Electronic Supporting Information

Dinitrogen Functionalization at a Ditantalum Center. Balancing N_2 Displacement and N_2 Functionalization in the Reaction of Coordinated N_2 with CS_2

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General Experimental Procedures

All manipulations were performed under an atmosphere of dry and oxygen-free dinitrogen by means of standard Schlenk or Glovebox techniques. Anhydrous toluene, diethylether and hexanes were purchased from Aldrich, sparged with dinitrogen and dried further by passage through towers containing activated alumina and molecular sieves. Benzene-d_6 was refluxed over sodium, vacuum transferred and freeze-pump-thaw degassed. ^{1}H, ^{31}P and ^{13}C NMR spectra were recorded on a Bruker AV-400 MHz spectrometer. Unless noted otherwise, all spectra were recorded at room temperature. ^{1}H NMR spectra were referenced to residual proton signals in C_6D_6 (7.16 ppm) or C_7D_8 (2.09); ^{31}P NMR spectra were referenced to external $P(OMe)_3$ (141.0 ppm with respect to 85% H_3PO_4 at 0.0 ppm). H_2 (99.99) and D_2 (HD 0.4%, lecture bottle) were purchased from Praxair or from Cambridge Isotopes Ltd. and passed through activated molecular sieves prior to use. $[PhP(CH_2SiMe_2NPh)_2]TaMe_3$ and $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) were prepared according to literature methods.[1-3] For the purposes of infrared signature comparison $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}S)(\mu\text{-}N)(NCS)$ (**2**) $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}S)_2(\mu\text{-}CH_2)$ (**3**) were prepared according to literature methods.[4,5]

General Procedures for Screening Reaction Conditions in Table 1.

Stock solutions (0.01 M) of **1** (0.038 g, 0.030 mmol) were prepared at room temperature using toluene, hexanes or diethyl ether (3.00 mL). For CS_2, the neat liquid and an empty vial were cooled to -35 ^{o}C, the liquid was weighed in the vial and diluted in the appropriate solvent to 0.01 M (0.012 g, 0.158 mmol in 15.00 mL). For each run, 1.00 mL of **1** solution was added to a vial containing a stir bar and 1.00 mL of CS_2 solution was added and stirred. After 1.5 h, the solvent was removed in vacuo and the material was dissolved in C_6D_6 and examined by ^{1}H and $^{31}P\{^1H\}$ NMR spectroscopy (5 seconds relaxation delay). Relative amounts of **2** and **3** were determined by integrations of the $^{31}P\{^1H\}$ NMR spectroscopic signals and are not absolute. It should be noted that entries 5 and 6 were performed in hexanes in which **1** is sparingly soluble precluding precise concentration preparation. As such, **1** was weighed into the reaction vessel, hexanes was added, and a precise amount of a measure CS_2 solution was added (varying rate of addition).

Entry 1: To a room temperature vial charged with 1.00 mL toluene solution of **1** (0.01 M, 0.01 mmol), 0.46 mL of a toluene solution of CS_2 (0.022 M, 0.01 mmol) was added drop-wise over 10 minutes. The reaction was stirred at room temperature for 1.5 h, at which point the solvent was removed *in vacuo*. 0.8 mL C_6D_6 was added to the brown residue and quantitatively transferred to an NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 0.07 : 1.00.

Entry 2: To a cooled (-35 ^{o}C) vial charged with 1.00 mL toluene solution of **1** (0.01 M, 0.01 mmol), 0.46 mL of a cooled (-35 ^{o}C) toluene solution of CS_2 (0.022 M, 0.01 mmol) was added all at once. The reaction was stirred at room temperature for 1.5 h, at which point the solvent was removed *in vacuo*. 0.8 mL C_6D_6 was added to the brown residue and quantitatively transferred to an NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 0.56 : 1.00. Reaction incomplete and considerable starting material evident.

Entry 3: To a room temperature vial charged with 1.00 mL diethyl ether solution of **1** (0.01 M,

0.01 mmol), 1.00 mL of a diethyl ether solution of CS_2 (0.01 M, 0.01 mmol) was added drop-wise over 10 minutes. The reaction was stirred at room temperature for 1.5 h, at which point the solvent was removed *in vacuo*. 0.8 mL C_6D_6 was added to the brown residue and quantitatively transferred to an NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 0.05 : 1.00.

Entry 4: To a cooled (-35 ^oC) vial charged with 1.00 mL diethyl ether solution of **1** (0.01 M, 0.01 mmol), 1.00 mL of a cooled (-35 ^oC) diethyl ether solution of CS_2 (0.01 M, 0.01 mmol) was added all at once. The reaction was stirred at room temperature for 1.5 h, at which point the solvent was removed *in vacuo*. 0.8 mL C_6D_6 was added to the brown residue and quantitatively transferred to an NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 0.09 : 1.00.

Entry 5: To a room temperature vial charged with **1** (0.013 g, 0.01 mmol) and hexanes (1.00 mL), 0.33 mL of a room temperature hexanes solution of CS_2 (0.13 M, 0.04 mmol) was added drop-wise over 10 minutes. The reaction was stirred at room temperature for 1.5 h, at which point the solvent was removed *in vacuo*. 0.8 mL C_6D_6 was added to the brown residue and quantitatively transferred to an NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 0.16 : 1.00.

Entry 6: To a room temperature vial charged with **1** (0.013 g, 0.01 mmol) and hexanes (1.00 mL), 0.33 mL of a room temperature hexanes solution of CS_2 (0.13 M, 0.04 mmol) was added all at once. The reaction was stirred at room temperature for 1.5 h, at which point the solvent was removed *in vacuo*. 0.8 mL C_6D_6 was added to the brown residue and quantitatively transferred to an NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.28 : 1.00.

Entry 7: To a room temperature vial charged with **1** (0.016 g, 0.013 mmol), room temperature CS_2 (0.130 g, 1.7 mmol, 134 equiv) was added all at once. The reaction was stirred at room temperature for 1.5 h, at which point the volatiles were removed *in vacuo*. 0.8 mL C_6D_6 was added to the brown residue and quantitatively transferred to an NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 0.00. = 0.00 : 1.00.

General Procedures for Time-dependent Speciation Experiments Monitored by ReactIR

An array of 9 experimental runs was designed with deliberate concentration variation of both $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) and CS_2 to establish order dependence in both reagents. In all cases, the IR instrument was blanked with pure C_6D_6 followed by addition of the appropriate CS_2 solution to the reaction flask. Once observing the CS_2 stretch, the appropriate tantalum solution was added and considered t = 0. Values outlined in the table are the molar concentrations of the reagents in each reaction mixture based on the total volume of the reaction mixture. The reactions were allowed to proceed at room temperature for 6 hours with IR spectra recorded every 15 seconds, at which point the sample was transfer to an NMR tube for $^{31}P\{^1H\}$ and ^1H NMR experiments.

Entry	**[1]** (mol/L)	**[CS_2]** (mol/L)	**Equiv.**
1	0.01	0.10	10
2	0.008	0.098	12.25
3	0.006	0.096	16
4	0.01	0.01	1
5	0.008	0.008	1
6	0.006	0.006	1
7	0.01	0.02	2
8	0.01	0.05	5
9	0.008	0.04	5

Entry 1: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.00 mL C_6D_6 was added and baseline established. Via syringe, the CS_2 stock solution (0.50 mL, 0.40 M, 0.20 mmol) was added. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.151 g, 0.12 mmol in 3.0 mL in C_6D_6, 0.04 M) was prepared and 0.5 mL (0.02 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 0.99.

Entry 2: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.00 mL C_6D_6 was added and baseline established. Via syringe, the CS_2 stock solution (0.50 mL, 0.392 M, 0.20 mmol) was added. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.081 g, 0.064 mmol in 2.0 mL in C_6D_6, 0.032 M) was prepared and 0.5 mL (0.016 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 0.44.

Entry 3: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 0.83 mL C_6D_6 was added and baseline established. Via syringe, the CS_2 stock solution (0.5 mL, 0.384 M, 0.19 mmol) was added. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.045 g, 0.036 mmol in 1.5 mL in C_6D_6, 0.024 M) was prepared and 0.67 mL (0.012 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 3.36.

Entry 4: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.0 mL C_6D_6 was added and baseline established. Via syringe, the CS_2 stock solution (0.5 mL, 0.04 M, 0.02 mmol) was added. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.151 g, 0.12 mmol in 3.0 mL in C_6D_6, 0.04 M) was prepared and 0.5 mL (0.02 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 7.62.

Entry 5: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.0 mL C_6D_6 was added and baseline established. Via syringe, the CS_2 stock solution (0.5 mL, 0.032

M, 0.016 mmol) was added. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.121 g, 0.10 mmol in 3.0 mL in C_6D_6, 0.032 M) was prepared and 0.5 mL (0.016 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 23.56.

Entry 6: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 0.83 mL C_6D_6 was added and baseline established. Via syringe, the CS_2 stock solution (0.5 mL, 0.024 M, 0.012 mmol) was added. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.01 g, 0.14 mmol in 8.0 mL in C_6D_6, 0.018 M) was prepared and 0.67 mL (0.012 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 48.56.

Entry 7: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.0 mL C_6D_6 was added and baseline established. Via syringe, the CS_2 stock solution (0.5 mL, 0.08 M, 0.04 mmol) was added. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.151 g, 0.12 mmol in 3.0 mL in C_6D_6, 0.04 M) was prepared and 0.5 mL (0.02 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 6.68.

Entry 8: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.0 mL C_6D_6 was added and baseline established. Via syringe, the CS_2 stock solution (0.5 mL, 0.20 M, 0.10 mmol) was added. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.151 g, 0.12 mmol in 3.0 mL in C_6D_6, 0.04 M) was prepared and 0.5 mL (0.02 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 3.37.

Entry 9: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.0 mL C_6D_6 was added and baseline established. Via syringe, the CS_2 stock solution (0.5 mL, 0.16 M, 0.08 mmol) was added. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.121 g, 0.10 mmol in 3.0 mL in C_6D_6, 0.032 M) was prepared and 0.5 mL (0.016 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^1H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 48.16.

The final set of 3 experiments were outlined to establish the precise CS_2 consumption. Rather than adding a solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) to an already IR measured CS_2 solution and observing initial baseline fluctuations, the baseline was established on **1** with subsequent addition of CS_2 at t = 0. By keeping the [**1**] constant throughout this series, the precise rate and amount and CS_2 consumed as a function of concentration was established. A stock solution of $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.04 M, 0.101 g in 2.0 mL) in C_6D_6 was prepared and used for all experiments. The total reaction volume in all cases is 2.0 mL (1.0 mL C_6D_6, 0.5 mL Ta (**1**) solution and 0.5 mL CS_2 solution). The reactions were allowed

to proceed at room temperature for 2.5 hours with IR spectra recorded every 15 seconds, at which point the sample was transfer to an NMR tube for $^{31}P\{^{1}H\}$ and ^{1}H NMR experiments.

Entry	**[1]** (mol/L)	**[CS_2]** (mol/L)	**Equiv.**
10	0.01	0.10	10
11	0.01	0.05	5
12	0.01	0.02	2

Entry 10: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.0 mL C_6D_6 was added and baseline established. Via syringe, the $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) stock solution (0.5 mL, 0.04 M, 0.02 mmol) was added. A stock solution of CS_2 (0.03 g, 0.40 mmol in 1.0 mL in C_6D_6, 0.4 M) was prepared and 0.5 mL (0.2 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^{1}H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 1.10.

Entry 11: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.0 mL C_6D_6 was added and baseline established. Via syringe, the $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) stock solution (0.5 mL, 0.04 M, 0.02 mmol) was added. A stock solution of CS_2 (0.015 g, 0.20 mmol in 1.0 mL in C_6D_6, 0.2 M) was prepared and 0.5 mL (0.1 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^{1}H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 1.38.

Entry 12: To an oven dried flask cooled under vacuum and equipped with a React IR probe, 1.0 mL C_6D_6 was added and baseline established. Via syringe, the $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) stock solution (0.5 mL, 0.04 M, 0.02 mmol) was added. A stock solution of CS_2 (0.012 g, 0.16 mmol in 2.0 mL in C_6D_6, 0.08 M) was prepared and 0.5 mL (0.04 mmol) was added at t = 0 and stirred as indicated above. Upon completion, 0.6 mL was extracted from the reaction flask and injected into a septum equipped NMR tube. Product ratio determined by $^{31}P\{^{1}H\}$ NMR spectroscopy; **2** (-4 ppm): **3** (-6 ppm) = 1.00 : 3.31.

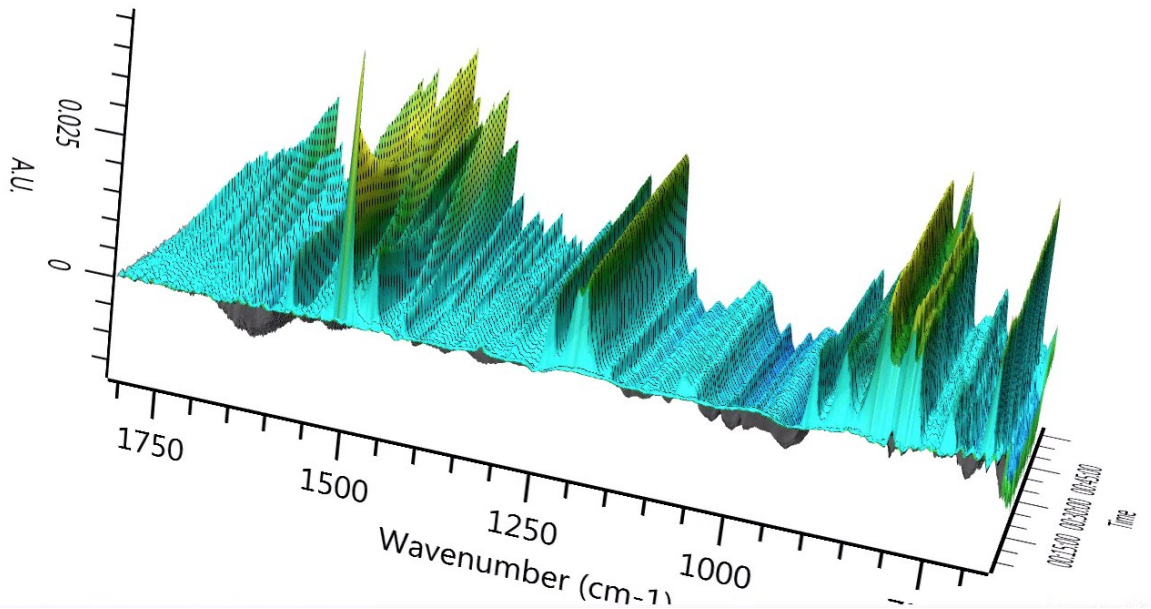


Figure S1: Waterfall plot showing the reaction progress using ReactIR in situ FTIR.

Chemometric Model for Determination of In Situ Concentration by ReactIR

Concentration measurements were possible by first identifying unique identifier bands for each component is the reaction solvent. Stock solutions of complex **1**, and both products **2** and **3** were created and analyzed by ReactIR. Extracted spectra were overlayed to provide a comparative spectral trace (Figure S2-A). Due to the significant structural similarity between these compounds (in particular **1** and **3**) identification of isolated bands was complicated, however, three unique bands were evident; 1227 cm^{-1} associated with **1**, 780 cm^{-1} associated with **2** and 1197 cm^{-1} associated with **3**. It was not possible to create a predicative reaction trend based on an intensity vs. time profile of these individual bands from the native spectra, particularly for compounds **1** and **3**, which show significant overlap. However, processing individual time-point spectra as the second derivative provided sufficient segregation of the signals to build a predictive concentration model (Figure S2-B)

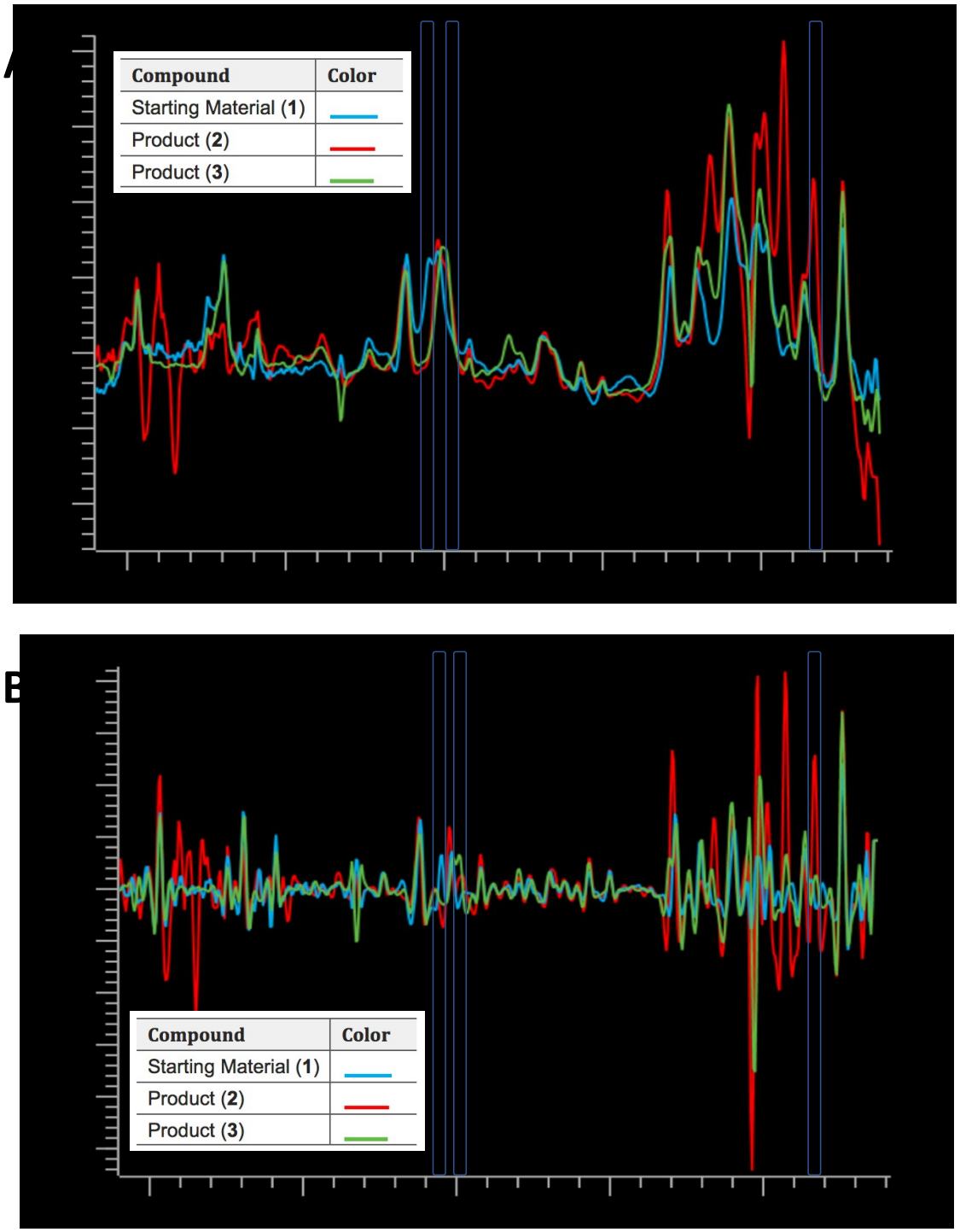


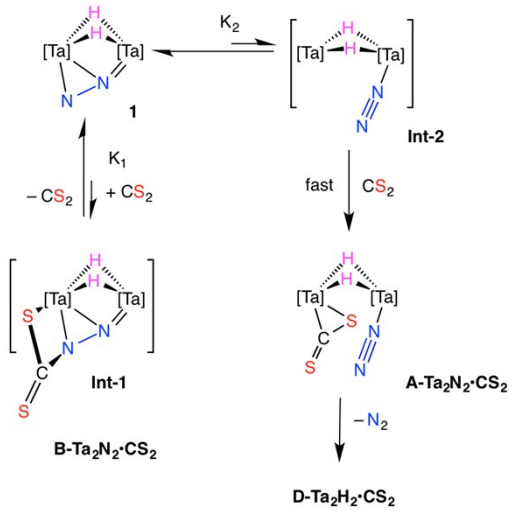
Figure S2: Reference IR spectra of individual components; A) Native absorption spectra for authentic samples with unique bands of interest highlighted; B) Second derivative of empirical spectral absorption as a function of wavenumber.

Using the identified bands, concentration vs. time profiles were created for all ReactIR experiments. Predictive trends were validated by confirming mass balance was preserved for all recorded experiments, allowing correlation coefficients to be approximated. Final product ratios were cross validated by comparing the predicted product ratio (**2** vs **3**) from authentic NMR

experiments as described above.

General Procedures for Time-dependent Speciation Experiments Monitored by ReactIR

Please cite - Hoops S., Sahle S., Gauges R., Lee C., Pahle J., Simus N., Singhal M., Xu L., Mendes P. and Kummer U. (2006). COPASI: a COmplex PAthway SImulator. Bioinformatics 22, 3067-74.



Simulation of the kinetic model was performed using Complex Pathway Simulator (COPASI).[ref above] The competitive mechanism was created using an input reaction array as follows:

Table S1: COPASI input reaction array.

Name	Reaction	Rate Law
01	1 + CS_2 <=>Int-1	Mass action (reversible)
02	Int-1 -> 2	Mass action (irreversible)
03	1 <=> Int-2	Mass action (reversible)
04	Int-2 + CS_2 -> 3	Mass action (irreversible)

Product forming reactions involving capture of Int_1 and Int_2 (Reactions 02 and 4) were designated as irreversible. Concentration data from three independent experiments were then loaded as experimental reference data. Initial values for the rate constants were randomized and then optimized using a genetic algorithm (20000 generation, population size = 400). Optimization was run until the RMS error was constant for 1000 generations. Parameter estimation was completed for a total of 10 independent runs, each with differently randomized starting values for the rate constants. Data is tabulated in Table S2 and graphed against experimental results (Figure S2).

		Experiment Number									
		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
k_1	**1 + CS_2 -> Int-1**	**0.88199**	**0.9654**	**0.935019**	**0.876661**	**0.971653**	**0.966355**	**0.88691**	**0.873768**	**0.871109**	**0.907254**
k_{-1}	**Int-1 -> 1 + CS_2**	**267.109**	**1.45E+02**	**33.1724**	**156.666**	**319.174**	**222.192**	**1**	**5.01491**	**37.534**	**140.346**
K_1		**0.003**	**0.007**	**0.028**	**0.006**	**0.003**	**0.004**	**0.887**	**0.174**	**0.023**	**0.006**
k_2	**Int-1 -> 2**	**27093.8**	**1328.36**	**456.769**	**31254.1**	**2809.06**	**1977.56**	**62.6322**	**229517**	**67744.6**	**3327.58**
k_3	**1 -> Int-2**	**0.06432**	**0.06395**	**0.06417**	**0.064137**	**0.064148**	**0.063827**	**0.064224**	**0.064192**	**0.064089**	**0.064274**
k_{-3}	**Int-2 -> 1**	**1.071**	**1.01E+00**	**1.29698**	**1.28E+00**	**1.00E+00**	**4.76E+01**	**3.00E+00**	**1.21E+00**	**1.23E+00**	**2.45E+01**
K_3		**0.060**	**0.063**	**0.049**	**0.050**	**0.064**	**0.001**	**0.021**	**0.053**	**0.052**	**0.003**
k_4	**Int-2 + CS_2 > 3**	**84512.5**	**154881**	**356245**	**227088**	**27890.4**	**425089**	**788930**	**644299**	**462003**	**782045**

Synthesis of Isotopically Labeled Complexes

Synthesis of [PhP(CH_2SiMe_2NPh-d_2)$_2$Ta]$_2$(μ-η^2:η^2-N_2)(μ-D)$_2$ (**d_{10}-1**).
To a vessel charged with [PhP(CH_2SiMe_2NPh)$_2$Ta]Me_3 (0.717 g, 1.09 mmol), diethyl ether (30 mL) was added. The resulting yellow solution was degassed by freeze/pump/thaw at 10^{-5} torr and pressurized with 4 atm of deuterium (Cambridge Isotopes Laboratory). The frozen solution was allowed to warm to RT with stirring over 12 h. The resulting purple solution was degassed by freeze/pump/thaw and pressurized with 4 atm of nitrogen gas. The frozen solution was allowed to warm to RT with stirring over 12 h. All volatiles were removed *in vacuo* from the resulting brown solution and the resulting solid was washed with hexanes to afford the product in 28 % yield (0.196 g, 0.15 mmol). ^{1}H NMR (400 MHz, C_6D_6): δ 8.25 (m, 2H), 7.31 – 7.04 (m, 16H), 6.89 (m, 2H), 6.81 (m, 2H), 6.75 (m, 2H), 1.59 (m, 4H), 1.48 (AMX, m, 2H), 0.64 (AMX, $^2J_{HH}$ = 13.3, $^2J_{HP}$ = 10.8 Hz, 2H), 0.10 (s, 6H), 0.02 (s, 6H), -0.05 (s, 6H), -0.21 (s, 6H). ^{31}P{^{1}H} NMR (162 MHz, C_6D_6): δ 10.9 (d, $^3J_{PP}$ = 19.7 Hz, 1P), 7.8 (m, 1P).

Isotope Effect Experiments

To a vial charged with **1** (0.094 g, 0.074 mmol) and ***d_{10}*-1** (0.094, 0.074 mmol), 15.00 mL of diethyl ether was added and the solution was stirred to homogeneous. In a separate vial, a CS_2 solution was prepared (0.133 g, 1.75 mmol in 20.00 mL diethyl ether) and added to the stirring solution of 1 (0.85 mL, 0.087 M), drop-wise over 10 minutes. The solution was stirred for 2.5 h and a 3.00 mL aliquot was extracted. Following removal of the volatiles *in vacuo*, the residue was dissolved in 0.90 mL C_6D_6. 0.70 mL of this solution was transferred to an NMR tube and 6 μL of toluene was added via micro syringe as an internal standard. ^{1}H and ^{31}P{^{1}H} NMR spectra were recorded (relaxation delay = 10 seconds) and the quantities of **1** and **3** were determined based on the resonances at ppm (hydrides) and ppm (methylene) compared to toluene (2.09 ppm). A second 0.90 mL aliquot was taken after 16 h (0.70 mL C_6D_6, 4 μL toluene added) and the characterization procedure was repeated. The concentrations of ***d_{10}*-1** and ***d_{10}*-3** were determined by assuming the remaining CS_2 (unreacted from **1**) had reacted to ***d_{10}*-3**, and the remaining ***d_{10}*-1** left unreacted. The ^{31}P{^{1}H} NMR spectrum showed resolution of the isotopomers **3** and ***d_{10}*-3** for qualitative relative integration which is in good agreement with the values measure in the ^{1}H NMR spectrum. The results are delineated in Table S1.

Table S1. 1 vs. ***d_{10}*-1** Competition experiment results based on ^{1}H and $^{31}P\{^{1}H\}$ NMR spectroscopy.

Trial 1								
Species	*moles init.*	*[initial] mol/L*	*integral*	*ratio*	*final moles*	*concentration mol/L*	*NMR technique*	
Ta2N2	1.10E-05	1.55E-02	5.4	0.054	4.21E-06	5.96E-03		1.01E-05
Ta2D2N2	1.10E-05	1.55E-02	-	-	6.76E-06	9.58E-03		
CS2	1.10E-05	1.55E-02	0	0	0.00E+00	0.00E+00		KIE
Ta2CH2	0.00E+00	0.00E+00	7.58	0.0758	5.90E-06	8.37E-03	1H	**1.17E+00**
Ta2CD2	0.00E+00	0.00E+00	-	-	5.06E-06	7.18E-03	31P	**1.30E+00**
Toluene	5.19E-05	7.36E-02	100					
total volume (L)								
7.06E-04								
Trial 2								
Species	*moles init.*	*[initial] mol/L*	*integral*	*ratio*	*final moles*	*concentration mol/L*	*NMR technique*	
Ta2N2	1.10E-05	1.56E-02	8.52	0.0852	4.22E-06	5.99E-03		1.04E-05
Ta2D2N2	1.10E-05	1.56E-02	-	-	6.15E-06	9.60E-03		
CS2	1.10E-05	1.56E-02	0	0	0.00E+00	0.00E+00		KIE
Ta2CH2	0.00E+00	0.00E+00	12.41	0.1241	6.15E-06	8.72E-03	1H	**1.28E+00**
Ta2CD2	0.00E+00	0.00E+00	-	-	4.82E-06	6.87E-03	31P	**1.26E+00**
Toluene	3.30E-05	4.70E-02	100					
total volume (L)								
7.04E-04								

Low Temperature $^{31}P\{^{1}H\}$ NMR Spectroscopy

A J-Young NMR tube charged with $[PhP(CH_2SiMe_2NPh)_2Ta]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)(\mu\text{-}H)_2$ (**1**) (0.010 g, 0.008 mmol) in 0.70 mL d^8-Toluene was frozen in liquid nitrogen and degassed. CS_2 (0.138 g, 1.80 mmol, 225 equiv.) was added via vacuum transfer and the sample was warmed to 195 K. The liquid solution was mixed thoroughly and placed in a precooled 400 MHz NMR spectrometer (195 K). An NMR spectrum was recorded to show exclusively starting material. After 10 minutes, no change was observed. The magnet was heated to 213 K and 233 K with spectra recorded after 10 minutes at both temperatures. While only starting material was observed at 213 K, a signal consistent with **2** began to appear very slowly at 233 K. Upon cooling back to 223 K in an attempt to observe buildup an intermediate, the production of **2** stopped. As the sample was warmed to 273 K and 298 K over the course of 2 hours, only **2** was observed.

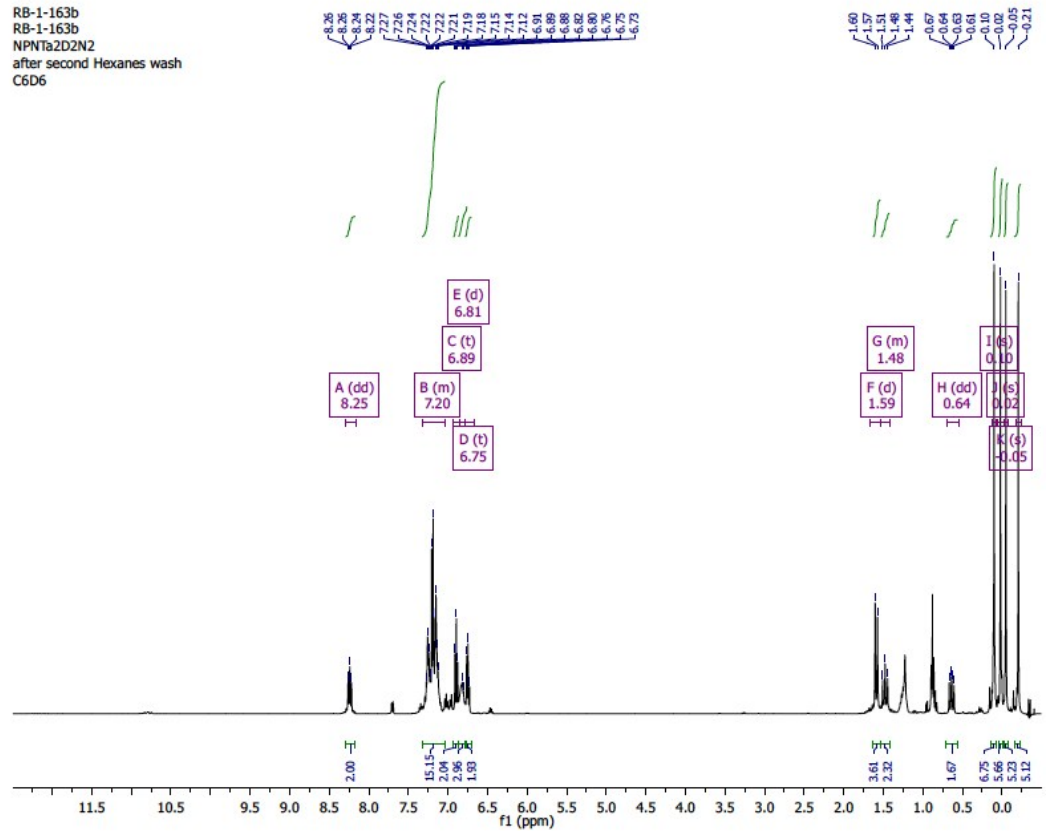


Figure S3. ^{1}H NMR spectra (in C_6D_6) of ***d*$_{10}$-1**.

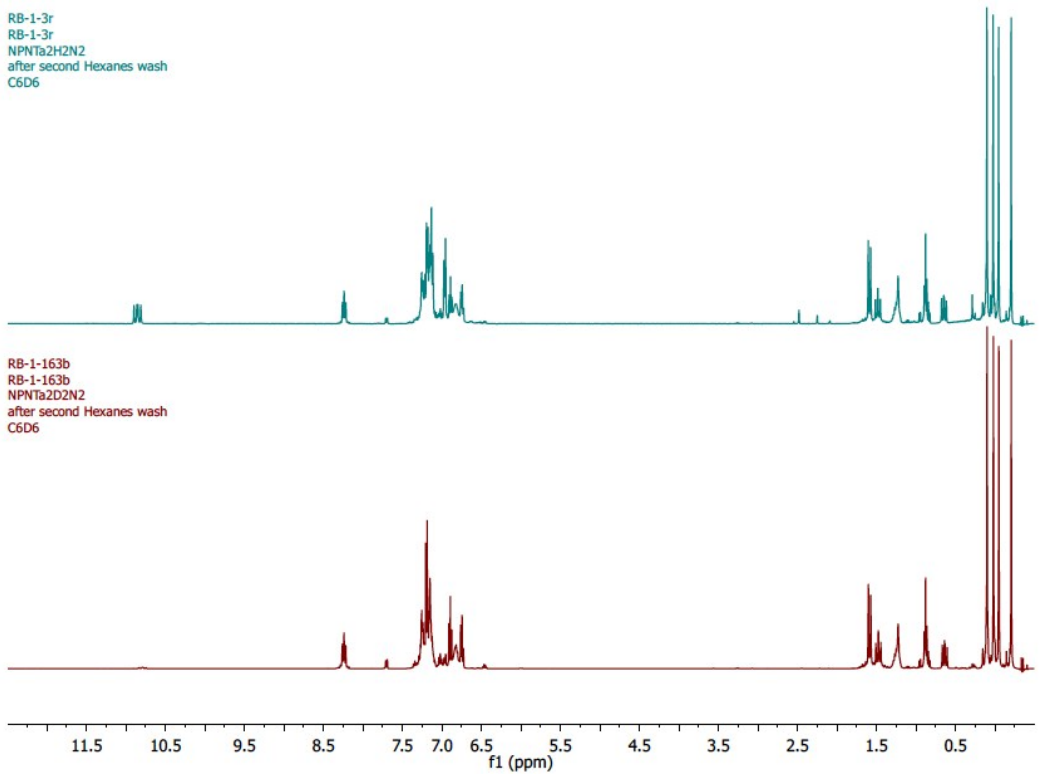


Figure S4. Stacked ^{1}H NMR spectra (in C_6D_6) of **1** (top) and ***d*$_{10}$-1** (bottom).

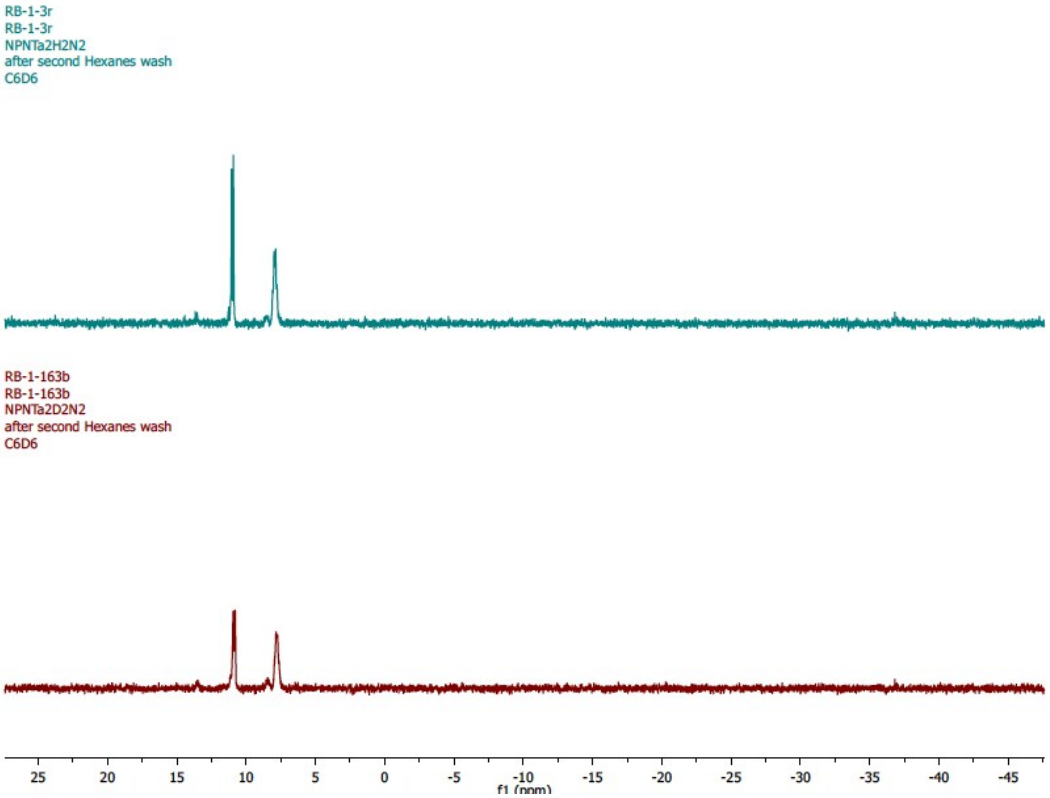


Figure S5. Stacked $^{31}P\{^{1}H\}$ NMR spectra (in C_6D_6) of **1** (top) and ***d*$_{10}$-1** (bottom).

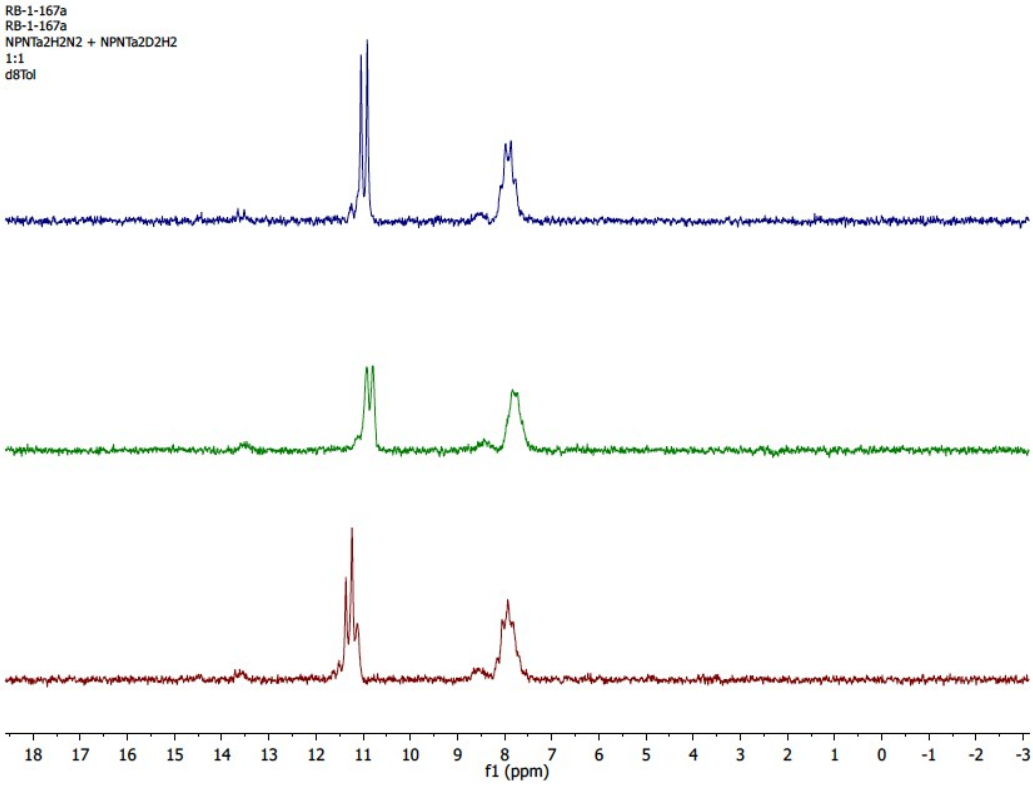


Figure S6. Stacked $^{31}P\{^{1}H\}$ NMR spectra (in C_6D_6) of **1** (top) and ***d*$_{10}$-1** (middle) and 1:1 mixture of **1** and ***d*$_{10}$-1** (bottom).

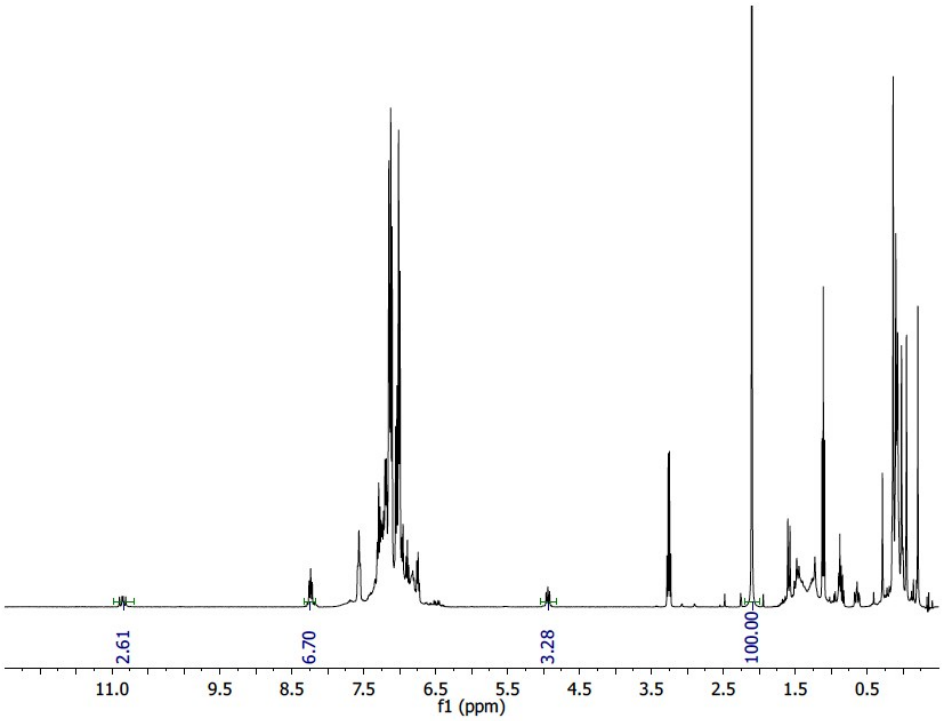


Figure S7. ^{1}H NMR spectra (in C_6D_6, toluene internal standard) **1** vs. ***d*$_{10}$-1** + CS_2 competition experiment.

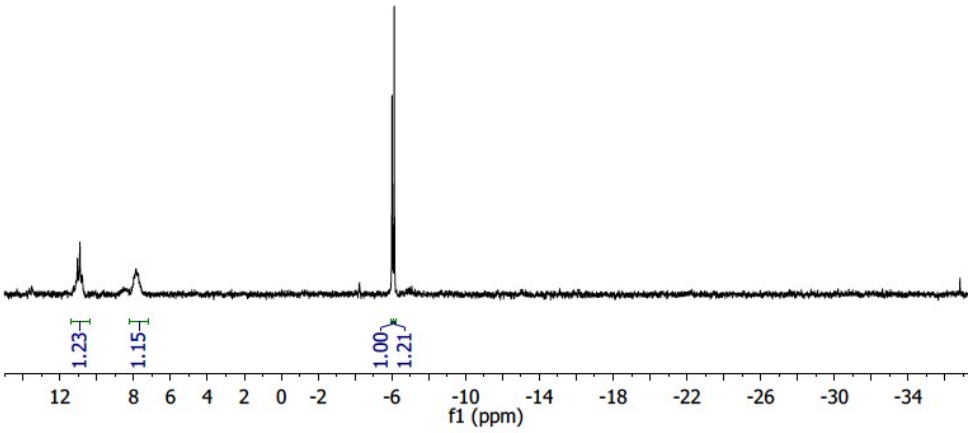


Figure S8. $^{31}P\{^{1}H\}$ NMR spectra (in C_6D_6) **1** vs. ***d*$_{10}$-1** + CS_2 competition experiment.

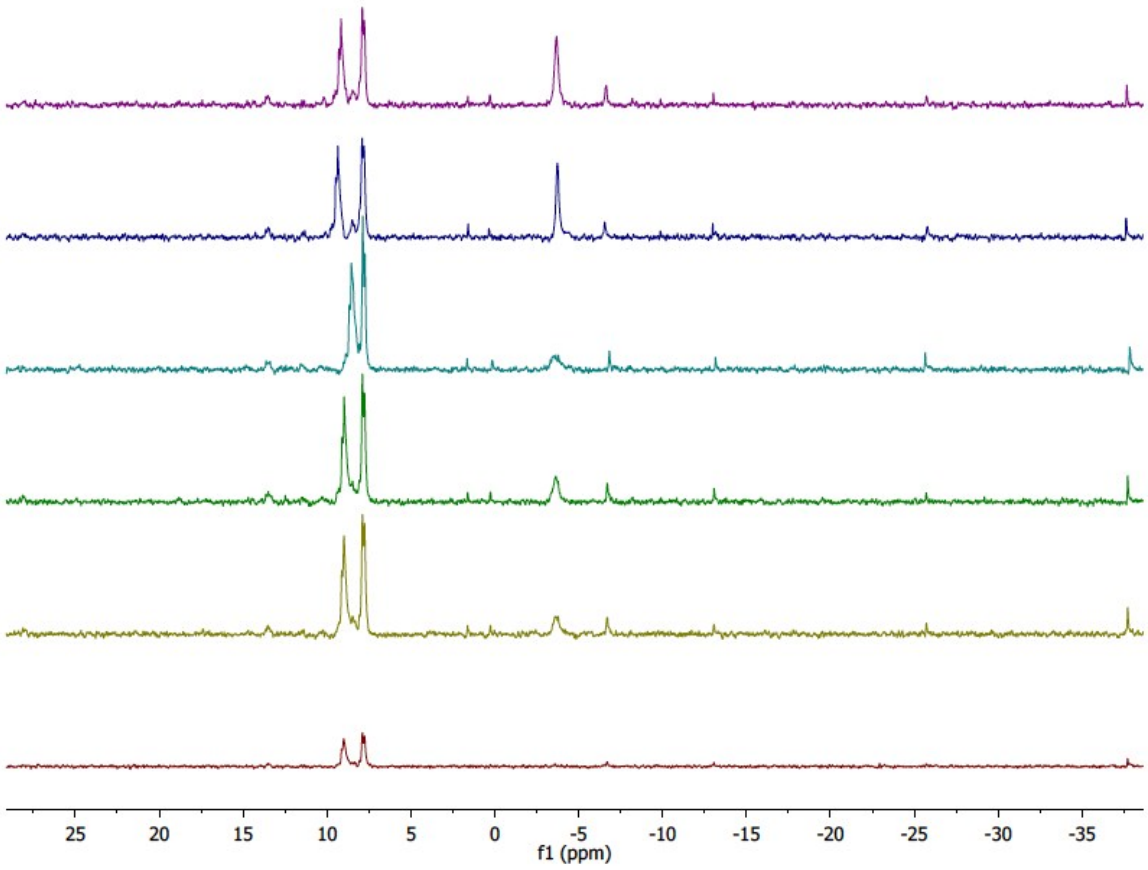


Figure S9. Stacked $^{31}P\{^{1}H\}$ NMR spectra (in d_8-Toluene) of **1** + 225 equiv CS_2 at varying temperatures: 233 K, 1 minute (a); 233 K, 15 minutes (b); 233 K, 25 minutes (c); 223 K, 15 minutes (d); 243 K, 5 minutes (e); 243 K, 15 minutes (f).

Computational Details

We used the small core Stuttgart-Dresden relativistic effective core potential in combination with its adapted basis set to treat the tantalum atoms,[6,7] while carbon, oxygen, nitrogen and hydrogen atoms were described with a 6-31G(d,p) double-ζ basis set;[8] silicon and phosphorus atoms were modeled with the Stuttgart-Dresden ECP in combination with its adapted basis set and additional *d* polarization functions.[9,10] Calculations were carried out at the DFT level of theory using the hybrid functional B3PW91.[11,12] We have also considered in the present study dispersion effects, in particular the third generation of Grimme's dispersion corrections with Becke-Johnson damping model[13] on the B3PW91 geometries (single point calculations).Geometry optimizations were performed without any symmetry restrictions and the nature of the extremes (minima and transition states) was verified with analytical frequency calculations. Gibbs free energies were obtained at T = 298.15 K within the harmonic approximation. IRC calculations were performed to confirm the connections of the

optimized transition states. DFT calculations were carried out with the Gaussian09 suite program.[14] The electronic density (at the DFT level) has been analyzed using the Natural Bond Orbital (NBO) technique.[15] Calculations have been realized in the gas-phase and the real NPN ligands have been computed.

Reactant **1**

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H	0.230541	4.958492	3.943810
H	-0.613652	4.047990	1.809784
H	3.830608	4.222935	-1.489888
H	3.390398	2.653730	-2.195192
H	3.300429	4.128096	-3.173200
H	1.716353	6.202340	-0.545537
H	1.344912	6.420227	-2.264707
H	0.043438	6.078008	-1.105025
H	-5.157947	0.801239	-1.629317
H	-4.862289	0.200524	-3.271629
H	-3.903260	-0.420102	-1.906970
H	-4.681220	3.774264	-2.616361
H	-3.237455	4.146565	-3.569486
H	-4.485152	3.076951	-4.232188
H	0.447121	-5.565061	-1.869672
H	1.871004	-5.055693	-0.947461
H	0.980726	-6.510659	-0.471017
H	-2.358170	-5.556450	-0.570970
H	-1.765643	-6.385095	0.878673
H	-2.623430	-4.843033	1.033988
H	2.758441	1.165510	3.828791
H	1.011341	0.974680	4.090631
H	2.171096	0.386247	5.306091
H	4.482309	-1.437027	3.219602
H	3.862940	-2.144501	4.719394
H	3.696426	-3.021245	3.186905
H	-1.798939	1.728589	-4.746850
H	-1.774145	0.158443	-3.903355
H	1.566608	-3.965193	1.869500
H	0.550122	-5.263407	2.551995
H	-0.009130	-1.688056	4.839175
H	1.095162	-3.085926	4.833779
H	-0.777326	3.905389	-2.938987
H	0.591632	3.698506	-4.061513
H	0.703516	0.046499	-0.386906
H	-1.197387	-0.317808	-0.673932

A-Ta_2N_2•CS_2

E = -2397.180981

C	3.057542	-1.717641	0.266703
C	2.601326	-0.843309	1.267567
C	3.406160	0.267117	1.580580
C	4.631669	0.466257	0.947002
C	5.084832	-0.425911	-0.024772
C	4.283439	-1.515959	-0.364765
N	1.406313	-1.128123	1.991292
Si	1.792527	-1.533598	3.706709
C	3.439383	-2.471698	3.784227
Ta	-0.454868	-1.113713	0.999535
S	-2.936709	-1.164792	1.529449
C	-1.757753	-0.479629	2.621447
S	-1.987691	0.221875	4.110494
Ta	-0.556727	1.591460	-0.162289
N	0.002669	1.931969	1.910510
N	0.256543	2.172181	2.972959
P	-0.533232	-3.214387	2.779980
C	0.404847	-2.704012	4.281237
N	-0.359591	-2.781280	-0.322426
Si	-0.056032	-4.492695	0.082915
C	-1.583320	-5.580299	-0.181835
P	-0.269276	1.441197	-2.740513
C	1.144508	0.705795	-3.669865
C	2.281173	0.260936	-2.989527
C	3.377350	-0.223486	-3.705167
C	3.340501	-0.276020	-5.096963
C	2.204111	0.160639	-5.779758
C	1.112461	0.652952	-5.069347
N	0.708249	3.265086	-0.441059
C	1.425508	3.974765	0.575501
C	2.785491	3.729047	0.815864
C	3.475487	4.438082	1.798871
C	2.825074	5.408294	2.559409
C	1.472762	5.660491	2.328193
C	0.780381	4.955175	1.346859
N	-2.394030	2.058515	-0.954904
C	-2.800741	3.030317	-0.027432
C	-2.888409	2.660373	1.330857
C	-3.148569	3.618913	2.320565
C	-3.385899	4.937154	1.962848
C	-3.344536	5.310391	0.608207
C	-3.038836	4.383184	-0.373434
C	-0.188921	3.220974	-3.236612
Si	0.944731	4.121122	-1.997531
C	2.735538	4.081428	-2.602820

C	-1.841850	0.768213	-3.441976
Si	-3.273134	1.465704	-2.382262
C	-4.531277	0.155095	-1.902362
C	0.394545	5.928437	-1.890760
C	-4.164388	2.860388	-3.303175
C	-2.005582	-4.127884	3.431686
C	-2.185984	-5.504288	3.248283
C	-3.300543	-6.152906	3.779233
C	-4.251687	-5.434556	4.500014
C	-4.080625	-4.063814	4.689359
C	-2.969732	-3.411588	4.158959
C	0.495472	-4.471567	1.903879
C	-0.782899	-2.710566	-1.682342
C	0.148690	-2.623535	-2.731055
C	-0.257651	-2.694963	-4.063518
C	-1.606473	-2.844237	-4.385328
C	-2.547491	-2.905241	-3.355296
C	-2.143406	-2.834804	-2.023422
C	1.877507	-0.070028	4.892360
C	1.344523	-5.249512	-0.949033
H	-1.921074	-2.911484	-5.423122
H	-3.603458	-3.019141	-3.587912
H	-2.871465	-2.903319	-1.220508
H	0.488439	-2.633652	-4.851102
H	1.199728	-2.515311	-2.484035
H	-1.458641	-6.086096	2.693247
H	-3.420165	-7.222706	3.629629
H	-5.119558	-5.940266	4.914575
H	-4.815143	-3.492418	5.250092
H	-2.854594	-2.343516	4.321659
H	-2.838546	1.605081	1.593116
H	-3.192137	3.302388	3.358488
H	-3.616372	5.679028	2.721917
H	-2.973088	4.682640	-1.414290
H	-3.537459	6.343000	0.328524
H	4.256354	-0.559896	-3.164391
H	2.310147	0.283973	-1.903812
H	4.194743	-0.655712	-5.650848
H	2.169311	0.120183	-6.865084
H	0.233015	0.992781	-5.610534
H	6.048153	-0.275948	-0.504088
H	4.619387	-2.227501	-1.115577
H	5.240811	1.323420	1.223150
H	3.063017	0.973999	2.329161
H	2.433795	-2.564345	0.000666
H	3.287674	2.964256	0.232156

H	4.528730	4.229320	1.970261
H	3.363288	5.958089	3.326217
H	0.949703	6.408216	2.918964
H	-0.275595	5.142597	1.173161
H	3.394190	4.585852	-1.889804
H	3.094805	3.058205	-2.741914
H	2.815090	4.604448	-3.562857
H	1.049142	6.502429	-1.228847
H	0.430826	6.387314	-2.885551
H	-0.627652	6.008055	-1.509299
H	-5.331209	0.602289	-1.303172
H	-4.982505	-0.305728	-2.787551
H	-4.052246	-0.621751	-1.302017
H	-4.893956	3.354476	-2.653518
H	-3.481778	3.620886	-3.694144
H	-4.714109	2.437165	-4.151718
H	1.093402	-5.257434	-2.013619
H	2.290022	-4.713279	-0.823373
H	1.503325	-6.287882	-0.634774
H	-1.841943	-5.611694	-1.244599
H	-1.384042	-6.608128	0.143006
H	-2.449315	-5.205680	0.370362
H	2.678448	0.631502	4.642045
H	0.923589	0.464018	4.903343
H	2.072386	-0.451562	5.902266
H	4.284370	-1.826012	3.530097
H	3.592269	-2.842509	4.804271
H	3.458550	-3.329887	3.105455
H	-1.946262	1.024727	-4.501356
H	-1.799690	-0.321374	-3.347629
H	1.514409	-4.070238	1.918744
H	0.510811	-5.450516	2.392055
H	-0.293381	-2.152306	4.918674
H	0.782959	-3.573274	4.828930
H	-1.197643	3.630461	-3.129519
H	0.135686	3.333155	-4.275493
H	0.664159	0.185155	-0.115681
H	-1.257489	-0.165830	-0.444869

D-Ta_2H_2•CS_2

E = -2287.750157

C	3.578712	0.110177	0.548324
C	2.832901	-1.069894	0.615853

C	3.146373	-2.133707	-0.241724
C	4.189235	-2.018220	-1.156382
C	4.926947	-0.835502	-1.224362
C	4.620781	0.224591	-0.374251
P	1.428533	-1.246374	1.801901
C	-0.056010	-1.422133	0.716780
Si	-0.721262	0.342096	0.409425
C	0.170282	1.094587	-1.081712
Ta	0.550128	0.433534	3.640711
N	-0.440134	1.217588	1.946412
C	-0.952054	2.549412	1.856150
C	-0.251481	3.552184	1.166177
C	-0.775120	4.838523	1.043322
C	-2.008713	5.156873	1.609662
C	-2.709127	4.173343	2.307847
C	-2.190005	2.885815	2.429661
Ta	2.625825	1.600498	5.072866
N	4.305634	0.580530	5.763930
C	4.678033	-0.710744	5.279358
C	5.175358	-0.869933	3.974968
C	5.579679	-2.119707	3.509392
C	5.504531	-3.240827	4.337549
C	5.006816	-3.096384	5.632277
C	4.593893	-1.848712	6.097663
N	3.263411	3.472899	4.283714
Si	2.914269	5.084173	4.964824
C	4.436670	6.197226	4.769910
C	3.959709	3.512147	3.051309
C	3.445570	4.192545	1.929500
C	4.185247	4.308015	0.754736
C	5.453727	3.734950	0.653547
C	5.962895	3.026346	1.742202
C	5.226455	2.915059	2.920295
C	1.418217	6.021106	4.286764
C	2.610414	4.775238	6.830948
P	3.150136	3.059066	7.212911
C	2.703020	2.725788	8.973072
C	2.692424	3.762260	9.915291
C	2.404037	3.495926	11.252018
C	2.123218	2.191705	11.659247
C	2.126807	1.157408	10.725625
C	2.411474	1.420863	9.385719
C	5.003627	3.039308	7.223039
Si	5.569323	1.256070	6.851399
C	7.265072	1.290326	6.009262
C	5.783827	0.284265	8.461275

N	-0.346047	-1.372251	4.135327
Si	0.394220	-2.995783	4.074216
C	-0.906885	-4.276372	3.579072
C	-1.667938	-1.285447	4.655821
C	-2.690970	-0.657123	3.928017
C	-3.988940	-0.581114	4.433090
C	-4.299481	-1.144457	5.668373
C	-3.291430	-1.771422	6.401587
C	-1.990317	-1.828594	5.912740
C	1.699639	-2.847624	2.681738
C	1.237458	-3.531195	5.673782
C	-2.563621	0.245522	-0.014282
H	5.829914	-4.213078	3.978284
H	4.933460	-3.960853	6.287208
H	4.191062	-1.743161	7.100299
H	5.958724	-2.213220	2.495130
H	5.241713	0.001254	3.330307
H	2.906834	4.783295	9.611830
H	2.395725	4.307959	11.973976
H	1.894116	1.984761	12.701063
H	1.891482	0.142310	11.032826
H	2.370211	0.618129	8.656966
H	-1.204141	-2.274212	6.512949
H	-3.514558	-2.204965	7.372974
H	-5.311868	-1.092824	6.058406
H	-2.455732	-0.235501	2.956524
H	-4.761843	-0.089508	3.847423
H	5.187728	1.148776	-0.417139
H	3.350352	0.938039	1.214235
H	5.739551	-0.742511	-1.939833
H	4.424898	-2.849156	-1.815830
H	2.576879	-3.058819	-0.196412
H	6.035884	3.841867	-0.257576
H	6.948474	2.570496	1.683588
H	3.766963	4.853523	-0.087776
H	2.452936	4.626398	1.993774
H	5.634888	2.385194	3.774173
H	0.715259	3.308252	0.737196
H	-0.214113	5.595626	0.500648
H	-2.416890	6.158901	1.512731
H	-3.667882	4.406783	2.763804
H	-2.733424	2.128318	2.985437
H	-0.236708	2.079595	-1.327495
H	1.244874	1.196796	-0.906889
H	0.029136	0.445961	-1.954305
H	-2.993012	1.248364	-0.100149

H	-2.695734	-0.261470	-0.976877
H	-3.132297	-0.306595	0.739677
H	0.507218	-3.802185	6.442146
H	1.876259	-4.402656	5.492175
H	1.862070	-2.721252	6.058705
H	-1.695583	-4.341940	4.333707
H	-1.377686	-4.028320	2.622832
H	-0.443227	-5.264863	3.485522
H	7.560121	0.285526	5.691309
H	7.287448	1.946187	5.134739
H	8.016868	1.651714	6.720270
H	6.178058	-0.717576	8.267300
H	6.506411	0.808982	9.097471
H	4.849890	0.191920	9.020819
H	1.592063	6.389318	3.271533
H	0.523030	5.394228	4.277892
H	1.225388	6.892340	4.924853
H	4.655451	6.380516	3.713728
H	4.253678	7.166169	5.248099
H	5.329870	5.757007	5.224021
H	1.653375	-3.696996	1.991855
H	2.706191	-2.800146	3.111539
H	5.330991	3.674563	6.394209
H	5.407132	3.432730	8.161097
H	1.537455	4.823883	7.047090
H	3.130318	5.520846	7.441378
H	-0.806706	-1.975776	1.289823
H	0.165375	-1.962869	-0.208410
H	2.157915	1.336516	3.175617
H	2.188182	-0.208233	4.410143
S	0.038664	2.510132	4.830440
C	0.797011	1.271919	5.999838
S	-0.062332	0.551169	7.237743

C-Ta_2N_2•CS_2

E= -2397.210539

Ta	0.667714	-1.998436	0.372337
Ta	-0.846849	1.749864	-0.476935
N	-0.388807	2.876446	1.181585
Si	-0.285882	4.671631	1.092386
C	-1.456455	5.126608	-0.357202
P	-2.671090	3.742388	-0.534631
C	-3.457948	3.882976	-2.192591
Si	-2.231959	3.082099	-3.421560

N	-0.844568	2.484616	-2.438324
N	0.146230	-3.673616	-0.690678
Si	-0.142899	-5.391665	-0.250795
C	0.877988	-5.598344	1.352868
P	1.931021	-4.087948	1.478156
C	3.302789	-4.282407	0.250947
Si	3.954180	-2.543708	-0.211571
N	2.564265	-1.393459	-0.071576
N	-1.156604	-1.133343	0.468759
C	-2.478562	-1.052616	0.381038
S	-3.554308	-2.238437	0.925609
S	-3.010133	0.480054	-0.357152
N	-0.271661	-0.144400	0.035299
C	2.739803	-4.132308	3.136743
C	3.554454	-5.214072	3.499171
C	4.143639	-5.259669	4.759414
C	3.923981	-4.224946	5.670130
C	3.112981	-3.148810	5.317367
C	2.519958	-3.099487	4.054827
C	5.314913	-2.066943	1.005573
C	4.672346	-2.617995	-1.958763
C	3.073625	-0.057974	-0.167245
C	3.398668	0.502646	-1.409211
C	4.011858	1.751741	-1.481019
C	4.302286	2.463064	-0.318514
C	3.947997	1.924781	0.918705
C	3.335141	0.676992	0.996853
C	0.520981	-6.542761	-1.596929
C	-1.959136	-5.755202	0.066711
C	-0.318858	-3.335735	-2.008933
C	-1.671375	-3.052300	-2.258956
C	-2.099003	-2.772005	-3.555735
C	-1.195546	-2.771143	-4.618851
C	0.150651	-3.045411	-4.376557
C	0.586188	-3.321634	-3.082569
C	0.244461	2.181873	-3.321109
C	0.367591	0.925097	-3.933111
C	1.400982	0.671246	-4.834077
C	2.329910	1.662532	-5.149280
C	2.217520	2.914174	-4.543237
C	1.188512	3.170085	-3.640273
C	-3.091879	1.664806	-4.321567
C	-1.697355	4.403697	-4.666584
C	-3.982579	4.124364	0.712767
C	-4.424297	3.146457	1.610441
C	-5.434317	3.442413	2.527000

C	-6.011425	4.709918	2.551338
C	-5.580225	5.687392	1.653512
C	-4.571037	5.396818	0.739490
C	1.441066	5.308465	0.659566
C	-0.917960	5.453070	2.688733
C	-0.085615	2.279247	2.436576
C	-0.960035	1.337817	3.003265
C	-0.689935	0.763510	4.242303
C	0.450811	1.126288	4.958677
C	1.327445	2.060374	4.407554
C	1.068053	2.625443	3.160640
H	0.766479	-1.751919	2.107620
H	0.841603	1.599671	-0.968817
H	-2.578235	4.761192	-5.212430
H	4.795807	3.429517	-0.375089
H	1.775415	3.325717	2.727832
H	-0.291300	5.180322	3.541894
H	-3.975663	2.026786	-4.858977
H	0.863731	-3.052535	-5.196898
H	-4.381163	3.295135	-2.152669
H	-1.940805	5.128025	2.899056
H	0.649836	0.692622	5.934764
H	-1.385526	0.035084	4.649955
H	-1.858771	1.057421	2.461647
H	2.224108	2.352982	4.948824
H	-4.247989	6.167011	0.043069
H	-6.030567	6.676306	1.664414
H	-6.798972	4.936992	3.264647
H	-5.769914	2.674146	3.217692
H	-3.993210	2.150907	1.576907
H	-2.376950	-3.048146	-1.431839
H	-3.148676	-2.553392	-3.730638
H	-1.537452	-2.559038	-5.627970
H	1.630268	-3.545775	-2.886117
H	2.937130	-2.342456	6.023714
H	1.886349	-2.261283	3.779040
H	4.383830	-4.261118	6.653855
H	4.772576	-6.102650	5.032202
H	3.728196	-6.028192	2.799257
H	3.129027	1.463847	-5.858184
H	2.932882	3.699312	-4.776565
H	1.472860	-0.311182	-5.293078
H	-0.344189	0.143815	-3.683572
H	1.103356	4.144148	-3.167169
H	3.058703	0.254395	1.957428
H	4.160880	2.472256	1.833110

H	4.252271	2.167913	-2.454462
H	3.150315	-0.037218	-2.316756
H	5.737400	-1.088083	0.765476
H	4.935925	-2.034911	2.031029
H	6.119950	-2.809455	0.961002
H	3.901655	-2.824175	-2.707029
H	5.158463	-1.674532	-2.221335
H	5.424697	-3.413305	-2.013323
H	-2.528257	-5.761324	-0.867919
H	-2.072966	-6.738050	0.538451
H	-2.392937	-4.988157	0.717015
H	0.027673	-6.343221	-2.552854
H	1.600392	-6.440367	-1.745395
H	0.314608	-7.583938	-1.324734
H	2.116848	5.284451	1.519537
H	1.878725	4.695735	-0.134295
H	1.381458	6.346546	0.311863
H	-0.914275	6.544961	2.596854
H	-2.419724	1.196548	-5.046561
H	-3.406407	0.903542	-3.600758
H	-0.982430	4.010344	-5.393562
H	-1.236957	5.263693	-4.169594
H	1.474260	-6.516261	1.362117
H	0.215301	-5.602308	2.225092
H	-0.886426	5.166158	-1.290532
H	-1.938201	6.096122	-0.194056
H	-3.708963	4.915847	-2.452844
H	2.861293	-4.743376	-0.637604
H	4.110330	-4.924441	0.618154

CS_2

E = -58.524500

C	0.289863	0.000000	0.384654
S	1.540975	0.000000	-0.557861
S	-0.961002	0.000000	1.327517

N_2

E = -109.474369

N	0.000000	0.000000	-0.052161
N	0.000000	0.000000	1.052161

TS-DD1 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.736334

C	0.934689	3.120572	-2.001011
C	1.953316	2.621722	-1.169337
C	3.202756	2.341821	-1.749849
C	3.433152	2.576444	-3.104485
C	2.417817	3.081057	-3.917486
C	1.166969	3.344493	-3.356766
N	1.764537	2.460927	0.234155
Si	1.852874	4.017062	1.092593
C	2.268985	3.527747	2.886808
P	1.511066	1.861721	3.212319
Ta	1.011883	0.599846	0.919753
S	-1.397458	1.398814	0.748796
Ta	-1.163888	-0.736248	-0.411200
N	-2.304664	0.000161	-2.026281
C	-3.109019	1.175551	-1.884794
C	-2.714594	2.393204	-2.463721
C	-3.511902	3.531238	-2.356024
C	-4.723099	3.480704	-1.667114
C	-5.125839	2.276574	-1.089056
C	-4.334081	1.135590	-1.200047
C	0.264468	2.192179	4.538016
C	0.634037	2.167218	5.887788
C	-0.295294	2.483093	6.877124
C	-1.599581	2.829399	6.526096
C	-1.972769	2.852454	5.183232
C	-1.047728	2.531060	4.191071
C	2.843538	0.847928	3.994736
Si	3.883028	0.030345	2.618753
C	4.878208	-1.378811	3.389751
C	5.095952	1.255331	1.842471
N	2.680431	-0.528573	1.422438
C	2.987290	-1.782747	0.817467
C	2.751078	-2.994157	1.486935
C	3.109378	-4.208600	0.907273
C	3.701738	-4.242669	-0.356836
C	3.923252	-3.046600	-1.038675
C	3.572104	-1.828631	-0.457339
C	-0.334840	-0.404423	2.107255
S	-1.013683	-1.117374	3.377011
P	-0.375891	-2.344672	-2.331069
C	1.101342	-2.171328	-3.427551

C	1.565164	-3.278389	-4.150767
C	2.644575	-3.151478	-5.021209
C	3.269511	-1.913972	-5.180072
C	2.812825	-0.809752	-4.463633
C	1.735009	-0.935269	-3.585387
N	-2.219224	-2.459337	0.012520
Si	-1.501897	-4.091996	-0.081807
C	-2.765969	-5.431716	-0.529082
C	-1.783849	-2.457493	-3.526779
Si	-2.523441	-0.700914	-3.654053
C	-1.645467	0.255733	-5.032301
C	-0.214590	-3.994838	-1.503574
C	-4.355460	-0.837612	-4.101885
C	-3.602687	-2.269618	0.276033
C	-4.017821	-1.547574	1.408069
C	-5.371839	-1.325669	1.660533
C	-6.344883	-1.822751	0.797226
C	-5.947242	-2.542939	-0.331519
C	-4.597994	-2.759720	-0.592438
C	-0.702329	-4.573629	1.551900
C	0.237923	4.998505	1.053250
C	3.247060	5.099549	0.410415
H	0.318673	-1.707405	-0.038735
H	4.417357	2.376022	-3.521915
H	0.506238	0.104190	-0.904726
H	-1.752769	-0.279713	-5.982895
H	4.563205	2.050612	1.314487
H	0.031528	5.362416	0.041955
H	2.996205	-4.017404	-5.575846
H	3.985960	-5.190957	-0.804426
H	2.924408	-5.133702	1.447170
H	2.280231	-2.965782	2.465038
H	4.367317	-3.055867	-2.030130
H	3.746508	-0.895470	-0.984877
H	1.646499	1.898742	6.175093
H	0.000941	2.456864	7.922302
H	-2.324028	3.074269	7.298011
H	-2.990327	3.109444	4.902551
H	-1.353163	2.517562	3.149017
H	-3.265588	-1.176306	2.096215
H	-5.660292	-0.762537	2.544187
H	-7.399173	-1.653372	0.996650
H	-4.303949	-3.304422	-1.483094
H	-6.693453	-2.932274	-1.019591
H	3.289284	0.158452	-4.579161
H	1.395449	-0.071389	-3.020332

H	4.109877	-1.812205	-5.861572
H	1.085362	-4.246510	-4.034403
H	2.599092	3.272502	-4.971380
H	0.367125	3.738735	-3.978974
H	-0.038761	3.318741	-1.562894
H	3.996538	1.963023	-1.112649
H	-1.764497	2.433286	-2.986234
H	-3.182230	4.462283	-2.810925
H	-5.345004	4.367482	-1.581767
H	-6.067095	2.220076	-0.547995
H	-4.653757	0.200095	-0.752655
H	-2.087831	1.248680	-5.156783
H	-0.578042	0.376378	-4.828352
H	-4.802909	0.152115	-4.231037
H	-4.472275	-1.389735	-5.041533
H	-4.911996	-1.359271	-3.317993
H	-1.466411	-4.646379	2.332757
H	-0.194652	-5.541245	1.473225
H	0.021145	-3.815009	1.856077
H	-3.620330	-5.428088	0.153914
H	-3.144386	-5.341617	-1.551696
H	-2.272082	-6.406887	-0.442593
H	5.732163	0.735724	1.117641
H	5.748213	1.704480	2.599908
H	5.424578	-1.945611	2.630393
H	5.609966	-0.953764	4.086681
H	4.246331	-2.077672	3.944675
H	-0.607144	4.376536	1.362372
H	0.298156	5.868082	1.717738
H	3.046296	5.397124	-0.622956
H	3.339759	6.011010	1.011832
H	4.209343	4.578443	0.430069
H	-0.347173	-4.815652	-2.217083
H	0.799578	-4.041211	-1.092412
H	3.435332	1.432643	4.706770
H	2.342597	0.031283	4.528589
H	1.909091	4.247433	3.626681
H	3.354713	3.436982	2.990947
H	-2.538640	-3.109703	-3.075234
H	-1.472771	-2.880619	-4.486422

Int-D1 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.737984

C	-1.647988	2.620093	6.524128
C	-0.300658	2.501416	6.866918
C	0.652177	2.267727	5.878211
C	0.262763	2.145986	4.538643
C	-1.088970	2.256843	4.199579
C	-2.038825	2.498771	5.192089
P	1.530615	1.903317	3.217736
C	2.843107	0.806516	3.912740
Si	3.878697	0.094998	2.468096
C	5.081841	1.383185	1.783591
N	2.688258	-0.408140	1.222719
C	2.981613	-1.680604	0.653144
C	2.654935	-2.875663	1.311951
C	3.018984	-4.107310	0.771965
C	3.705760	-4.173435	-0.441696
C	4.015371	-2.991990	-1.114659
C	3.657954	-1.758117	-0.573269
Ta	1.023902	0.793099	0.871337
C	-0.144992	-0.496208	1.988290
S	-0.755046	-1.285873	3.248712
Ta	-1.118884	-0.837365	-0.412177
S	-1.304439	1.447260	0.545003
P	-0.402006	-2.484890	-2.300942
C	-1.786359	-2.590132	-3.524934
Si	-2.502631	-0.830486	-3.672774
C	-4.339722	-0.950961	-4.107556
N	-2.243683	-2.507276	0.047203
C	-3.609634	-2.248997	0.321770
C	-3.964407	-1.475633	1.441495
C	-5.299597	-1.176492	1.714109
C	-6.313708	-1.648890	0.885320
C	-5.976744	-2.421030	-0.229461
C	-4.646504	-2.712823	-0.512295
N	-2.252706	-0.119074	-2.054959
C	-3.033018	1.077756	-1.950101
C	-2.599216	2.276557	-2.541093
C	-3.377257	3.431022	-2.475494
C	-4.605829	3.418016	-1.816025
C	-5.045895	2.233852	-1.224317
C	-4.274314	1.075938	-1.294516
C	-0.300954	-4.140386	-1.481536
Si	-1.582588	-4.164537	-0.047295
C	-0.778071	-4.689497	1.571341
C	1.090514	-2.313419	-3.376447
C	1.591791	-3.424360	-4.066659
C	2.673802	-3.286643	-4.932933

C	3.262398	-2.035562	-5.120920
C	2.768254	-0.927024	-4.436084
C	1.689155	-1.063664	-3.561993
C	-1.628364	0.100766	-5.070972
C	-2.905564	-5.454484	-0.473758
N	1.817476	2.673198	0.332473
Si	1.920184	4.185055	1.258842
C	0.305305	5.166466	1.267302
C	1.973533	2.824346	-1.075057
C	3.180174	2.451141	-1.695012
C	3.370811	2.639153	-3.062325
C	2.359579	3.194614	-3.847362
C	1.151980	3.553729	-3.247254
C	0.956013	3.370714	-1.879622
C	3.320189	5.283969	0.620168
C	2.318721	3.577211	3.021873
C	4.893644	-1.347948	3.144095
H	0.178185	-2.003077	-0.067782
H	4.321185	2.362575	-3.512981
H	0.619450	-0.153473	-0.844690
H	-1.756510	-0.441208	-6.015238
H	4.549145	2.210856	1.308613
H	0.085611	5.560750	0.270194
H	3.055978	-4.155627	-5.461984
H	3.995364	-5.134613	-0.857351
H	2.766473	-5.020037	1.305715
H	2.112932	-2.820526	2.251159
H	4.532806	-3.025889	-2.069313
H	3.894491	-0.835806	-1.095250
H	1.699058	2.176189	6.155983
H	0.009064	2.589342	7.904768
H	-2.390832	2.801757	7.296042
H	-3.087444	2.580746	4.920153
H	-1.398409	2.133652	3.164937
H	-3.178173	-1.132756	2.106360
H	-5.541565	-0.575355	2.586564
H	-7.353821	-1.421287	1.100441
H	-4.398224	-3.293227	-1.394316
H	-6.756671	-2.790873	-0.890333
H	3.218333	0.051472	-4.573274
H	1.320968	-0.198898	-3.017383
H	4.103962	-1.926789	-5.799889
H	1.140238	-4.403036	-3.927644
H	2.511407	3.350068	-4.911779
H	0.355626	3.985602	-3.848318
H	0.009607	3.630075	-1.415089

H	3.968814	2.027900	-1.080261
H	-1.631667	2.291884	-3.032490
H	-3.018472	4.346859	-2.939411
H	-5.212070	4.318174	-1.763815
H	-6.000808	2.206284	-0.705289
H	-4.622128	0.156305	-0.835679
H	-2.056804	1.099378	-5.197613
H	-0.556600	0.205887	-4.881753
H	-4.775618	0.040847	-4.257582
H	-4.467323	-1.523014	-5.033899
H	-4.899820	-1.447853	-3.310231
H	-1.528680	-4.742005	2.366430
H	-0.312744	-5.676433	1.469664
H	-0.019347	-3.963678	1.868984
H	-3.750060	-5.415609	0.220525
H	-3.293867	-5.352543	-1.491599
H	-2.450088	-6.448538	-0.391298
H	5.724400	0.916405	1.028974
H	5.727586	1.781228	2.574565
H	5.459559	-1.845901	2.351545
H	5.608296	-0.956955	3.877929
H	4.272282	-2.099165	3.638454
H	-0.534320	4.532602	1.568136
H	0.368532	6.015066	1.958016
H	3.124067	5.605862	-0.407159
H	3.412713	6.181248	1.242130
H	4.280882	4.759785	0.631377
H	-0.473845	-4.954543	-2.194178
H	0.709292	-4.230384	-1.068132
H	3.444460	1.314679	4.674222
H	2.322692	-0.042338	4.372877
H	1.960869	4.248955	3.806502
H	3.401933	3.461985	3.128507
H	-2.555797	-3.234279	-3.086033
H	-1.455459	-3.022700	-4.473443

TS-D1D2 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.726459

C	-1.983929	2.104266	6.328768
C	-0.699357	1.738310	6.730837
C	0.311969	1.583117	5.784935
C	0.039222	1.783150	4.427858
C	-1.250076	2.144330	4.024489

C	-2.255509	2.307592	4.976366
P	1.398871	1.720393	3.180834
C	2.730828	0.604253	3.788778
Si	3.901393	0.169339	2.333684
C	5.078726	1.598446	1.943974
N	2.848191	-0.227359	0.927587
C	3.167665	-1.491819	0.357956
C	2.751416	-2.694311	0.953928
C	3.156172	-3.922782	0.433079
C	3.964186	-3.980997	-0.702819
C	4.358640	-2.793463	-1.318208
C	3.964732	-1.563233	-0.795021
Ta	1.141064	0.966764	0.676503
C	-0.044283	-0.624897	1.620582
S	-0.318557	-1.284740	3.121979
Ta	-1.119825	-0.830052	-0.312461
S	-1.099142	1.649258	0.258939
P	-0.379812	-2.612123	-2.035445
C	-1.819870	-2.788220	-3.185454
Si	-2.561674	-1.058386	-3.495438
C	-4.406153	-1.256138	-3.870676
N	-2.231201	-2.490489	0.218101
C	-3.534572	-2.111061	0.612246
C	-3.701275	-1.223251	1.692035
C	-4.973144	-0.774905	2.057277
C	-6.101198	-1.215909	1.373215
C	-5.949494	-2.110969	0.308552
C	-4.687149	-2.547699	-0.073688
N	-2.292143	-0.163394	-1.980046
C	-3.036038	1.054338	-2.007459
C	-2.603945	2.156720	-2.764795
C	-3.348925	3.333870	-2.809976
C	-4.540720	3.444180	-2.094768
C	-4.974055	2.360812	-1.329733
C	-4.235760	1.180118	-1.288552
C	-0.276824	-4.208454	-1.118331
Si	-1.647809	-4.175463	0.228942
C	-0.944182	-4.703021	1.891798
C	1.060988	-2.501256	-3.185414
C	1.554342	-3.650472	-3.814608
C	2.577181	-3.554157	-4.755343
C	3.113529	-2.307836	-5.079374
C	2.630830	-1.161014	-4.451690
C	1.612535	-1.256220	-3.503125
C	-1.738948	-0.294734	-5.022758
C	-2.999253	-5.415825	-0.250075

N	1.967014	2.858211	0.544553
Si	1.925519	4.280131	1.601144
C	0.299885	5.235991	1.500787
C	2.163006	2.995756	-0.857518
C	3.344256	2.505684	-1.451351
C	3.566341	2.640569	-2.820498
C	2.616396	3.264662	-3.628809
C	1.434631	3.742321	-3.058073
C	1.201828	3.604966	-1.693055
C	3.364433	5.447301	1.224449
C	2.117916	3.445090	3.294453
C	4.959400	-1.293192	2.892175
H	0.216610	-1.781511	0.510096
H	4.490503	2.265907	-3.253179
H	0.642269	-0.282680	-0.804511
H	-1.882798	-0.953574	-5.887262
H	4.547568	2.457194	1.527586
H	0.217798	5.773000	0.550383
H	2.953569	-4.452701	-5.236864
H	4.283242	-4.939462	-1.102558
H	2.845032	-4.839947	0.928014
H	2.124031	-2.647957	1.840004
H	4.975947	-2.821600	-2.211805
H	4.276512	-0.636730	-1.268223
H	1.307584	1.292177	6.108022
H	-0.482793	1.571828	7.782621
H	-2.771108	2.226054	7.067762
H	-3.255910	2.585240	4.655693
H	-1.471118	2.264657	2.966901
H	-2.826662	-0.938268	2.271309
H	-5.073276	-0.088750	2.893848
H	-7.090813	-0.874464	1.663251
H	-4.577860	-3.219705	-0.918240
H	-6.823600	-2.459878	-0.235482
H	3.045866	-0.186642	-4.692824
H	1.250387	-0.361549	-3.005596
H	3.907278	-2.232702	-5.817795
H	1.141519	-4.626089	-3.572769
H	2.792747	3.377805	-4.694902
H	0.684414	4.220243	-3.682201
H	0.268728	3.945304	-1.256164
H	4.082071	2.030794	-0.813336
H	-1.658136	2.085083	-3.292929
H	-2.991627	4.171786	-3.404283
H	-5.121466	4.361816	-2.129973
H	-5.897851	2.431047	-0.760558

H	-4.576028	0.340964	-0.689765
H	-2.184361	0.674788	-5.264003
H	-0.663893	-0.156424	-4.878326
H	-4.862833	-0.287610	-4.094925
H	-4.552409	-1.910716	-4.737584
H	-4.934171	-1.685748	-3.014439
H	-1.736548	-4.743292	2.645982
H	-0.487814	-5.696974	1.816995
H	-0.201533	-3.980165	2.238560
H	-3.856436	-5.350733	0.426952
H	-3.361120	-5.287854	-1.274841
H	-2.586680	-6.428201	-0.166587
H	5.825270	1.269330	1.212540
H	5.614619	1.915746	2.845968
H	5.614915	-1.641249	2.088417
H	5.588622	-0.968970	3.729424
H	4.352729	-2.138926	3.224097
H	-0.553685	4.556054	1.579193
H	0.234587	5.974051	2.308221
H	3.293650	5.823897	0.198689
H	3.344393	6.311057	1.897990
H	4.332162	4.949068	1.336060
H	-0.392597	-5.067113	-1.789013
H	0.711585	-4.246552	-0.649915
H	3.251174	1.014012	4.661570
H	2.218188	-0.328658	4.061389
H	1.621829	3.983881	4.105518
H	3.180728	3.355024	3.540119
H	-2.571818	-3.379417	-2.652454
H	-1.533206	-3.314888	-4.100725

Int-D2 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.732755

C	-2.129455	2.213707	6.096765
C	-0.870779	1.810689	6.542881
C	0.164859	1.613109	5.631969
C	-0.060112	1.803539	4.265059
C	-1.322039	2.206049	3.816663
C	-2.350663	2.412653	4.734298
P	1.336994	1.708827	3.064636
C	2.655020	0.584864	3.687719
Si	3.880004	0.184862	2.264718
C	5.063337	1.624307	1.934992

N	2.891148	-0.196215	0.806937
C	3.189009	-1.470745	0.254833
C	2.776290	-2.660345	0.881569
C	3.155881	-3.901776	0.371508
C	3.929463	-3.988047	-0.786348
C	4.315628	-2.814679	-1.434124
C	3.950700	-1.571726	-0.920728
Ta	1.175050	0.994259	0.540661
C	-0.018208	-0.656611	1.448108
S	-0.317990	-1.212231	3.036774
Ta	-1.101838	-0.761688	-0.466047
S	-0.996193	1.743379	-0.031310
P	-0.358930	-2.571252	-2.153377
C	-1.836388	-2.760857	-3.253162
Si	-2.639486	-1.051153	-3.537667
C	-4.484222	-1.308093	-3.867701
N	-2.185227	-2.435080	0.085745
C	-3.472410	-2.060913	0.540300
C	-3.594322	-1.150182	1.606553
C	-4.853679	-0.713685	2.027198
C	-6.008376	-1.185820	1.412248
C	-5.898441	-2.101147	0.359370
C	-4.650874	-2.528721	-0.077650
N	-2.356462	-0.116628	-2.041418
C	-3.146097	1.073012	-2.067870
C	-2.778082	2.172116	-2.861579
C	-3.565548	3.321292	-2.903092
C	-4.733962	3.404850	-2.146917
C	-5.102078	2.323723	-1.345860
C	-4.322055	1.169678	-1.308446
C	-0.221743	-4.148185	-1.210744
Si	-1.605065	-4.123735	0.125595
C	-0.923242	-4.635053	1.800580
C	1.050073	-2.453377	-3.338293
C	1.529345	-3.599880	-3.983067
C	2.534061	-3.498856	-4.942538
C	3.065168	-2.250999	-5.269648
C	2.595084	-1.106809	-4.627663
C	1.594893	-1.206517	-3.660602
C	-1.867411	-0.273004	-5.083149
C	-2.940948	-5.375299	-0.367150
N	2.043338	2.877751	0.476563
Si	1.955883	4.288909	1.545156
C	0.337389	5.253321	1.402342
C	2.286939	3.026496	-0.915539
C	3.438717	2.451355	-1.490233

C	3.706716	2.590675	-2.852253
C	2.835175	3.306528	-3.670535
C	1.682551	3.872961	-3.118683
C	1.402646	3.728514	-1.764747
C	3.408622	5.459445	1.239004
C	2.080114	3.422009	3.224925
C	4.934393	-1.274512	2.840302
H	0.254147	-1.600674	0.743927
H	4.608523	2.148805	-3.268393
H	0.694294	-0.303313	-0.901595
H	-1.997452	-0.947483	-5.937750
H	4.546367	2.479761	1.495195
H	0.304687	5.838605	0.477850
H	2.900923	-4.394859	-5.435829
H	4.228816	-4.956321	-1.177667
H	2.850812	-4.806802	0.891957
H	2.174024	-2.594631	1.784742
H	4.906924	-2.864075	-2.344358
H	4.260049	-0.657665	-1.418799
H	1.139729	1.292454	5.988610
H	-0.693122	1.648622	7.602671
H	-2.935102	2.369136	6.809050
H	-3.330094	2.721814	4.379281
H	-1.504767	2.325001	2.751594
H	-2.696524	-0.848656	2.142365
H	-4.920650	-0.013152	2.854976
H	-6.987034	-0.853776	1.747081
H	-4.574502	-3.218095	-0.911788
H	-6.794033	-2.474003	-0.131197
H	3.006365	-0.131557	-4.871322
H	1.244097	-0.313568	-3.152131
H	3.845301	-2.172560	-6.022002
H	1.121246	-4.576670	-3.737804
H	3.048214	3.424336	-4.729437
H	0.991089	4.422866	-3.751528
H	0.486460	4.132857	-1.347047
H	4.121321	1.911937	-0.842556
H	-1.847523	2.124849	-3.418465
H	-3.257465	4.159105	-3.524144
H	-5.347079	4.301309	-2.178333
H	-6.007266	2.373728	-0.745628
H	-4.614469	0.330504	-0.685280
H	-2.350157	0.676748	-5.330109
H	-0.796240	-0.094024	-4.953372
H	-4.975308	-0.353888	-4.079927
H	-4.629941	-1.966405	-4.731849

H	-4.978987	-1.754060	-3.000202
H	-1.737772	-4.722175	2.526942
H	-0.419166	-5.606110	1.730385
H	-0.232555	-3.879264	2.185806
H	-3.794783	-5.331367	0.315558
H	-3.310242	-5.243433	-1.388750
H	-2.511437	-6.381620	-0.295062
H	5.845054	1.300615	1.238698
H	5.554297	1.942622	2.861853
H	5.605082	-1.618040	2.047013
H	5.548674	-0.943777	3.686122
H	4.329848	-2.123972	3.165553
H	-0.520202	4.573968	1.405073
H	0.232174	5.950476	2.241389
H	3.378415	5.848307	0.215785
H	3.362317	6.315203	1.921417
H	4.370548	4.958529	1.382915
H	-0.317304	-5.019474	-1.868293
H	0.767274	-4.159145	-0.741668
H	3.145308	0.982361	4.583562
H	2.134437	-0.354113	3.923837
H	1.568607	3.952895	4.031382
H	3.133546	3.309434	3.499689
H	-2.553457	-3.379055	-2.704420
H	-1.568435	-3.267357	-4.185658

TS-D2D3 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.723311

C	4.446194	2.313110	1.109931
Ta	3.041292	1.999392	4.591892
N	4.791773	1.011716	5.131971
C	5.347033	-0.166764	4.557030
C	4.894527	-1.446866	4.925335
C	5.512879	-2.590505	4.421531
C	6.595552	-2.487695	3.545406
C	7.044365	-1.222340	3.167203
C	6.421864	-0.074209	3.657076
H	7.597996	3.494244	1.522250
Si	5.667921	1.435095	6.644433
C	6.120178	-0.094003	7.657327
C	7.269038	2.359382	6.230724
C	4.587864	2.541442	7.783995
P	3.006051	3.102831	7.001304

C	1.680891	3.016482	8.291970
C	0.334765	3.013301	7.908212
C	-0.665232	3.075586	8.875497
C	3.145728	4.965279	6.854481
C	-0.335921	3.135120	10.230178
C	5.729053	6.186432	5.613941
C	2.009238	3.088726	9.648647
C	1.002903	3.140324	10.613934
Si	4.015305	5.464175	5.250548
C	3.006038	6.735336	4.286794
N	4.006636	3.930053	4.380147
C	4.628077	3.616179	3.196107
C	6.003836	3.823116	2.901728
C	6.548872	3.310057	1.742028
C	5.783867	2.528697	0.849846
C	3.852581	2.887108	2.255055
H	2.483329	0.810062	3.046608
Ta	0.773865	0.253825	3.649057
P	1.435124	-1.450592	1.793593
C	2.796616	-1.273636	0.557402
C	4.121769	-1.438386	0.981150
C	5.168172	-1.345152	0.066667
C	4.910893	-1.067367	-1.275531
C	3.597189	-0.881960	-1.700531
C	2.545194	-0.988918	-0.790778
C	1.648003	-3.104348	2.592610
H	-0.528899	0.556445	-1.656905
C	1.180287	-3.657937	5.650456
Si	0.359837	-3.181548	4.017253
C	-0.131814	-1.528065	0.818162
C	-0.934576	-4.501529	3.603997
Si	-1.024142	0.170640	0.764607
N	-0.292525	-1.539674	4.042828
C	-0.413774	1.151104	-0.742397
N	-0.697705	0.984206	2.311976
C	-1.499207	-0.598545	5.965435
C	-1.501449	-1.293793	4.739943
C	-2.741967	-1.716327	4.221301
C	-3.928969	-1.454725	4.898060
C	-3.914427	-0.751770	6.105501
C	-2.867224	-0.172536	0.511528
C	-2.696072	-0.327171	6.630821
C	-1.576347	2.093314	2.493721
C	-2.658189	2.018229	3.385655
C	-3.518430	3.101299	3.556675
C	-3.330147	4.280624	2.835809

C	-2.260145	4.367350	1.946396
C	-1.391568	3.290177	1.780411
S	0.813793	2.734808	4.281834
C	1.862481	0.176297	5.387099
S	2.164936	0.086985	7.074785
H	2.000900	-0.828928	4.832732
H	7.065394	3.267818	5.658843
H	3.477063	6.956425	3.322988
H	3.383900	-0.662770	-2.743246
H	7.085354	-3.381483	3.169233
H	5.160596	-3.569662	4.737171
H	4.084882	-1.518822	5.645774
H	7.890897	-1.124069	2.491455
H	6.764258	0.912843	3.362001
H	3.047821	3.103661	9.966954
H	1.270613	3.188230	11.666115
H	-1.119201	3.177335	10.982028
H	-1.706759	3.070611	8.565840
H	0.071972	2.941306	6.856449
H	-0.548204	-0.306142	6.406196
H	-2.664802	0.206471	7.576972
H	-4.842943	-0.546532	6.630932
H	-2.758963	-2.250588	3.276328
H	-4.872286	-1.793781	4.477041
H	6.186221	-1.487526	0.414575
H	4.349391	-1.637904	2.024427
H	5.729880	-0.997269	-1.986279
H	1.530171	-0.848762	-1.144061
H	6.243229	2.118034	-0.043607
H	3.832716	1.745059	0.417473
H	2.765272	2.992486	2.297080
H	6.617603	4.381351	3.600148
H	-0.536925	3.376625	1.116529
H	-2.090690	5.282527	1.384191
H	-4.006078	5.121046	2.967484
H	-4.345853	3.016979	4.256935
H	-2.815454	1.102036	3.945886
H	-1.007294	2.061619	-0.866785
H	0.637029	1.440524	-0.646740
H	-3.424458	0.763860	0.414943
H	-3.028020	-0.760328	-0.399575
H	-3.281597	-0.723003	1.360925
H	0.414990	-3.772513	6.425527
H	1.719450	-4.608372	5.564783
H	1.872977	-2.884258	5.996265
H	-1.740755	-4.503314	4.343675

H	-1.380024	-4.359971	2.614387
H	-0.461957	-5.490359	3.622176
H	7.932680	1.723478	5.636468
H	7.800876	2.636158	7.148348
H	6.815227	-0.749627	7.126251
H	6.601251	0.228020	8.588707
H	5.222250	-0.664963	7.911043
H	2.002534	6.344287	4.092328
H	2.913645	7.676201	4.840444
H	6.249343	6.487340	4.699050
H	5.611434	7.085784	6.230104
H	6.366237	5.486484	6.162328
H	1.526569	-3.909181	1.859502
H	2.665928	-3.147519	2.993702
H	5.153338	3.402121	8.156851
H	4.315347	1.910095	8.634284
H	2.112397	5.327904	6.827573
H	3.612735	5.369698	7.758621
H	-0.785185	-2.186328	1.397939
H	0.015981	-1.977626	-0.168891

Int-D3 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.791748

C	1.088143	3.117046	-3.276191
Ta	0.843297	0.749827	1.258947
N	2.598088	-0.385785	1.387354
C	2.858280	-1.711927	0.954709
C	2.513551	-2.816544	1.754066
C	2.840121	-4.112819	1.358724
C	3.507849	-4.338445	0.153616
C	3.835049	-3.251044	-0.657700
C	3.512343	-1.952905	-0.263779
H	4.392578	2.345718	-3.372241
Si	3.885308	0.248753	2.461674
C	4.918688	-1.139432	3.222802
C	5.072262	1.439260	1.595452
C	3.036704	1.150165	3.932731
P	1.590977	2.144365	3.359524
C	0.498155	2.451767	4.811072
C	-0.883984	2.561290	4.616988
C	-1.715121	2.853671	5.698392
C	2.264419	3.808029	2.889019
C	-1.175589	3.027006	6.971985

C	3.080963	5.175387	0.239371
C	1.036840	2.625200	6.091580
C	0.200712	2.909867	7.168842
Si	1.765543	4.100607	1.072070
C	0.109348	5.008536	1.032598
N	1.696467	2.464084	0.358791
C	1.894554	2.538286	-1.054183
C	3.162124	2.304798	-1.612214
C	3.392573	2.501103	-2.973213
C	2.359803	2.914198	-3.814697
C	0.853834	2.930058	-1.914911
H	0.589623	-0.125664	-0.591718
Ta	-1.168214	-0.838924	-0.383505
P	-0.124785	-2.447899	-2.223863
C	1.359398	-2.236597	-3.299264
C	1.965945	-0.985172	-3.441616
C	3.042839	-0.829972	-4.315812
C	3.525415	-1.917043	-5.041182
C	2.926940	-3.168863	-4.896879
C	1.847271	-3.326712	-4.031987
C	-0.043199	-4.138855	-1.489631
H	-1.393958	-0.288409	-5.752351
C	-1.113881	-4.997107	1.339260
Si	-1.580560	-4.318465	-0.361744
C	-1.532491	-2.467853	-3.433681
C	-2.768941	-5.567906	-1.149610
Si	-2.406758	-0.765278	-3.531444
N	-2.218749	-2.667568	-0.284943
C	-1.496459	0.281377	-4.821237
N	-2.392204	-0.044261	-1.894276
C	-3.801682	-1.876441	1.433842
C	-3.546983	-2.490585	0.193384
C	-4.652937	-2.896172	-0.580042
C	-5.954525	-2.703705	-0.128939
C	-6.192743	-2.088198	1.102286
C	-4.173499	-1.062281	-4.138593
C	-5.110456	-1.674333	1.875015
C	-3.290345	1.057778	-1.824320
C	-4.502700	0.949543	-1.124612
C	-5.389350	2.021843	-1.066322
C	-5.094801	3.223875	-1.711246
C	-3.891707	3.344829	-2.404475
C	-2.997186	2.276851	-2.456265
S	-1.394630	1.413703	0.554733
C	-0.446510	-1.140218	1.551091
S	-0.230649	-0.469285	3.126994

H	-0.077643	-2.177447	1.421201
H	4.540648	2.293608	1.170578
H	-0.194962	5.218405	0.002827
H	3.298587	-4.021917	-5.458232
H	3.774148	-5.348216	-0.146654
H	2.580212	-4.950288	2.001586
H	2.005252	-2.633982	2.697270
H	4.346289	-3.409755	-1.603363
H	3.765070	-1.105046	-0.892976
H	2.108056	2.534877	6.252569
H	0.623657	3.038451	8.161434
H	-1.826966	3.247588	7.813206
H	-2.787245	2.933849	5.543155
H	-1.308321	2.394612	3.630079
H	-2.961743	-1.559149	2.043914
H	-5.276922	-1.192528	2.834872
H	-7.210100	-1.933555	1.450434
H	-4.474880	-3.354711	-1.547403
H	-6.788874	-3.026095	-0.746864
H	3.498982	0.148747	-4.420408
H	1.609611	-0.133066	-2.869001
H	4.366322	-1.790527	-5.717723
H	1.387432	-4.305617	-3.928736
H	2.542188	3.079389	-4.872932
H	0.272133	3.436203	-3.919992
H	-0.136298	3.073262	-1.492813
H	3.971081	1.995220	-0.959562
H	-2.046615	2.381735	-2.968556
H	-3.640101	4.278822	-2.901164
H	-5.791348	4.056629	-1.668346
H	-6.319540	1.913656	-0.514063
H	-4.734792	0.015744	-0.622949
H	-2.050346	1.196722	-5.048650
H	-0.495972	0.560916	-4.478771
H	-4.697762	-0.112552	-4.279539
H	-4.165318	-1.593340	-5.097371
H	-4.741242	-1.653836	-3.414787
H	-1.986298	-4.977433	2.000928
H	-0.771687	-6.035031	1.259774
H	-0.320137	-4.409938	1.808138
H	-3.693164	-5.657676	-0.571434
H	-3.034006	-5.313978	-2.180473
H	-2.286469	-6.552416	-1.161623
H	5.598258	0.924620	0.784367
H	5.824070	1.807618	2.303098
H	5.452372	-1.708140	2.455841

H	5.660340	-0.698406	3.898949
H	4.303839	-1.839359	3.794531
H	-0.680299	4.407205	1.492608
H	0.182842	5.963601	1.565613
H	2.815577	5.399019	-0.797790
H	3.170526	6.125624	0.778280
H	4.061485	4.689590	0.238678
H	-0.030616	-4.913877	-2.263533
H	0.886111	-4.198665	-0.912652
H	3.743891	1.759653	4.506958
H	2.632416	0.364246	4.581160
H	1.857244	4.567533	3.561568
H	3.353523	3.798410	2.993843
H	-2.264329	-3.185694	-3.053247
H	-1.185936	-2.798933	-4.418188

Isomer D3 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.809733

C	-0.573553	5.826486	2.484951
C	0.236993	4.691898	2.506968
C	-0.316508	3.412772	2.669404
C	-1.709964	3.307273	2.814579
C	-2.517386	4.440819	2.793870
C	-1.954534	5.707378	2.627941
N	0.516456	2.248958	2.713927
Si	1.086097	1.796802	4.337323
C	0.006484	0.497671	5.187626
C	2.858220	1.150124	4.020420
P	2.887787	0.331599	2.350754
C	3.212250	-1.454917	2.706970
C	3.927169	-2.254031	1.805052
C	4.121140	-3.611440	2.056966
C	3.596006	-4.193650	3.209383
C	2.869698	-3.410969	4.105237
C	2.674326	-2.054151	3.854145
Ta	0.717937	1.249062	0.898323
C	0.857362	-0.816996	0.276950
S	-0.227583	-0.956864	1.730185
N	2.244654	2.262865	-0.062971
Si	3.924387	2.519670	0.474000
C	4.393792	0.968969	1.481765
S	-1.198892	1.629744	-0.334238
Ta	-1.064342	-0.875478	-0.825078

N	-2.158381	-0.543874	-2.586424
C	-3.228814	0.384210	-2.726947
C	-2.992001	1.660543	-3.270276
C	-4.031414	2.572859	-3.435206
C	-5.331768	2.238094	-3.056196
C	-5.576320	0.979989	-2.508579
C	-4.539590	0.061510	-2.346826
P	0.154808	-2.775576	-2.001920
C	0.090553	-4.368799	-1.060546
Si	-1.534349	-4.322765	-0.060356
C	-2.650067	-5.712008	-0.721088
N	-2.115876	-2.665296	-0.305769
C	-3.431243	-2.338692	0.089902
C	-3.680677	-1.253026	0.955430
C	-4.982187	-0.874207	1.288034
C	-6.074248	-1.585548	0.801639
C	-5.847963	-2.670160	-0.049716
C	-4.555362	-3.029824	-0.414870
C	1.901383	-2.672816	-2.618558
C	2.458525	-3.787066	-3.260853
C	3.766039	-3.751040	-3.740193
C	4.536024	-2.599109	-3.580939
C	3.990846	-1.488223	-2.940138
C	2.680957	-1.523077	-2.459100
C	-0.854520	-2.985961	-3.542633
Si	-1.593735	-1.296575	-4.087374
C	-3.057665	-1.671151	-5.227009
C	-0.306214	-0.303529	-5.055553
C	-1.214140	-4.680973	1.766566
C	1.895505	3.061825	-1.206813
C	2.014948	2.542024	-2.504111
C	1.695580	3.318406	-3.615078
C	1.252464	4.631700	-3.456108
C	1.129682	5.158045	-2.171488
C	1.449460	4.383642	-1.057528
C	5.111099	2.665812	-0.990041
C	4.111158	4.068349	1.545980
C	1.192332	3.304629	5.473775
H	1.715257	-1.486163	0.253643
H	0.166481	-0.502350	-2.023510
H	-0.121123	6.806869	2.357383
H	0.052734	-0.870883	-5.922022
H	3.487574	4.011992	2.442700
H	-0.991643	0.911723	5.366744
H	4.182080	-4.621865	-4.239588
H	0.999907	5.234717	-4.323663

H	1.789804	2.891316	-4.610031
H	2.346992	1.516883	-2.630914
H	0.773560	6.175183	-2.030115
H	1.326450	4.788059	-0.058062
H	4.688181	-4.211144	1.350260
H	3.750853	-5.250485	3.407443
H	2.450232	-3.855237	5.003631
H	2.095243	-1.465454	4.558364
H	-2.840525	-0.730020	1.406019
H	-5.133577	-0.025641	1.949877
H	-7.086082	-1.301947	1.076175
H	-4.402121	-3.836944	-1.121958
H	-6.689107	-3.229110	-0.452827
H	4.583941	-0.585679	-2.819015
H	2.254546	-0.659390	-1.958951
H	5.554942	-2.567819	-3.957073
H	-2.586969	6.590307	2.607860
H	-3.593648	4.333070	2.899774
H	-2.148360	2.319320	2.919558
H	1.313576	4.784311	2.401951
H	-1.974672	1.934631	-3.533256
H	-3.820314	3.553601	-3.854490
H	-6.142066	2.951122	-3.182022
H	-6.582685	0.704252	-2.203235
H	-4.735659	-0.917268	-1.922669
H	-0.747003	0.629309	-5.421523
H	0.549242	-0.053048	-4.423071
H	-3.530443	-0.745811	-5.569622
H	-2.726441	-2.231414	-6.108600
H	-3.816964	-2.262029	-4.705484
H	-2.146629	-4.604889	2.336235
H	-0.813229	-5.691276	1.906500
H	-0.506558	-3.956872	2.180386
H	-3.580718	-5.796035	-0.152917
H	-2.901321	-5.585723	-1.779365
H	-2.113928	-6.663090	-0.616241
H	3.821617	4.961836	0.983855
H	5.154340	4.191755	1.858844
H	4.891062	3.551423	-1.592969
H	6.142118	2.748665	-0.628124
H	5.048172	1.791305	-1.644362
H	-0.111650	-0.401577	4.577178
H	0.428545	0.215979	6.159515
H	0.201128	3.726245	5.665148
H	1.625760	3.010147	6.436413
H	1.815352	4.095496	5.045831

H	0.157192	-5.245107	-1.713122
H	0.952158	-4.368396	-0.384208
H	5.226474	1.124624	2.175361
H	4.696750	0.214609	0.748061
H	3.259076	0.488680	4.793781
H	3.513245	2.026158	3.959488
H	-1.707140	-3.615706	-3.263406
H	-0.284719	-3.489266	-4.330585
H	4.343573	-1.826956	0.897690
H	1.870355	-4.691986	-3.392527

TS-3 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.766864

C	-1.042034	5.820497	2.564933
C	-0.159015	4.740902	2.543848
C	-0.602828	3.437450	2.815284
C	-1.960972	3.254515	3.125330
C	-2.839521	4.334395	3.151234
C	-2.387630	5.624216	2.868595
N	0.315078	2.337603	2.827314
Si	0.952501	2.059387	4.469536
C	-0.156054	0.917179	5.495516
C	2.679349	1.280459	4.214757
P	2.623880	0.276919	2.652591
C	2.932883	-1.464120	3.200603
C	3.729055	-2.340020	2.452222
C	3.912876	-3.660052	2.863012
C	3.300301	-4.126113	4.024617
C	2.500224	-3.263901	4.773024
C	2.314144	-1.945391	4.362878
Ta	0.508129	1.068526	1.166086
C	0.600069	-1.187358	0.729266
S	-0.482474	-1.062675	2.137737
N	1.990508	1.969510	0.011477
Si	3.649251	2.286482	0.580077
C	4.100844	0.780163	1.659992
S	-1.652523	1.494423	0.304094
Ta	-1.392517	-0.849755	-0.408856
N	-2.275418	-0.420733	-2.255558
C	-3.239952	0.631082	-2.360640
C	-2.862154	1.894958	-2.846650
C	-3.798614	2.917630	-2.976140
C	-5.129992	2.707935	-2.615757

C	-5.512572	1.461072	-2.123729
C	-4.581115	0.430651	-2.002038
P	-0.084576	-2.533603	-1.864682
C	-0.039286	-4.134451	-0.920714
Si	-1.650570	-4.274781	0.098313
C	-2.698272	-5.680922	-0.629175
N	-2.376726	-2.665665	-0.053275
C	-3.739984	-2.422346	0.205035
C	-4.106037	-1.447782	1.155966
C	-5.444588	-1.108873	1.364524
C	-6.452861	-1.758172	0.659914
C	-6.108005	-2.740770	-0.274204
C	-4.776339	-3.061899	-0.509341
C	1.634768	-2.381673	-2.543016
C	2.183249	-3.444867	-3.274603
C	3.472046	-3.358934	-3.793861
C	4.231775	-2.207597	-3.585376
C	3.695453	-1.149826	-2.855285
C	2.402851	-1.233920	-2.333145
C	-1.127787	-2.851715	-3.361670
Si	-1.965589	-1.198306	-3.820754
C	-3.572697	-1.578640	-4.743473
C	-0.829349	-0.198650	-4.957588
C	-1.276104	-4.720742	1.894652
C	1.594093	2.799330	-1.090983
C	2.002672	2.500432	-2.401093
C	1.632186	3.311093	-3.472377
C	0.840577	4.439590	-3.262836
C	0.425011	4.745760	-1.967758
C	0.799980	3.940352	-0.894335
C	4.930332	2.406357	-0.806926
C	3.734379	3.893637	1.573466
C	1.174148	3.670530	5.436489
H	1.409794	-1.909486	0.698863
H	0.454068	-0.386486	-0.304961
H	-0.671253	6.819432	2.348242
H	-0.599827	-0.765267	-5.867405
H	3.014963	3.884006	2.396595
H	-1.117260	1.408264	5.680390
H	3.882288	-4.189321	-4.362106
H	0.549739	5.069963	-4.098427
H	1.962677	3.054288	-4.475607
H	2.612105	1.620710	-2.576547
H	-0.200663	5.615290	-1.784880
H	0.460137	4.183088	0.107263
H	4.542279	-4.321444	2.273717

H	3.446265	-5.153614	4.345570
H	2.015380	-3.616513	5.679139
H	1.679421	-1.293002	4.954177
H	-3.326081	-0.986339	1.757939
H	-5.691615	-0.343243	2.094853
H	-7.495561	-1.507392	0.831960
H	-4.521119	-3.794022	-1.267817
H	-6.886441	-3.248094	-0.838865
H	4.282311	-0.249617	-2.696738
H	1.989425	-0.402535	-1.768274
H	5.236746	-2.136185	-3.992102
H	-3.076427	6.464053	2.885393
H	-3.886703	4.164581	3.388266
H	-2.319742	2.248835	3.320979
H	0.892437	4.900785	2.323576
H	-1.819300	2.071487	-3.091150
H	-3.481020	3.887906	-3.349628
H	-5.858245	3.508595	-2.712333
H	-6.544829	1.282554	-1.832953
H	-4.884645	-0.540519	-1.624347
H	-1.313943	0.735851	-5.256756
H	0.111743	0.052981	-4.460020
H	-4.096899	-0.657682	-5.015315
H	-3.362904	-2.135574	-5.663824
H	-4.245903	-2.177259	-4.121844
H	-2.203886	-4.742086	2.476667
H	-0.809060	-5.709640	1.965542
H	-0.610996	-3.981064	2.348946
H	-3.649630	-5.790041	-0.099931
H	-2.911516	-5.544412	-1.694285
H	-2.147953	-6.622756	-0.517068
H	3.495808	4.744940	0.927294
H	4.738769	4.050949	1.982587
H	4.673871	3.195692	-1.519021
H	5.907353	2.647720	-0.372437
H	5.032779	1.467195	-1.358111
H	-0.359250	-0.023730	4.976250
H	0.297241	0.696564	6.468966
H	0.213867	4.163368	5.612000
H	1.627102	3.451579	6.410515
H	1.823114	4.377103	4.910479
H	0.095695	-4.983853	-1.599254
H	0.825357	-4.089006	-0.251241
H	4.984113	0.929118	2.289853
H	4.310318	-0.026518	0.949217
H	3.024375	0.674438	5.057248

H	3.402086	2.089546	4.064188
H	-1.918094	-3.545436	-3.055118
H	-0.553474	-3.302075	-4.176357
H	4.221598	-2.001428	1.545926
H	1.602433	-4.348156	-3.443517

Int-D4 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.840936

Ta	1.046645	0.040239	3.165345
P	0.955026	-1.655769	1.107969
C	1.960098	-1.542994	-0.439791
C	1.418152	-1.670015	-1.723700
C	2.239737	-1.589998	-2.848101
C	3.610090	-1.384728	-2.702335
C	4.158598	-1.256996	-1.426270
C	3.340014	-1.330378	-0.301503
C	1.230397	-3.347168	1.786525
Si	0.492315	-3.378995	3.550283
C	1.691284	-4.348516	4.644100
H	-1.960067	0.449175	-1.716375
C	-0.820647	-1.588383	0.614535
C	-1.280084	0.989305	-1.046937
Si	-1.371772	0.235330	0.687311
C	-1.164998	-4.296969	3.539621
C	-3.169161	0.312399	1.272963
N	0.278077	-1.669928	4.063026
N	-0.266225	1.014327	1.851606
C	-0.502279	2.426344	1.861015
C	0.121080	3.264740	0.923159
C	0.332508	-1.951780	6.526095
C	-0.199725	4.620035	0.850889
C	-1.140301	5.169465	1.721564
C	-1.744545	4.351476	2.677481
C	-0.325351	-1.973040	7.755380
C	-1.428851	2.996683	2.748860
C	-0.360237	-1.641527	5.346301
C	-1.728280	-1.343671	5.439987
C	-2.381694	-1.355528	6.669835
C	-1.685986	-1.678119	7.835406
S	0.598675	1.413976	5.066365
Ta	2.941398	1.670658	4.683311
P	2.662841	3.305330	6.794194
H	2.624613	6.563647	2.508379

C	1.503411	4.004333	9.274712
C	1.626174	3.003100	8.301489
C	2.088726	6.251931	3.409373
C	2.207300	4.979719	6.186375
Si	3.178724	5.231116	4.567841
C	0.748270	3.786100	10.424115
C	0.977892	1.779531	8.497819
C	0.105065	2.562430	10.613752
C	0.221187	1.562847	9.650555
C	4.744973	6.259721	4.875754
C	4.367434	3.462684	7.489684
Si	5.120108	1.720142	7.451718
C	4.789081	0.847947	9.099265
C	6.996889	1.894477	7.247582
C	6.688442	3.406755	1.923633
C	6.243714	3.867702	0.684107
C	6.127275	-0.646185	5.249433
C	6.712402	-1.909287	5.204045
C	6.140121	-2.979973	5.892470
C	4.974299	-2.768017	6.627552
C	4.389340	-1.502494	6.675339
C	4.950311	-0.416731	5.983392
N	4.362243	0.882779	6.059823
C	4.457314	3.686060	2.870902
N	3.582029	3.590329	3.990737
C	4.022811	4.143859	1.613772
C	4.905897	4.234137	0.538402
C	5.809667	3.323751	3.002094
C	3.179246	1.133310	2.539199
S	3.485074	-0.449978	3.362494
H	7.727392	3.113725	2.054928
H	7.249120	2.409896	6.315271
H	1.804811	-1.689308	-3.838968
H	6.598576	-3.964278	5.858716
H	4.518593	-3.589962	7.174304
H	3.487349	-1.332271	7.256116
H	7.620740	-2.057442	4.625160
H	6.562793	0.182194	4.698322
H	1.997801	4.963157	9.138005
H	0.660023	4.571666	11.169912
H	-0.488017	2.392613	11.508386
H	-0.285445	0.611313	9.781913
H	1.044820	1.003625	7.741907
H	1.395336	-2.162599	6.468220
H	0.231911	-2.223562	8.654939
H	-2.198990	-1.699492	8.792851

H	-2.266524	-1.093880	4.530407
H	-3.440812	-1.115116	6.716258
H	5.225335	-1.091802	-1.303378
H	3.773400	-1.217107	0.689240
H	4.248228	-1.322276	-3.579392
H	0.353538	-1.830529	-1.859940
H	6.928753	3.937135	-0.156137
H	4.541083	4.585713	-0.423827
H	2.974514	4.393951	1.484812
H	6.151543	2.963249	3.968327
H	0.844550	2.833362	0.236734
H	0.284038	5.246788	0.105909
H	-1.394960	6.223737	1.660174
H	-2.472634	4.767869	3.369061
H	-1.894665	2.358290	3.493174
H	-1.580992	2.040535	-1.040474
H	-0.269766	0.924853	-1.461725
H	-3.507218	1.350237	1.349299
H	-3.825986	-0.206342	0.565282
H	-3.283282	-0.155666	2.255606
H	1.278460	-4.527472	5.640548
H	1.886917	-5.323417	4.181590
H	2.645529	-3.823813	4.751051
H	-1.595104	-4.328228	4.545053
H	-1.899951	-3.830407	2.876744
H	-1.013562	-5.329604	3.205311
H	7.495410	0.921198	7.246676
H	7.402051	2.482197	8.079730
H	5.213236	-0.160217	9.106739
H	5.250311	1.414486	9.916526
H	3.716680	0.774106	9.301796
H	1.195585	5.697480	3.109691
H	1.768883	7.159523	3.936259
H	5.273668	6.424819	3.931696
H	4.473874	7.240779	5.282372
H	5.445947	5.786245	5.569197
H	0.810135	-4.121244	1.136101
H	2.313773	-3.495006	1.854658
H	4.939542	4.094467	6.804250
H	4.373190	3.916932	8.484994
H	1.133693	4.967597	5.969224
H	2.416588	5.764952	6.919485
H	-1.355029	-2.129842	1.401805
H	-1.042700	-2.081105	-0.336752
H	2.340780	1.037794	1.776417
H	4.015202	1.453492	1.918333

TS-4 (after **D-Ta_2H_2•CS_2** in Figure 8)

E = -2287.791822

Ta	3.068820	1.554501	4.862747
P	2.933743	3.066854	6.988077
C	2.235327	4.661736	6.399229
Si	2.970711	4.995888	4.662546
C	4.438482	6.189558	4.786992
C	6.408223	3.585081	1.676608
C	5.768496	3.803109	0.456454
C	1.648527	5.821163	3.605989
C	3.628908	3.757133	1.590522
C	4.377296	3.890500	0.421180
C	4.262580	3.537375	2.825107
C	5.664333	3.458379	2.848544
N	3.515626	3.407226	4.035762
N	4.824757	0.972852	5.898548
C	2.055404	2.572374	8.532524
C	1.709208	3.525498	9.497217
Si	5.663504	1.820513	7.232691
C	1.091660	3.131720	10.682520
C	5.725870	0.827726	8.844280
C	7.437081	2.291758	6.766952
C	4.663747	3.413966	7.533445
C	1.771811	1.222053	8.763679
C	1.161824	0.830133	9.955046
C	0.820941	1.782961	10.913790
C	5.607886	-0.168748	5.531077
C	7.241148	-1.228564	4.070722
C	6.465273	-0.124974	4.421020
C	5.557078	-1.355470	6.279529
C	7.185049	-2.400443	4.824792
H	7.791977	-3.259570	4.553212
H	0.945022	-0.220232	10.127917
C	6.336075	-2.456568	5.930109
Ta	0.842434	0.189823	3.377197
N	-0.333867	-1.458976	4.056097
C	-1.386255	-1.155789	4.969310
C	-2.670880	-0.847299	4.490948
C	-3.721445	-0.574234	5.366412
C	-3.516137	-0.609260	6.744820
C	-2.246057	-0.916968	7.235147
C	-1.194802	-1.184753	6.362045

C	0.899138	-3.975473	5.301048
Si	-0.057938	-3.197822	3.866225
C	-1.690973	-4.136004	3.654194
C	0.970019	-3.360540	2.260493
P	1.000081	-1.699098	1.451092
C	-0.601885	-1.477037	0.563561
C	-2.768014	0.684255	0.159906
C	2.072654	-1.923385	-1.202891
C	3.126156	-2.030356	-2.111040
C	0.002215	1.059752	-1.124651
Si	-0.914078	0.397993	0.396962
C	3.656889	-1.817856	0.618178
C	4.705671	-1.930009	-0.291903
C	4.443653	-2.034289	-1.658252
C	2.326663	-1.816656	0.169017
N	-0.366488	1.113109	1.944111
C	-0.928593	2.410525	2.155649
C	-1.883020	2.624836	3.165028
C	-2.479625	3.872058	3.331565
C	-0.588118	3.497380	1.331661
C	-1.201113	4.740502	1.490058
C	-2.151355	4.936490	2.490244
S	0.682143	1.511757	5.363527
S	2.967326	-0.889021	4.259417
C	2.708251	0.845988	2.644585
H	3.772409	1.065598	3.054496
H	2.941635	1.048868	1.587866
H	-0.269230	0.471115	-2.008867
H	2.039879	6.096234	2.622131
H	7.492414	3.517652	1.719582
H	7.464394	2.928937	5.877513
H	2.913435	-2.113294	-3.173593
H	6.273767	-3.365513	6.523315
H	4.873396	-1.411986	7.120998
H	7.894321	-1.169400	3.203389
H	6.506400	0.784499	3.827931
H	1.915821	4.578917	9.325608
H	0.821140	3.877937	11.424501
H	0.339694	1.476535	11.838431
H	2.014705	0.483039	8.005181
H	-0.199915	-1.395309	6.742665
H	-2.070277	-0.941814	8.307739
H	-4.333401	-0.397979	7.428749
H	-2.830252	-0.826952	3.416530
H	-4.704650	-0.336448	4.967205
H	5.730034	-1.931529	0.070254

H	3.866613	-1.724486	1.681819
H	5.263236	-2.118824	-2.366668
H	1.053415	-1.925674	-1.575685
H	6.347970	3.904128	-0.456733
H	3.866986	4.057550	-0.524010
H	2.544927	3.808687	1.564762
H	6.155914	3.295859	3.802938
H	0.167236	3.358561	0.564149
H	-0.924066	5.560635	0.832368
H	-2.626959	5.905110	2.615624
H	-3.214588	4.007510	4.121044
H	-2.152774	1.797514	3.814240
H	-0.269295	2.099716	-1.328166
H	1.087413	1.001454	-0.999683
H	-2.995510	1.748720	0.053748
H	-3.114858	0.170182	-0.743723
H	-3.337044	0.300993	1.012441
H	0.313777	-3.937931	6.225329
H	1.128731	-5.026358	5.089987
H	1.837886	-3.436876	5.463276
H	-2.332653	-4.010160	4.531323
H	-2.248894	-3.789149	2.778496
H	-1.494630	-5.206966	3.529911
H	8.039173	1.401383	6.564238
H	7.906721	2.839359	7.592121
H	6.322220	-0.081720	8.730415
H	6.189543	1.437753	9.628485
H	4.724481	0.545900	9.183192
H	0.783238	5.168668	3.464900
H	1.310430	6.739904	4.099898
H	4.834996	6.404113	3.789814
H	4.109180	7.137849	5.226861
H	5.260873	5.800084	5.394037
H	0.586614	-4.125405	1.577157
H	2.008902	-3.603012	2.507764
H	5.058560	4.201743	6.885527
H	4.697333	3.759550	8.570659
H	1.152665	4.525046	6.307405
H	2.441068	5.484937	7.091178
H	-1.360451	-1.857280	1.256821
H	-0.685659	-2.036958	-0.373120

Complex **3**

E = -2287.859944

C	-3.824391	0.722471	-5.458967
C	-2.438250	0.795950	-5.311729
C	3.694861	0.929760	-4.546019
C	-4.644484	1.065116	-4.384974
C	5.032834	1.145159	-4.211134
C	1.540747	-3.265209	-4.002587
C	-1.877428	1.204379	-4.104931
C	2.892931	0.111037	-3.756198
C	-4.084362	1.474873	-3.175453
C	4.284225	-3.712442	-2.742800
C	5.561026	0.529947	-3.077240
C	-0.587166	4.437489	-2.876665
C	-2.691520	1.548832	-3.012365
C	3.412679	-0.515899	-2.610907
C	4.760183	-0.293504	-2.286605
C	-3.520807	4.663497	-2.129667
C	-4.840074	-3.098535	-1.639956
C	-4.289926	-1.846774	-1.377950
C	1.754020	-4.038188	-0.970030
C	-4.940848	-4.055029	-0.628808
C	-6.118750	0.821148	0.389321
C	-3.810724	-1.526186	-0.097561
C	-1.458313	4.116148	0.122025
C	-4.470472	-3.745625	0.645551
C	4.271469	2.142739	0.716063
C	3.560228	-2.886820	1.069677
C	-3.900975	-2.499193	0.909431
C	4.604076	3.429190	1.131667
C	-0.133255	-0.244709	1.050863
C	-3.692564	2.543536	1.220516
C	3.383681	1.357136	1.466365
C	-0.513707	-4.073515	1.591968
C	5.823380	-0.922929	1.845870
C	0.850615	-3.838469	1.820729
C	4.062803	3.955885	2.305557
C	-4.603877	0.111609	2.931521
C	2.839313	1.894768	2.640999
C	-1.274690	-4.765452	2.530725
C	1.424533	-4.288523	3.015277
C	-1.262586	2.873992	2.807956
C	3.178234	3.182835	3.055116
C	-0.854933	4.139191	3.245183
C	3.450923	-1.296855	3.752636
C	-0.693896	-5.215591	3.716368
C	0.655627	-4.970973	3.958042

C	-1.259160	1.808267	3.718500
C	-0.467761	4.338741	4.569958
C	-0.875566	2.009720	5.043106
C	-0.479755	3.276473	5.472358
H	-4.259990	0.401727	-6.401128
H	-1.788319	0.530167	-6.141474
H	3.270754	1.408266	-5.425097
H	5.655860	1.787559	-4.827084
H	-5.725823	1.015031	-4.486086
H	2.008415	-2.707367	-4.820425
H	1.508498	-4.321861	-4.292075
H	1.844867	-0.041240	-3.996222
H	4.779826	-3.122701	-3.519898
H	-0.855143	4.215156	-3.914765
H	0.518178	-2.901959	-3.873091
H	-0.800085	1.248534	-3.977243
H	4.226827	-4.749124	-3.093941
H	-3.824637	4.448234	-3.158553
H	-0.517361	5.526658	-2.774772
H	6.601792	0.688517	-2.805549
H	-4.720253	1.746131	-2.339047
H	0.390783	3.997655	-2.668501
H	-5.196658	-3.323908	-2.641724
H	4.919397	-3.694505	-1.851714
H	-3.363593	5.745349	-2.048014
H	-4.216211	-1.102914	-2.165249
H	-4.352985	4.395159	-1.471751
H	5.167981	-0.775357	-1.403532
H	0.700437	-4.235547	-1.193135
H	2.258961	-4.989637	-0.773025
H	-6.103964	1.272499	-0.606616
H	-6.530384	-0.188369	0.295195
H	-5.379806	-5.027656	-0.832212
H	4.142989	-2.901338	0.143264
H	4.674166	1.736505	-0.206621
H	-0.380242	4.292814	0.198399
H	-6.797344	1.406380	1.020313
H	-2.000907	4.984776	0.510270
H	5.287796	4.024278	0.531502
H	-4.077704	3.068744	0.341129
H	6.189317	-0.930605	0.814845
H	-0.985679	-3.713388	0.680492
H	3.851575	-3.764142	1.656349
H	-4.548969	-4.478546	1.445080
H	-0.538399	-1.166723	1.481992
H	6.363573	-1.694168	2.406414

H	-3.510507	-2.274919	1.896911
H	0.159458	0.455693	1.838979
H	6.069601	0.049248	2.283630
H	-4.023350	3.085122	2.112435
H	-5.193819	-0.809347	2.936474
H	-0.837507	4.975851	2.553851
H	-2.325390	-4.950160	2.330204
H	4.324228	4.959968	2.628098
H	2.474975	-4.113801	3.222111
H	-5.141600	0.856591	3.529706
H	2.131804	1.304725	3.214921
H	-3.648781	-0.089052	3.423267
H	2.373330	-1.449623	3.862479
H	-1.544567	0.815644	3.384699
H	2.735535	3.582701	3.963231
H	3.970639	-2.116773	4.262233
H	3.720430	-0.366160	4.260470
H	-1.290943	-5.754096	4.447210
H	1.117654	-5.315958	4.879217
H	-0.157048	5.327913	4.895435
H	-0.880430	1.174155	5.737805
H	-0.179066	3.433510	6.504583
N	2.597766	-1.379264	-1.810887
N	-2.115261	1.995518	-1.781011
N	-3.281312	-0.222722	0.169011
N	3.061094	0.028643	1.034995
Si	2.535213	-3.056060	-2.411470
Si	-1.904546	3.761632	-1.704789
Si	-4.394734	0.769987	1.166541
Si	3.960345	-1.232360	1.931207
P	1.788972	-2.933394	0.514097
P	-1.829551	2.579527	1.071283
S	-0.682213	-1.351865	-1.757840
S	0.993656	1.747175	-1.031779
Ta	-1.475307	0.412927	-0.561323
Ta	1.574564	-0.327646	-0.319284

TS-1 (after **C-Ta_2N_2•CS_2** in Figure 7)

E= -2397.186564

Ta	0.674014	-1.963889	0.615540
Ta	-1.008744	1.627317	-0.044236
N	-0.462724	2.873979	1.485583
Si	-0.422488	4.666291	1.335563
C	-1.595021	5.041260	-0.129813

P	-2.840881	3.674105	-0.244213
C	-3.540112	3.749586	-1.947328
Si	-2.328738	2.770390	-3.057556
N	-0.943833	2.256136	-2.012742
N	0.212678	-3.614894	-0.563991
Si	-0.153995	-5.324968	-0.163666
C	0.850324	-5.643245	1.431167
P	1.905784	-4.145729	1.647552
C	3.289673	-4.321208	0.426844
Si	3.982503	-2.589209	0.018137
N	2.621766	-1.421058	0.178790
N	-1.222078	-1.498637	1.002829
C	-2.484753	-1.224232	1.067491
S	-3.662037	-2.270822	1.697138
S	-3.035653	0.394098	0.448477
N	-0.168005	-0.156946	0.278186
C	2.693466	-4.292840	3.312984
C	3.534018	-5.372643	3.616836
C	4.094222	-5.494499	4.885386
C	3.818433	-4.539416	5.865076
C	2.979818	-3.466506	5.572020
C	2.417195	-3.341188	4.300938
C	5.357211	-2.184576	1.248464
C	4.702451	-2.619324	-1.731309
C	3.146189	-0.090075	0.182983
C	3.461742	0.563128	-1.017495
C	4.081013	1.811934	-1.003487
C	4.390963	2.434915	0.204320
C	4.051108	1.804899	1.401745
C	3.429589	0.558661	1.394376
C	0.448431	-6.477837	-1.539783
C	-1.985410	-5.622292	0.154638
C	-0.302328	-3.250714	-1.851421
C	-1.657050	-2.920887	-2.032650
C	-2.153210	-2.649229	-3.306604
C	-1.315142	-2.699649	-4.421364
C	0.033276	-3.014815	-4.250323
C	0.535802	-3.281209	-2.978381
C	0.188943	1.966897	-2.849061
C	0.344571	0.721736	-3.474737
C	1.404617	0.499776	-4.352580
C	2.327148	1.509731	-4.624950
C	2.186098	2.746670	-3.996245
C	1.130368	2.972018	-3.116229
C	-3.236397	1.277097	-3.765230
C	-1.748672	3.895545	-4.461261

C	-4.188012	4.182618	0.913953
C	-4.582653	3.339214	1.958142
C	-5.611272	3.726829	2.818539
C	-6.251562	4.950905	2.639873
C	-5.865340	5.793642	1.596286
C	-4.838314	5.411956	0.737747
C	1.284762	5.352184	0.895002
C	-1.078621	5.462159	2.913671
C	-0.068579	2.345316	2.752104
C	-0.918821	1.478681	3.455933
C	-0.554578	0.980965	4.704937
C	0.656231	1.350434	5.289579
C	1.508364	2.211463	4.598817
C	1.156320	2.696970	3.341567
H	0.934999	-1.743413	2.337626
H	0.675403	1.158306	-0.394219
H	-2.623697	4.231982	-5.029369
H	4.890763	3.399766	0.213328
H	1.843517	3.333785	2.795004
H	-0.447885	5.213955	3.771631
H	-4.086152	1.602960	-4.376116
H	0.695077	-3.065979	-5.111443
H	-4.508314	3.238380	-1.924364
H	-2.095569	5.121158	3.127277
H	0.931362	0.973896	6.270758
H	-1.230565	0.306126	5.222819
H	-1.869734	1.196448	3.014258
H	2.459323	2.504907	5.036803
H	-4.547762	6.074240	-0.074532
H	-6.365304	6.747427	1.450986
H	-7.054121	5.248397	3.309139
H	-5.912511	3.063575	3.624294
H	-4.099290	2.375576	2.087080
H	-2.312935	-2.889163	-1.167618
H	-3.205152	-2.404912	-3.425789
H	-1.709590	-2.500081	-5.413790
H	1.581242	-3.540507	-2.840242
H	2.759107	-2.722198	6.332050
H	1.764278	-2.504236	4.069254
H	4.255610	-4.635254	6.855190
H	4.744152	-6.335672	5.110843
H	3.750299	-6.127497	2.864447
H	3.145888	1.335118	-5.317443
H	2.897269	3.544663	-4.195278
H	1.500225	-0.472465	-4.827239
H	-0.362839	-0.073632	-3.261118

H	1.015977	3.937365	-2.631528
H	3.163672	0.066824	2.324594
H	4.281118	2.279604	2.352068
H	4.318862	2.295173	-1.946401
H	3.209766	0.086959	-1.959496
H	5.804458	-1.208526	1.043488
H	4.978240	-2.178812	2.274583
H	6.144678	-2.943943	1.179581
H	3.928788	-2.817586	-2.478923
H	5.174916	-1.663438	-1.975254
H	5.465225	-3.402444	-1.809967
H	-2.566209	-5.547234	-0.769739
H	-2.135918	-6.627995	0.564557
H	-2.381579	-4.886281	0.863140
H	-0.039384	-6.240443	-2.489775
H	1.530904	-6.416039	-1.690550
H	0.201278	-7.514964	-1.286510
H	1.946120	5.393612	1.765307
H	1.763437	4.729721	0.132918
H	1.187448	6.371600	0.503352
H	-1.095465	6.552325	2.805511
H	-2.575839	0.673916	-4.394450
H	-3.612224	0.643284	-2.956060
H	-1.077275	3.374029	-5.148152
H	-1.227431	4.781645	-4.085767
H	1.441214	-6.563657	1.387137
H	0.178599	-5.695844	2.294573
H	-1.022965	5.020468	-1.063076
H	-2.067302	6.024098	-0.026594
H	-3.691729	4.776681	-2.293434
H	2.842969	-4.741421	-0.479025
H	4.077491	-4.996058	0.777540

Int-CC1 (after **C-Ta_2N_2•CS_2** in Figure 7)

E= -2397.321126

Ta	0.954753	-1.484249	0.250168
Ta	-1.117420	1.528799	-0.467975
N	-0.545698	2.799245	1.082214
Si	-0.671742	4.584566	1.115113
C	-1.871480	5.008070	-0.315391
P	-2.938132	3.515512	-0.529541
C	-3.700578	3.581680	-2.211916
Si	-2.470508	2.727877	-3.403291
N	-1.062087	2.243080	-2.394553

N	0.149265	-3.073771	-0.825258
Si	-0.561979	-4.625269	-0.280183
C	0.361701	-5.004559	1.347577
P	1.741871	-3.778828	1.463016
C	3.073939	-4.384989	0.323334
Si	4.099878	-2.869354	-0.197208
N	2.928465	-1.516858	-0.367604
N	-0.632431	-1.746784	1.631779
C	-1.384694	-1.956479	2.530643
S	-2.419173	-2.257884	3.730331
S	-2.794844	0.110746	-0.172954
N	0.580589	0.401216	-0.384780
C	2.432159	-3.953831	3.168962
C	3.074077	-5.130252	3.578777
C	3.545956	-5.258086	4.882469
C	3.375692	-4.213216	5.791756
C	2.731710	-3.043947	5.393135
C	2.260920	-2.910834	4.086261
C	5.385862	-2.494686	1.134905
C	4.999311	-3.231298	-1.822892
C	3.630713	-0.282433	-0.566334
C	4.013272	0.112650	-1.857489
C	4.753124	1.277191	-2.053963
C	5.114121	2.078421	-0.971586
C	4.716598	1.707515	0.312987
C	3.983263	0.539792	0.517360
C	-0.211389	-5.980550	-1.555393
C	-2.421470	-4.536548	0.020914
C	-0.066156	-2.794795	-2.210089
C	-1.338083	-2.449139	-2.699141
C	-1.555431	-2.301017	-4.067919
C	-0.508521	-2.468130	-4.975510
C	0.766234	-2.773701	-4.497885
C	0.984726	-2.935203	-3.131782
C	0.160491	2.199158	-3.140452
C	0.461606	1.117694	-3.982309
C	1.595077	1.147658	-4.791632
C	2.456239	2.244839	-4.767244
C	2.184323	3.307589	-3.907300
C	1.047513	3.285392	-3.101522
C	-3.314697	1.242743	-4.199409
C	-1.924077	3.956130	-4.731657
C	-4.315019	3.756574	0.680369
C	-4.612839	2.750371	1.605438
C	-5.658148	2.922101	2.514270
C	-6.412105	4.093575	2.501911

C	-6.123238	5.098333	1.577069
C	-5.078816	4.931807	0.671273
C	0.970287	5.471142	0.785352
C	-1.369116	5.177620	2.765257
C	0.046298	2.258418	2.265695
C	-0.723940	1.515806	3.172526
C	-0.166383	1.034549	4.355127
C	1.169189	1.292977	4.663117
C	1.948939	2.017335	3.762060
C	1.398615	2.486368	2.570853
H	1.634773	-1.121341	1.833533
H	1.432577	0.967169	-0.469641
H	-2.798247	4.284676	-5.305137
H	5.693382	2.984180	-1.127347
H	2.016466	3.025187	1.859280
H	-0.718431	4.873918	3.590587
H	-4.209063	1.557284	-4.749265
H	1.592362	-2.903833	-5.192639
H	-4.625049	2.997055	-2.160509
H	-2.364384	4.762234	2.946111
H	1.597521	0.934208	5.594975
H	-0.785160	0.454527	5.033966
H	-1.766471	1.319214	2.941035
H	2.994088	2.218882	3.984711
H	-4.863188	5.720385	-0.046062
H	-6.711786	6.011759	1.561655
H	-7.226410	4.225049	3.209252
H	-5.880957	2.134717	3.228810
H	-4.034252	1.830815	1.601153
H	-2.147292	-2.293230	-1.992770
H	-2.551098	-2.052693	-4.425078
H	-0.684226	-2.360188	-6.042252
H	1.970349	-3.189310	-2.756559
H	2.591581	-2.230135	6.098970
H	1.762841	-1.997479	3.773521
H	3.742297	-4.313957	6.809687
H	4.043527	-6.173864	5.190215
H	3.203825	-5.955460	2.882538
H	3.332662	2.269126	-5.409038
H	2.852226	4.164151	-3.868729
H	1.800948	0.304534	-5.445545
H	-0.199282	0.256560	-3.995862
H	0.817761	4.124489	-2.450658
H	3.669538	0.248066	1.514622
H	4.985676	2.325208	1.166173
H	5.038157	1.562542	-3.062304

H	3.713179	-0.500486	-2.701044
H	5.976172	-1.609844	0.881097
H	4.909713	-2.324272	2.104836
H	6.071186	-3.343958	1.236227
H	4.307852	-3.500605	-2.626958
H	5.582340	-2.364709	-2.148441
H	5.693497	-4.067168	-1.679105
H	-2.966640	-4.405198	-0.918684
H	-2.768927	-5.468428	0.481799
H	-2.673641	-3.708423	0.688231
H	-0.676384	-5.740413	-2.516207
H	0.860182	-6.123225	-1.727022
H	-0.628669	-6.933015	-1.209908
H	1.645376	5.394982	1.642647
H	1.480839	5.059380	-0.090902
H	0.782876	6.536096	0.603354
H	-1.443174	6.270763	2.775855
H	-2.642366	0.739268	-4.900309
H	-3.611868	0.526802	-3.426970
H	-1.211776	3.504313	-5.427422
H	-1.452450	4.841090	-4.293184
H	0.727287	-6.035165	1.398669
H	-0.296634	-4.822466	2.203760
H	-1.300426	5.127953	-1.242387
H	-2.439633	5.924979	-0.130130
H	-3.947349	4.602645	-2.519362
H	2.569363	-4.788868	-0.559839
H	3.692044	-5.173104	0.764309

TS-2 (after **C-Ta_2N_2•CS_2** in Figure 7)

E = -2397.283038

C	1.398615	2.486368	2.570853
C	0.046298	2.258418	2.265695
C	-0.723940	1.515806	3.172526
C	-0.166383	1.034549	4.355127
C	1.169189	1.292977	4.663117
C	1.948939	2.017335	3.762060
N	-0.545698	2.799245	1.082214
Si	-0.671742	4.584566	1.115113
C	-1.369116	5.177620	2.765257
Ta	-1.117420	1.528799	-0.467975
N	0.580589	0.401216	-0.384780
Ta	0.954753	-1.484249	0.250167
N	-0.632431	-1.746784	1.631779

C	-1.384693	-1.956479	2.530643
S	-2.419172	-2.257885	3.730331
N	0.149265	-3.073770	-0.825259
C	-0.066156	-2.794794	-2.210090
C	-1.338083	-2.449138	-2.699142
C	-1.555432	-2.301016	-4.067919
C	-0.508522	-2.468129	-4.975511
C	0.766233	-2.773700	-4.497886
C	0.984726	-2.935202	-3.131783
P	1.741872	-3.778828	1.463014
C	2.432160	-3.953832	3.168960
C	3.074078	-5.130253	3.578775
C	3.545958	-5.258087	4.882466
C	3.375694	-4.213217	5.791754
C	2.731712	-3.043948	5.393133
C	2.260921	-2.910835	4.086259
N	2.928465	-1.516857	-0.367605
C	3.630713	-0.282432	-0.566335
C	4.013272	0.112651	-1.857490
C	4.753124	1.277192	-2.053964
C	5.114121	2.078422	-0.971586
C	4.716598	1.707515	0.312987
C	3.983263	0.539792	0.517359
P	-2.938132	3.515513	-0.529540
C	-4.315019	3.756575	0.680370
C	-4.612839	2.750372	1.605439
C	-5.658148	2.922102	2.514271
C	-6.412105	4.093576	2.501912
C	-6.123238	5.098334	1.577070
C	-5.078816	4.931808	0.671274
N	-1.062087	2.243081	-2.394553
C	0.160491	2.199159	-3.140452
C	0.461605	1.117695	-3.982309
C	1.595076	1.147659	-4.791632
C	2.456238	2.244840	-4.767244
C	2.184323	3.307590	-3.907300
C	1.047513	3.285392	-3.101522
S	-2.794845	0.110746	-0.172954
C	-1.871480	5.008070	-0.315391
C	0.970287	5.471142	0.785352
C	-3.700578	3.581681	-2.211915
Si	-2.470509	2.727878	-3.403291
C	-1.924078	3.956131	-4.731656
C	-3.314698	1.242744	-4.199409
Si	-0.561979	-4.625269	-0.280184
C	-2.421470	-4.536548	0.020913

C	0.361702	-5.004559	1.347575
C	-0.211389	-5.980549	-1.555395
C	3.073939	-4.384989	0.323332
Si	4.099878	-2.869353	-0.197210
C	4.999311	-3.231297	-1.822894
C	5.385862	-2.494686	1.134903
H	1.668027	-0.343858	1.386796
H	1.322141	0.543489	0.673453
H	-2.798248	4.284677	-5.305136
H	5.693382	2.984181	-1.127347
H	2.016466	3.025187	1.859280
H	-0.718431	4.873918	3.590587
H	-4.209064	1.557285	-4.749265
H	1.592361	-2.903832	-5.192640
H	-4.625049	2.997056	-2.160508
H	-2.364384	4.762234	2.946112
H	1.597521	0.934208	5.594975
H	-0.785160	0.454527	5.033966
H	-1.766471	1.319214	2.941035
H	2.994088	2.218882	3.984711
H	-4.863188	5.720386	-0.046061
H	-6.711786	6.011760	1.561656
H	-7.226410	4.225050	3.209253
H	-5.880957	2.134718	3.228811
H	-4.034252	1.830815	1.601154
H	-2.147292	-2.293229	-1.992770
H	-2.551099	-2.052692	-4.425078
H	-0.684227	-2.360187	-6.042253
H	1.970349	-3.189309	-2.756561
H	2.591583	-2.230136	6.098969
H	1.762842	-1.997479	3.773520
H	3.742299	-4.313958	6.809685
H	4.043529	-6.173865	5.190212
H	3.203826	-5.955460	2.882535
H	3.332661	2.269127	-5.409038
H	2.852226	4.164151	-3.868729
H	1.800947	0.304535	-5.445545
H	-0.199283	0.256561	-3.995862
H	0.817761	4.124489	-2.450658
H	3.669538	0.248066	1.514621
H	4.985676	2.325208	1.166173
H	5.038157	1.562543	-3.062304
H	3.713179	-0.500485	-2.701045
H	5.976172	-1.609843	0.881095
H	4.909713	-2.324272	2.104834
H	6.071187	-3.343957	1.236225

H	4.307852	-3.500604	-2.626960
H	5.582340	-2.364708	-2.148443
H	5.693497	-4.067167	-1.679107
H	-2.966640	-4.405198	-0.918685
H	-2.768926	-5.468428	0.481798
H	-2.673641	-3.708423	0.688230
H	-0.676384	-5.740412	-2.516209
H	0.860182	-6.123224	-1.727024
H	-0.628669	-6.933014	-1.209910
H	1.645376	5.394982	1.642647
H	1.480839	5.059380	-0.090902
H	0.782876	6.536096	0.603354
H	-1.443174	6.270763	2.775855
H	-2.642367	0.739269	-4.900309
H	-3.611869	0.526803	-3.426970
H	-1.211777	3.504314	-5.427422
H	-1.452450	4.841091	-4.293183
H	0.727288	-6.035165	1.398667
H	-0.296633	-4.822466	2.203758
H	-1.300426	5.127953	-1.242387
H	-2.439633	5.924979	-0.130129
H	-3.947349	4.602646	-2.519361
H	2.569363	-4.788867	-0.559841
H	3.692045	-5.173104	0.764307

Int-C1C2 (after **C-Ta_2N_2•CS_2** in Figure 7)

E = -2397.309333

C	1.398615	2.486368	2.570853
C	0.046298	2.258418	2.265695
C	-0.723940	1.515806	3.172526
C	-0.166383	1.034549	4.355127
C	1.169189	1.292977	4.663117
C	1.948939	2.017335	3.762060
N	-0.545698	2.799245	1.082214
Si	-0.671742	4.584566	1.115113
C	-1.369116	5.177620	2.765257
Ta	-1.117420	1.528799	-0.467975
N	0.580589	0.401216	-0.384780
Ta	0.954753	-1.484249	0.250167
N	-0.632431	-1.746784	1.631779
C	-1.384693	-1.956479	2.530643
S	-2.419172	-2.257885	3.730331
N	0.149265	-3.073770	-0.825259
C	-0.066156	-2.794794	-2.210090

C	-1.338083	-2.449138	-2.699142
C	-1.555432	-2.301016	-4.067919
C	-0.508522	-2.468129	-4.975511
C	0.766233	-2.773700	-4.497886
C	0.984726	-2.935202	-3.131783
P	1.741872	-3.778828	1.463014
C	2.432160	-3.953832	3.168960
C	3.074078	-5.130253	3.578775
C	3.545958	-5.258087	4.882466
C	3.375694	-4.213217	5.791754
C	2.731712	-3.043948	5.393133
C	2.260921	-2.910835	4.086259
N	2.928465	-1.516857	-0.367605
C	3.630713	-0.282432	-0.566335
C	4.013272	0.112651	-1.857490
C	4.753124	1.277192	-2.053964
C	5.114121	2.078422	-0.971586
C	4.716598	1.707515	0.312987
C	3.983263	0.539792	0.517359
P	-2.938132	3.515513	-0.529540
C	-4.315019	3.756575	0.680370
C	-4.612839	2.750372	1.605439
C	-5.658148	2.922102	2.514271
C	-6.412105	4.093576	2.501912
C	-6.123238	5.098334	1.577070
C	-5.078816	4.931808	0.671274
N	-1.062087	2.243081	-2.394553
C	0.160491	2.199159	-3.140452
C	0.461605	1.117695	-3.982309
C	1.595076	1.147659	-4.791632
C	2.456238	2.244840	-4.767244
C	2.184323	3.307590	-3.907300
C	1.047513	3.285392	-3.101522
S	-2.794845	0.110746	-0.172954
C	-1.871480	5.008070	-0.315391
C	0.970287	5.471142	0.785352
C	-3.700578	3.581681	-2.211915
Si	-2.470509	2.727878	-3.403291
C	-1.924078	3.956131	-4.731656
C	-3.314698	1.242744	-4.199409
Si	-0.561979	-4.625269	-0.280184
C	-2.421470	-4.536548	0.020913
C	0.361702	-5.004559	1.347575
C	-0.211389	-5.980549	-1.555395
C	3.073939	-4.384989	0.323332
Si	4.099878	-2.869353	-0.197210

C	4.999311	-3.231297	-1.822894
C	5.385862	-2.494686	1.134903
H	1.668027	-0.343858	1.386796
H	-2.798248	4.284677	-5.305136
H	5.693382	2.984181	-1.127347
H	2.016466	3.025187	1.859280
H	-0.718431	4.873918	3.590587
H	-4.209064	1.557285	-4.749265
H	1.592361	-2.903832	-5.192640
H	-4.625049	2.997056	-2.160508
H	-2.364384	4.762234	2.946112
H	1.597521	0.934208	5.594975
H	-0.785160	0.454527	5.033966
H	-1.766471	1.319214	2.941035
H	2.994088	2.218882	3.984711
H	-4.863188	5.720386	-0.046061
H	-6.711786	6.011760	1.561656
H	-7.226410	4.225050	3.209253
H	-5.880957	2.134718	3.228811
H	-4.034252	1.830815	1.601154
H	-2.147292	-2.293229	-1.992770
H	-2.551099	-2.052692	-4.425078
H	-0.684227	-2.360187	-6.042253
H	1.970349	-3.189309	-2.756561
H	2.591583	-2.230136	6.098969
H	1.762842	-1.997479	3.773520
H	3.742299	-4.313958	6.809685
H	4.043529	-6.173865	5.190212
H	3.203826	-5.955460	2.882535
H	3.332661	2.269127	-5.409038
H	2.852226	4.164151	-3.868729
H	1.800947	0.304535	-5.445545
H	-0.199283	0.256561	-3.995862
H	0.817761	4.124489	-2.450658
H	3.669538	0.248066	1.514621
H	4.985676	2.325208	1.166173
H	5.038157	1.562543	-3.062304
H	3.713179	-0.500485	-2.701045
H	5.976172	-1.609843	0.881095
H	4.909713	-2.324272	2.104834
H	6.071187	-3.343957	1.236225
H	4.307852	-3.500604	-2.626960
H	5.582340	-2.364708	-2.148443
H	5.693497	-4.067167	-1.679107
H	-2.966640	-4.405198	-0.918685
H	-2.768926	-5.468428	0.481798

H	-2.673641	-3.708423	0.688230
H	-0.676384	-5.740412	-2.516209
H	0.860182	-6.123224	-1.727024
H	-0.628669	-6.933014	-1.209910
H	1.645376	5.394982	1.642647
H	1.480839	5.059380	-0.090902
H	0.782876	6.536096	0.603354
H	-1.443174	6.270763	2.775855
H	-2.642367	0.739269	-4.900309
H	-3.611869	0.526803	-3.426970
H	-1.211777	3.504314	-5.427422
H	-1.452450	4.841091	-4.293183
H	0.727288	-6.035165	1.398667
H	-0.296633	-4.822466	2.203758
H	-1.300426	5.127953	-1.242387
H	-2.439633	5.924979	-0.130129
H	-3.947349	4.602646	-2.519361
H	2.569363	-4.788867	-0.559841
H	3.692045	-5.173104	0.764307
H	1.901725	-1.120407	1.777126

Complex **2**

E = -2396.188463

C	1.398615	2.486368	2.570853
C	0.048224	2.258743	2.266130
C	-0.726982	1.516365	3.169949
C	-0.151473	0.982839	4.320947
C	1.199216	1.190372	4.601251
C	1.968203	1.957119	3.727388
N	-0.492428	2.709727	1.018211
Si	-0.557648	1.405289	-0.218891
C	-2.183083	0.453296	-0.157646
Ta	-1.331399	4.580885	0.877293
S	-3.400676	4.924231	1.592746
N	-0.081242	6.208177	0.512583
Si	1.474821	6.195320	-0.372202
C	2.995162	6.235611	0.758266
C	-0.425477	7.499526	1.020027
C	0.322057	8.099255	2.047335
C	0.024435	9.388083	2.485702
C	-1.037414	10.097066	1.924963
C	-1.805173	9.498631	0.926055
C	-1.500318	8.216446	0.474295
C	1.570731	7.640472	-1.581893

C	1.479412	4.527530	-1.312161
P	-0.297874	4.092503	-1.563839
C	-0.409683	2.281105	-1.913730
N	-1.642728	5.054757	2.836915
Ta	-3.244052	5.775078	3.844405
N	-2.388626	5.617969	5.721053
Si	-3.132239	6.060293	7.296451
C	-2.371156	7.644258	7.989605
N	-4.271102	6.766148	2.276006
C	-4.856500	7.474421	1.518717
S	-5.670064	8.413073	0.490471
N	-4.922706	4.560644	4.042398
Si	-6.671026	4.945888	3.971076
C	-7.634245	3.794983	5.125843
P	-5.092311	7.155211	5.270876
C	-4.978359	6.350436	6.938227
C	-4.638671	3.160351	4.020160
C	-4.818178	2.394254	2.855119
C	-4.654528	1.010379	2.884090
C	-4.284658	0.363443	4.064065
C	-4.066755	1.118673	5.216734
C	-4.241769	2.500324	5.195072
C	-5.111208	8.974331	5.599235
C	-5.939759	9.529046	6.584003
C	-5.972271	10.906641	6.783499
C	-5.181049	11.744519	5.996431
C	-4.360816	11.200312	5.010602
C	-4.322798	9.819812	4.810455
C	-6.769285	6.743282	4.608543
C	-0.961078	5.571068	5.848953
C	-0.329012	4.395627	6.282950
C	1.051053	4.360039	6.473462
C	1.830386	5.488446	6.222128
C	1.214438	6.653881	5.765955
C	-0.166458	6.698660	5.580901
C	-0.766553	4.958985	-3.128242
C	-1.882320	5.802499	-3.149292
C	-2.247458	6.450960	-4.330101
C	-1.505725	6.258290	-5.493572
C	-0.395049	5.412995	-5.479817
C	-0.025854	4.767243	-4.302653
C	0.898920	0.222787	0.008806
C	-7.399678	4.819672	2.236321
C	-2.936662	4.682334	8.579342
H	0.878737	-0.535836	-0.781813
H	2.905642	5.458754	6.374271

H	1.131493	7.540139	2.506252
H	1.497029	8.593908	-1.050551
H	-2.226499	-0.286729	-0.964893
H	-3.775217	0.629038	6.142675
H	-1.330923	2.128416	-2.485638
H	0.761050	7.596391	-2.315573
H	-1.263797	11.104726	2.262476
H	-2.649300	10.026028	0.490813
H	-2.095777	7.757960	-0.309495
H	0.626253	9.838501	3.271495
H	0.840435	4.109624	-4.303368
H	0.183528	5.256986	-6.386395
H	-1.792195	6.762838	-6.412308
H	-3.115442	7.104228	-4.335632
H	-2.468877	5.937129	-2.244752
H	-5.080356	2.898779	1.930562
H	-4.817417	0.435893	1.976338
H	-4.166542	-0.716419	4.084313
H	-4.089926	3.090200	6.092739
H	-3.747513	11.848898	4.391470
H	-3.679880	9.394502	4.045030
H	-5.208047	12.819749	6.150978
H	-6.617146	11.326994	7.550553
H	-6.568568	8.887577	7.196921
H	1.646641	0.762231	5.494063
H	3.019094	2.137177	3.938305
H	-0.768195	0.399916	4.999694
H	-1.781269	1.362304	2.961977
H	2.001927	3.060980	1.873480
H	-0.650202	7.602315	5.223886
H	1.809709	7.539991	5.560200
H	1.517955	3.439190	6.810296
H	-0.934065	3.511873	6.457492
H	-1.301448	7.521724	8.180764
H	-2.503518	8.480430	7.296913
H	-2.858718	7.905165	8.935865
H	-3.399370	3.745738	8.253994
H	-1.880139	4.488435	8.786812
H	-3.412162	4.986484	9.518831
H	-7.427088	3.780265	1.895455
H	-8.428071	5.199079	2.235900
H	-6.817160	5.405367	1.520551
H	-7.527829	2.751954	4.813087
H	-7.297170	3.870401	6.164481
H	-8.700362	4.046426	5.096815
H	3.134340	7.223578	1.206652

H	2.915773	5.500687	1.565494
H	3.894033	6.006235	0.173638
H	2.525658	7.624002	-2.118924
H	-2.292781	-0.073506	0.794837
H	-3.022967	1.145566	-0.271230
H	0.852220	-0.290490	0.973155
H	1.857456	0.747994	-0.047847
H	-7.550602	6.884927	5.362130
H	-6.957644	7.427498	3.774288
H	1.909997	3.751873	-0.669705
H	2.051925	4.571594	-2.243896
H	0.435622	1.916548	-2.505629
H	-5.476962	5.380098	6.851344
H	-5.469080	6.926553	7.728747

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