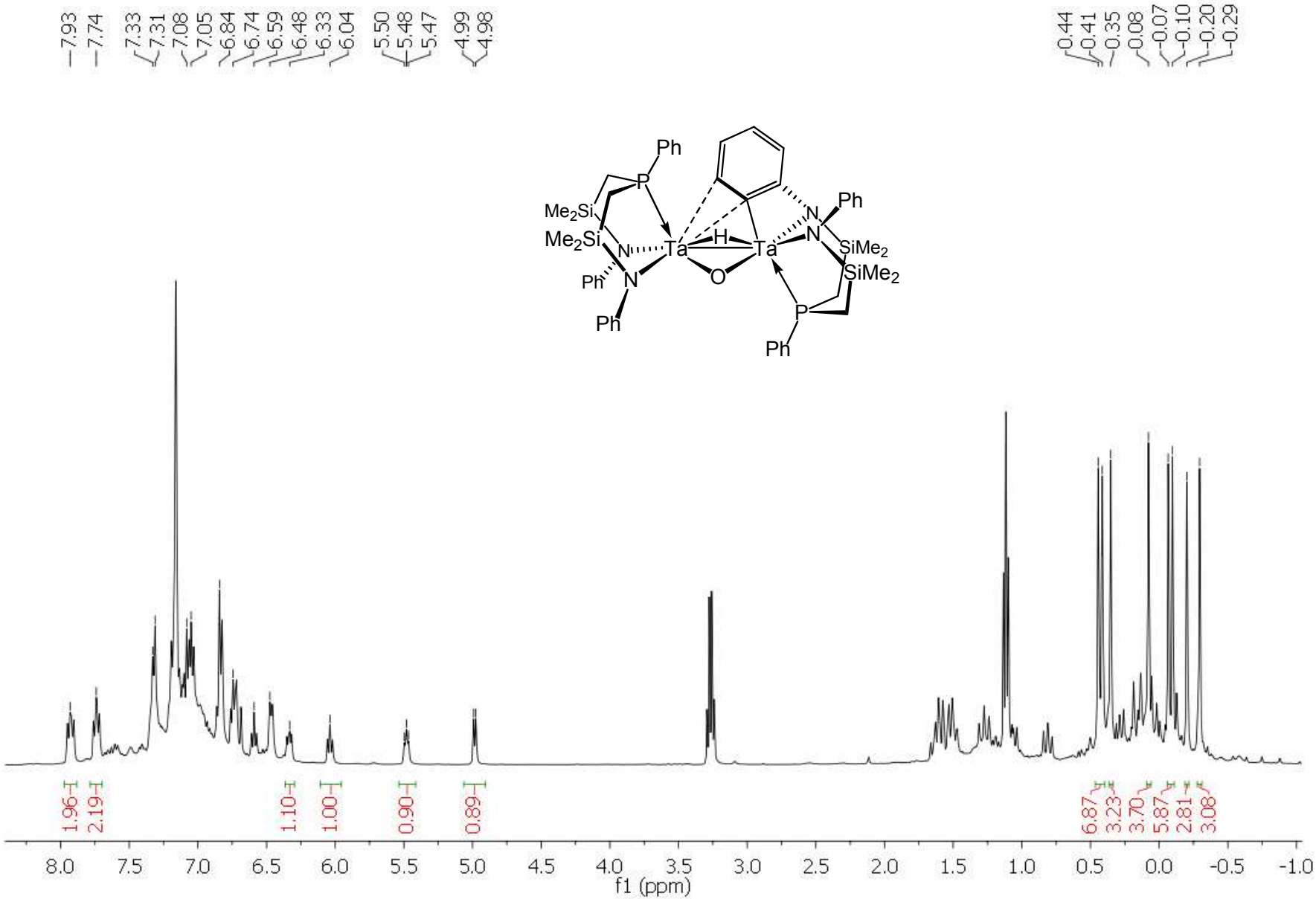

Figure S8. ^{1}H spectrum (400 MHz, RT) of ^{13}C-**4** in C_6D_6 (residual Et_2O at δ 3.25 and 1.1)

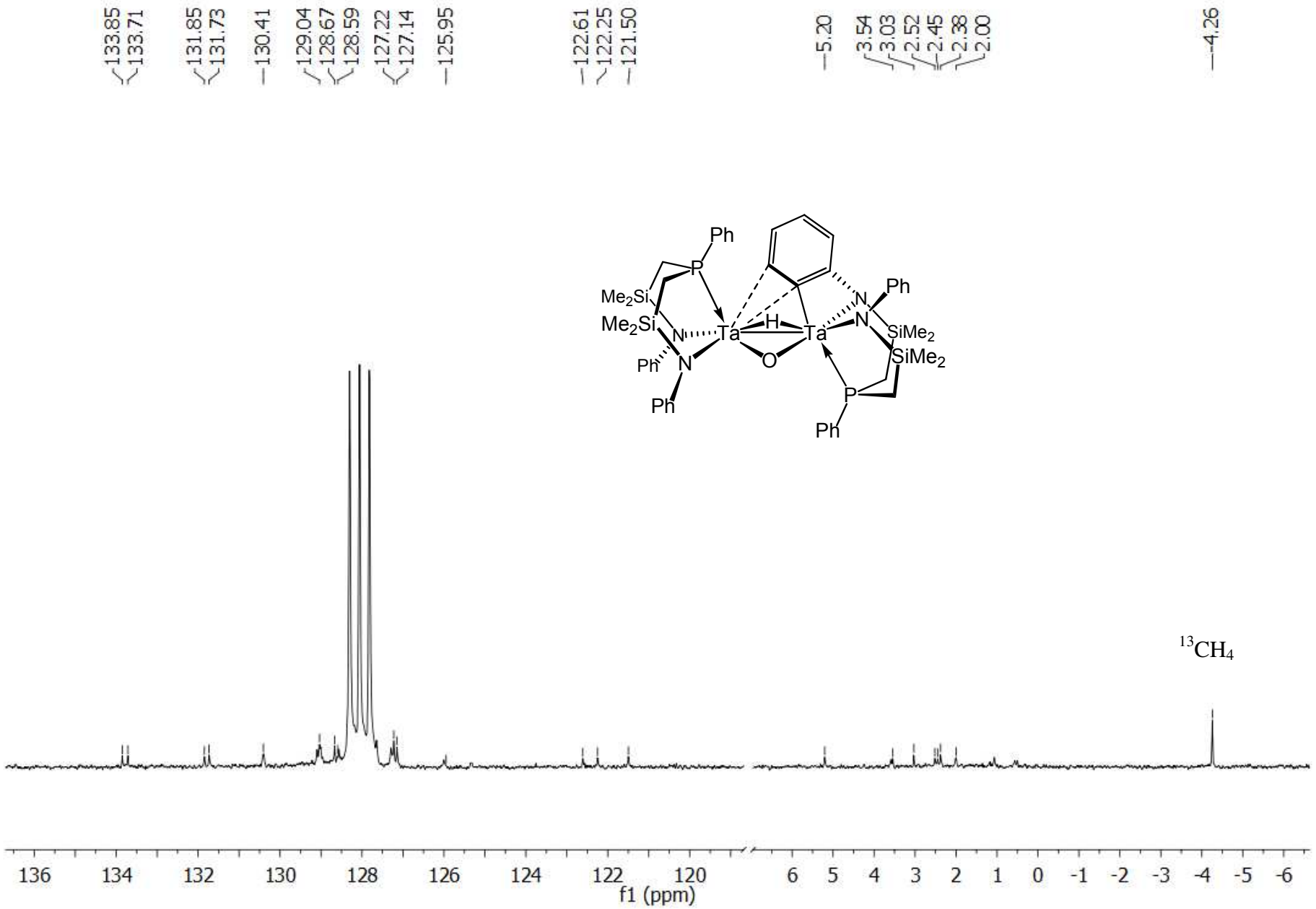

Figure S9. $^{13}C\{^{1}H\}$ spectrum (101 MHz, RT) from ^{13}C-**4** in C_6D_6

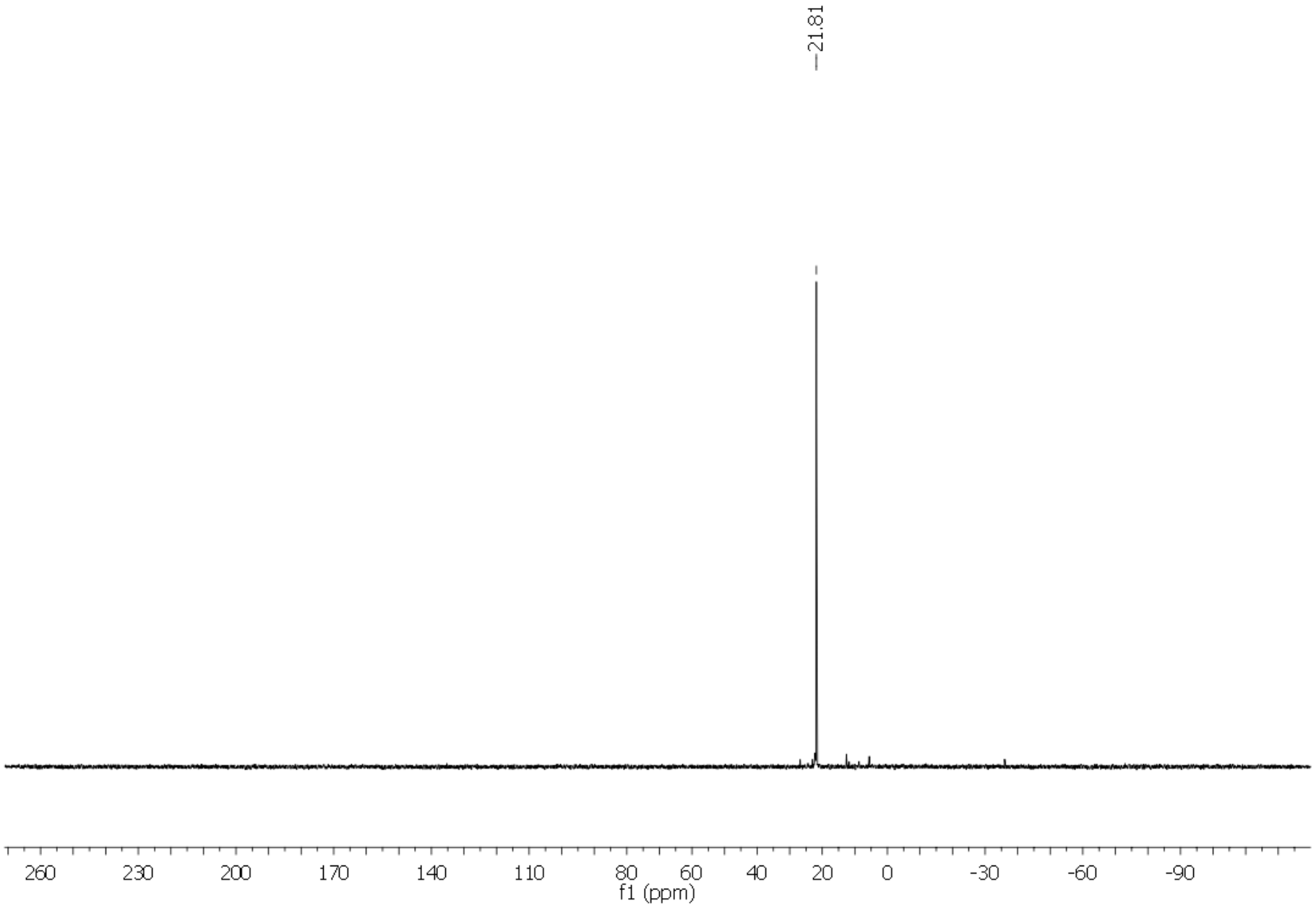

Figure S10. $^{31}P\{^{1}H\}$ spectrum (161 MHz, RT) of **1** in C_6D_6.

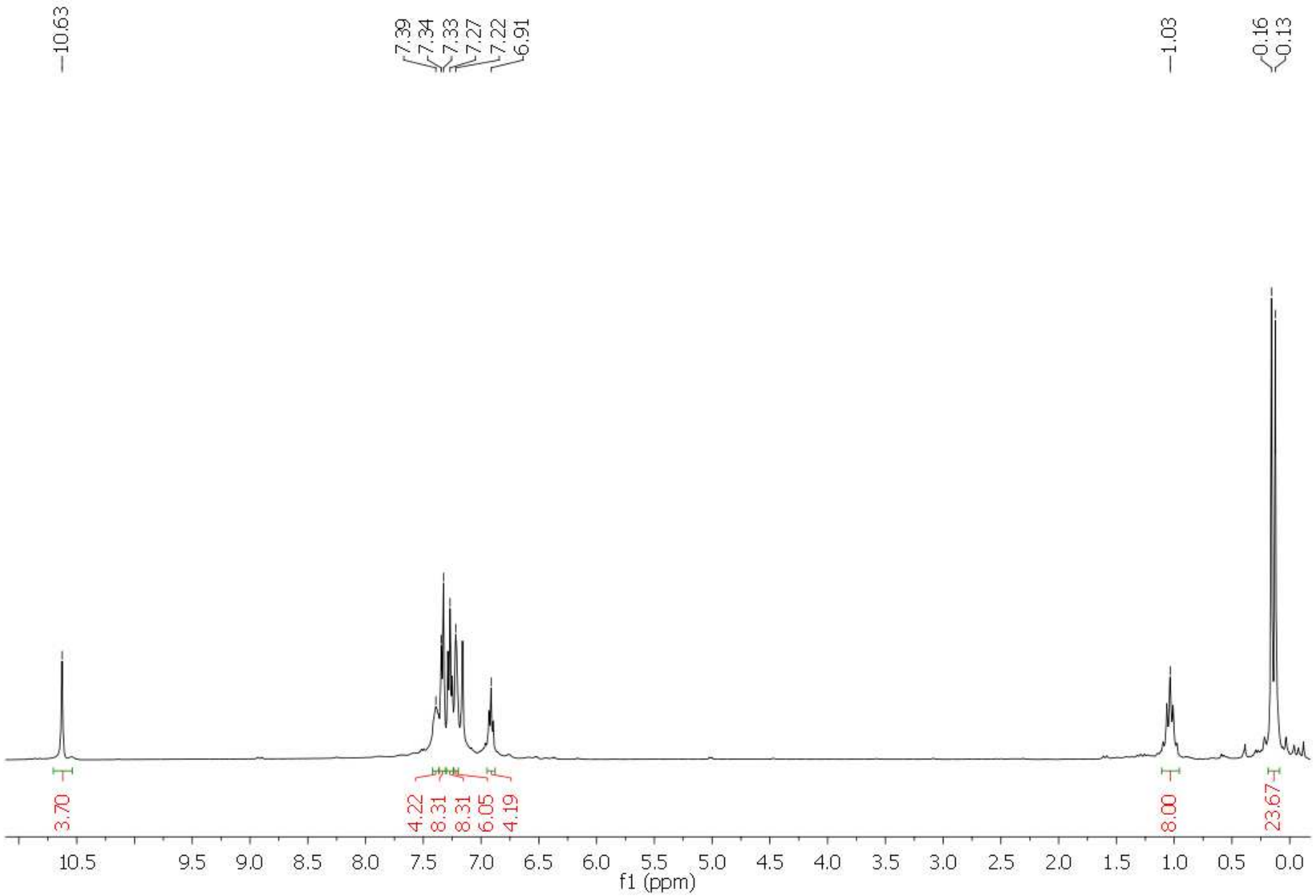

Figure S11. ^{1}H spectrum (400 MHz, C_6D_6) of **1**

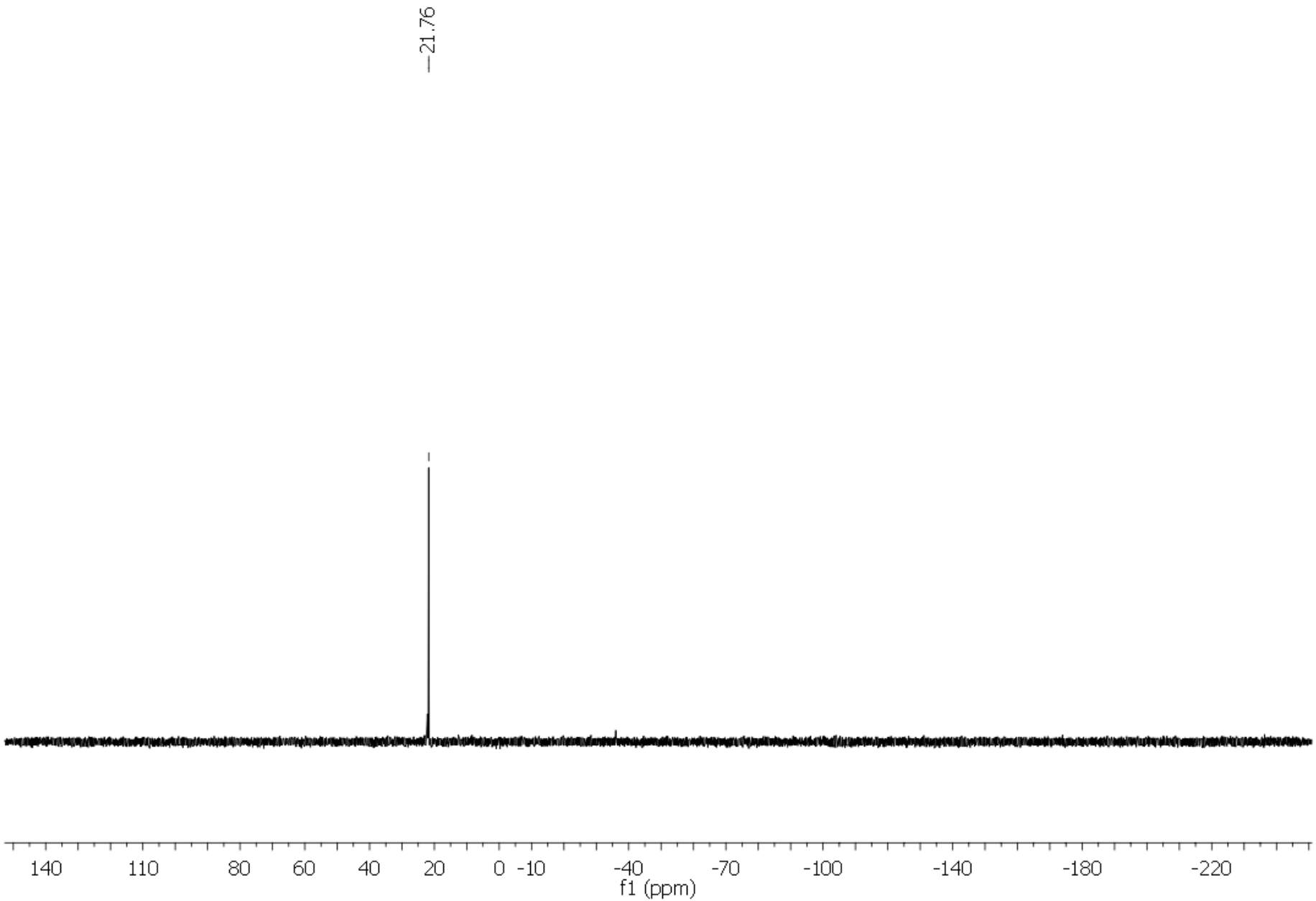

Figure S12. $^{31}P\{^{1}H\}$ spectrum (161 MHz, C_6D_6) of **1-*d*$_x$**

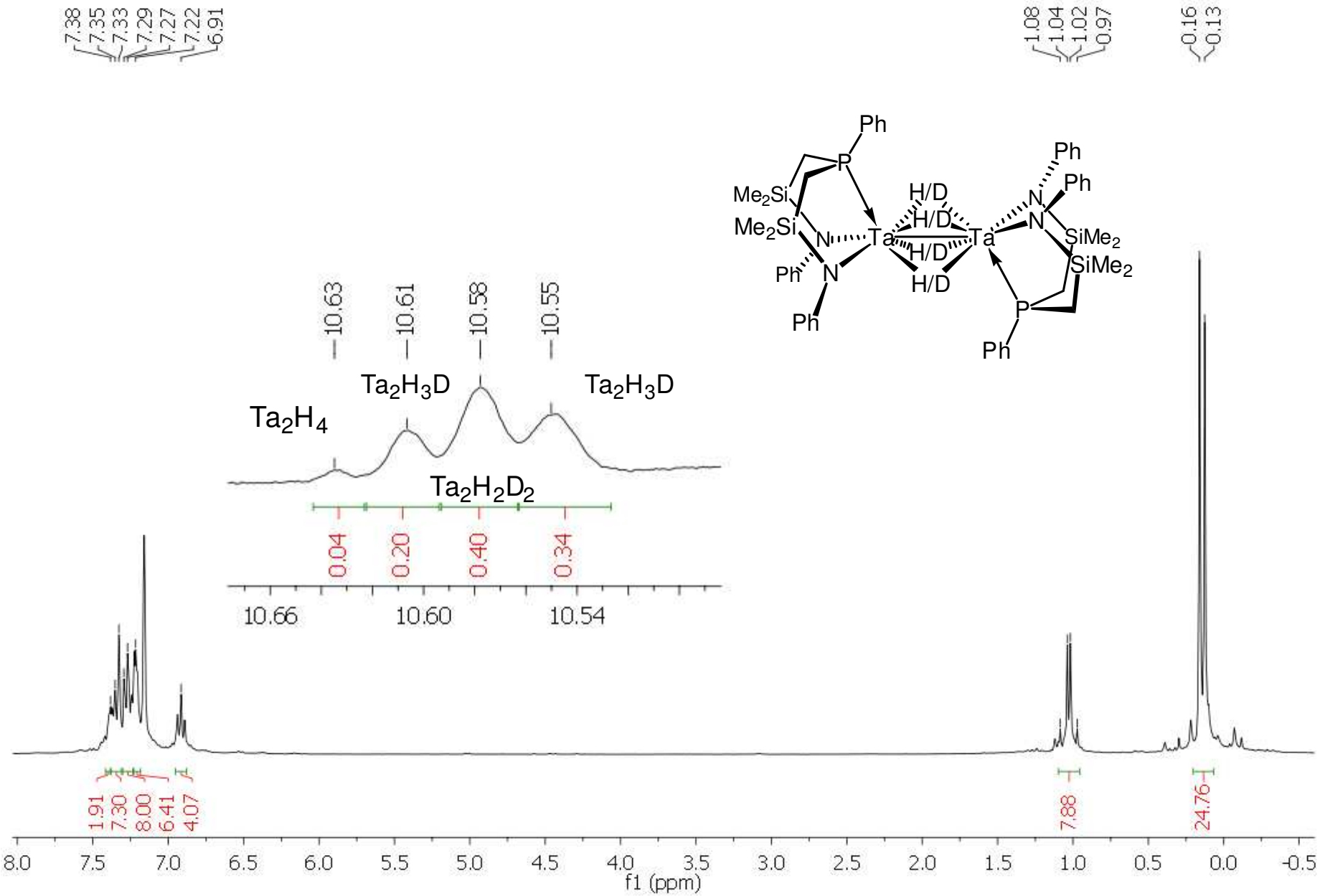

Figure S13. ^{1}H spectrum (400 MHz, C_6D_6) of **1-*d*$_x$**

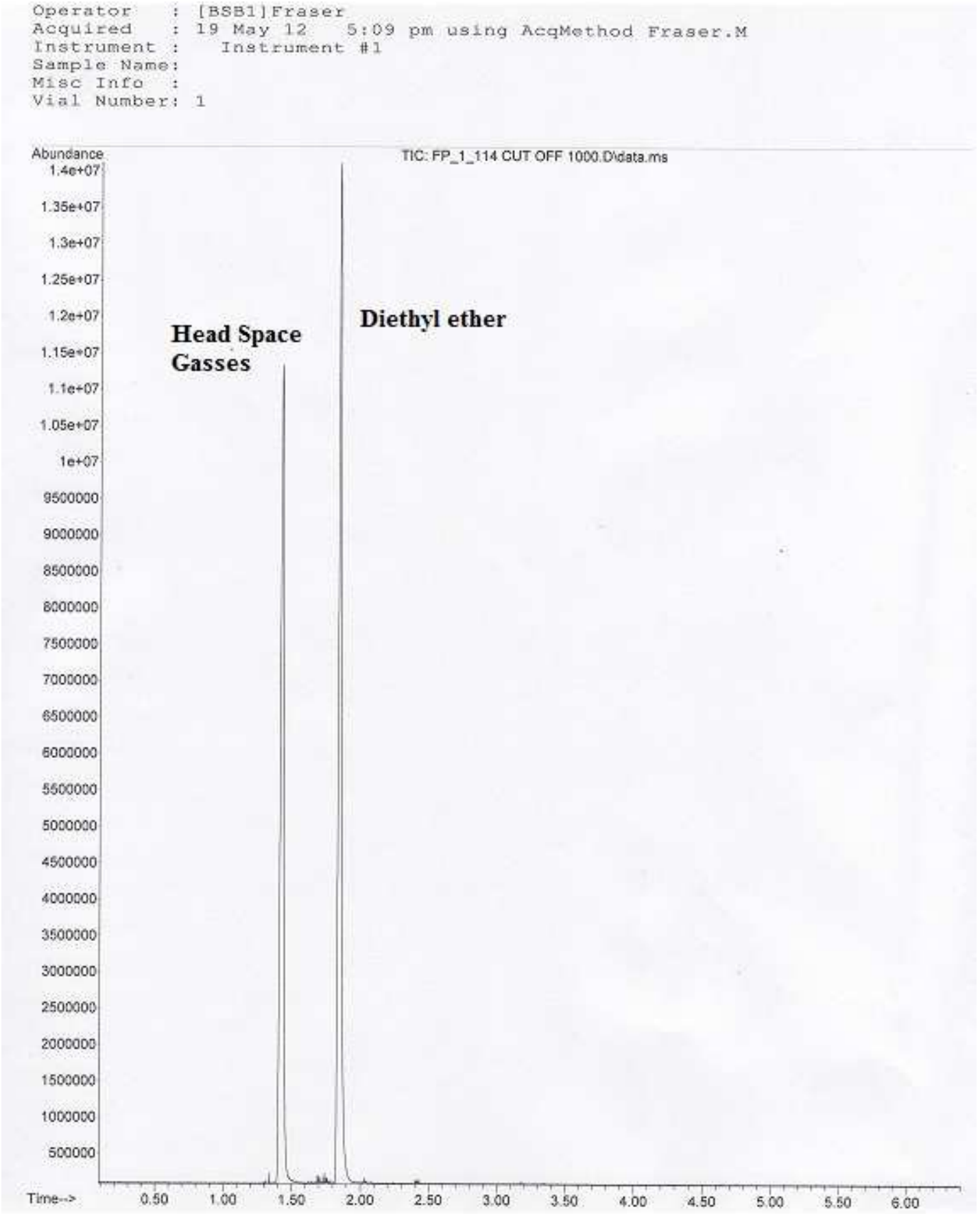

Figure S14. Typical Chromatogram of carbon monoxide hydrogenation

```
Operator    : Fraser
Instrument :   Instrument #1
Acquired    : 16 May 2012  16:42      using AcqMethod FRASER.M
Sample Name: FP_1_111 Headspace analysis
Misc Info   :
```

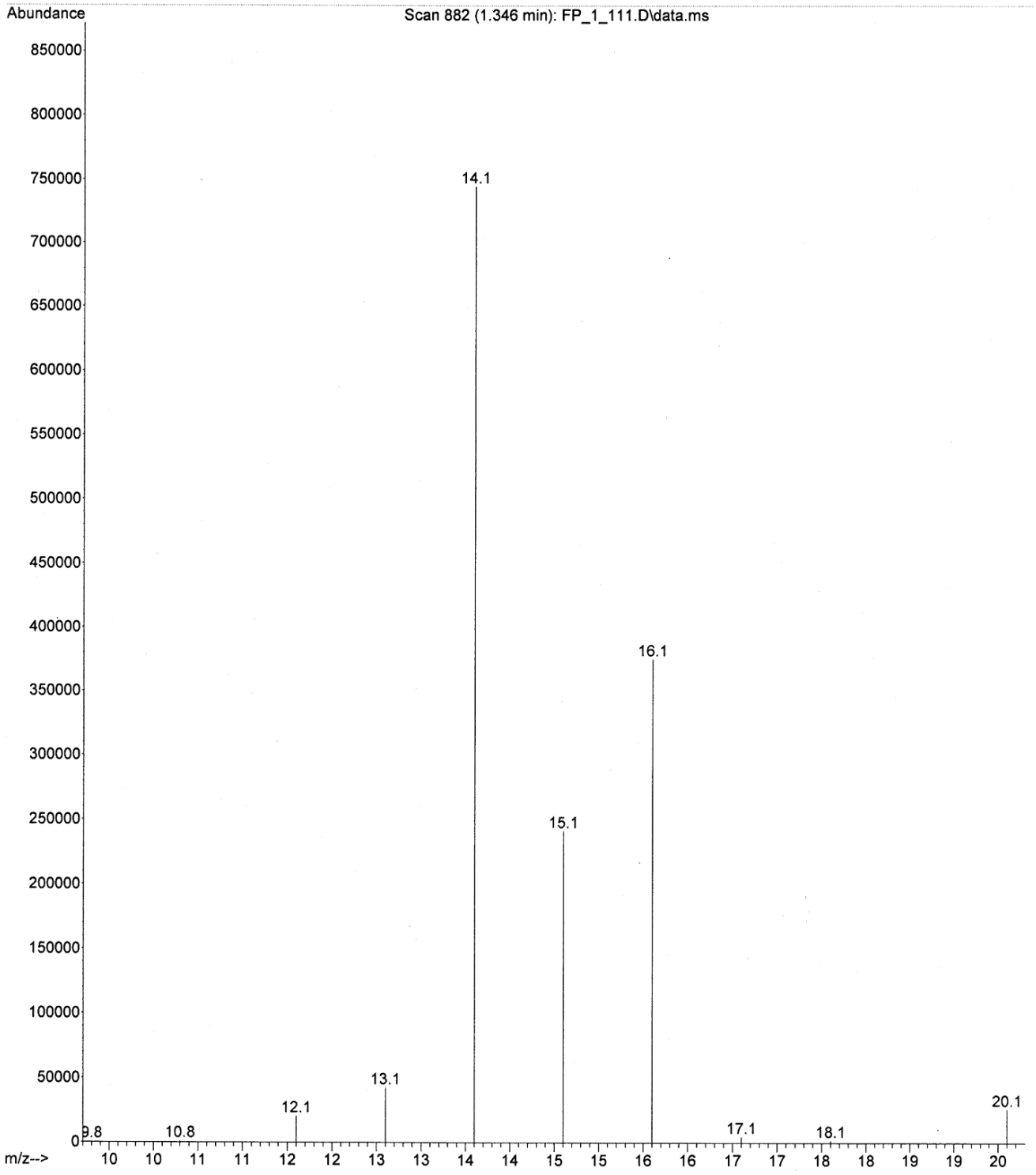

Figure S15. Mass spectrum of the head-space gases (CH_4) from the reaction of CO with **1**

```
Operator    : Fraser
Acquired    : 19 May 2012  17:38      using AcqMethod Fraser.M
Instrument :   Instrument #1
Sample Name:
Misc Info   :
Vial Number: 1
```

Figure S16. Mass spectrum of the head-space gases (CD_4) from the reaction of CO with **1-*d*$_{12}$**

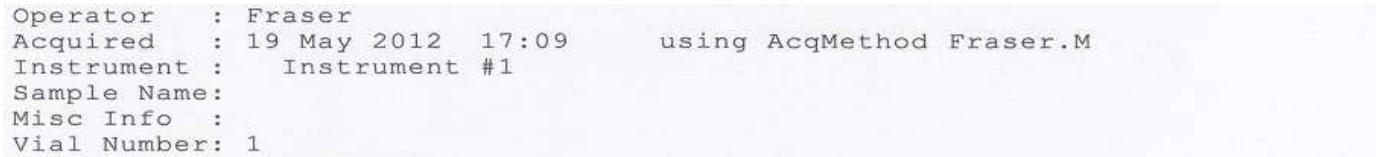

Figure S17. Mass spectrum of the head-space gases (CD_4, CD_3H, and CD_2H_2) from the reaction of CO with **1-d_x**

Computational Details

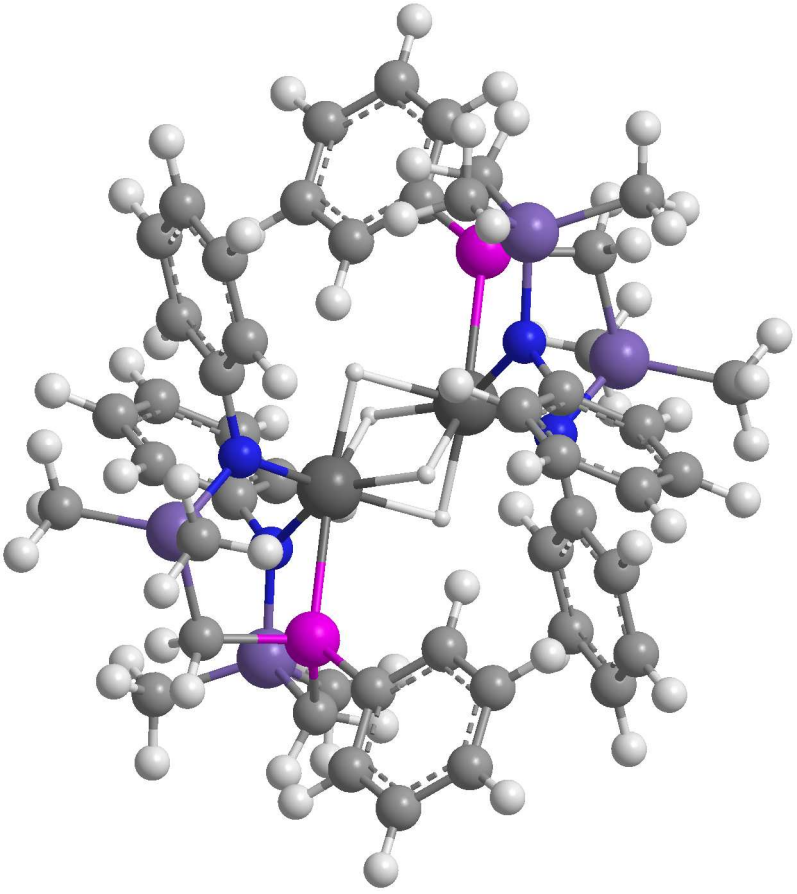

Figure S18. Full optimized structure of **1**. In the body of the paper (Figure 3), the ligand backbone and substituents have been removed for clarity.

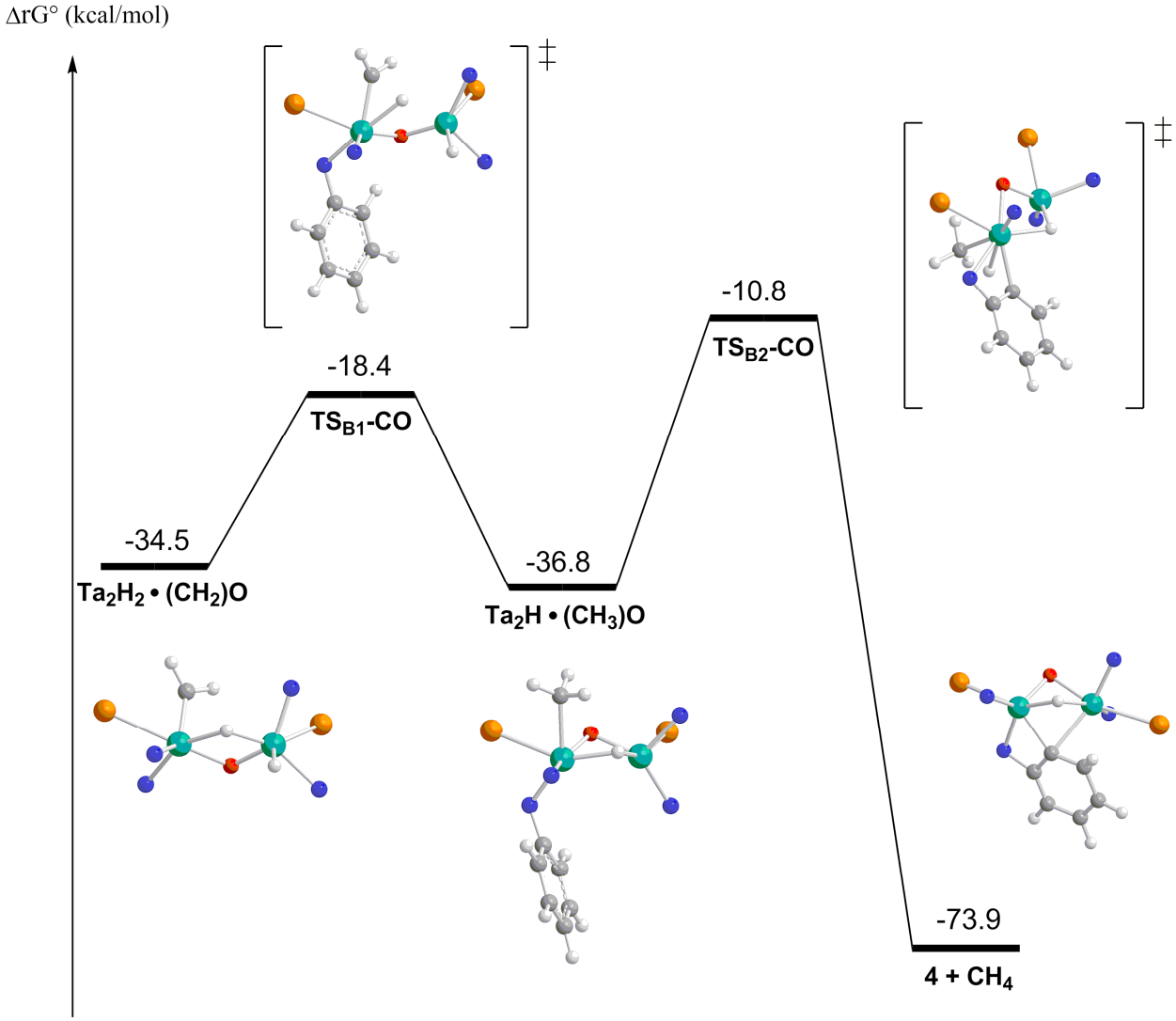

Figure S19. Gibbs free energy profile of pathway **B**.

The Gibbs free energy profile of pathway **B** is presented in Figure S19. The first step of the reaction is the same as for pathway **A**. The second step is the formation of methane directly from C-H activation of the ortho CH bond of the phenyl group. The transition state lies at +26.0 kcal/mol with respect to **Ta_2H•$(CH_3)O$**, which is almost the same as the second step of pathway **A** (+27.9 kcal/mol). The advantage of this pathway is that the product **4** and the methane molecule are formed at the same time, and avoids the formation of a Ta(III) intermediate.

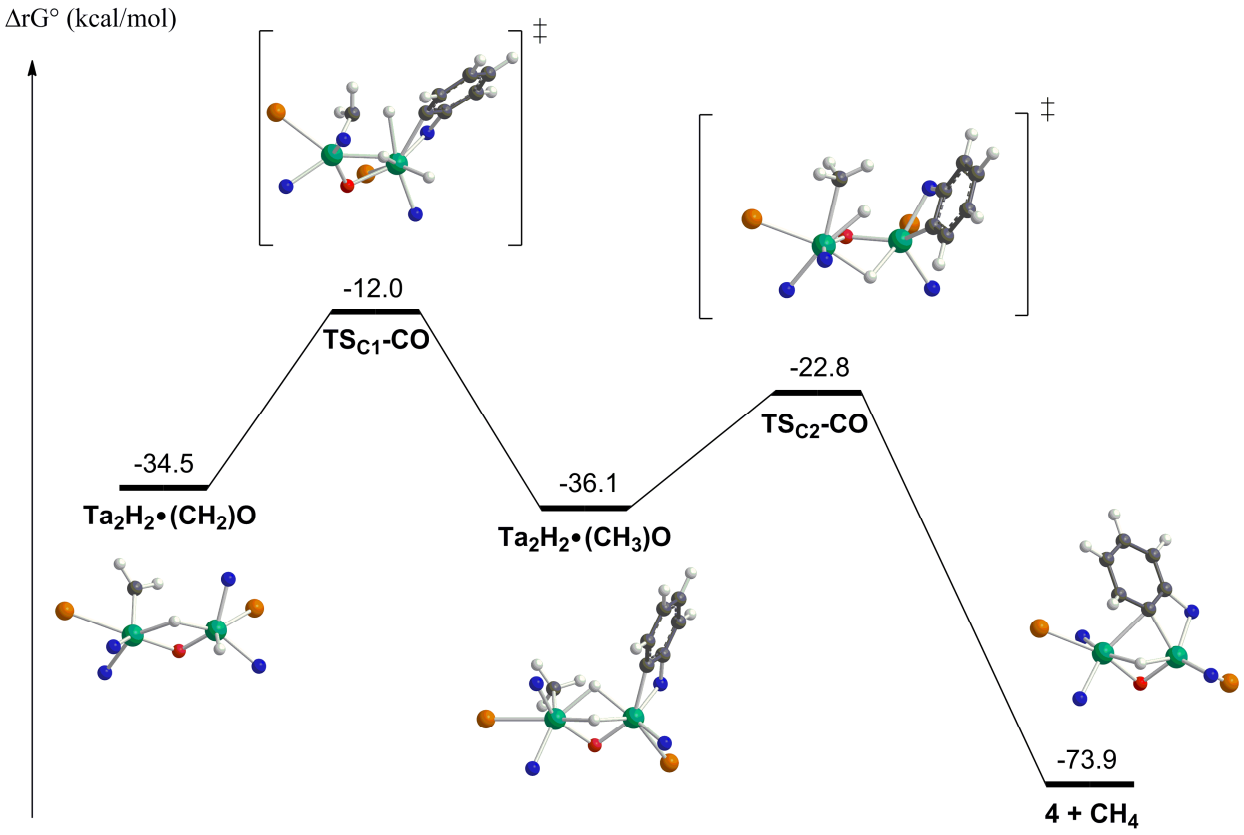

Figure S20. Gibbs free energy profile of pathway **C**.

The Gibbs free energy profile of pathway **C** is presented in Figure S20. In this pathway, the two elementary steps of pathway **B** are inverted, that is the first step of the reaction is the C-H activation of the ortho CH bond of the phenyl group. It leads to the Ta(V) complex **Ta_2H_2•(CH_3)O** where the methyl group is formed as well as the Ta_2-Ph interaction. The activation barrier is equal to +22.5 kcal/mol and the reaction is slightly exergonic by -1.6 kcal/mol. The second step corresponds to the migration of a bridging hydride to form product **4** with concomitant release of methane. The transition state lies at only +13.3 kcal/mol with respect to **Ta_2H_2•(CH_3)O.** To summarize, the relevant energetic values of the three pathways are compared in Table Y1. As on can see, none of pathways is obviously preferred. Pathways **A** and **B** are equivalent since the last transition state can be considered without barrier. Although the first step of pathway **C** is slightly more kinetically difficult than the two others, the second step is from far the easiest. To conclude, all three profiles can account for the formation of the experimental product.

	TS_1	TS_2	TS_3
Pathway A	+16.1	+27.6	+2.1
Pathway B	+16.1	+26.0	-
Pathway C	+22.5	+13.3	-

Table S2. Relevant energetic values of the three pathways, all with respect to $\mathbf{Ta_2H_2{\bullet}(CH_2)O}$.

Cartesian coordinates of all optimized molecules

CO

E = -113.258297
G = -113.272376

C	0.000000	0.000000	0.031465
O	0.000000	0.000000	1.168535

CH_4

E = -40.508109
G = -40.482693

C	-0.000004	0.000000	0.000009
H	-0.000001	0.000000	1.091768
H	1.029319	0.000000	-0.363923
H	-0.514658	-0.891417	-0.363925
H	-0.514658	0.891417	-0.363925

Complex **1**

E = -2230.358469
G = -2229.457381

Ta	3.071778	5.586970	9.738125
N	2.561361	4.710100	11.581500
C	1.219045	4.478070	11.996999
H	3.583955	1.698640	12.254099
C	0.621631	5.210415	13.036207
C	-0.686353	4.944375	13.441286
C	-1.434285	3.948185	12.814620
C	-0.856631	3.220764	11.773376
C	0.452474	3.477762	11.373715
Si	3.753376	4.138294	12.779673
C	3.497840	2.302674	13.163019
C	3.742159	5.106962	14.408476
C	5.469991	4.365710	11.975062
P	5.425488	5.822072	10.829421
Ta	1.615671	7.400983	8.601817
H	3.498886	7.052054	8.499538
C	-1.943882	10.542267	9.644121
H	6.825565	6.405257	8.966664
Si	-1.253013	8.818525	10.034717
C	-1.980565	7.520483	8.828599
P	-0.737907	7.165857	7.510195
H	7.601278	4.644919	6.516574
C	6.505845	4.623224	6.558607
N	4.187012	4.228770	8.545134
C	3.472099	3.281250	7.761103
N	2.126393	8.278224	6.758718
Si	0.934559	8.849639	5.560182
C	-0.782220	8.622121	6.364415
C	0.946319	7.880664	3.931559
C	1.189904	10.685236	5.176606
C	4.066893	7.779245	5.304539
C	5.374928	8.045989	4.900079
C	6.122216	9.042222	5.527445
C	5.543864	9.768969	6.568768
C	4.234705	9.511280	6.967805
C	3.468771	8.510926	6.343808
C	3.246702	3.472723	6.385283
C	2.589313	2.507732	5.626240
C	2.125809	1.331470	6.219649
C	2.321736	1.136795	7.586211
C	-0.661781	4.548595	6.483585
C	-2.640917	5.816877	5.909110
C	-3.145603	4.719772	5.216882
C	-1.171299	3.450629	5.788519
C	-2.409686	3.534777	5.156532
C	-1.394759	5.737340	6.545793
C	6.631585	2.445983	8.694760
Si	5.940337	4.169685	8.304671
C	6.082386	7.250530	11.793883
C	5.349249	8.439158	11.856478
C	7.328703	7.171060	12.430263
C	5.858761	9.537068	12.551636
C	7.097309	9.452986	13.183319
C	7.833389	8.268114	13.122574
N	0.500392	8.758998	9.794955
C	1.215082	9.706238	10.579546
C	1.698252	10.890588	9.995149
C	2.365091	11.850784	10.755619
C	2.560863	11.655479	12.122113
C	2.097447	10.478866	12.714897
C	1.440293	9.514143	11.955306
H	1.098494	8.590330	12.411506
H	2.249745	10.309733	13.778126
H	3.064143	12.411111	12.719268
H	2.722418	12.759776	10.277794
H	1.526928	11.047976	8.933945
C	2.988826	2.097251	8.346133
C	6.668041	5.467583	9.510868
C	-1.819146	8.365459	11.780706
H	-2.138008	6.582873	9.372943
H	-2.936110	7.838191	8.397313
H	-0.981382	9.496668	6.991664
H	-1.581261	8.538421	5.620814

H	-1.513155	11.281143	10.327681
H	-3.031694	10.558508	9.775976
H	-1.719581	10.865835	8.623205
H	-1.443912	7.378832	12.067703
H	-2.914588	8.343667	11.822379
H	-1.472365	9.097779	12.516216
H	1.878432	8.027040	3.378731
H	0.123045	8.226516	3.295245
H	0.810437	6.808707	4.106643
H	1.103721	11.289350	6.085469
H	0.444711	11.039803	4.455829
H	2.182794	10.856930	4.749664
H	-3.223917	6.733807	5.956782
H	-4.112864	4.787692	4.726255
H	-2.805124	2.678481	4.616702
H	-0.590470	2.534189	5.746787
H	0.304116	4.484839	6.977746
H	3.499572	6.984613	4.830051
H	5.812737	7.465383	4.091670
H	7.140738	9.248245	5.210675
H	6.112597	10.546839	7.072376
H	3.784451	10.079026	7.777335
H	1.188627	5.935828	9.840490
H	2.710530	7.390600	10.249395
H	7.623566	5.149708	9.942079
H	5.668937	3.491211	11.347673
H	6.269229	4.449308	12.718461
H	6.200399	1.707062	8.011538
H	7.719304	2.429755	8.562178
H	6.407976	2.122466	9.715849
H	6.130607	5.609971	6.272032
H	6.158761	3.891148	5.822997
H	2.810069	4.960821	14.961403
H	4.565401	4.760696	15.044605
H	3.878404	6.178903	14.233571
H	4.243003	1.947959	13.883754
H	2.504939	2.131042	13.589964
H	3.160271	1.940341	9.407386
H	1.964336	0.228086	8.064522
H	1.622337	0.575624	5.622928
H	2.436886	2.676391	4.562954
H	3.588525	4.396283	5.928590
H	7.911821	6.254222	12.382294
H	8.800776	8.200246	13.612960
H	7.492744	10.309241	13.723217
H	5.277803	10.453413	12.593679
H	4.383236	8.502874	11.362537
H	1.189490	6.004979	13.510164
H	-1.123614	5.525482	14.249632
H	-2.452767	3.742703	13.131870
H	-1.425878	2.442911	11.270321
H	0.902193	2.909523	10.564234
H	1.976872	5.597353	8.090544

Complex **Ta_2H_4•CO**

E = -2343.653049
G = -2342.742150

Ta	-1.344229	-0.001800	-0.287724
C	-3.077385	-0.809922	3.993587
N	-2.330849	-1.348097	1.032098
C	-1.864923	-2.692795	1.104283
C	-2.171869	-3.614894	0.090742
C	-1.775821	-4.947909	0.183367
C	-1.063099	-5.397806	1.294307
C	-0.738780	-4.490705	2.303986
C	-1.127764	-3.156147	2.209340
Si	-3.636552	-1.032835	2.199870
C	-4.926202	-2.421674	2.161056
C	-4.038268	-2.148689	-3.542056
Si	-3.555177	-0.493776	-2.765787
C	-4.454089	0.596159	1.613104
C	-4.667655	-0.188400	-1.242482
C	-3.837245	0.881368	-4.029806
P	-3.788777	0.946243	-0.068166
C	-4.369873	2.643436	-0.519660
C	-5.731493	2.965683	-0.434934
C	-6.174155	4.245327	-0.758843
C	-5.260372	5.216737	-1.170704
C	-3.905653	4.903875	-1.254440
C	-3.458932	3.622270	-0.928910
C	-0.958801	-0.772290	-3.278694
C	-0.607706	-2.093258	-3.586253
C	-0.469733	0.263983	-4.084659
C	0.324298	-0.020981	-5.193352
C	0.191719	-2.371757	-4.692773
C	0.651040	-1.339137	-5.509015
N	-1.845540	-0.496845	-2.186010
Ta	1.437392	0.069709	0.424161
N	2.873722	-1.419705	-0.005672
C	2.678405	-2.471149	-0.950803
C	3.430184	-2.522331	-2.137313
C	3.316561	-3.598671	-3.015703
C	2.440132	-4.645682	-2.737846
C	1.666862	-4.591564	-1.577590
C	1.782095	-3.521104	-0.693997
Si	4.467839	-1.547243	0.787965
C	5.827960	-0.580953	-0.117032

C	5.018060	-3.346900	0.975989
C	4.257516	-0.828200	2.549479
P	3.020212	0.545039	2.477952
C	3.957385	2.108112	2.178986
Si	2.894638	3.166914	0.990307
C	4.042937	4.396026	0.124173
C	1.585448	4.126597	1.963429
C	2.238981	2.325650	-1.501854
N	2.250107	1.956955	-0.134562
C	3.029369	1.986440	-3.781554
C	1.516571	3.443654	-1.960079
C	1.570133	3.835269	-3.295003
C	2.332902	3.113576	-4.214819
C	2.983419	1.597058	-2.444523
H	3.494036	5.072696	-0.536150
C	1.705974	-0.468095	4.734273
C	2.308919	0.671159	4.181698
C	2.320023	1.854704	4.926943
C	1.752354	1.895807	6.201117
C	1.169569	0.755572	6.747435
C	1.147557	-0.427839	6.008866
C	-0.066040	0.950187	1.552203
O	-1.082713	1.283043	2.071732
H	0.886690	-0.749962	1.919874
H	0.130232	-1.237782	-0.114216
H	0.319692	0.454852	-1.114813
H	-1.276327	1.749916	-0.556632
H	0.463536	-3.400950	-4.907121
H	6.070475	-1.059999	-1.070983
H	2.356466	-5.489597	-3.417362
H	0.971016	-5.393154	-1.344988
H	1.183310	-3.488470	0.211125
H	6.745257	-0.555245	0.482812
H	-4.139903	1.424069	2.257098
H	-3.933992	-2.976375	-2.834260
H	-3.921142	-0.469062	4.605314
H	3.915693	-3.613272	-3.922887
H	4.106664	-1.704211	-2.368009
H	3.827322	-1.623105	3.168686
H	5.192809	-0.498863	3.013955
H	4.850639	1.817554	1.614999
H	4.290479	2.591609	3.101652
H	5.523390	0.448788	-0.328243
H	4.245522	-3.935818	1.480392
H	5.936660	-3.399438	1.571286
H	5.212002	-3.811477	0.005360
H	0.965142	4.719570	1.283329
H	2.058847	4.819513	2.669196
H	0.923821	3.461025	2.524025
H	4.790715	3.873583	-0.480622
H	4.567962	5.001574	0.871693
H	2.763948	2.757901	4.521823
H	1.769773	2.824355	6.765222
H	0.730878	0.787861	7.740757
H	0.689073	-1.321403	6.423528
H	1.660356	-1.389667	4.159880
H	0.903258	3.995408	-1.252523
H	1.012006	4.710587	-3.619298
H	2.379671	3.424930	-5.254729
H	-5.547361	0.537896	1.618555
H	-4.791128	-1.139769	-0.715681
H	-5.655083	0.190913	-1.525862
H	-4.482224	-3.371821	2.472738
H	-5.746761	-2.191685	2.850169
H	-5.351635	-2.564696	1.162615
H	-2.277760	-0.067955	4.062615
H	-2.720101	-1.752474	4.418886
H	-3.195237	0.747459	-4.904765
H	-4.880556	0.864049	-4.365662
H	-3.633224	1.866016	-3.599418
H	-5.083638	-2.110748	-3.869304
H	-3.416513	-2.366391	-4.414889
H	-2.733286	-3.267491	-0.770953
H	-2.034368	-5.639767	-0.614623
H	-0.761646	-6.438529	1.371816
H	-0.175700	-4.823846	3.172572
H	-0.852495	-2.446815	2.983428
H	-2.403089	3.372245	-0.987669
H	-3.190329	5.657636	-1.571913
H	-5.606130	6.215499	-1.422840
H	-7.231578	4.485550	-0.688654
H	-6.451794	2.218202	-0.110495
H	-0.705998	1.290228	-3.822274
H	0.696254	0.796568	-5.803943
H	1.269539	-1.558709	-6.374973
H	-0.956850	-2.893288	-2.941403
H	3.618889	1.405815	-4.486344
H	3.534995	0.725749	-2.103889

TS_1-CO

E = -2343.651311
G = -2342.739131

Ta	-1.024149	-3.706798	2.883856
C	-2.569360	-4.778258	7.120560
N	-1.958172	-5.188093	4.104396
C	-1.484698	-6.526720	4.039654
C	-1.778147	-7.343863	2.935020
C	-1.386638	-8.680490	2.899826
C	-0.691313	-9.243278	3.970104

C	-0.376157	-8.441990	5.068040
C	-0.757503	-7.101984	5.099194
Si	-3.207990	-4.956396	5.347339
C	-4.457474	-6.382271	5.311373
C	-3.759196	-5.628233	-0.552501
Si	-3.251596	-4.073198	0.395810
C	-4.099963	-3.334309	4.862482
C	-4.351754	-3.928438	1.951877
C	-3.508260	-2.559271	-0.704636
P	-3.482785	-2.862458	3.191701
C	-4.111514	-1.146960	2.897648
C	-5.487382	-0.904318	2.786187
C	-5.963424	0.393257	2.616532
C	-5.069480	1.463434	2.562838
C	-3.701155	1.230551	2.682236
C	-3.221649	-0.069245	2.848559
C	-0.656179	-4.435533	-0.111714
C	-0.309947	-5.753226	-0.439496
C	-0.146233	-3.389540	-0.892669
C	0.664668	-3.659733	-1.993048
C	0.502458	-6.017644	-1.539940
C	0.984604	-4.974453	-2.329044
N	-1.551070	-4.172898	0.977010
Ta	1.776938	-3.566881	3.502224
N	3.147885	-5.183991	3.366025
C	3.032462	-6.138259	2.305234
C	3.775342	-5.989397	1.122366
C	3.747158	-6.966625	0.127892
C	2.967877	-8.110096	0.287499
C	2.199559	-8.253286	1.444139
C	2.228240	-7.281634	2.440541
Si	4.611072	-5.491467	4.321184
C	6.192315	-4.915073	3.444472
C	4.810126	-7.320230	4.762663
C	4.398094	-4.511444	5.947996
P	3.328067	-3.040481	5.616103
C	4.422046	-1.629476	5.156040
Si	3.469355	-0.596532	3.856097
C	4.714445	0.478177	2.924185
C	2.185971	0.506906	4.698980
C	2.658679	-1.410098	1.440238
N	2.740167	-1.825117	2.801385
C	3.573388	-1.408746	-0.815899
C	1.693828	-0.480799	1.013550
C	1.684003	-0.011782	-0.297785
C	2.627484	-0.468306	-1.220037
C	3.590090	-1.873058	0.498396
H	4.220597	1.092098	2.165574
C	1.761286	-3.595826	7.863263
C	2.556532	-2.621220	7.243011
C	2.712827	-1.380631	7.868820
C	2.096892	-1.123524	9.094065
C	1.318753	-2.101381	9.707971
C	1.151634	-3.339964	9.088240
C	0.266668	-2.900648	4.649951
O	-0.835134	-2.639875	5.117232
H	0.892178	-4.141313	5.033921
H	0.564664	-4.880090	2.833658
H	0.622074	-3.067045	2.062805
H	-1.095161	-1.959768	2.580981
H	0.767075	-7.045231	-1.771185
H	6.384005	-5.532490	2.561565
H	2.951322	-8.876572	-0.482707
H	1.572985	-9.130695	1.580005
H	1.627696	-7.396508	3.337419
H	7.058414	-5.004251	4.110323
H	-3.799517	-2.528690	5.540359
H	-3.682381	-6.525252	0.069660
H	-3.392372	-4.494456	7.787160
H	4.335838	-6.827665	-0.775380
H	4.379084	-5.096029	0.994661
H	3.850105	-5.152731	6.647215
H	5.340159	-4.217228	6.421846
H	5.279505	-2.068204	4.633775
H	4.802019	-1.082274	6.023505
H	6.114309	-3.874009	3.115207
H	3.929074	-7.691637	5.295412
H	5.687674	-7.466952	5.402443
H	4.939013	-7.929281	3.863359
H	1.650763	1.095812	3.946703
H	2.652220	1.207740	5.401013
H	1.449940	-0.095581	5.239300
H	5.465510	-0.136653	2.418788
H	5.230361	1.148165	3.621282
H	3.310133	-0.602124	7.406708
H	2.229021	-0.154239	9.567016
H	0.840843	-1.899716	10.662437
H	0.539546	-4.106543	9.554849
H	1.607425	-4.558777	7.382122
H	0.945998	-0.146634	1.726722
H	0.934551	0.715602	-0.600960
H	2.622405	-0.096533	-2.241026
H	-5.190856	-3.425270	4.882070
H	-4.424181	-4.922887	2.404031
H	-5.359976	-3.574464	1.714575
H	-3.974857	-7.332006	5.560735
H	-5.252692	-6.205911	6.044549
H	-4.922294	-6.493820	4.326394
H	-1.800638	-4.002469	7.166689
H	-2.151541	-5.718574	7.493244
H	-2.876360	-2.615587	-1.595533
H	-4.553138	-2.501275	-1.030425

H	-3.264168	-1.638570	-0.166575
H	-4.799171	-5.534503	-0.885540
H	-3.131030	-5.772430	-1.436017
H	-2.328072	-6.908969	2.106665
H	-1.636561	-9.288421	2.033600
H	-0.397102	-10.288742	3.948807
H	0.173265	-8.861699	5.907382
H	-0.492814	-6.478645	5.947960
H	-2.155541	-0.259475	2.934309
H	-3.001219	2.060846	2.644727
H	-5.441168	2.475833	2.430257
H	-7.032040	0.569531	2.528038
H	-6.195450	-1.728123	2.835885
H	-0.375940	-2.366031	-0.614793
H	1.056146	-2.833384	-2.578926
H	1.615892	-5.183218	-3.188409
H	-0.673238	-6.563048	0.184741
H	4.309883	-1.779886	-1.524247
H	4.338577	-2.591500	0.819940

Complex **Ta_2H_3•HCO**

E = -2343.668287
G = -2342.755305

Ta	-1.397022	-0.216520	-0.261814
C	-2.867204	-1.548354	3.754778
N	-2.281559	-1.927471	0.731783
C	-1.730056	-3.211018	0.515094
C	-1.830622	-3.835327	-0.742759
C	-1.365615	-5.131527	-0.949875
C	-0.785134	-5.855088	0.093032
C	-0.664135	-5.250454	1.344262
C	-1.116783	-3.948127	1.549205
Si	-3.518490	-1.857543	2.001459
C	-4.575550	-3.431037	1.998013
C	-3.821182	-1.941933	-4.119274
Si	-3.481370	-0.511265	-2.927257
C	-4.626739	-0.369904	1.533760
C	-4.656631	-0.655540	-1.428843
C	-3.817699	1.122879	-3.819835
P	-3.944303	0.332053	-0.032782
C	-4.723889	2.006086	-0.171627
C	-6.115423	2.132749	-0.279049
C	-6.708450	3.391586	-0.332233
C	-5.916208	4.538776	-0.271151
C	-4.533028	4.420156	-0.154902
C	-3.936090	3.159608	-0.105535
C	-0.829001	-0.708105	-3.261322
C	-0.215821	-1.930168	-3.576816
C	-0.447236	0.432531	-3.986352
C	0.495758	0.345963	-5.009489
C	0.732147	-2.010218	-4.594162
C	1.087664	-0.876135	-5.324461
N	-1.834644	-0.628308	-2.248307
Ta	1.389865	0.137965	0.416526
N	2.672890	-1.513679	0.566394
C	2.867541	-2.353978	-0.581260
C	3.876583	-2.048533	-1.507701
C	4.132874	-2.886580	-2.591360
C	3.389816	-4.052474	-2.767008
C	2.373763	-4.356359	-1.860650
C	2.106980	-3.515963	-0.782172
Si	3.534129	-2.181854	1.983693
C	5.326072	-2.630390	1.570152
C	2.691453	-3.707102	2.708824
C	3.511139	-0.787462	3.299336
P	3.008297	0.743252	2.406775
C	4.496735	1.335495	1.482639
Si	3.882811	2.428730	0.038126
C	5.040756	2.206684	-1.439693
C	3.905422	4.233257	0.592254
C	1.531329	2.877330	-1.107752
N	2.196338	1.892465	-0.308163
C	1.151206	3.950492	-3.252776
C	0.671822	3.814239	-0.515502
C	0.066196	4.805600	-1.282914
C	0.305857	4.883755	-2.655472
C	1.759123	2.954847	-2.488691
H	4.785217	2.899978	-2.246250
C	1.360260	2.576970	3.754705
C	2.649930	2.039261	3.670585
C	3.639211	2.474757	4.562506
C	3.343100	3.437558	5.523673
C	2.056354	3.973051	5.602024
C	1.067924	3.541840	4.719928
C	-0.206743	0.154868	1.708397
O	-1.393896	0.729330	1.691806
H	-0.084488	-0.659041	2.468743
H	0.365197	-1.090959	-0.650479
H	0.047660	0.935772	-0.675388
H	-1.765405	1.457959	-0.692409
H	1.200968	-2.966202	-4.809376
H	5.363443	-3.411304	0.805349
H	3.595176	-4.713379	-3.604645
H	1.773948	-5.253071	-1.989966
H	1.298067	-3.746139	-0.095805
H	5.826190	-3.011738	2.467747
H	-4.542876	0.415349	2.291869
H	-3.750607	-2.910425	-3.614370
H	-3.704623	-1.388741	4.444519

H	4.919994	-2.627957	-3.295118
H	4.468430	-1.150225	-1.356224
H	2.741516	-0.994621	4.050948
H	4.473484	-0.673578	3.808667
H	4.983825	0.442426	1.079244
H	5.209481	1.864989	2.123293
H	5.898367	-1.773406	1.201890
H	1.653707	-3.490117	2.976962
H	3.221585	-4.041135	3.608198
H	2.687180	-4.531220	1.989965
H	3.540839	4.898775	-0.194508
H	4.931970	4.526896	0.840111
H	3.283792	4.380304	1.480354
H	4.989662	1.188458	-1.836663
H	6.075406	2.407906	-1.138883
H	4.644151	2.061968	4.511538
H	4.115280	3.769734	6.212211
H	1.826391	4.724268	6.352596
H	0.064140	3.952995	4.779964
H	0.589384	2.235329	3.069148
H	0.483042	3.747333	0.551619
H	-0.594382	5.523808	-0.803963
H	-0.164046	5.660620	-3.251892
H	-5.681688	-0.641937	1.425146
H	-4.649153	-1.698247	-1.093914
H	-5.684997	-0.366498	-1.667698
H	-3.983176	-4.313562	2.255264
H	-5.389162	-3.344715	2.726969
H	-5.017886	-3.602829	1.011081
H	-2.246040	-0.647865	3.752470
H	-2.279254	-2.388483	4.136943
H	-3.212353	1.211901	-4.726675
H	-4.873045	1.179638	-4.111166
H	-3.594965	1.974454	-3.170213
H	-4.826266	-1.852395	-4.546391
H	-3.101622	-1.936545	-4.943563
H	-2.291720	-3.278476	-1.551530
H	-1.472159	-5.585213	-1.932679
H	-0.436253	-6.871617	-0.065311
H	-0.209907	-5.793619	2.169522
H	-1.005739	-3.484597	2.525623
H	-2.857218	3.059881	-0.025975
H	-3.912596	5.310893	-0.105004
H	-6.378442	5.521409	-0.312852
H	-7.788301	3.477640	-0.419559
H	-6.743931	1.245979	-0.317013
H	-0.885807	1.389223	-3.721922
H	0.769610	1.242914	-5.559856
H	1.821538	-0.943557	-6.123008
H	-0.477121	-2.810948	-3.000319
H	1.338856	3.992166	-4.322661
H	2.395670	2.212270	-2.959306

TS_2-CO

E = -2343.650060
G = -2342.737050

C	-1.152623	-4.560185	0.626550
C	-1.588660	-3.465861	-0.153113
C	-1.612118	-3.655759	-1.549190
C	-1.239539	-4.865765	-2.129156
C	-0.841443	-5.943151	-1.338267
C	-0.801926	-5.776664	0.046177
N	-2.019158	-2.256025	0.421564
Si	-3.051883	-2.410311	1.858151
C	-2.188626	-2.557509	3.538981
C	-4.087353	-0.792902	1.928893
P	-3.729669	0.137356	0.386369
C	-4.533441	1.797733	0.562465
C	-3.862649	2.955849	0.154361
C	-4.472411	4.205047	0.275933
C	-5.755198	4.308661	0.810066
C	-6.430098	3.159087	1.221839
C	-5.823170	1.911521	1.098192
Ta	-1.233496	-0.345736	-0.283499
C	-0.296375	1.045036	1.352033
O	-0.866887	-0.066688	1.846977
Ta	1.364921	0.192445	0.407107
N	2.526582	-1.476794	1.018864
C	2.871072	-2.339681	-0.061990
C	2.361339	-3.644391	-0.177136
C	2.732696	-4.464433	-1.239085
C	3.608457	-4.003574	-2.223155
C	4.106669	-2.705734	-2.133671
C	3.746268	-1.887400	-1.063722
N	2.492877	1.665351	-0.490070
Si	4.090026	2.241792	0.111782
C	4.365280	1.392496	1.800842
P	2.710732	0.993106	2.535835
C	2.963876	-0.417114	3.693037
Si	3.029328	-2.011762	2.626712
C	1.899027	-3.290866	3.438536
C	2.126011	2.380808	-1.674633
C	2.616102	2.002020	-2.932232
C	2.315237	2.752922	-4.066366
C	1.516574	3.891330	-3.971032
C	1.004766	4.263337	-2.728581
C	1.306894	3.516737	-1.591904
C	4.111995	4.121232	0.322225
C	5.526625	1.792437	-1.036646

C	2.286783	2.465159	3.573590
C	2.655330	2.546788	4.921680
C	2.328676	3.672404	5.676468
C	1.631293	4.729172	5.093078
C	1.257936	4.656049	3.751796
C	1.578813	3.528159	2.998080
C	4.796663	-2.688823	2.588898
N	-2.014085	-0.175328	-2.223534
Si	-3.761942	-0.261872	-2.626565
C	-4.647912	-0.687941	-0.990001
C	-1.204103	-0.035920	-3.392708
C	-1.330020	1.063813	-4.258515
C	-0.599306	1.134012	-5.442954
C	0.292138	0.120104	-5.788328
C	0.461443	-0.954781	-4.916252
C	-0.275103	-1.033960	-3.736786
C	-4.519767	1.350505	-3.280222
C	-4.104020	-1.616868	-3.900958
C	-4.274729	-3.847856	1.662442
H	3.220921	1.103877	-3.010117
H	0.406265	-1.320797	-0.313302
H	0.313932	0.436121	-1.189839
H	-1.399390	1.395152	0.184358
H	-0.604157	1.995459	1.808930
H	5.392214	2.242738	-2.024475
H	1.166691	-1.747220	-5.153889
H	4.855186	-3.564534	1.935395
H	3.890489	-4.645877	-3.052729
H	2.310699	-5.462994	-1.306886
H	1.634078	-3.995865	0.546939
H	5.114456	-2.994187	3.592004
H	-3.744649	-0.170937	2.761995
H	-3.861406	-2.609434	-3.510860
H	-2.929214	-2.470525	4.343335
H	4.784590	-2.326293	-2.894476
H	4.139985	-0.878886	-0.987668
H	2.096077	-0.454036	4.360646
H	3.869076	-0.296319	4.297075
H	4.858719	0.430635	1.626888
H	4.983089	1.991179	2.477817
H	5.508500	-1.946236	2.214761
H	0.859183	-2.954363	3.397916
H	2.176290	-3.438630	4.488881
H	1.966648	-4.259957	2.935285
H	3.913582	4.624388	-0.628341
H	5.103505	4.433090	0.670354
H	3.375351	4.463854	1.053466
H	5.641428	0.712355	-1.163277
H	6.459815	2.183037	-0.614153
H	3.196069	1.729322	5.390063
H	2.618602	3.721876	6.722518
H	1.375475	5.604815	5.683087
H	0.709364	5.473793	3.292442
H	1.278926	3.468011	1.955932
H	0.914605	3.807058	-0.621402
H	0.371261	5.142499	-2.640177
H	1.286467	4.476238	-4.856989
H	-5.155105	-1.002439	2.050661
H	-4.540694	-1.763808	-0.819247
H	-5.710155	-0.423567	-0.998429
H	-3.765022	-4.812521	1.601958
H	-4.956001	-3.876025	2.520612
H	-4.876345	-3.733129	0.754703
H	-1.465438	-1.744122	3.640667
H	-1.671201	-3.512671	3.669415
H	-4.228726	1.548215	-4.315345
H	-5.612298	1.258931	-3.252983
H	-4.241566	2.211991	-2.666562
H	-5.162786	-1.609215	-4.183333
H	-3.511534	-1.450114	-4.805807
H	-1.950574	-2.834842	-2.171467
H	-1.277306	-4.969191	-3.211105
H	-0.568607	-6.892449	-1.790447
H	-0.486267	-6.598689	0.684932
H	-1.081153	-4.445096	1.704441
H	-2.860669	2.873751	-0.258871
H	-3.941839	5.097012	-0.046288
H	-6.228565	5.281846	0.907437
H	-7.429858	3.234172	1.641045
H	-6.357705	1.023158	1.425200
H	-1.990900	1.878928	-3.984381
H	-0.723598	1.996028	-6.093498
H	0.855694	0.172781	-6.715851
H	-0.136692	-1.878280	-3.069741
H	2.699607	2.437079	-5.031938

Complex **Ta_2H_2•H_2CO**

E = -2343.669017
G = -2342.747303

C	0.403376	3.891252	12.049550
C	0.890823	3.628323	10.760049
C	-0.012400	3.154350	9.796121
C	-1.352576	2.943686	10.112249
C	-1.823110	3.196715	11.400660
C	-0.937732	3.674739	12.365513
N	2.275559	3.778995	10.444788
Si	3.207853	2.298439	10.830973
C	4.136610	2.427616	12.474599
Ta	3.207876	5.507627	9.767877

N	4.763361	6.000118	11.128429
C	4.471310	6.693473	12.332791
C	3.538473	6.164757	13.241009
C	3.272396	6.794087	14.454764
C	3.943250	7.964046	14.805108
C	4.864539	8.507590	13.911123
C	5.115767	7.891307	12.688523
Ta	1.771614	7.481818	8.677109
N	-0.179833	6.974725	7.928089
Si	-0.502360	6.321640	6.321207
C	-2.331528	6.330052	5.829958
N	1.602198	9.461638	9.270591
Si	1.127716	10.825326	8.220136
C	2.530490	12.076263	7.962651
C	1.772223	9.918937	10.615862
C	0.752201	9.728448	11.561541
C	0.873614	10.242587	12.850310
C	2.008820	10.962199	13.222295
C	3.034689	11.140919	12.296189
C	2.923251	10.618916	11.009038
C	-0.364967	11.750252	8.917395
C	0.604137	10.060750	6.544930
P	1.567451	8.525016	6.205764
C	0.503037	7.448346	5.130348
C	2.968955	9.026460	5.100235
C	3.302433	10.359662	4.837762
C	4.388031	10.673384	4.018907
C	5.157316	9.660820	3.451455
C	4.835745	8.327559	3.706458
C	3.753532	8.014372	4.524605
C	3.700150	6.963413	7.880941
O	2.859567	5.816042	7.676881
P	5.088902	3.765623	8.932074
C	6.593378	3.999358	9.991194
Si	6.492732	5.706892	10.841324
C	7.481626	5.599032	12.450024
C	4.433195	2.092119	9.382589
C	2.114962	0.756841	10.883084
C	5.712306	3.554185	7.198298
C	4.915638	3.997861	6.134795
C	5.318304	3.770755	4.818009
C	6.515277	3.109419	4.551188
C	7.312374	2.666869	5.607029
C	6.911839	2.884388	6.923353
C	7.316782	6.960679	9.679227
C	-1.240690	7.287794	8.814636
C	-1.347084	6.689335	10.084036
C	-2.372671	7.035784	10.962353
C	-3.334030	7.979739	10.605538
C	-3.254586	8.574703	9.346582
C	-2.223651	8.240661	8.472568
C	0.135372	4.553403	6.112053
H	-2.421930	6.544182	11.930194
H	-0.623684	5.934880	10.370949
H	-2.450823	5.752798	4.905866
H	3.854759	1.732466	8.523789
H	6.996755	4.920215	13.158761
H	2.741157	-0.126179	11.055152
H	-4.134256	8.242940	11.291529
H	-3.995643	9.310048	9.041908
H	-2.173963	8.723602	7.501114
H	1.154999	6.855143	4.482316
H	-0.127620	8.075012	4.490977
H	-0.426734	9.719743	6.682117
H	0.615015	10.765513	5.707026
H	-2.946313	5.859144	6.603212
H	-2.726685	7.333605	5.653256
H	1.170127	4.481757	6.456901
H	0.087609	4.244377	5.061143
H	-0.476272	3.859071	6.696279
H	2.745154	12.597180	8.900463
H	2.235520	12.832539	7.225099
H	3.452650	11.597764	7.620157
H	-1.199920	11.061392	9.076656
H	-0.685548	12.535319	8.222812
H	-0.123249	12.219998	9.875112
H	2.717901	11.165310	5.268055
H	4.628204	11.715180	3.824193
H	6.001752	9.907144	2.813969
H	5.429869	7.528764	3.271183
H	3.517042	6.970255	4.715706
H	3.731133	10.741259	10.293614
H	3.933048	11.685254	12.576744
H	2.097277	11.369257	14.225619
H	5.251200	1.388260	9.569282
H	6.598834	3.216116	10.755228
H	7.506016	3.905045	9.396750
H	3.425056	2.436316	13.307204
H	4.800765	1.566669	12.614050
H	4.728892	3.344901	12.532404
H	1.571384	0.616354	9.944486
H	1.379735	0.814716	11.690720
H	7.232620	7.981812	10.063608
H	8.382979	6.729384	9.570271
H	6.868787	6.943564	8.680246
H	8.484992	5.213115	12.236041
H	7.584800	6.570879	12.937785
H	1.086259	4.271462	12.802936
H	-1.289124	3.881471	13.373420
H	-2.867600	3.029490	11.646964
H	-2.032930	2.578004	9.347363
H	0.358350	2.957078	8.794897

H	3.987056	4.521541	6.349754
H	4.691589	4.111831	3.998047
H	6.826875	2.935803	3.524794
H	8.244908	2.146402	5.406126
H	7.535822	2.518804	7.734712
H	5.809301	8.348855	11.988289
H	5.383118	9.430065	14.159094
H	3.744494	8.450850	15.755419
H	2.544395	6.358312	15.134759
H	3.041263	5.235909	12.981758
H	0.070359	10.083736	13.565431
H	-0.138528	9.181470	11.266172
H	4.206787	7.303147	6.975395
H	2.620989	7.242503	10.411325
H	4.560153	6.674536	8.571019
H	1.383776	5.972470	9.802274

TS_3-CO

E = -2343.633688
G = -2342.716670

C	-2.174511	7.195539	8.286373
C	-1.001664	6.492138	8.625579
C	-1.027818	5.720487	9.797424
C	-2.168694	5.660325	10.594006
C	-3.323860	6.357341	10.240910
C	-3.320179	7.123867	9.076019
N	0.159038	6.563135	7.807325
Si	-0.006161	6.020365	6.127073
C	1.524375	5.067339	5.558824
Ta	1.793986	7.744596	8.488695
O	3.511244	6.311171	7.917764
C	3.599490	8.266557	7.529165
Ta	3.376189	5.908766	9.787356
P	5.013599	3.916093	9.165874
C	6.314026	3.988690	7.858248
C	6.219114	4.983740	6.877138
C	7.171175	5.049455	5.858841
C	8.215490	4.128011	5.812515
C	8.309583	3.131695	6.785383
C	7.362753	3.061110	7.804445
N	2.446582	4.165202	10.636712
Si	2.451830	2.510992	9.963382
C	0.951585	2.099812	8.882375
C	1.746690	4.343803	11.854929
C	2.249996	5.224360	12.832632
C	1.590878	5.426609	14.042161
C	0.416769	4.734841	14.334379
C	-0.093901	3.851022	13.385399
C	0.549621	3.667294	12.163428
C	2.652096	1.199310	11.315424
C	3.997304	2.415182	8.833883
N	5.053153	6.494900	10.866352
Si	6.345351	5.390905	11.439430
C	8.045399	5.898077	10.785991
C	5.339917	7.846440	11.238678
C	4.917678	8.371235	12.469461
C	5.236221	9.677726	12.835221
C	5.980046	10.491758	11.981545
C	6.404547	9.982183	10.754548
C	6.093501	8.673721	10.390135
N	0.974561	9.447979	9.290381
C	0.698964	9.584143	10.685487
C	-0.513385	9.127356	11.223107
C	-0.792963	9.291159	12.578554
C	0.124506	9.917904	13.421139
C	1.335918	10.366762	12.895595
C	1.625022	10.198464	11.542805
P	1.036618	8.778553	6.079075
C	2.177506	9.448678	4.780667
C	2.423787	10.815046	4.609161
C	3.318329	11.259096	3.634713
C	3.982230	10.344829	2.820433
C	3.749883	8.979475	2.987072
C	2.859415	8.535294	3.961193
C	-1.530967	4.935297	5.855977
C	-0.099652	7.644289	5.116973
Si	0.678134	10.906491	8.313682
C	0.023223	10.228778	6.644614
C	2.233690	11.958665	8.095162
C	-0.688501	11.972161	9.070309
C	5.896241	3.659127	10.765973
C	6.412642	5.307363	13.327685
H	-2.144375	5.065919	11.503175
H	-0.131823	5.181371	10.082261
H	-1.551947	4.583005	4.818678
H	3.703277	2.460254	7.779690
H	5.459317	4.966684	13.743408
H	1.125414	1.164492	8.337524
H	-4.212572	6.305883	10.863747
H	-4.209685	7.675734	8.781291
H	-2.181206	7.806388	7.387296
H	0.247111	7.559232	4.083537
H	-1.111593	8.061497	5.103104
H	-0.960569	9.810831	6.889312
H	-0.117611	10.971210	5.852005
H	-1.494590	4.057691	6.509497
H	-2.464751	5.463997	6.060807
H	2.444520	5.557056	5.890623
H	1.533591	4.962766	4.467355

H	1.517882	4.060448	5.989921
H	2.568523	12.315490	9.074966
H	2.047654	12.836290	7.465239
H	3.045309	11.370851	7.656377
H	-1.599849	11.388705	9.232149
H	-0.927443	12.810703	8.406438
H	-0.377165	12.380588	10.036257
H	1.918315	11.544039	5.233082
H	3.492216	12.324849	3.512841
H	4.676738	10.692399	2.060760
H	4.263025	8.257137	2.357881
H	2.694825	7.467691	4.084949
H	2.580948	10.520670	11.140206
H	2.065792	10.848494	13.541415
H	-0.099305	10.049884	14.476304
H	4.564539	1.492180	8.994626
H	5.168181	3.206195	11.447444
H	6.764810	2.997682	10.687222
H	1.799304	1.167692	11.997150
H	2.751997	0.212122	10.849860
H	3.549845	1.382782	11.914783
H	0.782493	2.897073	8.152274
H	0.032060	1.980650	9.462813
H	8.313182	6.901974	11.127549
H	8.808367	5.200981	11.150934
H	8.068968	5.888871	9.692353
H	7.193787	4.606890	13.644707
H	6.645185	6.286519	13.757091
H	3.185472	5.742700	12.636405
H	2.007258	6.123701	14.764690
H	-0.091806	4.883097	15.282333
H	-1.011185	3.303504	13.588789
H	0.101640	3.006222	11.427530
H	5.395900	5.692984	6.921919
H	7.095171	5.825209	5.101674
H	8.956647	4.182934	5.019723
H	9.121248	2.409991	6.750686
H	7.444313	2.279412	8.555813
H	6.435276	8.271616	9.440521
H	6.985678	10.602982	10.077360
H	6.227106	11.509766	12.269267
H	4.897837	10.060342	13.794661
H	4.325919	7.748804	13.133175
H	-1.736486	8.925031	12.974901
H	-1.227800	8.637505	10.568403
H	3.743376	8.379883	6.454699
H	3.123181	7.766136	9.934703
H	4.557153	8.307699	8.049387
H	1.626461	6.588424	10.091936

Complex **Ta_2H_2•(CH_2)O**

E = -2343.697560
G = -2342.784701

C	-4.807883	0.166145	-1.583537
C	-3.602110	-0.553915	-1.480517
C	-3.598028	-1.706242	-0.673578
C	-4.749674	-2.118183	-0.004755
C	-5.937211	-1.396574	-0.121595
C	-5.957958	-0.251145	-0.917762
N	-2.430158	-0.124986	-2.149740
Si	-2.307433	-0.282702	-3.903614
C	-1.048545	-1.595604	-4.426904
Ta	-0.841696	0.625766	-0.987935
O	-0.528804	-1.229837	-0.219114
C	0.881173	0.581037	-1.984486
Ta	0.675490	-1.019636	1.224665
P	2.260986	-3.108212	0.601464
C	3.062896	-3.291418	-1.047660
C	2.248838	-3.104748	-2.174134
C	2.771235	-3.276711	-3.454085
C	4.111924	-3.622391	-3.621922
C	4.928037	-3.800822	-2.506145
C	4.406629	-3.639498	-1.222860
N	0.184312	-2.529509	2.615935
Si	0.139015	-4.302629	2.364773
C	-1.566308	-4.932711	1.847235
C	-0.467009	-2.228790	3.857332
C	0.287353	-2.050885	5.026863
C	-0.332046	-1.794741	6.247499
C	-1.722565	-1.721641	6.330544
C	-2.482092	-1.896531	5.175071
C	-1.864192	-2.146393	3.950984
C	0.695115	-5.243645	3.910139
C	1.367401	-4.679742	0.943996
N	2.563552	-0.197950	1.415115
Si	4.006398	-1.061198	2.030994
C	5.552467	-0.693189	1.009205
C	2.828208	1.203898	1.264712
C	2.531390	2.092426	2.308647
C	2.827311	3.449594	2.190409
C	3.420745	3.944061	1.029428
C	3.710936	3.067172	-0.016020
C	3.420054	1.709654	0.099233
N	-1.714979	2.304132	-0.086738
C	-2.034906	2.147074	1.300643
C	-3.121770	1.357246	1.705933
C	-3.447469	1.236864	3.056922
C	-2.706371	1.907938	4.026645
C	-1.621405	2.692885	3.633615

C	-1.283820	2.806561	2.288570
P	-1.098385	2.397991	-3.047737
C	0.261431	3.439269	-3.763069
C	0.368717	4.808080	-3.486589
C	1.416434	5.563872	-4.011036
C	2.379811	4.965029	-4.819577
C	2.286789	3.602878	-5.101104
C	1.239442	2.847347	-4.578483
C	-3.968136	-0.715935	-4.706366
C	-1.724521	1.435499	-4.518176
Si	-2.303866	3.864145	-0.706115
C	-2.426997	3.603931	-2.592109
C	-1.159797	5.306094	-0.251675
C	-4.032973	4.259254	-0.047094
C	3.578813	-2.923217	1.875106
C	4.342822	-0.641683	3.841111
H	-4.717922	-3.015320	0.609039
H	-2.667526	-2.254923	-0.573046
H	-3.828961	-0.833257	-5.787180
H	0.817035	-4.939561	0.033590
H	3.462058	-0.844371	4.457690
H	-1.524148	-6.007732	1.637598
H	-6.833707	-1.720897	0.399314
H	-6.874060	0.325976	-1.018058
H	-4.828777	1.066234	-2.191660
H	-0.916502	1.343406	-5.248915
H	-2.536447	1.997074	-4.992795
H	-3.372898	3.076601	-2.759581
H	-2.426730	4.509090	-3.206749
H	-4.358544	-1.659941	-4.313289
H	-4.728437	0.053052	-4.543942
H	-0.071630	-1.353759	-3.998918
H	-0.957777	-1.643798	-5.518293
H	-1.357033	-2.582119	-4.064642
H	-1.226960	5.500509	0.823565
H	-1.451423	6.227075	-0.770395
H	-0.115258	5.082499	-0.486323
H	-4.730546	3.444401	-0.263809
H	-4.413849	5.174360	-0.515122
H	-4.019840	4.411709	1.035852
H	-0.368219	5.298067	-2.860626
H	1.474329	6.625820	-3.787396
H	3.194252	5.555010	-5.230726
H	3.029947	3.123532	-5.732812
H	1.188206	1.787270	-4.809310
H	-0.418898	3.386812	1.982654
H	-1.028568	3.213830	4.381573
H	-2.964074	1.814623	5.077562
H	2.056638	-5.496699	1.179478
H	3.117682	-3.252442	2.811955
H	4.453735	-3.553926	1.689710
H	0.021174	-5.054891	4.750031
H	0.693797	-6.320634	3.706875
H	1.705510	-4.958238	4.220056
H	-1.912126	-4.419241	0.944862
H	-2.303218	-4.772020	2.639284
H	5.816234	0.366452	1.061540
H	6.397114	-1.272304	1.400487
H	5.411115	-0.958978	-0.042225
H	5.183957	-1.227185	4.228927
H	4.591652	0.418908	3.945038
H	1.369849	-2.113895	4.961560
H	0.275392	-1.655397	7.138481
H	-2.206766	-1.525758	7.283116
H	-3.566191	-1.831477	5.221774
H	-2.456574	-2.250639	3.047124
H	1.208561	-2.812830	-2.049721
H	2.129870	-3.129405	-4.318155
H	4.520667	-3.749799	-4.620423
H	5.973470	-4.068914	-2.631888
H	5.055060	-3.788889	-0.365058
H	3.629733	1.029237	-0.719364
H	4.162846	3.440756	-0.931138
H	3.652354	5.001653	0.938571
H	2.591281	4.122086	3.011385
H	2.053440	1.703222	3.202618
H	-4.295047	0.621627	3.347132
H	-3.718242	0.853288	0.950977
H	1.443111	1.343819	-2.520797
H	0.216273	0.739510	0.729006
H	1.466891	-0.343249	-1.890407
H	-0.055273	-0.177502	2.585225

TS_{A1}-CO or **TS_{B1}-CO**

E = -2343.669396
G = -2342.759085

C	1.403696	2.684988	-4.357387
C	0.298895	3.320656	-3.767817
C	0.286566	4.718998	-3.704247
C	1.347019	5.463834	-4.219976
C	2.436866	4.823205	-4.804992
C	2.461444	3.430532	-4.872567
P	-1.061222	2.273372	-3.080199
C	-2.445067	3.420664	-2.662741
Si	-2.310991	3.777843	-0.787930
C	-4.044685	4.193870	-0.151241
Ta	-0.852748	0.596291	-1.016302
N	-1.687659	2.271170	-0.071474
C	-1.936675	2.247365	1.335863

C	-3.026645	1.538895	1.863865
C	-3.296716	1.564277	3.230746
C	-2.492799	2.301746	4.097981
C	-1.403085	3.004119	3.583532
C	-1.123893	2.975001	2.219694
N	-2.519685	-0.117913	-2.098774
Si	-2.623903	-0.237025	-3.857969
C	-1.601971	1.239101	-4.522634
C	-3.560092	-0.749422	-1.362606
C	-4.777191	-0.084606	-1.125614
C	-5.807947	-0.698768	-0.417589
C	-5.650049	-1.994071	0.075104
C	-4.446982	-2.663746	-0.146675
C	-3.412290	-2.051259	-0.852930
C	-1.888024	-1.854341	-4.515232
C	-4.403467	-0.094998	-4.490197
O	-0.346066	-1.236362	-0.429543
Ta	0.768183	-0.935092	1.106829
N	2.675548	-0.180619	1.461763
C	2.916588	1.231824	1.464466
C	2.438862	2.033798	2.512845
C	2.707554	3.401434	2.540565
C	3.453699	3.997949	1.524777
C	3.927062	3.210833	0.474722
C	3.663239	1.843401	0.444086
C	1.117339	0.825624	-1.548458
P	2.334565	-3.044264	0.491279
C	3.637329	-2.936284	1.791690
Si	4.096218	-1.097091	2.035398
C	4.421649	-0.766020	3.866585
N	0.151365	-2.412379	2.460878
C	-0.649750	-2.094549	3.607948
C	-0.042649	-1.848375	4.848767
C	-0.809520	-1.584397	5.980924
C	-2.202203	-1.570731	5.901813
C	-2.815215	-1.810983	4.673602
C	-2.050437	-2.067536	3.536996
C	3.161068	-3.248624	-1.144372
C	2.405204	-2.907632	-2.275906
C	2.943250	-3.067757	-3.551436
C	4.241475	-3.552801	-3.708603
C	5.000774	-3.882174	-2.586669
C	4.463195	-3.734277	-1.308704
C	1.382376	-4.582821	0.825839
Si	0.192043	-4.192987	2.275916
C	0.820671	-5.043695	3.847398
C	-1.488805	-4.935837	1.827591
C	5.667254	-0.724902	1.049630
C	-1.194320	5.272784	-0.454363
H	-4.312404	-3.674487	0.230687
H	-2.466317	-2.559012	-1.011756
H	-4.414351	-0.189995	-5.581956
H	0.793253	-4.794463	-0.073070
H	3.545932	-1.029638	4.467618
H	-1.376903	-6.006123	1.618598
H	-6.454262	-2.475074	0.624799
H	-6.738379	-0.161452	-0.250834
H	-4.900333	0.924252	-1.508728
H	-0.694823	0.873343	-5.013934
H	-2.156428	1.847248	-5.245394
H	-3.356653	2.826488	-2.792022
H	-2.513292	4.299103	-3.311723
H	-5.037744	-0.884290	-4.076096
H	-4.853106	0.868684	-4.230740
H	-0.844755	-1.953253	-4.199416
H	-1.926317	-1.897859	-5.609692
H	-2.441686	-2.714008	-4.122998
H	-1.209401	5.514137	0.612953
H	-1.548685	6.156641	-0.998129
H	-0.156787	5.078948	-0.740798
H	-4.737979	3.364799	-0.323448
H	-4.432791	5.080035	-0.666737
H	-4.032698	4.402681	0.922181
H	-0.551085	5.239430	-3.253139
H	1.316209	6.548691	-4.165060
H	3.261255	5.404714	-5.208298
H	3.306795	2.920569	-5.326725
H	1.441207	1.600448	-4.408371
H	-0.256071	3.492470	1.823293
H	-0.761566	3.575937	4.250023
H	-2.708035	2.322626	5.162445
H	2.035758	-5.438114	1.025740
H	3.155864	-3.289155	2.709410
H	4.502768	-3.577511	1.598808
H	0.157705	-4.829924	4.690484
H	0.844703	-6.129441	3.700342
H	1.828234	-4.716385	4.122676
H	-1.892673	-4.450589	0.934115
H	-2.212160	-4.821153	2.639296
H	5.966952	0.321489	1.151524
H	6.487094	-1.347913	1.426310
H	5.533626	-0.944366	-0.013879
H	5.278515	-1.346599	4.226120
H	4.636893	0.294380	4.031243
H	1.041943	-1.862706	4.908175
H	-0.315444	-1.391777	6.930188
H	-2.800810	-1.369928	6.785960
H	-3.899227	-1.794239	4.593344
H	-2.530859	-2.230630	2.577157
H	1.401477	-2.506790	-2.150963
H	2.349718	-2.804843	-4.422617
H	4.662215	-3.671093	-4.703316

H	6.013388	-4.258320	-2.704663
H	5.065308	-4.001740	-0.445334
H	4.023332	1.234312	-0.378862
H	4.504483	3.662504	-0.327921
H	3.663096	5.063703	1.549693
H	2.329512	4.002609	3.363586
H	1.845211	1.568588	3.293645
H	-4.144862	1.006425	3.617971
H	-3.662070	0.973978	1.187338
H	1.607939	1.753424	-1.845496
H	0.784552	0.859516	0.011150
H	1.841650	0.005112	-1.487691
H	-0.092075	0.016760	2.326600

Complex **Ta_2H•$(CH_3)O$**

E = -2343.705975
G = -2342.788390

Ta	0.758381	-0.932245	0.761353
C	1.860757	1.258993	3.646791
C	2.516668	1.032811	2.425873
C	1.945894	2.492625	4.286959
C	2.696762	3.529362	3.731823
C	3.348842	3.320183	2.517868
C	3.256922	2.089522	1.868968
N	2.441820	-0.236405	1.778935
P	2.301200	-2.934831	-0.023389
C	3.288231	-3.001668	-1.581156
C	3.038839	-2.046134	-2.573945
C	3.750907	-2.090433	-3.773913
C	4.707401	-3.080664	-3.988192
C	4.955239	-4.036002	-3.001135
C	4.248493	-3.997364	-1.802004
C	5.289499	-0.522721	0.615805
Si	3.971107	-1.144531	1.826809
C	3.537694	-2.952414	1.355581
C	4.704947	-1.150277	3.571871
C	1.373234	-4.537041	0.075727
Si	0.028331	-4.329896	1.420522
C	0.530466	-5.275565	2.982671
C	-1.606599	-5.048397	0.803897
C	-0.697058	-2.200515	2.948267
C	0.036174	-2.086617	4.143521
C	-0.598546	-1.768669	5.342831
C	-1.977433	-1.561868	5.374973
C	-2.712404	-1.653206	4.192150
C	-2.080468	-1.957305	2.988032
N	-0.050057	-2.582368	1.729900
Ta	-0.764959	0.964382	-0.680116
N	-2.430199	-0.047871	-1.567171
N	-1.747805	2.550640	0.235615
C	-3.400513	-0.541413	-0.650471
C	-4.222464	0.333411	0.083870
C	-5.234386	-0.149200	0.911513
C	-5.471773	-1.518663	1.025282
H	-2.240879	0.795087	2.161250
C	-1.903413	2.847997	1.605456
C	-3.631523	-1.923563	-0.493692
C	-4.659687	-2.402833	0.314099
C	-2.163735	1.815072	2.526012
C	-2.334867	2.081034	3.880849
C	-2.265509	3.386658	4.366692
C	-2.004998	4.420876	3.471325
C	-1.821965	4.158135	2.115578
Si	-2.202058	3.810727	-0.960253
C	-3.972997	4.405846	-0.640572
C	-1.054803	5.328553	-1.015618
C	-2.268279	3.004608	-2.709676
C	-4.389876	-1.015236	-3.686291
P	-0.965235	1.762415	-3.186770
Si	-2.582172	-0.725980	-3.210331
C	-1.568116	-2.303709	-3.488099
C	-1.840516	0.616229	-4.347259
C	0.288707	2.617337	-4.243224
C	0.038748	3.803741	-4.940090
C	1.015190	4.355902	-5.768782
C	2.249581	3.725933	-5.913419
C	2.506190	2.540706	-5.224611
C	1.534243	1.991962	-4.391480
C	0.924075	2.418293	-1.072021
H	1.214496	2.735814	-0.062465
H	1.780061	1.913736	-1.528491
H	0.725110	3.325124	-1.652614
H	0.214752	0.850702	1.026158
O	0.711430	-0.433908	-1.062572
H	-4.817831	-3.475454	0.395149
H	-2.987191	-2.622299	-1.017733
H	-4.448819	-1.321354	-4.736825
H	0.905319	-4.695621	-0.902089
H	3.991390	-1.551301	4.298815
H	-1.527877	-6.133791	0.675695
H	-6.273111	-1.891052	1.657074
H	-5.849246	0.557971	1.462495
H	-4.049710	1.400127	0.000133
H	-1.091962	0.183636	-5.018237
H	-2.586192	1.142770	-4.951457
H	-3.198002	2.426399	-2.735544
H	-2.361221	3.806572	-3.451607
H	-4.856486	-1.794082	-3.077957
H	-4.976110	-0.098428	-3.565214

H	-0.553496	-2.160628	-3.103144
H	-1.507420	-2.536039	-4.557761
H	-2.005557	-3.172066	-2.985996
H	-1.528165	6.187352	-0.527791
H	-0.843254	5.610101	-2.052811
H	-0.100378	5.133413	-0.521353
H	-4.697370	3.596144	-0.771353
H	-4.232077	5.210656	-1.338281
H	-4.076538	4.792949	0.377112
H	-0.919333	4.306337	-4.848828
H	0.808020	5.279590	-6.302400
H	3.010112	4.158550	-6.557435
H	3.470099	2.049444	-5.325732
H	1.744797	1.082298	-3.835444
H	-1.582737	4.982136	1.451423
H	-1.931123	5.445948	3.826319
H	-2.408293	3.592320	5.423760
H	2.038248	-5.383279	0.280096
H	3.036430	-3.407660	2.216811
H	4.424678	-3.547723	1.114717
H	-0.201861	-5.127934	3.782014
H	0.581239	-6.348698	2.766125
H	1.507702	-4.960807	3.361519
H	-1.892245	-4.608437	-0.155549
H	-2.408721	-4.849511	1.521463
H	5.643891	0.473121	0.897798
H	6.153388	-1.197645	0.615690
H	4.897489	-0.472187	-0.404666
H	5.613060	-1.762456	3.606729
H	4.967972	-0.135600	3.885950
H	1.107776	-2.260476	4.114806
H	-0.012977	-1.687886	6.255050
H	-2.473495	-1.325600	6.312314
H	-3.785399	-1.482308	4.198956
H	-2.648922	-2.018299	2.065320
H	2.288872	-1.279614	-2.388881
H	3.556212	-1.348378	-4.543679
H	5.260027	-3.111530	-4.923363
H	5.699135	-4.810716	-3.166553
H	4.446444	-4.747505	-1.039798
H	3.737783	1.942217	0.906797
H	3.926688	4.121559	2.063741
H	2.764377	4.489882	4.234880
H	1.418179	2.644464	5.224756
H	1.274233	0.455389	4.082035
H	-2.527751	1.252754	4.556487

TS_{A2}-CO

E = -2343.660824

G = -2342.743881

Ta	0.838897	-0.800429	0.705614
C	1.529448	1.530114	3.269651
C	2.576332	1.168093	2.403669
C	1.544975	2.740997	3.956464
C	2.619626	3.620312	3.820495
C	3.669622	3.275000	2.971897
C	3.644698	2.073921	2.265701
N	2.525110	-0.061420	1.699950
P	2.274852	-2.861778	-0.133694
C	3.201640	-3.009646	-1.721613
C	2.862906	-2.139090	-2.765161
C	3.513298	-2.244658	-3.995771
C	4.496802	-3.212741	-4.189182
C	4.833954	-4.083038	-3.151052
C	4.188584	-3.983186	-1.921105
C	5.215962	-0.461815	0.212056
Si	4.041241	-1.002543	1.600185
C	3.545957	-2.816898	1.215041
C	4.950944	-1.006773	3.259138
C	1.335425	-4.442697	0.081198
Si	0.044579	-4.164327	1.466798
C	0.590894	-5.064384	3.040773
C	-1.616054	-4.877594	0.920742
C	-0.662609	-2.008646	2.928747
C	0.069668	-1.770713	4.106034
C	-0.579096	-1.449410	5.297830
C	-1.970078	-1.367437	5.340254
C	-2.706132	-1.582002	4.172849
C	-2.063129	-1.887507	2.975661
N	0.009524	-2.407207	1.728926
Ta	-0.802856	0.998560	-0.558217
N	-2.462069	-0.124718	-1.383241
N	-1.801041	2.687040	0.208621
C	-3.469119	-0.620202	-0.524647
C	-4.170512	0.251649	0.333752
C	-5.190133	-0.206727	1.164681
C	-5.563841	-1.550605	1.164429
H	-2.116059	0.898419	2.143081
C	-1.941285	2.978653	1.575927
C	-3.853924	-1.978348	-0.498034
C	-4.885967	-2.430950	0.321277
C	-2.091713	1.926494	2.503565
C	-2.248356	2.174936	3.863947
C	-2.274181	3.482314	4.351375
C	-2.119667	4.535336	3.451624
C	-1.949493	4.290203	2.091467
Si	-2.341043	3.858133	-1.024143
C	-4.138460	4.366483	-0.717547
C	-1.288495	5.428508	-1.222478

C	-2.301046	2.951502	-2.719416
C	-4.240665	-0.848087	-3.737104
P	-0.856744	1.813673	-2.978106
Si	-2.479544	-0.751263	-3.044375
C	-1.596670	-2.415863	-3.280411
C	-1.481379	0.499117	-4.110402
C	0.450317	2.724329	-3.912383
C	0.221034	3.890524	-4.649501
C	1.261130	4.489684	-5.359693
C	2.536488	3.927895	-5.342156
C	2.773224	2.766065	-4.607372
C	1.738062	2.170416	-3.890825
C	1.189835	2.518630	-0.438085
H	1.523765	3.038099	0.466326
H	2.052669	2.048107	-0.911330
H	0.797611	3.289345	-1.104680
H	0.713370	1.505857	0.424166
O	0.692204	-0.348938	-1.128763
H	-5.154469	-3.484687	0.303785
H	-3.326253	-2.688640	-1.126547
H	-4.222581	-1.189562	-4.778158
H	0.823810	-4.639166	-0.867235
H	4.307316	-1.408548	4.048413
H	-1.539781	-5.961534	0.778197
H	-6.368724	-1.903884	1.802683
H	-5.703624	0.502234	1.809646
H	-3.902492	1.302737	0.333050
H	-0.605487	-0.002187	-4.535001
H	-2.066556	0.926671	-4.931845
H	-3.170619	2.285083	-2.736303
H	-2.417390	3.670670	-3.537929
H	-4.863825	-1.539259	-3.163414
H	-4.721847	0.135274	-3.709246
H	-0.616953	-2.367268	-2.794393
H	-1.444965	-2.617133	-4.347547
H	-2.151886	-3.260287	-2.861329
H	-1.436381	6.137495	-0.402968
H	-1.586558	5.934213	-2.148826
H	-0.219501	5.207710	-1.287545
H	-4.799466	3.495679	-0.765939
H	-4.470395	5.093664	-1.466895
H	-4.251733	4.821232	0.270990
H	-0.767022	4.339819	-4.677420
H	1.072615	5.396645	-5.927745
H	3.345386	4.397359	-5.895118
H	3.768224	2.330205	-4.581221
H	1.923520	1.280087	-3.295281
H	-1.797375	5.128928	1.420636
H	-2.123105	5.562724	3.807964
H	-2.414378	3.675137	5.411198
H	2.001913	-5.285622	0.294612
H	3.060182	-3.225119	2.108125
H	4.421988	-3.433842	0.985861
H	-0.110825	-4.877193	3.859081
H	0.621132	-6.145329	2.863048
H	1.584436	-4.747021	3.372125
H	-1.942704	-4.425185	-0.019362
H	-2.388340	-4.687978	1.672208
H	5.706364	0.492607	0.424297
H	6.000686	-1.214783	0.074056
H	4.675660	-0.362921	-0.734475
H	5.850731	-1.628987	3.199145
H	5.251302	0.002536	3.552723
H	1.152249	-1.853445	4.072404
H	0.006992	-1.270670	6.195514
H	-2.476674	-1.131710	6.272161
H	-3.789664	-1.505120	4.185796
H	-2.636200	-2.040240	2.066031
H	2.093887	-1.388238	-2.594705
H	3.250141	-1.567692	-4.804178
H	5.001353	-3.292690	-5.148284
H	5.598614	-4.840435	-3.301301
H	4.453385	-4.669043	-1.119745
H	4.450113	1.846218	1.574490
H	4.511165	3.951028	2.840935
H	2.634127	4.561389	4.362636
H	0.705313	2.994141	4.597003
H	0.695569	0.847581	3.408576
H	-2.365036	1.333431	4.540413

Complex **Ta_2O**

E = -2303.201186
G = -2302.328155

C	-1.273559	1.856366	-3.487853
C	-0.022664	1.401940	-3.915862
C	0.590730	2.010742	-5.018496
C	-0.041628	3.055139	-5.688798
C	-1.297611	3.494094	-5.268164
C	-1.911274	2.894227	-4.170184
P	0.759422	-0.058335	-3.087602
Ta	0.192983	-1.268578	-0.867858
Ta	0.192844	0.867984	1.000299
P	0.206273	0.533738	3.548776
C	-0.591103	-0.809470	4.534385
C	-0.644767	-0.740436	5.933023
C	-1.240007	-1.765294	6.663776
C	-1.785626	-2.866915	6.002527
C	-1.730284	-2.941671	4.612510
C	-1.133476	-1.918302	3.874166

C	1.977035	0.581488	4.099624
Si	2.938293	1.807466	2.985923
N	1.946708	1.942624	1.520406
C	1.845853	3.023779	0.644180
C	2.252569	4.350933	0.904211
C	1.993791	5.363017	-0.011057
C	1.288041	5.107746	-1.192087
C	0.858029	3.812660	-1.456545
C	1.148619	2.775195	-0.564581
C	4.651772	1.106281	2.610451
C	3.189719	3.398624	3.996818
C	-0.610827	2.100153	4.098835
Si	-2.076098	2.441202	2.909422
N	-1.554551	1.953573	1.267512
C	-2.515652	2.346987	0.291807
C	-2.524432	3.649134	-0.235904
C	-3.521356	4.055206	-1.121760
C	-4.529701	3.171951	-1.508045
C	-4.519776	1.869030	-1.006633
C	-3.527533	1.460795	-0.117284
C	-2.466739	4.290165	3.041140
C	-3.588793	1.453720	3.472268
C	2.590577	0.170309	-3.257429
Si	3.435211	-1.148112	-2.157105
N	2.098794	-1.964013	-1.318427
C	2.350817	-3.221959	-0.704155
C	1.786827	-4.399297	-1.229068
C	2.004321	-5.635128	-0.621945
C	2.799429	-5.729578	0.520025
C	3.372785	-4.572536	1.048259
C	3.151272	-3.335363	0.448253
C	4.655799	-0.261928	-1.018956
C	4.375929	-2.392406	-3.231759
C	0.337492	-1.413861	-4.306180
Si	-1.332135	-2.205796	-3.826225
N	-1.316327	-2.089172	-2.060532
C	-2.306405	-2.750411	-1.291350
C	-1.956687	-3.822448	-0.448525
C	-2.912536	-4.449650	0.350552
C	-4.243059	-4.037074	0.314650
C	-4.606547	-2.981121	-0.523637
C	-3.653500	-2.339655	-1.309504
C	-1.358127	-4.021731	-4.364008
C	-2.779326	-1.334301	-4.680824
O	-0.082403	-1.098218	0.998598
H	2.361665	-0.435379	3.958421
H	2.071214	0.834848	5.161487
H	0.114353	2.911320	3.973036
H	-0.925544	2.072487	5.147287
H	2.833160	1.170219	-2.881866
H	2.916945	0.098071	-4.300780
H	1.111159	-2.181622	-4.192364
H	0.363695	-1.034705	-5.333254
H	4.579968	0.120201	2.143578
H	5.240186	1.011398	3.529978
H	5.199100	1.762259	1.925702
H	3.952406	4.049279	3.558112
H	3.543279	3.115846	4.995508
H	2.271423	3.980254	4.119898
H	-1.604641	4.895481	2.743182
H	-2.719693	4.541123	4.077970
H	-3.314295	4.568766	2.408837
H	-4.427884	1.624146	2.790531
H	-3.902393	1.756987	4.477537
H	-3.376316	0.380501	3.487945
H	4.117461	0.441637	-0.376695
H	5.388036	0.301548	-1.609007
H	5.208332	-0.963925	-0.386470
H	4.803490	-3.188697	-2.614117
H	5.198382	-1.901996	-3.763989
H	3.720778	-2.860722	-3.973535
H	-0.494826	-4.567667	-3.970964
H	-1.347517	-4.105294	-5.456447
H	-2.264249	-4.516474	-3.998563
H	-3.726866	-1.822307	-4.430214
H	-2.658259	-1.385665	-5.769092
H	-2.844709	-0.281113	-4.396516
H	2.771757	4.585080	1.825243
H	2.344082	6.370227	0.202807
H	1.090086	5.907587	-1.899441
H	-1.739162	4.336850	0.061366
H	-3.510302	5.071799	-1.507801
H	-5.314569	3.493902	-2.187366
H	-5.298556	1.168171	-1.297555
H	-3.528498	0.450658	0.281864
H	-0.221118	0.113224	6.457326
H	-1.279207	-1.704636	7.748142
H	-2.251904	-3.665406	6.573475
H	-2.153484	-3.797311	4.093918
H	-1.076157	-1.973420	2.790767
H	1.180624	-4.324724	-2.127414
H	1.556508	-6.528637	-1.050034
H	2.971351	-6.692703	0.992011
H	3.992047	-4.631748	1.939907
H	3.579431	-2.433702	0.876404
H	-0.927033	-4.173058	-0.444709
H	-2.613640	-5.276749	0.989821
H	-4.989954	-4.532514	0.928464
H	-5.640753	-2.647397	-0.557782
H	-3.931494	-1.497938	-1.936273
H	1.567229	1.673385	-5.354852
H	0.445631	3.525252	-6.538967

H	-1.793093	4.306767	-5.792754
H	-2.880186	3.237487	-3.822858
H	-1.733497	1.412914	-2.607912
H	0.316816	3.594596	-2.369776
H	0.992629	1.714667	-0.890777

TS_{A3}-CO

E = -2303.197066
G = -2302.324800

C	-3.796157	6.044093	1.196496
C	-2.563874	5.591868	0.714939
C	-2.060738	6.111375	-0.484463
C	-2.783789	7.064638	-1.197393
C	-4.019278	7.503223	-0.719951
C	-4.522364	6.993271	0.475344
P	-1.650258	4.257870	1.617676
Ta	-2.128232	3.048464	3.877399
Ta	-2.182573	5.112019	5.847477
P	-2.229343	4.726069	8.449690
C	-3.183467	3.420669	9.338847
C	-3.362580	3.461412	10.728000
C	-4.075018	2.453082	11.371960
C	-4.613692	1.398214	10.633130
C	-4.433843	1.351478	9.252352
C	-3.718105	2.357448	8.601350
C	-0.487824	4.620285	9.067718
Si	0.625829	5.723308	7.962183
N	-0.287782	5.855889	6.459452
C	-0.259499	6.877210	5.498294
C	0.493234	8.057298	5.489664
C	0.339470	8.959002	4.432811
C	-0.591669	8.722817	3.417832
C	-1.383415	7.572517	3.447693
C	-1.222385	6.631088	4.472588
C	2.294633	4.871090	7.721570
C	0.916550	7.373242	8.859193
C	-2.951551	6.337402	8.996268
Si	-4.394334	6.770591	7.810385
N	-3.944577	6.138045	6.195537
C	-4.923380	6.487308	5.217730
C	-4.901608	7.742385	4.586349
C	-5.909036	8.107465	3.694349
C	-6.954890	7.230480	3.406230
C	-6.974067	5.972876	4.012657
C	-5.973059	5.605123	4.908807
C	-4.589817	8.652578	7.821530
C	-5.991918	5.975201	8.432173
C	0.152504	4.631616	1.457889
Si	1.088343	3.395048	2.586711
N	-0.192935	2.443714	3.382153
C	0.149495	1.190048	3.951203
C	-0.533015	0.019622	3.568299
C	-0.225341	-1.215179	4.136645
C	0.782094	-1.321629	5.095434
C	1.475334	-0.173547	5.478403
C	1.162854	1.064068	4.920949
C	2.182334	4.399008	3.756310
C	2.169288	2.256285	1.526486
C	-1.958933	2.791486	0.500024
Si	-3.579129	1.913842	1.004458
N	-3.593595	2.077373	2.772900
C	-4.606081	1.424848	3.527126
C	-4.281840	0.353072	4.378323
C	-5.263405	-0.278085	5.141530
C	-6.592432	0.135131	5.065075
C	-6.927797	1.196569	4.223081
C	-5.949572	1.839005	3.468513
C	-3.503876	0.089251	0.504226
C	-5.070946	2.687872	0.135909
O	-2.369982	3.120410	5.744879
H	-0.189954	3.571113	8.955705
H	-0.420105	4.881130	10.129224
H	-2.172363	7.097869	8.875861
H	-3.267305	6.329672	10.044629
H	0.298525	5.650831	1.832535
H	0.500553	4.582692	0.420574
H	-1.131160	2.093890	0.667174
H	-1.956153	3.101482	-0.550483
H	2.161143	3.878629	7.281406
H	2.818423	4.758549	8.677392
H	2.933930	5.454623	7.051511
H	1.780947	7.907716	8.453606
H	1.120405	7.181895	9.918937
H	0.050616	8.038643	8.793891
H	-3.679443	9.145006	7.465065
H	-4.790757	8.998249	8.842290
H	-5.421570	8.971662	7.187135
H	-6.810354	6.161604	7.730281
H	-6.276927	6.393644	9.404006
H	-5.877231	4.893110	8.543569
H	1.558066	4.968348	4.451370
H	2.794130	5.105316	3.183202
H	2.860304	3.762999	4.334086
H	2.659224	1.499118	2.146403
H	2.950186	2.830059	1.015398
H	1.576493	1.735031	0.767823
H	-2.592779	-0.395519	0.867916
H	-3.530986	-0.013203	-0.586362
H	-4.362686	-0.453590	0.913129

H	-5.990082	2.149517	0.388253
H	-4.939194	2.628325	-0.950710
H	-5.197060	3.739766	0.404463
H	1.201623	8.268279	6.285077
H	0.954090	9.855463	4.405916
H	-0.704186	9.436580	2.605858
H	-4.085089	8.423031	4.805376
H	-5.875291	9.088089	3.225825
H	-7.746519	7.522673	2.721488
H	-7.780387	5.276304	3.796612
H	-5.988278	4.628156	5.382596
H	-2.945459	4.278315	11.312442
H	-4.211129	2.490293	12.449475
H	-5.171829	0.613644	11.136961
H	-4.851362	0.533262	8.672676
H	-3.562866	2.321247	7.526274
H	-1.306486	0.096867	2.809769
H	-0.768511	-2.101035	3.816111
H	1.025696	-2.284715	5.534601
H	2.262419	-0.238334	6.225842
H	1.688925	1.956160	5.246922
H	-3.250139	0.013872	4.425854
H	-4.984862	-1.106480	5.788337
H	-7.358739	-0.363035	5.652247
H	-7.959642	1.533016	4.158648
H	-6.207981	2.683163	2.837093
H	-1.099581	5.775491	-0.865091
H	-2.382834	7.464553	-2.125018
H	-4.584830	8.245589	-1.276760
H	-5.475797	7.336429	0.864072
H	-4.174532	5.663985	2.142918
H	-2.124267	7.406987	2.672655
H	-1.293227	5.327829	4.159658

Complex **4**

E = -2303.238226
G = -2302.364733

C	-0.534262	4.796530	9.088568
H	0.106671	3.931630	8.881706
H	-0.512366	4.995869	10.165055
C	-3.432268	5.365195	9.483424
H	-2.955791	6.340788	9.628555
H	-3.665968	4.948085	10.467687
C	0.071102	4.142356	0.500679
H	0.390825	5.186518	0.582941
H	0.323819	3.757365	-0.492614
C	-2.316597	2.447966	0.197588
H	-1.485100	1.746679	0.319129
H	-2.573146	2.499867	-0.864781
C	1.989423	6.184101	7.943505
H	2.349190	5.290112	7.427705
H	2.394452	6.176573	8.961938
H	2.397824	7.062713	7.434512
C	-0.410807	7.915571	8.724006
H	-0.039481	8.721767	8.081978
H	0.006261	8.064953	9.726430
H	-1.498739	8.018574	8.781593
C	-5.890038	7.168737	8.991084
H	-5.253774	8.054883	8.902149
H	-6.177463	7.053300	10.042101
H	-6.796845	7.347031	8.406623
C	-6.099671	4.110835	8.571375
H	-7.021831	4.229652	7.994850
H	-6.375855	3.965161	9.622363
H	-5.600083	3.203633	8.218899
C	2.573910	4.026400	2.277035
H	2.389450	5.040441	2.643006
H	3.177187	4.089529	1.363777
H	3.151733	3.482355	3.029090
C	1.322152	1.397549	1.325213
H	1.827398	0.845621	2.123661
H	1.989208	1.418522	0.455924
H	0.423384	0.836650	1.051761
C	-3.568000	0.026595	1.651919
H	-2.620639	-0.167607	2.164882
H	-3.577489	-0.547911	0.718555
H	-4.380380	-0.341480	2.285219
C	-5.393627	2.135952	0.356706
H	-6.256346	1.847868	0.963320
H	-5.396024	1.520972	-0.550753
H	-5.517101	3.180824	0.056249
C	-0.423365	6.393346	5.182736
C	0.692015	6.959901	4.602505
H	1.596535	7.173817	5.164863
C	0.617039	7.288708	3.211977
H	1.477552	7.769725	2.750717
C	-0.507315	7.063225	2.455259
H	-0.544652	7.401837	1.422331
C	-1.685258	6.474191	3.050226
C	-1.634918	6.168956	4.434754
C	-5.162944	6.699986	5.909741
C	-4.666780	7.923704	5.430036
H	-3.650712	8.208061	5.687993
C	-5.450808	8.749129	4.627392
H	-5.039295	9.688359	4.266182
C	-6.754923	8.381768	4.293951
H	-7.368461	9.030014	3.674385
C	-7.260236	7.171509	4.767861
H	-8.273043	6.867809	4.513443

C	-6.474768	6.338065	5.562256
H	-6.861018	5.379817	5.895131
C	-2.494640	2.584714	9.124898
C	-2.640122	2.274958	10.483483
H	-2.631328	3.063754	11.231807
C	-2.791734	0.951376	10.888593
H	-2.905534	0.718243	11.943918
C	-2.795643	-0.072205	9.939606
H	-2.914803	-1.104838	10.256677
C	-2.644350	0.231384	8.588349
H	-2.642461	-0.564505	7.848623
C	-2.493820	1.555923	8.174206
H	-2.372101	1.797995	7.120174
C	0.416531	2.472761	4.398298
C	0.140597	1.114468	4.619185
H	-0.567906	0.615961	3.964233
C	0.754880	0.418914	5.657177
H	0.525220	-0.632953	5.808322
C	1.664940	1.063301	6.495256
H	2.152542	0.519463	7.299466
C	1.941484	2.413749	6.286957
H	2.652511	2.924919	6.931518
C	1.321633	3.116330	5.253406
H	1.522720	4.172096	5.098089
C	-4.802909	2.550673	3.625700
C	-4.737008	1.511336	4.567216
H	-3.792854	0.994287	4.701486
C	-5.854279	1.162900	5.323293
H	-5.781383	0.352074	6.043693
C	-7.060304	1.844628	5.158220
H	-7.933805	1.564549	5.740448
C	-7.130072	2.891914	4.240025
H	-8.060732	3.437007	4.103853
C	-6.011931	3.247048	3.487330
H	-6.062954	4.070648	2.782051
C	-2.563693	5.322489	-0.256700
C	-1.963331	5.807240	-1.423744
H	-0.970589	5.469144	-1.708154
C	-2.631573	6.731019	-2.226649
H	-2.155363	7.104235	-3.129348
C	-3.904477	7.175972	-1.872078
H	-4.422373	7.897678	-2.497619
C	-4.508057	6.698905	-0.708891
H	-5.495683	7.049218	-0.422083
C	-3.838956	5.780971	0.098879
H	-4.302776	5.422467	1.014942
N	-0.704987	5.926448	6.471891
N	-4.347776	5.871964	6.737907
N	-0.187306	3.155428	3.291022
N	-3.679368	2.849913	2.787483
O	-2.244174	3.239648	5.332303
Si	0.097221	6.238145	8.001703
Si	-4.980436	5.624505	8.389843
Si	0.937979	3.163629	1.897633
Si	-3.768971	1.873202	1.289721
P	-2.238266	4.315207	8.534979
P	-1.734403	4.088075	0.842215
Ta	-2.595985	5.053932	5.951917
Ta	-2.083183	3.993613	3.468738
H	-2.644552	6.660256	2.571588
H	-3.598644	5.029411	4.315370

TS_{B2}-CO

E = -2343.665014
G = -2342.746884

C	0.471134	3.667081	-6.105998
C	-0.480729	3.900640	-5.101890
C	-0.964339	5.201283	-4.919306
C	-0.499089	6.249302	-5.713828
C	0.454463	6.010840	-6.700247
C	0.938032	4.716622	-6.893153
P	-1.091876	2.461790	-4.116616
C	0.409266	1.687131	-3.360598
Si	-0.117880	-0.004278	-2.611116
C	1.021111	-1.375378	-3.246368
Ta	-2.437957	0.382709	-5.075699
N	-1.792113	-0.245066	-3.128057
C	-2.810380	-0.761993	-2.307470
C	-3.039812	-0.320536	-0.985948
C	-4.074794	-0.842895	-0.216193
C	-4.940176	-1.804724	-0.739881
C	-4.742308	-2.242094	-2.047709
C	-3.691522	-1.741360	-2.813475
Ta	-1.179059	-1.230377	-7.062032
C	-2.721007	1.922298	-7.042950
P	1.229590	-0.995135	-8.098636
C	2.089718	-2.552507	-7.589160
Si	0.808113	-3.966824	-7.395803
C	0.553053	-4.784177	-9.095223
C	2.444510	0.361107	-7.772592
C	2.851880	1.276758	-8.749311
C	3.768957	2.282230	-8.440052
C	4.284660	2.391027	-7.150401
C	3.872175	1.492496	-6.166019
C	2.956285	0.488968	-6.472202
C	1.011279	-1.095490	-9.935843
Si	-0.705147	-0.365869	-10.359132
C	-0.601429	1.520434	-10.422561
C	-1.255520	-1.038639	-12.036670

N	-1.738012	-0.987436	-9.054845
C	-3.057397	-1.402346	-9.361433
C	-3.469438	-2.715325	-9.065201
C	-4.764646	-3.144696	-9.357422
C	-5.672674	-2.284841	-9.971580
C	-5.276235	-0.979930	-10.274000
C	-3.993890	-0.539013	-9.964060
N	-0.671992	-3.244395	-6.715168
C	-1.487254	-4.197015	-6.036662
C	-2.058709	-5.291716	-6.710638
C	-2.828697	-6.236858	-6.031999
C	-3.049687	-6.113611	-4.662497
C	-2.490895	-5.031274	-3.981042
C	-1.720326	-4.088463	-4.655946
O	-0.556915	0.083521	-5.812433
C	1.563560	-5.246184	-6.225012
N	-3.975075	1.643683	-4.215234
Si	-3.967233	3.061496	-3.192397
C	-4.565563	4.590442	-4.138775
C	-4.539583	0.139121	-5.847603
C	-5.006178	0.893580	-4.735999
C	-6.331417	0.731007	-4.279686
C	-7.161724	-0.142644	-4.968646
C	-6.708486	-0.888780	-6.071073
C	-5.394875	-0.754259	-6.506165
C	-2.109384	3.164626	-2.740106
C	-4.972507	2.933695	-1.593182
C	0.165573	0.086927	-0.735276
H	-2.656563	-4.914649	-2.913254
H	-1.290608	-3.245445	-4.124229
H	1.510973	-4.911167	-9.613044
H	1.111213	1.514350	-4.181213
H	-4.760937	1.994286	-1.075142
H	2.074311	-1.118294	-3.081203
H	-3.649715	-6.847944	-4.132567
H	-3.258931	-7.070253	-6.582280
H	-1.900395	-5.397075	-7.780602
H	2.508845	-2.377130	-6.591583
H	2.912534	-2.803022	-8.267992
H	0.975079	-2.162049	-10.180627
H	1.856797	-0.660734	-10.476831
H	0.105222	-5.776835	-8.983526
H	-0.109935	-4.189429	-9.731712
H	1.767281	-4.805448	-5.244169
H	2.505526	-5.628757	-6.633710
H	0.886985	-6.092966	-6.078884
H	-1.577200	1.957045	-10.658327
H	0.105059	1.847640	-11.194515
H	-0.279635	1.931280	-9.461068
H	-1.330331	-2.130341	-12.011553
H	-0.529055	-0.761590	-12.808692
H	-2.231163	-0.643022	-12.331493
H	2.634309	-0.195164	-5.692432
H	4.263909	1.572941	-5.155777
H	5.001569	3.171351	-6.911685
H	4.084131	2.976353	-9.214630
H	2.462144	1.214480	-9.760091
H	-3.704546	0.485893	-10.180501
H	-5.976585	-0.294768	-10.744605
H	-6.676890	-2.622709	-10.209834
H	0.873307	2.357381	-2.629435
H	-1.972888	2.466157	-1.907245
H	-1.752825	4.146461	-2.414490
H	-0.246787	-0.781978	-0.214148
H	1.248617	0.095952	-0.562602
H	-0.248226	0.990048	-0.276421
H	0.849399	-1.535218	-4.313319
H	0.818577	-2.313498	-2.718513
H	-5.612786	4.452861	-4.429799
H	-4.508655	5.494775	-3.522018
H	-3.985448	4.752958	-5.051568
H	-4.729409	3.766479	-0.922604
H	-6.047551	2.979722	-1.795828
H	-2.401521	0.447781	-0.564230
H	-4.212241	-0.484602	0.801584
H	-5.749251	-2.206811	-0.136893
H	-5.396802	-2.995223	-2.478474
H	-3.522603	-2.134899	-3.812188
H	-1.708455	5.408621	-4.157808
H	-0.883594	7.253436	-5.556180
H	0.818806	6.828127	-7.316625
H	1.682492	4.517251	-7.658221
H	0.849330	2.662859	-6.275993
H	-3.629593	0.927276	-6.560240
H	-5.042256	-1.326120	-7.358690
H	-7.387038	-1.566525	-6.581116
H	-8.192154	-0.259355	-4.639215
H	-6.692107	1.269623	-3.408397
H	-5.055256	-4.162482	-9.111033
H	-2.755335	-3.400371	-8.616970
H	-3.122382	1.673047	-8.031232
H	-1.636310	1.990776	-7.155370
H	-2.372902	-1.515426	-5.630169
H	-3.118337	2.891658	-6.733654

TS_{C1}-CO

E = -2343.661521
G = -2342.748879

C	2.272068	-3.222875	-2.680420

C	2.746147	-2.306726	-1.734394
C	3.657804	-1.323892	-2.148649
C	4.098958	-1.273583	-3.469549
C	3.620469	-2.192729	-4.404831
C	2.704188	-3.164190	-4.006391
P	2.211791	-2.338664	0.041685
C	1.176108	-3.841244	0.238422
Si	0.404475	-3.798894	1.990302
C	-1.303181	-4.612327	1.828715
Ta	0.809787	-0.340634	1.386734
N	0.411924	-2.106214	2.515341
C	0.057220	-1.999354	3.893701
C	1.008091	-1.631894	4.859916
C	0.666954	-1.536261	6.206481
C	-0.632778	-1.814284	6.630531
C	-1.589130	-2.174655	5.683070
C	-1.251136	-2.264634	4.333651
Ta	-1.048571	0.623381	-0.772137
C	1.067860	1.120955	-0.681119
P	-0.805973	1.604629	-3.212841
C	-1.094406	0.263918	-4.448978
Si	-2.372863	-0.924105	-3.653507
C	-3.975969	-0.862380	-4.659868
C	0.614798	2.599542	-3.837531
C	1.839866	1.947865	-4.041823
C	2.943478	2.654560	-4.510741
C	2.844729	4.021446	-4.770859
C	1.634330	4.677223	-4.562023
C	0.524077	3.970954	-4.099044
C	-2.300622	2.692875	-3.222696
Si	-2.664133	3.479090	-1.506522
C	-1.774585	5.151373	-1.429416
C	-4.523294	3.778199	-1.379028
N	-2.110787	2.323857	-0.249136
C	-2.613986	2.631347	1.050920
C	-3.469626	1.727799	1.700728
C	-3.967519	2.004756	2.971303
C	-3.642799	3.197664	3.616034
C	-2.801951	4.106128	2.976953
C	-2.289113	3.826720	1.711178
N	-2.527166	-0.290179	-2.012069
C	-3.656494	-0.716525	-1.257034
C	-4.939742	-0.200037	-1.525766
C	-6.043743	-0.589492	-0.774361
C	-5.899483	-1.501471	0.273392
C	-4.637333	-2.018910	0.554314
C	-3.527027	-1.636143	-0.200230
O	-0.458914	-1.040151	-0.090148
C	-1.718716	-2.695140	-3.676213
N	2.881449	-0.131811	1.938952
Si	4.315032	-1.144278	1.959591
C	5.794154	-0.261162	1.164360
C	2.785053	1.159264	2.456263
C	3.622749	1.833080	3.359750
C	3.277237	3.128664	3.745426
C	2.105604	3.740100	3.286291
C	1.256849	3.048046	2.419386
C	1.603647	1.769391	1.988644
C	3.807500	-2.681676	0.945078
C	4.861400	-1.729829	3.679431
C	1.414746	-4.887667	3.171415
H	-4.508948	-2.730216	1.366024
H	-2.540089	-2.027631	0.022669
H	-3.787504	-1.265229	-5.661703
H	0.347537	-3.749713	-0.471944
H	4.078660	-2.318728	4.166599
H	-1.191831	-5.603415	1.372497
H	-6.761544	-1.801304	0.862339
H	-7.021657	-0.173180	-1.002772
H	-5.056089	0.516793	-2.333045
H	-0.140818	-0.247554	-4.615235
H	-1.429880	0.687125	-5.401361
H	-3.130927	2.011440	-3.428250
H	-2.268005	3.441583	-4.021134
H	-4.759423	-1.469585	-4.197170
H	-4.359685	0.156322	-4.775452
H	-0.737812	-2.742497	-3.194523
H	-1.626145	-3.078523	-4.698311
H	-2.398881	-3.353910	-3.126049
H	-2.120493	5.742067	-0.576782
H	-1.996536	5.729589	-2.334768
H	-0.689429	5.036462	-1.350848
H	-5.075382	2.835170	-1.419043
H	-4.868088	4.424277	-2.194174
H	-4.764610	4.268273	-0.431198
H	-0.408688	4.501448	-3.942586
H	1.547988	5.741897	-4.760291
H	3.708494	4.571943	-5.132565
H	3.884979	2.136153	-4.667498
H	1.941437	0.886994	-3.829894
H	-1.606891	4.526458	1.239570
H	-2.527306	5.035195	3.469674
H	-4.033995	3.412669	4.606082
H	1.723955	-4.769193	0.044039
H	3.622026	-3.516840	1.627331
H	4.582526	-2.994589	0.239642
H	0.926494	-4.929577	4.149927
H	1.491686	-5.911187	2.787560
H	2.425962	-4.500431	3.327984
H	-1.968077	-4.020827	1.192765
H	-1.781197	-4.746283	2.803094
H	6.020296	0.664888	1.702258

H	6.688422	-0.893696	1.192716
H	5.599793	0.005850	0.121410
H	5.754593	-2.359896	3.592121
H	5.109884	-0.890989	4.336790
H	2.012715	-1.392410	4.528295
H	1.423201	-1.238699	6.929111
H	-0.897854	-1.740604	7.681587
H	-2.611883	-2.378021	5.992182
H	-2.011335	-2.506073	3.597134
H	4.027639	-0.596610	-1.430703
H	4.822239	-0.518591	-3.766546
H	3.965202	-2.155342	-5.434521
H	2.331380	-3.889297	-4.725021
H	1.574319	-3.999302	-2.382374
H	1.412449	1.452989	0.621384
H	0.331987	3.504973	2.079851
H	1.857868	4.747445	3.610500
H	3.933004	3.670818	4.423303
H	4.523199	1.367777	3.752500
H	-4.616799	1.281105	3.456482
H	-3.744303	0.805319	1.197596
H	1.309892	2.166607	-0.912311
H	-0.618204	0.922757	1.101744
H	1.733193	0.489625	-1.280058
H	-0.031121	0.147522	2.841696

Complex **Ta_2H_2•$(CH_3)O$**

E = -2343.706463
G = -2342.787301

C	1.117634	0.753187	2.813538
C	2.521648	0.655645	2.730260
C	3.366281	1.369308	3.582762
C	2.778735	2.177719	4.564337
C	1.394033	2.264620	4.683793
C	0.564340	1.553778	3.801489
N	2.862652	-0.268883	1.700314
Si	4.414099	-1.006109	1.305180
C	5.770814	-0.800802	2.608939
Ta	0.892012	-0.697186	1.147072
O	0.518326	-0.832087	-0.773639
Ta	-0.420551	0.876058	-0.999077
N	-1.917770	-0.186843	-2.090181
C	-2.654769	-1.183100	-1.371844
C	-3.933076	-0.894470	-0.864743
C	-4.719067	-1.891270	-0.289137
C	-4.243300	-3.199483	-0.196697
C	-2.961601	-3.491726	-0.664994
C	-2.170805	-2.496526	-1.237194
P	2.276865	-2.987643	0.477584
C	3.964949	-2.866567	1.230691
C	2.616503	-3.573901	-1.247663
C	3.141972	-4.856089	-1.459147
C	3.439361	-5.292843	-2.747406
C	3.218266	-4.450268	-3.837561
C	2.692993	-3.176271	-3.633400
C	2.385508	-2.736009	-2.344353
C	1.404136	-4.384555	1.314888
Si	0.471772	-3.685151	2.829808
C	1.633164	-3.659181	4.327117
C	-0.986927	-4.826471	3.198160
N	-0.084026	-2.050376	2.367268
C	-1.196939	-1.656422	3.185159
C	-1.020251	-1.300053	4.530871
C	-2.118588	-1.008182	5.338954
C	-3.411402	-1.057701	4.820225
C	-3.592001	-1.388614	3.476865
C	-2.498365	-1.683864	2.666498
C	1.552415	1.732443	-1.646335
P	-0.921525	2.240554	-3.326899
C	-2.489255	3.107276	-2.906687
Si	-2.475950	3.639138	-1.069901
N	-1.439970	2.485118	-0.160193
C	-1.634131	2.824697	1.219431
C	-2.611848	2.169865	1.983878
C	-2.923888	2.612000	3.267307
C	-2.263726	3.712911	3.815577
C	-1.256527	4.338159	3.082713
C	-0.936139	3.892361	1.801140
C	-1.331912	1.045622	-4.669884
Si	-2.210855	-0.422293	-3.827513
C	-1.488450	-2.030001	-4.517725
C	0.167884	3.498844	-4.136502
C	1.286437	3.064537	-4.863124
C	2.135748	3.980284	-5.477341
C	1.885719	5.348316	-5.371901
C	0.779163	5.791077	-4.652162
C	-0.074324	4.873685	-4.038979
C	-4.055661	-0.380630	-4.253155
C	-1.864071	5.427659	-0.926738
C	-4.278889	3.610164	-0.497074
C	5.067322	-0.422890	-0.367673
H	-2.574893	-4.505204	-0.590658
H	-1.168266	-2.713729	-1.589919
H	-4.190733	-0.500817	-5.334135
H	0.653839	-4.760627	0.610131
H	5.397808	-0.998259	3.618002
H	-0.628426	-5.845167	3.384734
H	-4.859657	-3.978897	0.241963
H	-5.711887	-1.645211	0.079291

H	-4.309455	0.120190	-0.955608
H	-0.395688	0.703930	-5.122734
H	-1.935088	1.526471	-5.446433
H	-3.269929	2.345826	-2.998568
H	-2.724180	3.921550	-3.599714
H	-4.588880	-1.194567	-3.753889
H	-4.528391	0.561191	-3.957010
H	-0.426292	-2.124652	-4.272617
H	-1.595850	-2.049166	-5.608706
H	-2.007162	-2.904080	-4.113996
H	-2.036604	5.809032	0.083150
H	-2.422264	6.065283	-1.623375
H	-0.796944	5.523864	-1.145096
H	-4.696786	2.599843	-0.539363
H	-4.877294	4.254232	-1.152527
H	-4.380245	3.976768	0.527392
H	-0.930813	5.241336	-3.485567
H	0.572546	6.854373	-4.566728
H	2.549279	6.063295	-5.849918
H	2.995897	3.623505	-6.036999
H	1.502260	2.003920	-4.955187
H	-0.144247	4.370514	1.233295
H	-0.707087	5.172498	3.510369
H	-2.516638	4.063851	4.812226
H	2.083283	-5.204276	1.571638
H	3.893022	-3.220071	2.265467
H	4.679658	-3.496299	0.692746
H	1.075456	-3.418406	5.237310
H	2.101823	-4.639686	4.471806
H	2.420518	-2.907563	4.213635
H	-1.684496	-4.852444	2.355786
H	-1.537033	-4.490383	4.081271
H	5.255743	0.655430	-0.342157
H	6.004696	-0.928417	-0.626009
H	4.343382	-0.617135	-1.164304
H	6.573181	-1.516664	2.395053
H	6.210542	0.200768	2.592695
H	-0.013851	-1.227634	4.929234
H	-1.957031	-0.733583	6.378379
H	-4.266723	-0.836926	5.453291
H	-4.592094	-1.427856	3.052453
H	-2.640621	-1.946523	1.624441
H	1.945817	-1.757314	-2.178053
H	2.517798	-2.519466	-4.481471
H	3.453083	-4.789336	-4.842883
H	3.845400	-6.289171	-2.900461
H	3.320821	-5.518204	-0.615425
H	2.365696	1.421402	-0.987896
H	-0.513033	1.638418	3.899297
H	0.954258	2.897828	5.450773
H	3.418703	2.742278	5.239188
H	4.446706	1.306699	3.501799
H	-3.684415	2.088409	3.839535
H	-3.128303	1.318224	1.552884
H	1.556577	2.826656	-1.698158
H	1.786440	1.361498	-2.655107
H	-0.896712	0.138190	0.787419
H	0.765025	1.097848	0.525056

TS_{C2}-CO

E = -2343.679898
G = -2342.766124

C	1.222257	0.804918	2.561430
C	2.623414	0.768799	2.400425
C	3.473152	1.658480	3.062225
C	2.895868	2.566030	3.959509
C	1.517888	2.588535	4.169654
C	0.678518	1.716096	3.458779
N	2.940413	-0.280850	1.496146
Si	4.508082	-0.999496	1.139405
C	5.803837	-0.744884	2.496163
Ta	0.950294	-0.768978	1.034506
O	0.593560	-0.802113	-0.897512
Ta	-0.514016	0.830549	-0.909011
N	-2.041883	-0.258911	-1.973745
C	-2.809157	-1.230955	-1.268068
C	-4.059820	-0.896395	-0.718119
C	-4.864410	-1.862032	-0.115669
C	-4.443195	-3.190397	-0.044482
C	-3.193541	-3.533281	-0.563001
C	-2.381715	-2.567653	-1.156015
P	2.409243	-2.999974	0.286225
C	4.077120	-2.861065	1.077804
C	2.791973	-3.526285	-1.449118
C	3.564957	-4.670916	-1.689120
C	3.853066	-5.065598	-2.992827
C	3.372146	-4.319816	-4.070058
C	2.598440	-3.185270	-3.837028
C	2.303071	-2.786445	-2.531571
C	1.560944	-4.454001	1.053025
Si	0.610519	-3.857855	2.596092
C	1.729716	-3.933499	4.121599
C	-0.865534	-5.005772	2.861123
N	0.084025	-2.187068	2.240174
C	-0.978798	-1.800219	3.132399
C	-0.697962	-1.355778	4.432841
C	-1.732251	-1.074943	5.324461
C	-3.061801	-1.223996	4.932161
C	-3.346948	-1.639212	3.631004

C	-2.317341	-1.922460	2.736557
C	1.562629	2.129817	-0.810420
P	-0.691731	2.063529	-3.264696
C	-2.217587	3.048256	-2.937592
Si	-2.324401	3.664353	-1.129366
N	-1.557957	2.432828	-0.078357
C	-1.872507	2.740927	1.278603
C	-2.783236	1.946204	1.993041
C	-3.169645	2.294564	3.284705
C	-2.667337	3.447948	3.890822
C	-1.745026	4.230449	3.199743
C	-1.340518	3.874245	1.913845
C	-1.174202	0.850846	-4.563949
Si	-2.279850	-0.467221	-3.714045
C	-1.746575	-2.155682	-4.391423
C	0.556429	3.185876	-4.035009
C	1.778767	2.622493	-4.430326
C	2.765820	3.409667	-5.016075
C	2.550830	4.775519	-5.203589
C	1.344842	5.345829	-4.804143
C	0.351761	4.556449	-4.222931
C	-4.086330	-0.207710	-4.232626
C	-1.509128	5.375677	-1.050312
C	-4.159608	3.855820	-0.719399
C	5.202539	-0.427716	-0.522514
H	-2.848822	-4.563477	-0.511141
H	-1.403943	-2.829071	-1.547457
H	-4.204863	-0.379769	-5.308398
H	0.820627	-4.802967	0.323933
H	5.361305	-0.849706	3.491123
H	-0.519959	-6.039300	2.978122
H	-5.076558	-3.945939	0.411581
H	-5.832416	-1.575646	0.288609
H	-4.395777	0.134123	-0.789730
H	-0.263654	0.371452	-4.939193
H	-1.669350	1.354336	-5.400830
H	-3.031734	2.326088	-3.054273
H	-2.372631	3.847358	-3.670612
H	-4.732360	-0.917214	-3.706175
H	-4.449666	0.800520	-4.009819
H	-0.712521	-2.386186	-4.117005
H	-1.822174	-2.156822	-5.485416
H	-2.385253	-2.957371	-4.010163
H	-1.715206	5.868455	-0.096860
H	-1.922090	6.008302	-1.845744
H	-0.424156	5.322578	-1.183059
H	-4.678414	2.896014	-0.805327
H	-4.632250	4.566452	-1.407011
H	-4.297606	4.224100	0.300933
H	-0.580324	5.020109	-3.917689
H	1.170883	6.409085	-4.944775
H	3.322513	5.391668	-5.656228
H	3.706290	2.957949	-5.319029
H	1.962987	1.561442	-4.278005
H	-0.587369	4.461192	1.399030
H	-1.319688	5.115084	3.666813
H	-2.980219	3.722102	4.894450
H	2.255754	-5.274628	1.260092
H	3.982048	-3.202045	2.114526
H	4.815705	-3.486949	0.568628
H	1.155380	-3.694890	5.021904
H	2.147055	-4.939374	4.245899
H	2.555320	-3.218486	4.054236
H	-1.549512	-4.963860	2.008470
H	-1.427402	-4.729812	3.757528
H	5.361132	0.655706	-0.510838
H	6.160946	-0.910690	-0.743886
H	4.507704	-0.657664	-1.335962
H	6.590273	-1.501054	2.389397
H	6.281544	0.237236	2.435683
H	0.336758	-1.212298	4.727261
H	-1.493555	-0.731455	6.327769
H	-3.866913	-1.011669	5.630581
H	-4.377592	-1.750369	3.304187
H	-2.538834	-2.244321	1.724717
H	1.685364	-1.914989	-2.331831
H	2.218631	-2.606693	-4.675112
H	3.598713	-4.626996	-5.087478
H	4.452672	-5.954737	-3.168605
H	3.943694	-5.260889	-0.857709
H	2.206256	2.362617	0.047354
H	-0.393912	1.756741	3.623514
H	1.089527	3.295769	4.875617
H	3.537190	3.259060	4.499777
H	4.548441	1.645664	2.910192
H	-3.865796	1.655589	3.820197
H	-3.174733	1.050434	1.521495
H	1.201463	3.086959	-1.191673
H	2.183514	1.640782	-1.564368
H	-0.876269	0.006527	0.797566
H	0.931045	1.281874	0.167490