Supporting Information

Catalytic hydrogenation of azobenzene in the presence of a cuboidal Mo_3S_4 cluster *via* an uncommon sulfur-based H_2 activation mechanism

Eva Guillamón,[a,1] Mónica Oliva,[a,1] Juan Andrés,[a] Rosa Llusar,[*,a] Elena Pedrajas,[a] Vicent S. Safont,[a] Andres G. Algarra[*, b] and Manuel G. Basallote[*, b]

[a] Departament de Química Física i Analítica, Universitat Jaume I, Av. Sos Baynat s/n, 12071 Castelló, Spain. [b] Departamento de Ciencia de los Materiales e Ingeniería Metalúrgica y Química Inorgánica, Facultad de Ciencias, Universidad de Cádiz, Apartado 40, Puerto Real, 11510 Cádiz, Spain.

*E-mails: rosa.llusar@uji.es, andres.algarra@uca.es, manuel.basallote@uca.es

Table of contents

Materials and Methods

The $[Mo_3S_4Cl_3(dmen)_3]Cl$ (**1**Cl) cluster catalyst was prepared according to the published procedure replacing HBF_4 by HCl.[1] Complexes $[Mo_3S_4Cl_3(edpp)_3]Cl$,[2] $[Mo_3S_4Cl_3(dnbpy)_3](PF_6)$,[3] $[Mo_3S_4Cl_3(dmpe)_3](PF_6)$,[4] and $[Mo_3S_4H_3(dmpe)_3](BPh_4)$[5] were synthesized by literature methods. All other reagents were obtained from commercial sources and used as received.

$[Mo_3S_4Br_3(dmen)_3]Br$ was obtained following the procedure employed for the synthesis of its chlorine analogue but using the $[Mo_3S_4Br_4(PPh_3)_3(H_2O)_2]$ derivative as starting material.[3] In this case, $[Mo_3S_4Br_4(PPh_3)_3(H_2O)_2]$ (50.0 mg, 0.032 mmol) was reacted with 3.5 equivalents of dmen ligand (12.7 μL, 0.112 mmol) in CH_3CN and after stirring, the reaction mixture was acidified with HBr. The desired product was precipitated with ether. (Yield: 90%) ^{1}H-NMR (CD_3CN): d = 2.85 (d, 9H, CH_3), 3.13 (m, 6H, CH_2), 3.65 (m, 3H, CH_2), 3.78 (d, 9H, CH_3), 3.88 ppm (m, 3H, CH_2). ESI(+)-MS (CH_3CN, 20V): m/z = 920 $[M^+]$

$[Mo_3S_4(tacn)_3]Cl_4$ (tacn = 1,4,7-triazacyclononane) was obtained by adapting the procedure employed for the synthesis of the $[Mo_3S_4Cl_3(dmen)_3]Cl$ cluster salt. A method for the preparation of this compound in low quantities has been already described but the procedure was tedious and difficult to scale up.[6] In this case, $[Mo_3S_4Cl_4(PPh_3)_3(H_2O)_2]$ (40.0 mg, 0.029 mmol) was dissolved in 8 mL of DMF an reacted with an excess (56.0 mg, 0.435 mmol) of the tacn ligand under reflux conditions for four hours. The reaction mixture was allowed to cool down and the solid containing the desired product separated from the solution by filtration. The solid was washed with DMF and Et_2O, yielding 13 mg (47 %) of the $[Mo_3S_4(tacn)_3]Cl_4$ cluster. ^{1}H-NMR (D_2O): 3.20-3.35, 4.01-4.11 (m, 18H, - NC*H*H-H*H*CN-), 3.36-3.5, 3.51-3.59, 4.50-4.61 (m, 18H, - NCH*H*-*H*HCN-); $^{13}C\{^1H\}$-NMR (D_2O): 52.49 (s, CH_2), 52.90 (s, CH_2), 54.19 (s, CH_2); ESI(+)-MS (CH_3OH, 20V): m/z = 402 $[M^{2+}]$, 268 $[M^{3+}]$

Mass spectra were registered using a triple quadrupole mass spectrometer with an orthogonal Z-spray electrospray source (Waters, Manchester). The temperature of the source block was set to 100 °C, and the desolvation temperature was set to 120 °C. A capillary voltage of 3.3 kV was used in the positive scan mode, and the cone voltage was set to *U*c = 20 V. Sample solutions in CH_3CN or CH_3OH were injected with a syringe pump directly connected to the ESI source at a flow rate of 10 $\mu L min^{-1}$. The observed

isotopic pattern of each compound perfectly matched the theoretical isotope pattern calculated from their elemental composition by using the MassLynx 4.1 program. Gas chromatography analyses were performed on an Agilent 7820A GC System equipped with a FID and a capillary column Agilent (HP-5, 30m x 0.32mm x 0.25 μm).The GC yields were determined using *n*-hexadecane as an internal standard. ^{1}H NMR spectra were recorded on a Bruker Avance III HD 400 MHz spectrometer using D_2O or CD_3CN as solvent. High pressure ^{1}H NMR spectra were recorded on a Bruker Avance 500 Ultrashield spectrometer using a sapphire NMR tube fitted with a titanium head, shown in Figure S1. To avoid the possibility of H/D exchange with deuterated methanol, the high pressure spectra were recorded in CD_3CN. Sample solutions in CD_3CN (0,2 mL) were introduced and the tube pressurized with H_2 at 20 bars and spectra were registered at temperatures ranging between 70 and -25 ^{0}C. These high pressure NMR experiments were performed at the ICIQ of Tarragona (Spain) by Dr. Marta Giménez Pedrós (tube pressurization) and by the NMR section of the Institute (spectra recording).

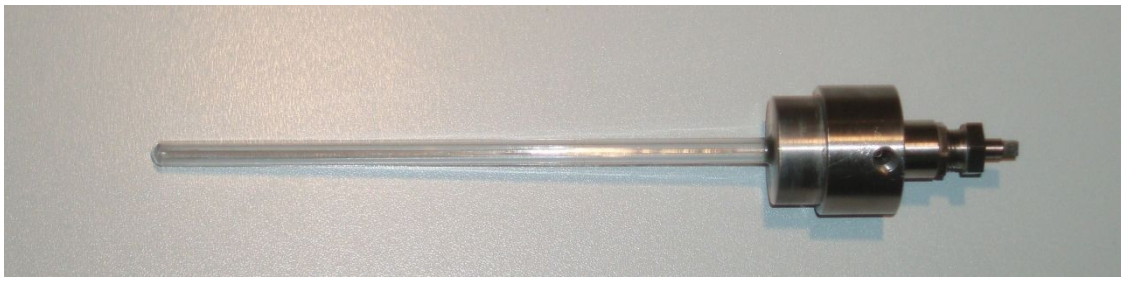

Figure S1. High pressure NMR tube

General procedure for the catalytic hydrogenation of azobenzene

A 4 mL glass vial containing a stirring bar was sequentially charged with the trinuclear catalyst (4.2 mg, 0.005 mmol) of $[Mo_3S_4Cl_3(dmen)_3]Cl$, azobenzene (18.4 mg, 0.1 mmol), *n*-hexadecane (15 µL; added as an internal standard) and 2 mL of dry CH_3OH or CD_3OD. Afterwards, the reaction vial was capped with a septum equipped with a needle and set in the alloy plate, which was then placed into a 300 mL autoclave. Once sealed, the autoclave was purged three times with 20 bar of hydrogen, then pressurized to 10 bar and placed into an aluminum block, which was preheated at 60 °C. The reaction was monitored at different times from 0,5 up to 8 hours. After each time, the autoclave was cooled to room temperature and the hydrogen was released. Ethyl acetate (2 mL) was then added, and a sample was taken to be analyzed using GC.

For the reaction done in the presence of copper (I), CuCl (1 mg, 0,01 mmol) was added to the glass vial containing $[Mo_3S_4Cl_3(dmen)_3]Cl$ (4.2 mg, 0.005 mmol), azobenzene (18.4 mg, 0.1 mmol), *n*-hexadecane (15 µL; added as an internal standard) and 2 mL of dry CH_3OH. Addition of CuCl causes a color change from green to red due to the formation of the heterobimetallic $[Mo_3CuS_4Cl_4(dmen)_3]^+$ cluster as confirmed by single crystal X-ray diffraction experiments. (*Vide infra*)

For the reaction done in the presence of chloride, (n-Bu_4N)Cl (4.2 mg/22.5 mg, 0.015 mmol/ 0.081 mmol) was added to a glass vial containing $[Mo_3S_4Cl_3(dmen)_3]Cl$ (4.2 mg, 0.005 mmol), azobenzene (18.4 mg, 0.1 mmol), *n*-hexadecane (15 µL; added as an internal standard) and 2 mL of dry CH_3OH. Cluster integrity after the catalytic protocol was shown by electrospray ionization mass spectrometry ESI-MS (m/z=787).

For the reaction done in the presence of a base, pyridine (1 µL/5 µL, 0.012 mmol/0.060 mmol) or Et_3N (0.7 µL/1.4 µL/2.1 µL, 0.005 mmol/0.010 mmol/0.015 mmol) was added to a glass vial containing $[Mo_3S_4Cl_3(dmen)_3]Cl$ (4.2 mg, 0.005 mmol), azobenzene (18.4 mg, 0.1 mmol), *n*-hexadecane (15 µL; added as an internal standard) and 2 mL of dry CH_3OH. Cluster integrity after the catalytic protocol was shown by electrospray ionization mass spectrometry ESI-MS (m/z=787) (Figure S3) for the reaction done in the presence of pyridine. In the case of Et_3N, partial substitution of the outer chlorine ligands by methoxo and hydroxo groups is observed (Figure S4).

The general catalytic protocol was adapted (Table 1, entries 8-13) when the $[Mo_3S_4Cl_3(dmen)_3]Cl$ cluster catalyst was replaced by $Mo_3S_4Br_3(dmen)_3]Br$ (5.1 mg,

0.005 mmol), $[Mo_3S_4Cl_3(dnbpy)_3]PF)_6$ (9.8 mg, 0.005 mmol), $[Mo_3S_4(tacn)_3]Cl_4$ (4.9 mg, 0.005 mmol), $[Mo_3S_4Cl_3(edpp)_3]Cl$ (6.2 mg, 0.005 mmol), $[Mo_3S_4Cl_3(dmpe)_3]BPh_4$ (6.6 mg, 0.005 mmol) and $[Mo_3S_4H_3(dmpe)_3]BPh_4$ (6.0 mg, 0.005 mmol). In the case of $[Mo_3S_4(tacn)_3]Cl_4$ (Table 1, entry 10), $HBF_4 \cdot Et_2O$ (1μL, 0.007 mmol) was added to avoid ligand deprotonation in solution. For the $[Mo_3S_4H_3(dmpe)_3]BPh_4$ cluster hydride (Table 1, entry 13) THF was used as solvent due to its low solubility in MeOH. In all cases, cluster integrity after the catalytic protocol was shown by electrospray ionization mass spectrometry ESI-MS.

Cluster monitoring after the catalytic reaction

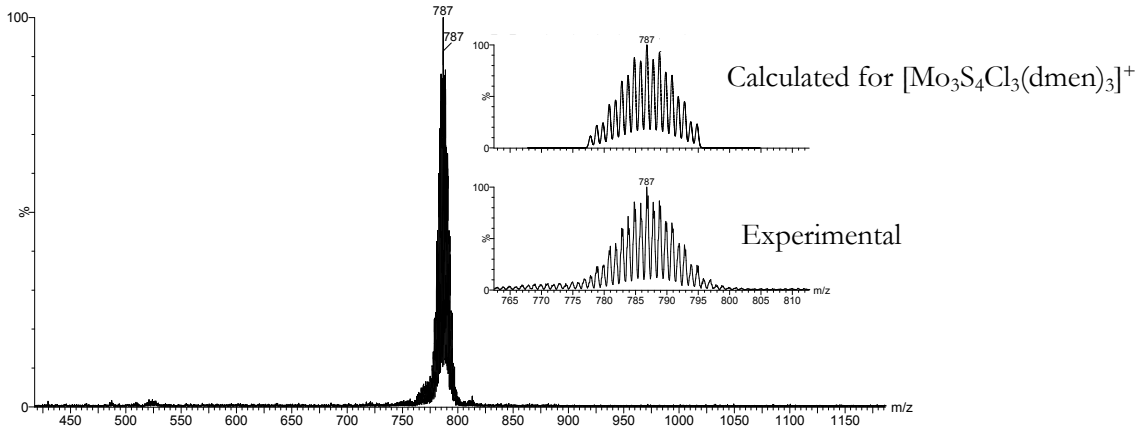

Figure S2. ESI mass spectrum of the catalyst in CH_3CN at 20 V after azobenzene hydrogenation in CH_3OH for experiment done with and without (*n*-Bu_4N)Cl.

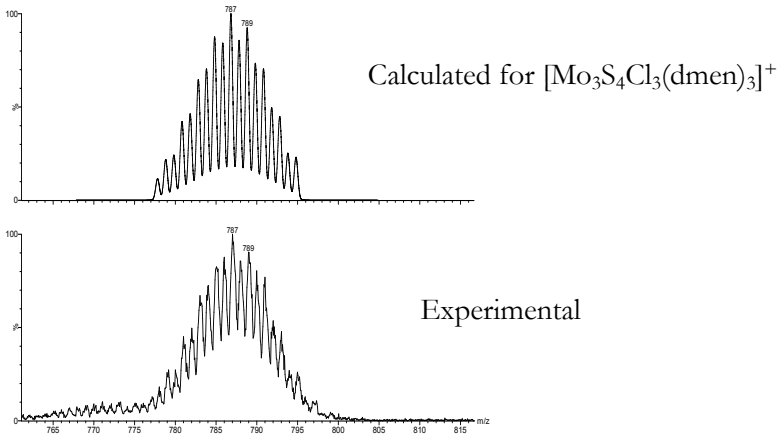

Figure S3. ESI mass spectrum of the catalyst in CH_3CN at 20 V after azobenzene hydrogenation in CH_3OH in the presence of 12 equivalents of pyridine.

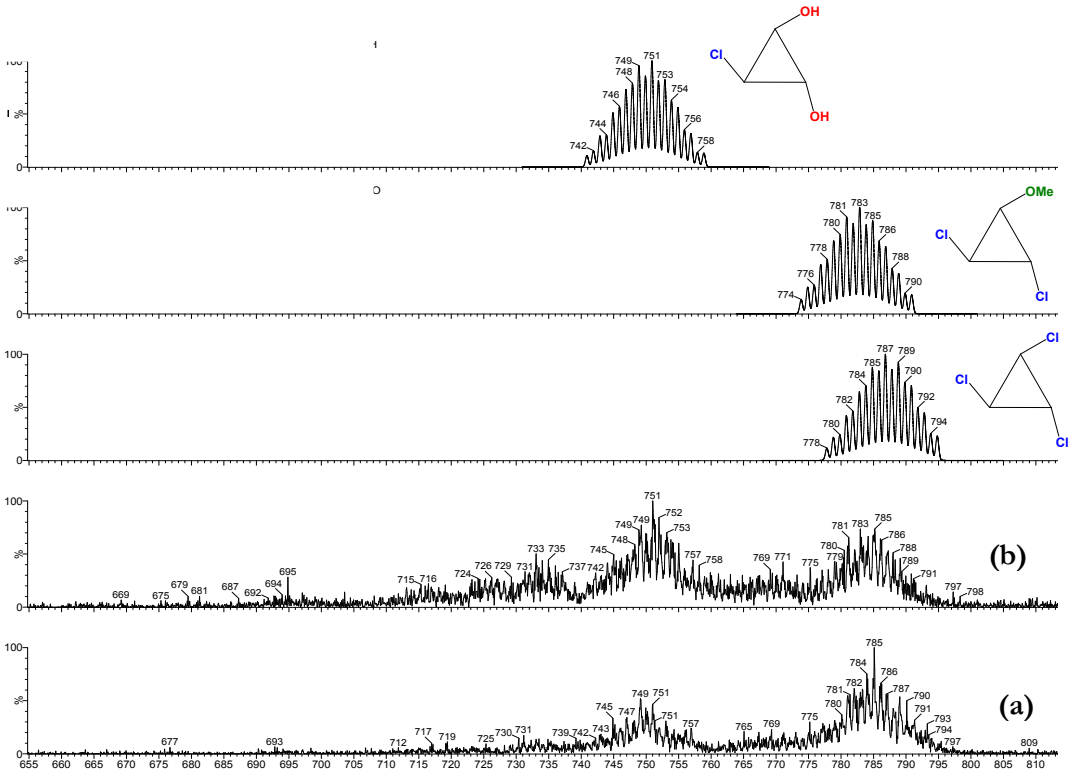

Figure S4. ESI mass spectrum of the catalyst in CH_3CN at 20 V after azobenzene hydrogenation in CH_3OH in the presence of 1 **(a)** and 2 **(b)** equivalents of Et_3N.

Cluster monitoring under H_2 pressure

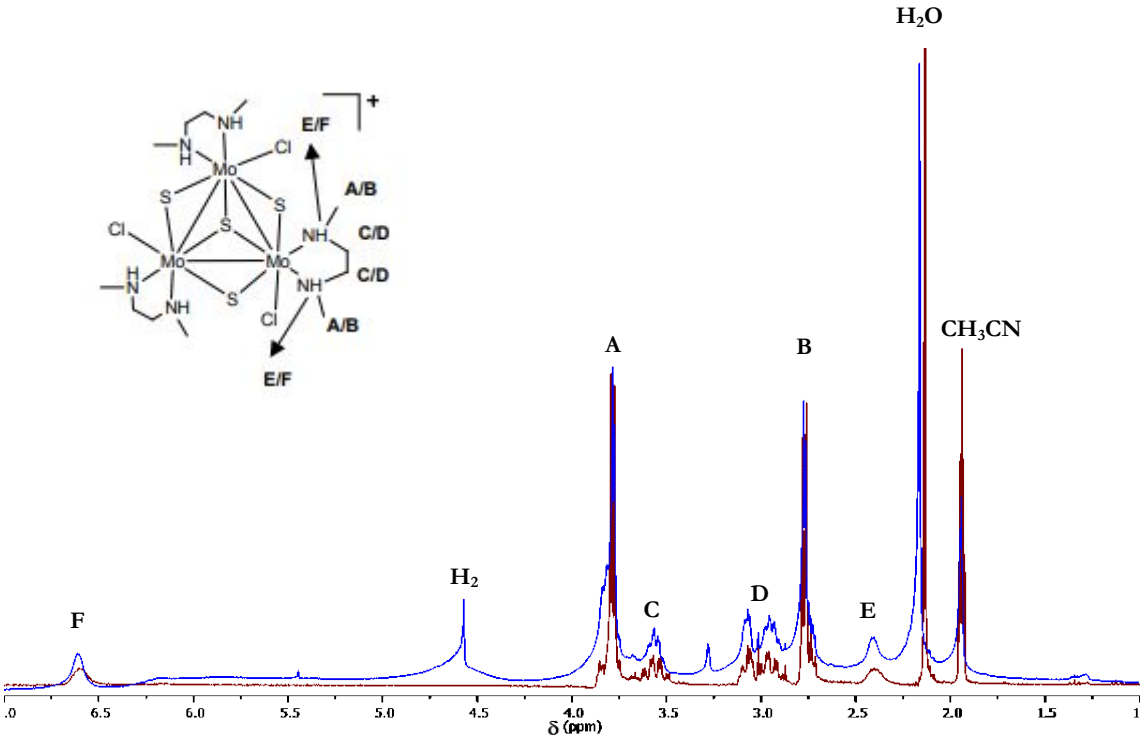

Figure S5. ^{1}H-NMR spectrum of the catalyst in CD_3CN under 20 bar of hydrogen pressure in CD_3CN at 70 ^oC (blue) and at atmospheric pressure at 25 ^oC (red)

Crystal structure determination of $[Mo_3CuS_4Cl_4(dmen)_3](CuCl_2)$

Single crystals of $[Mo_3CuS_4Cl_4(dmen)_3](CuCl_2)$ suitable for X-ray analysis were obtained by slow evaporation of a reaction mixture after the catalytic process. The diffraction data were collected on an Agilent Supernova diffractometer equipped with an Atlas CCD detector using Mo-K_α radiation (λ = 0.71073 Å). No instrument or crystal instabilities were observed during data collection. Absorption corrections based on the multiscan method were applied.[7] A suitable crystal with dimensions 0.27 × 0.21 × 0.19 mm^3 was selected and kept at a steady T = 270(7) K during data collection. The structure was solved with the Superflip[8] solution program using iterative methods and refined by the full-matrix method based on F^2 with the program SHELXL-15 using the Olex2 software package.using Olex2 as the graphical interface.[9] Hydrogen atoms were refined in their geometrically calculated positions using a riding model was used for this purpose. The refined value of the Flack parameter equals 0.54, so the crystal consists of a racemic mixture of the two enantiomers. (TWIN LAW (-1, 0, 0, 0, -1, 0, 0, 0, -1)). The structural figures were drawn using the Diamond visual crystal structure information system software.[10] CCDC 1979773 contains the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

Crystal Data for $[Mo_3CuS_4Cl_4(dmen)_3](CuCl_2)$. $C_{12}H_{36}Cl_6Cu_2Mo_3N_6S_4$, Mr = 1020.78 g/mol, cubic, space group $P2_13$, a = b= c 15.3959(3) Å, $\alpha = \beta = \gamma = 90°$, V = 3649.3(2) $Å^3$, T = 270(7) K, Z = 4, μ(Mo Ka) = 2.832 mm^{-1}. Reflections collected/unique = 12094/2494 (R_{int} = 0.0545) which were used in all calculations. Final refinement converged with R_1 = 0.0548 and wR_2 = 0.1144 for all data, GOF = 1.063, max/min residual electron density 0.7/–0.3 e/$Å^3$.

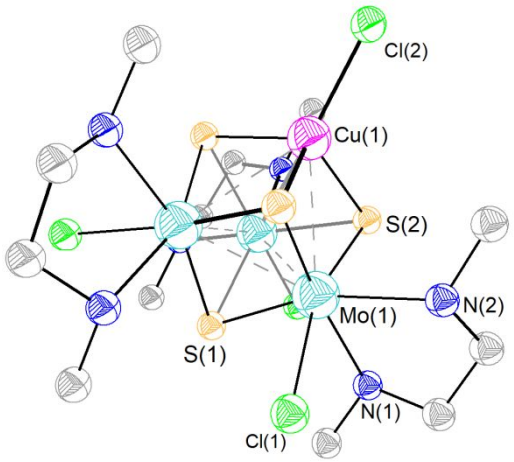

Figure S6. ORTEP representation of $[Mo_3(CuCl)S_4Cl_3(dmen)]^+$ (ellipsoids at 50% probability) with the atom-numbering scheme. Hydrogen atoms have been omitted for clarity. Intermetallic distances: Mo – Mo = 2.746 Å, Mo – Cu = 2.829 Å, Mo – (μ_3-S(1)) = 2.324 Å, Mo – $(\mu_3\text{-S})_{trans\text{-N}}$ = 2.316 Å, Mo – $(\mu_3\text{-S})_{trans\text{-Cl}}$ = 2.315 Å, Mo – $N_{(trans\text{-S(1)})}$ = 2.262 Å, Mo – $N_{(cis\text{-S(1)})}$ = 2.281 Å, Mo – Cl(1) = 2.467 Å, Cu – (μ_3-S) = 2.295 Å, Cu – Cl(2) = 2.207 Å.

Computational details

DFT calculations were run with Gaussian 09 (revision B.01).[11] Geometry optimizations were carried out without symmetry restrictions at the BP86 level,[12] with Mo and S atoms described using the SDD relativistic ECP and associated basis set,[13] with added polarization functions for the latter (ζ=0.503),[14] and the remaining atoms described with the 6-31G(d,p) basis set.[15] Solvent effects (methanol) were included in these optimizations through the PCM method.[16] The electronic state of the system was checked by comparing the energies of the singlet and triplet states. This showed that in all cases the singlet state is more favourable, and therefore all reported data correspond to this state. Analytical frequency calculations were used to characterize each stationary point as a minimum or a transition state (TS). These calculations, carried out at 333.15 K and 10 atm, also allowed obtaining the thermal and entropic corrections required to calculated Gibbs energy differences. Additionally, the Intrinsic Reaction Coordinate paths[17] were followed along both directions of each TS vector to confirm the nature of the species connected by a given TS.

The Gibbs energies discussed in the text were obtained by adding standard state, symmetry, and dispersion corrections to the previous energies. The standard state correction, employed to change the reference state from 10 atm to 1 M, was included by adding the term RT ln (2.45 L/mol · 1 mol/L) = 0.59 kcal/mol to the Gibbs energy of each species, where 2.45 corresponds to the volume of an ideal gas at 10 atm and 0 °C.[18] The effect of the symmetry of the molecules on their rotational entropies was accounted for via the term RT ln(σ), where σ represents the symmetry number of the molecule.[19] Specifically, a symmetry number of 3 was employed for the Mo_3S_4 clusters having a C_3 symmetry, and a symmetry number of 2 was used for azobenzene, 1,2-diphenylhydrazine and H_2. All the remaining species feature a symmetry number of 1 and therefore they do not require of symmetry correction. Finally, dispersion corrections were included via Grimme's D3 parameter set (with Becke-Johnson damping).[20]

The pK_a of **1-H$_2$** were computationally estimated via the isodesmic proton exchange reaction in Eq. 1, whereby acetic acid (pK_a = 9.63) has been used as reference Bronsted acid (HRef). The solution phase free energy (ΔG^*_{sol}) of such reaction is related to the pK_a of the studied species (HA) through Eq. 2.

HA + Ref$^-$ → A$^-$ + HRef (Eq. 1)

$$\mathrm{p}K_a(\mathrm{HA}) = \frac{\Delta G^*_{sol}}{RTln(10)} + \mathrm{p}K_a(\mathrm{HRef}) \qquad \text{(Eq. 2)}$$

Based on a recent computational benchmark on the prediction of pK_a values in methanol,[21] these optimizations were carried out in the gas phase with the X3LYP functional[22] and the def2-TZVP basis set.[23] Harmonic frequency calculations at the same level of theory were used to obtain the thermal corrections to the free energy, whereas single-point calculations including implicit solvation via the SMD method[24] provided the solvation contribution (CH_3OH).

Experimental and optimized bond distances for $[Mo_3S_4Cl_3(dmen)_3]^+$ (1) and optimized bond distances for $[Mo_3S_2(SH)_2Cl_3(dmen)_3]^+$ (1-H_2)

Table S1. Selected experimental and optimized bond distances (Å) for $[Mo_3S_4Cl_3(dmen)_3]^+$ (**1**) and optimized bond distances (Å) for $[Mo_3S_2(SH)_2Cl_3(dmen)_3]^+$ (**1-H_2**)

	$[Mo_3S_4Cl_3(dmen)_3](BF_4)$ experimental (ref. 1)	$[Mo_3S_4Cl_3(dmen)_3]^+$ optimized	$[Mo_3S_2(SH)_2Cl_3(dmen)_3]^+$ optimized
Mo-Mo	2.759[3]	2.797[2]	2.687 (x1), 2.776 (x2)
Mo-(μ_3-S1)	2.335[4]	2.379[1]	2.381[4]
Mo-(μ-S)[b]	2.301[5]	2.337[1]	2.357
Mo-(μ-S)[c]	2.288[7]	2.322[1]	2.345
Mo-(μ-S-H)[b]	-	-	2.415[21]
Mo-(μ-S-H)[c]	-	-	2.417[20]
Mo-N(1)[d]	2.278[6]	2.310[0]	2.329[4]
Mo-N(2)[e]	2.298[18]	2.335[1]	2.318[17]
Mo-Cl(1)	2.492[14]	2.531[0]	2.523[13]

[a] Standard deviations for averaged values are given in square brackets. [b] Mo-μ-S distance *trans* to Mo-N bond. [c] Mo-μ-S distance *trans* to Mo-Cl bond.[d] Distance *trans* to the Mo-(μ_3-S) bond. [e] Distance *cis* to the Mo-(μ_3-S) bond.

Potential energy profile for the catalytic conversion of azobenzene to aniline

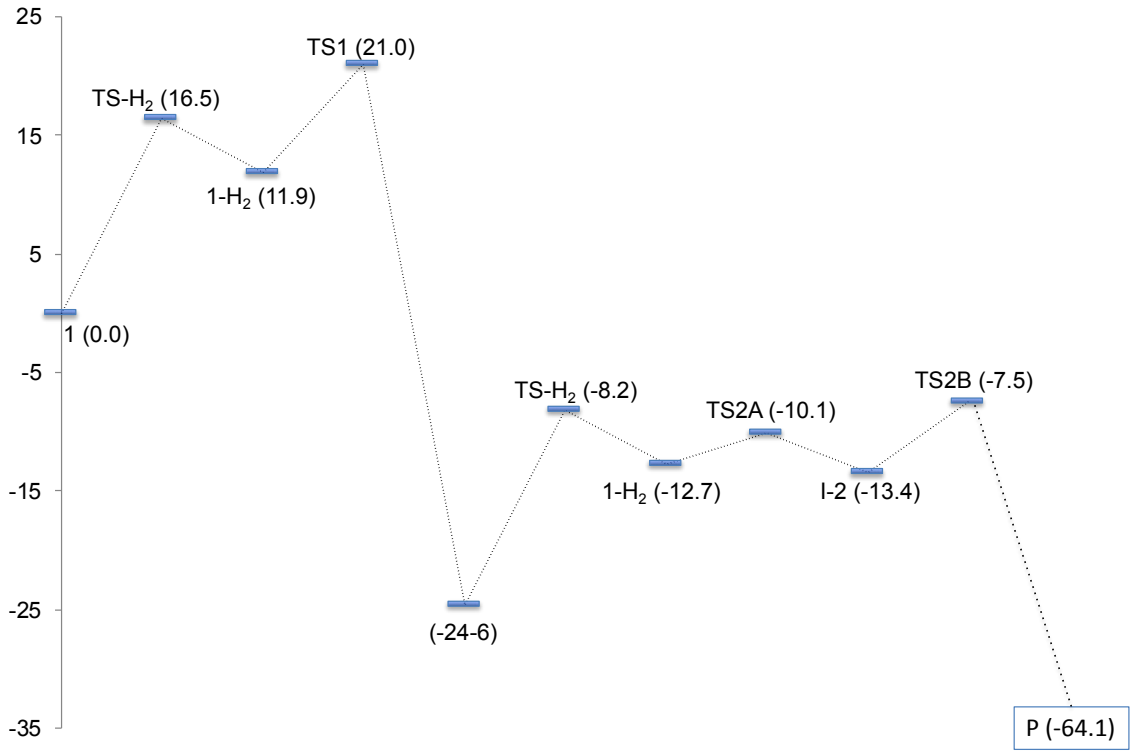

Figure S7. Potential energy profile (kcal/mol) for the two-cycle catalytic conversion of azobenzene to aniline.

Optimized structures of TS1, TS-2A, I-2 and TS-2B

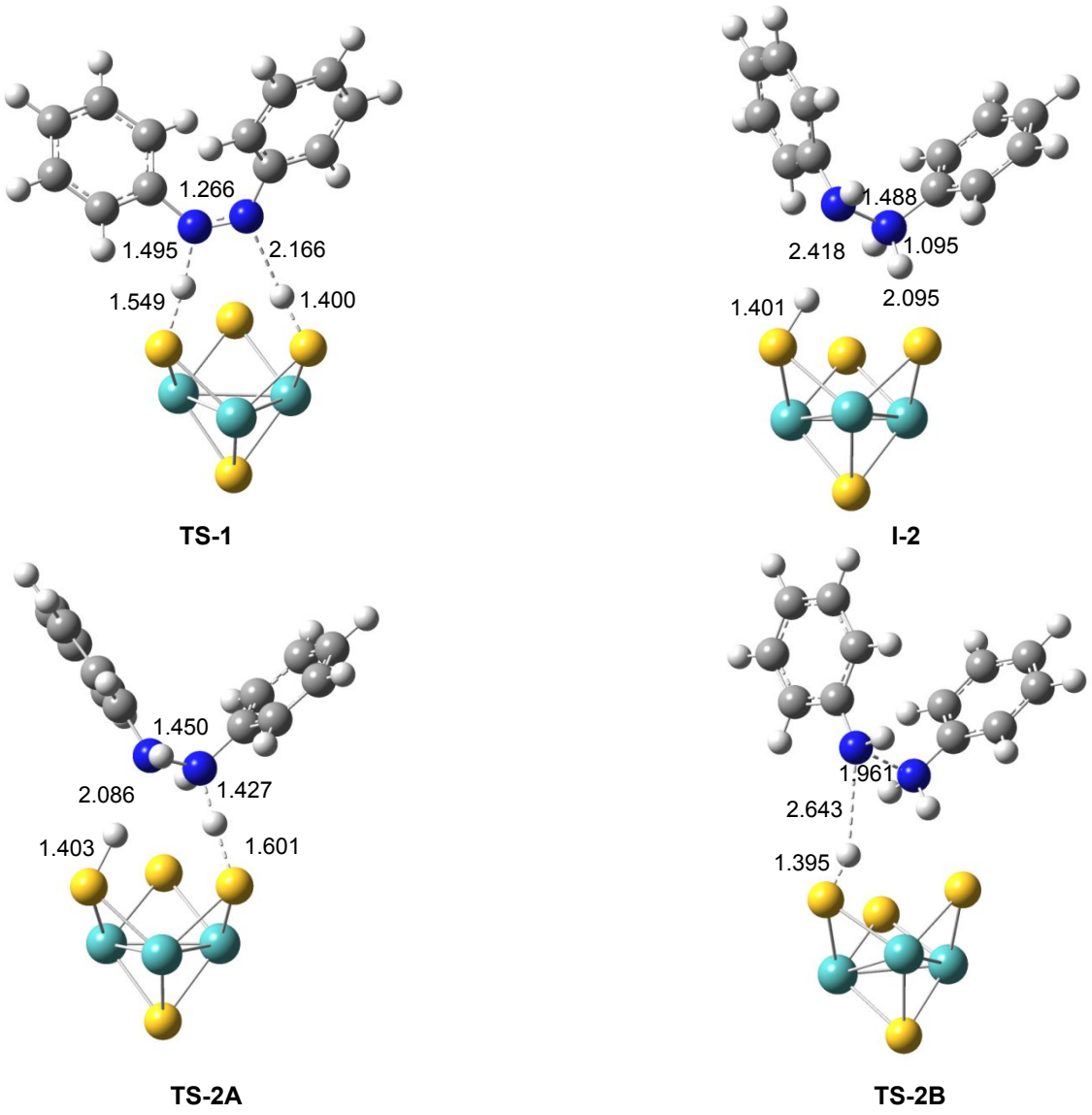

Figure S8. Optimised structures of **TS-1, TS-2A, I-2** and **TS-2B**. Cl and dmen ligands are omitted for simplicity.

Microkinetic modeling

To test the validity of the computationally-derived mechanism in Figure 4, microkinetic modeling procedures[25] were used to calculate the concentration-time profiles for azobenzene, 1,2-diphenylhydrazine and aniline. These were then compared with the experimental curves in Figure 1. For that purpose, the programs Copasi[26] and Specfit[27] were used and both led to similar results. The initial concentrations of cluster (0.0025 M) and azobenzene (0.05 M) were used in the modeling experiment. The concentration of H_2 was taken as that corresponding to the solubility of H_2 in methanol at 60ºC and 10 bar (0.049 M),[28] and it was kept constant during the reaction. The rate constants for each step were estimated from the free energies of activation in Figure 4 using the Eyring equation. Given the small energy differences involved, the formation of intermediate I-2 from the adduct resulting from H_2 addition to the cluster was considered to be a diffusion-controlled process, and so the rate constant for its formation was calculated using the equation $k_{diff} = (8\, k_B\, T\, N_A)/(3\, \eta)$,[29] which yields a value of 2.1×10^{10} M^{-1} s^{-1}, whereas for the reverse process a value of 1.9×10^{9} M^{-1} s^{-1} was taken, i.e. corresponding to a fast equilibrium with $K_e = 11$ M^{-1} (the value for a free energy difference of -1.6 kcal mol^{-1}).

The concentration-time profiles obtained in this way are shown in Figure S9 and compared with the experimental ones in Figure 1 (percentages now expressed in concentrations and time in seconds). Figure S9 shows the sequential conversion of azobenzene to 1,2-diphenylhydrazine and then to aniline. In addition, the concentration of the cluster remains constant and the calculated concentration-time profiles for intermediates **1-H_2** and **I-2** (curves not shown) show that these species are formed at very low concentrations, so that they can be considered to exist under steady-state conditions. Thus, it can be considered that the mechanism in Figure 4 roughly reproduces the experimental kinetic features, but the time scale for the reaction is significantly different.

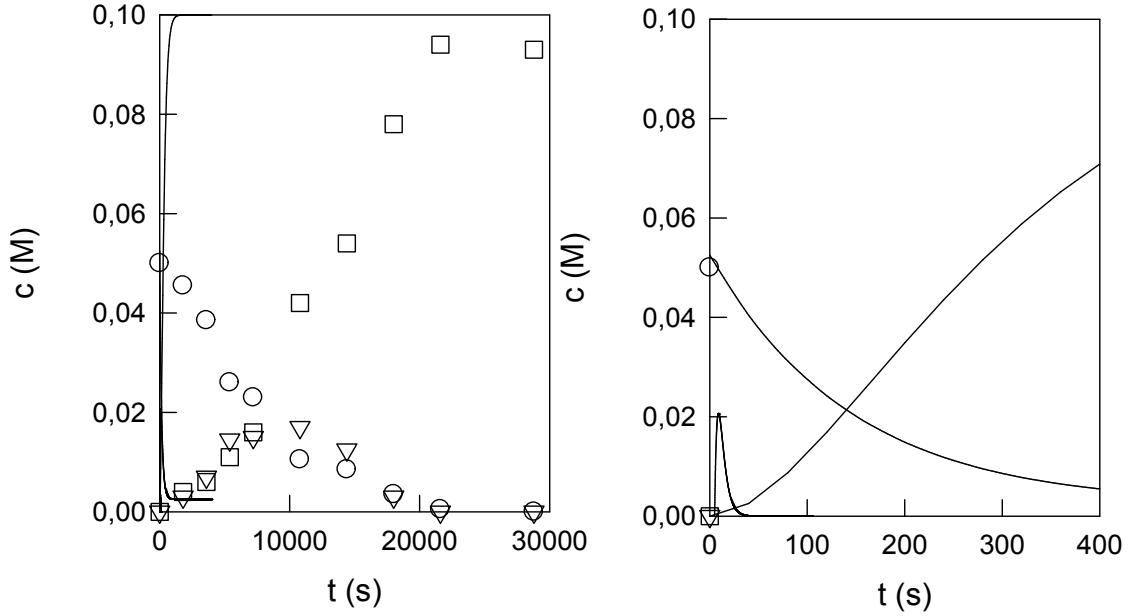

Figure S9. Concentration-time profiles for azobenzene (circles), 1,2-diphenylhydrazine (triangles) and aniline (squares) during the course of the cluster-catalyzed hydrogenation process. The symbols correspond to the experimental data (Figure 1 with the percentages converted to concentrations and times expressed in seconds), and the lines correspond to the concentrations calculated from the computed mechanism in Figure 4. The Figure at the right is an expansion showing the disappearance of azobenzene, the formation and disappearance of 1,2-diphenylhydrazine, and the formation of aniline at the early stages of the reaction.

At this point, the fitting capabilities of the Specfit program were used and a good agreement between the experimental and calculated kinetic profiles was obtained (Figure 5 of the main manuscript) by simply refining the rate constant for the initial step corresponding to H_2 activation, which yields a value of 1.31 ± 0.06 M^{-1} s^{-1}. This rate constant corresponds to a free energy of activation of 19.4 kcal mol^{-1}, only 2.5 kcal mol^{-1} larger than the computed value in Figure 4. Thus, the kinetic results can be well reproduced with the computed mechanism by simply introducing a minimal change in the free energy of activation for the addition of H_2 to the cluster, the difference being clearly below the experimental, computational and fitting errors and so, the microkinetic modeling provides strong support for the proposed mechanism.

Figure S10 shows the concentration-time profiles for all species participating in the reaction, both in the presence and in the absence of azobenzene. Of special relevance are the very low concentrations achieved by the species 1-H_2 and I-2, which are typical of intermediates formed under steady-state conditions and consequently experimentally unobservable.

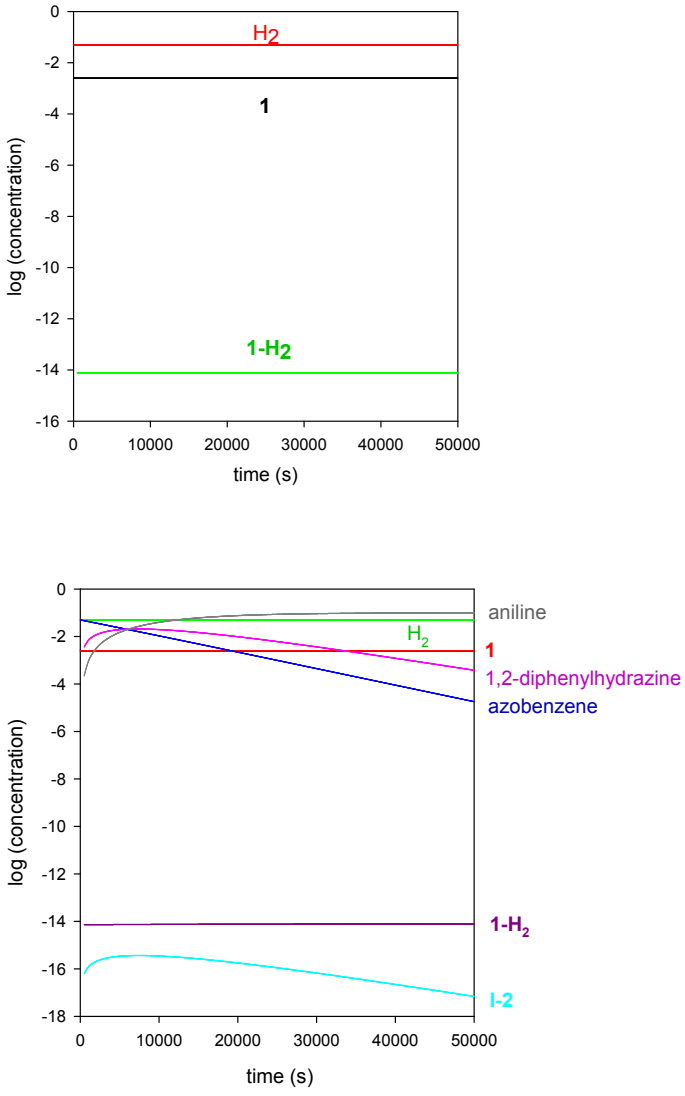

Figure S10. Calculated concentration-time profiles for all species in the reaction mixture in the presence (bottom) and the absence (top) of azobenzene. The concentrations were calculated from the computed mechanism in Figure 4 using the same conditions that those used for Figure 4 in the main text.

Computational tests on alternative mechanistic pathways

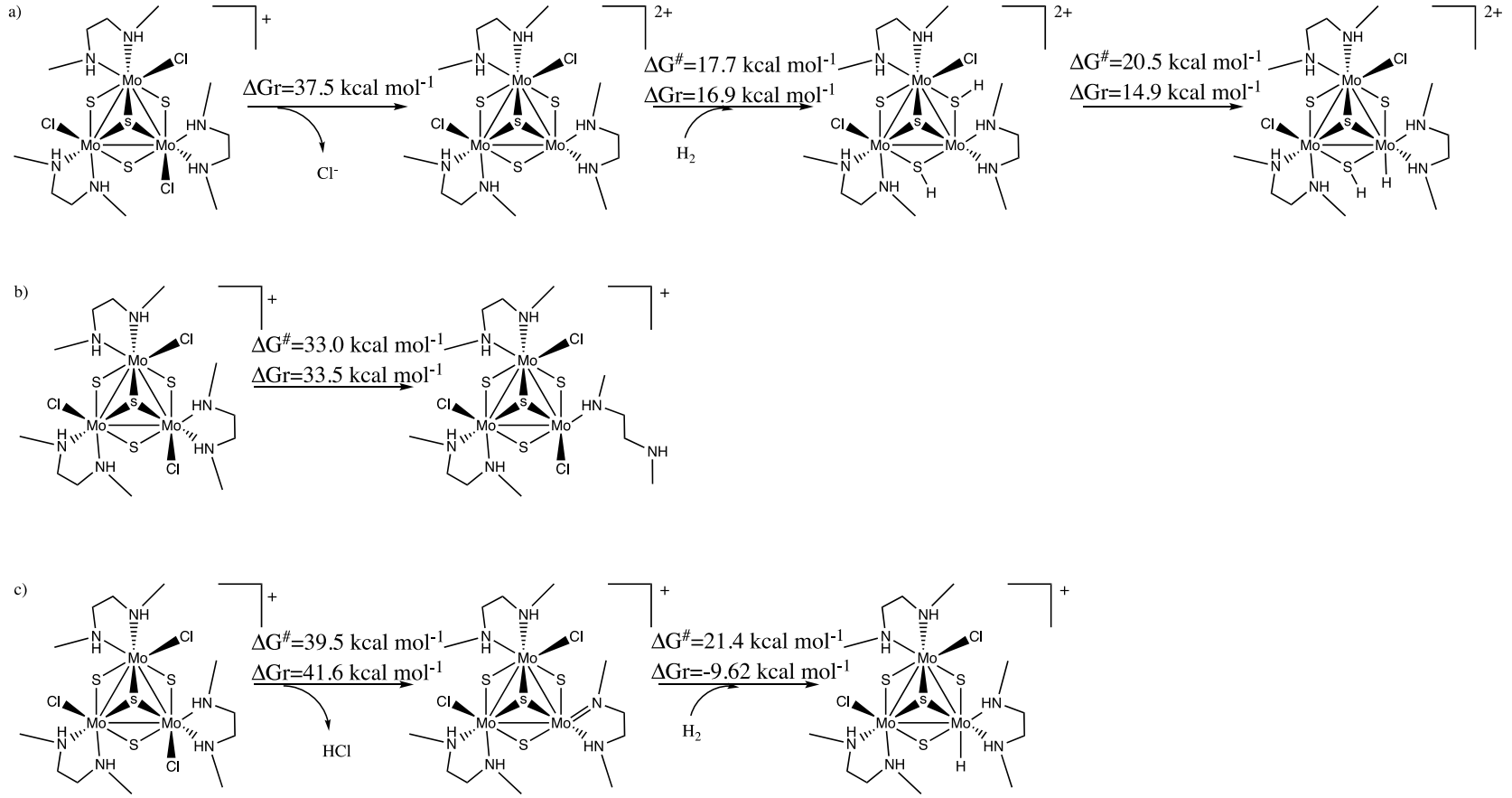

Figure S11. Computational tests on alternative mechanistic pathways. Activation ($\Delta G^{\#}$) and reaction (ΔG_r) free energies are reported for each elementary step.

References

1. Pedrajas, E.; Sorribes, I.; Junge, K.; Beller, M.; Llusar, R., A Mild and Chemoselective Reduction of Nitro and Azo Compounds Catalyzed by a Well-Defined Mo_3S_4 Cluster Bearing Diamine Ligands. *ChemCatChem* **2015,** *7*, 2675-2681.

2. Beltrán, T. F.; Safont, V. S.; Llusar, R., Synthesis, Structure, and Gas-Phase Fragmentation of Trinuclear Mo_3S_4 Clusters Bearing Aminophosphine Ligands: A Combined Experimental and Theoretical Study. *Eur. J. Inorg. Chem.* **2016**, 5171-5179.

3. Pedrajas, E.; Sorribes, I.; Gushchin, A. L.; Laricheva, Y. A.; Junge, K.; Beller, M.; Llusar, R., Chemoselective Hydrogenation of Nitroarenes Catalyzed by Molybdenum Sulphide Clusters. *ChemCatChem* **2017,** *9*, 1128-1134.

4. Estevan, F.; Feliz, M.; Llusar, R.; Mata, J. A.; Uriel, S., High yield synthesis of trinuclear $[M_3S_4X_3(diphos)_3]^+$ (M=Mo, W; X=Cl, Br and diphos=dmpe, dppe) molecular clusters from solid state materials. Synthesis and structure of $[W_3S_4H_3(dppe)_3](BPh_4)$. *Polyhedron* **2001,** *20*, 527-535.

5. Algarra, A. G.; Basallote, M. G.; Fernández-Trujillo, M. J.; Feliz, M.; Guillamón, E.; Llusar, R.; Sorribes, I.; Vicent, C., Chiral $[Mo_3S_4H_3(diphosphine)_3]^+$ Hydrido Clusters and Study of the Effect of the Metal Atom on the Kinetics of the Acid-Assisted Substitution of the Coordinated Hydride: Mo vs W. *Inorg. Chem.* **2010,** *49*, 5935-5942.

6. Cotton, F. A.; Dori, Z.; Llusar, R.; Schwotzer, W., Oxidative fragmentation of the cuboid molybdenum-sulfur Mo_4S_4 cluster core: synthesis and structures of $[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)_3([9]aneN_3)_3]^{4+}$ and $\{[MoO([9]aneN_3)]_2(\mu\text{-}S)_2\}^{2+}$ ($[9]aneN_3$ = 1,4,7-triazacyclononane). *Inorg. Chem.* **1986,** *25*, 3654-3658.

7. (a) CrysAlis, version 171.36.24, Agilent Technologies: Santa Clara, CA, 2012; (b) R. C. Clark, J. S. Reid, *Acta Crystallogr. A* **1995**, *51*, 887-897.

8. Palatinus, L.; Chapuis, G. SUPERFLIP - a computer program for the solution of crystal structures by charge flipping in arbitrary dimensions. *J. Appl. Crystallogr*. **2007**, *40*, 786-790.

9. (a) Sheldrick, G., A short history of SHELX. *Acta Crystallogr. A* **2008**, *64*, 112-122; (b) Sheldrick, G., Crystal structure refinement with SHELXL. *Acta Crystallogr. C* **2015**, *71*, 3-8; (c) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann,

H., OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr*. **2009**, *42*, 339-341.

10. Brandenburg, K.; Putz, H. DIAMOND; Crystal Impact GbR: Bonn, Germany, 2005.

11. Gaussian 09, Revision B.01; M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc.: Wallingford CT, 2013.

12. (a) Perdew, J. P., Density-functional approximation for the correlation energy of the inhomogeneous electron gas. *Phys. Rev. B* **1986**, *33*, 8822-8824; (b) Becke, A. D., Density-functional exchange-energy approximation with correct asymptotic behaviour. *Phys. Rev. A* **1988**, *38*, 3098.

13. Andrae, D.; Häubermann, U.; Dolg, M.; Stoll, H.; Preub, H., Energy-adjusted ab initio pseudopotentials for the second and third row transition elements. *Theor. Chim. Acta* **1990**, *77*, 123-141.

14. Hollwarth, A.; Bohme, M.; Dapprich, S.; Ehlers, A. W.; Gobbi, A.; Jonas, V.; Kohler, K. F.; Stegmann, R.; Veldkamp, A.; Frenking, G., A Set Of D-Polarization Functions For Pseudo-Potential Basis-Sets Of The Main-Group Elements Al-Bi And F-Type Polarization Functions For Zn, Cd, Hg. *Chem. Phys. Lett*. **1993**, *208*, 237-240.

15. (a) Hehre, W. J.; Ditchfield, R.; Pople, J. A., Self---Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian---Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1972**, *56*, 2257-2261. (b)

Harihanan, P. C.; Pople, J. A., Influence of polarization functions on molecular-orbital hydrogenation energies. *Theor. Chim. Acta* **1973**, *28*, 213-222.

16. (a) Cossi, M.; Scalmani, G.; Rega, N.; Barone, V., New developments in the polarizable continuum model for quantum mechanical and classical calculations on molecules in solution. *J. Chem. Phys*. **2002**, *117*, 43-54; (b) Tomasi, J.; Mennucci, B.; Cammi, R., Quantum mechanical continuum solvation models. *Chem. Rev*. **2005**, *105*, 2999-3093.

17. (a) Gonzalez, C.; Schlegel, H. B., Reaction path following in mass-weighted internal coordinates. *J. Phys. Chem.* **1990,** *94*, 5523-5527; (b) Gonzalez, C.; Schlegel, H. B., Improved algorithms for reaction path following: Higher-order implicit algorithms. *J. Chem. Phys.* **1991,** *95*, 5853-5860.

18. Harvey, J.; Himo, F.; Maseras, F.; Perrin, L., Scope and Challenge of Computational Methods for Studying Mechanism and Reactivity in Homogeneous Catalysis. *ACS Catal*. **2019**, *9*, 6803-6813.

19. (a) Fernández-Ramos, A., Ellingson, B. A., Meana-Pañeda, R., Marques, J. M. C., & Truhlar, D. G. (2007). Symmetry numbers and chemical reaction rates. *Theor. Chem. Acc.*, *118*, 813-826; (b) Gilson, M. K.; Irikura, K. K., Symmetry numbers for rigid, flexible, and fluxional molecules: theory and applications. *J. Phys. Chem. B* **2010**, *114* (49), 16304-16317.

20. (a) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H., A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010,** *132* (15), 154104; (b) Grimme, S.; Ehrlich, S.; Goerigk, L., Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* **2011,** *32* (7), 1456-1465.

21. Miguel, E. L. M.; Silva, P. L.; Pliego, J. R., Theoretical Prediction of pKa in Methanol: Testing SM8 and SMD Models for Carboxylic Acids, Phenols, and Amines. *J. Phys. Chem. B* **2014,** *118*, 5730-5739.

22. (a) Xu, X.; Goddard, W. A., The X3LYP extended density functional for accurate descriptions of nonbond interactions, spin states, and thermochemical properties. *Proc. Natl. Acad. Sci. U.S.A.* **2004,** *101*, 2673-2677; b) Xu, X.; Zhang, Q.; Muller, R. P.; Goddard, W. A., An extended hybrid density functional (X3LYP) with improved

descriptions of nonbond interactions and thermodynamic properties of molecular systems. *J. Chem. Phys.* **2004,** *122*, 014105.

23. Weigend, F.; Ahlrichs, R., Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005,** *7*, 3297-3305.

24. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009,** *113*, 6378-6396.

25. Besora, M.; Maseras, F., Microkinetic modeling in homogeneous catalysis. *WIREs Computational Molecular Science* **2018,** *8* (6), e1372.

26. Hoops S., Sahle S., Gauges R., Lee C., Pahle J., Simus N., Singhal M., Xu L., Mendes P. and Kummer U., COPASI: a COmplex PAthway SImulator. *Bioinformatics* **2006***, 22*, 3067-3074.

27. Binstead, R. A.; Jung, B.; Zuberbühler, A. D. SPECFIT-32; Spectrum Software Associates, Chapel Hill, NC, USA, 2000.

28. Liu; Takemura, F.; Yabe, A., Solubility of Hydrogen in Liquid Methanol and Methyl Formate at 20 °C to 140 °C. *Journal of Chemical & Engineering Data* **1996,** *41*, 1141-1143.

29. K. J. Laidler, Chemical Kinetics, 3rd Ed., Harper & Row, New York, 1987.

Cartesian coordinates of the optimized species

BP86-optimized structures

Azobenzene

E(UB-P86) = -572.764064606 a. u.
Free energy= -572.621449 a. u.
D3(BJ) dispersion correction = -0.04339292 a. u.
Cartesian

C	3.719204	-4.058289	2.327515
C	4.401878	-3.772005	1.119832
C	5.428591	-4.633292	0.672901
C	5.773018	-5.768584	1.419713
C	5.093668	-6.050039	2.617436
C	4.067927	-5.192055	3.066883
N	4.141581	-2.655190	0.280919
N	3.208630	-1.884881	0.700032
C	2.948653	-0.767789	-0.138610
C	3.631530	-0.481320	-1.346113
C	3.283249	0.652823	-2.085128
C	2.257795	1.511034	-1.635475
C	1.578322	1.229458	-0.437845
C	1.922281	0.093772	0.308580
H	2.927675	-3.380206	2.657679
H	3.541578	-5.415691	4.000762
H	5.359816	-6.935706	3.203312
H	6.569179	-6.432812	1.069281
H	5.939568	-4.388012	-0.263614
H	1.411181	-0.151639	1.244997
H	0.782424	1.893883	-0.087189
H	1.992023	2.397002	-2.221064
H	3.809730	0.876546	-3.018913
H	4.422924	-1.159472	-1.676436

1
E(UB-P86) = -2434.50146471 a. u.
Free energy = -2434.060137 a. u.
D3(BJ) dispersion correction = -0.25410335 a. u.
Cartesian

Mo	1.582817	-0.305185	0.107855
Mo	-1.062594	-1.215597	0.116353
Mo	-0.525090	1.530888	0.109482
Cl	3.232204	1.017203	-1.283910
Cl	-0.746297	-3.313829	-1.263308
Cl	-2.500408	2.299852	-1.274115
S	-0.006255	-0.000700	-1.635470
S	-1.984538	0.381386	1.528341
S	1.316588	1.535937	1.521702

S	0.669718	-1.899058	1.528490
N	3.561767	-0.785679	1.197938
H	4.182544	-0.097809	0.741467
N	2.493609	-2.042411	-1.160975
H	1.896862	-2.830220	-0.859853
N	-2.467672	-2.678986	1.220021
H	-2.182034	-3.564892	0.772532
N	-3.022750	-1.142806	-1.149895
H	-3.403738	-0.228898	-0.855056
N	-1.088960	3.487113	1.200858
H	-1.996817	3.683839	0.749440
N	0.520126	3.184339	-1.165782
H	1.502370	3.056940	-0.871438
C	3.691198	-0.603998	2.671869
H	3.459931	0.437672	2.933045
H	4.717946	-0.844934	2.998959
H	2.980904	-1.269504	3.184482
C	4.028657	-2.146947	0.790362
H	3.411525	-2.885984	1.328907
H	5.080954	-2.297378	1.094154
C	3.896548	-2.310829	-0.715353
H	4.544335	-1.587483	-1.238351
H	4.205810	-3.326926	-1.019542
C	2.425422	-2.012868	-2.651517
H	1.372519	-2.036929	-2.962597
H	2.948754	-2.889750	-3.072061
H	2.900816	-1.089517	-3.012454
C	-2.373267	-2.866823	2.695846
H	-1.354948	-3.183830	2.959027
H	-3.094441	-3.632439	3.031802
H	-2.594193	-1.913798	3.198926
C	-3.880654	-2.407463	0.811073
H	-4.535205	-3.243513	1.118905
H	-4.214492	-1.501900	1.345645
C	-3.957844	-2.219115	-0.695738
H	-4.992580	-1.979113	-0.999452
H	-3.657743	-3.145267	-1.214017
C	-2.964004	-1.109466	-2.640772
H	-2.462532	-0.185696	-2.958769
H	-3.985031	-1.131679	-3.061048
H	-2.398335	-1.983070	-2.995201
C	-1.303084	3.508252	2.675861
H	-2.092819	2.791998	2.940601
H	-1.599197	4.519671	3.005304
H	-0.370759	3.219246	3.183233
C	-0.142554	4.569543	0.788709
H	0.807763	4.403300	1.323913
H	-0.535048	5.557081	1.093646
C	0.058884	4.535472	-0.717922
H	-0.892854	4.738369	-1.237005

H	0.785946	5.308270	-1.025434
C	0.518830	3.110643	-2.656414
H	1.062389	2.209859	-2.971089
H	1.015886	4.001217	-3.079955
H	-0.520925	3.062841	-3.010601

H_2

E(UB-P86) = -1.17659590120 a. u.
Free energy = -1.177527 a.u.
D3(BJ) dispersion correction = -0.00011003 a. u.
Cartesian

H	0.000000	0.000000	-0.025448
H	0.000000	0.000000	0.725448

Aniline

E(UB-P86) = -287.609705694 a. u.
Free energy = -287.526877 a. u .
D3(BJ) dispersion correction = -0.02051285 a. u.
Cartesian

C	6.339621	-0.854888	-0.039651
C	5.194924	-0.549900	0.709891
C	5.063836	0.711454	1.343372
C	6.114140	1.652103	1.195127
C	7.253257	1.335029	0.442229
C	7.379920	0.080913	-0.181888
N	3.955752	0.996963	2.148327
H	6.027652	2.633280	1.676427
H	8.049715	2.080743	0.340702
H	8.270640	-0.161090	-0.769821
H	6.414966	-1.836108	-0.521583
H	4.391055	-1.288260	0.812293
H	3.748907	1.989506	2.259364
H	3.113912	0.465707	1.926285

1,2-Diphenylhydrazine
E(UB-P86) = -573.979931784 a. u.
Free energy = -573.814071 a. u.
D3(BJ) dispersion correction = -0.04791857 a. u.
Cartesian

C	6.379511	-1.318443	0.534419
C	5.196231	-0.792181	1.083732
C	5.081156	0.577144	1.359002
C	6.162250	1.450390	1.089512
C	7.351157	0.925237	0.535801
C	7.449379	-0.447572	0.263882
N	6.045265	2.809508	1.446159
H	8.181288	1.604495	0.324012

H	8.377521	-0.838387	-0.167804
H	6.464079	-2.387973	0.318631
H	4.348116	-1.451932	1.296995
H	4.154380	0.977709	1.786520
N	6.924473	3.730808	0.862436
C	6.513597	4.453436	-0.278233
C	7.163507	5.672770	-0.587277
C	6.810499	6.387455	-1.738561
C	5.805327	5.910552	-2.600609
C	5.159476	4.702650	-2.290690
C	5.503209	3.972549	-1.141295
H	7.944012	6.053617	0.081582
H	7.322125	7.330499	-1.959355
H	5.530118	6.474087	-3.497320
H	4.374440	4.315971	-2.949591
H	4.998027	3.028286	-0.919618
H	7.390591	4.301967	1.570408
H	5.078127	3.144393	1.526912

TS-H_2

E(UB-P86) = -2435.65184479 a. u.

Imaginary Frequency = 1090.90i cm^{-1}

Free energy = -2435.197874 a. u.

D3(BJ) dispersion correction = -0.26425867 a. u.

Cartesian

C	-1.692333	3.354077	2.622195
N	-1.412396	3.344341	1.159212
C	-0.516709	4.482367	0.789488
C	-0.276519	4.482633	-0.710678
N	0.279257	3.169860	-1.163245
C	0.301856	3.118905	-2.654832
Mo	-0.681932	1.429300	0.060500
S	1.099368	1.512798	1.646794
Mo	1.598306	-0.156945	0.066708
N	2.634538	-1.821738	-1.185320
C	2.595983	-1.765247	-2.676652
Mo	-0.961158	-1.263548	0.072968
N	-2.867677	-1.384775	-1.225813
C	-2.766946	-1.392063	-2.715265
Cl	-2.696993	2.023766	-1.312646
S	0.019852	-0.010773	-1.703897
S	-1.954715	0.197573	1.592167
Cl	3.143172	1.377178	-1.224267
S	0.783312	-1.687382	1.650545
N	3.622464	-0.496136	1.158333
C	4.156681	-1.837954	0.776282
C	4.044991	-2.017331	-0.727842
Cl	-0.347613	-3.385347	-1.165497
N	-2.263400	-2.841936	1.168422

C	-3.683371	-2.672231	0.737706
C	-3.739776	-2.514214	-0.772328
C	3.776414	-0.264496	2.622028
C	-2.176824	-3.041513	2.642203
H	-2.310734	3.486920	0.670440
H	1.267357	3.103057	-0.862017
H	4.191063	0.214786	0.669619
H	2.077765	-2.650697	-0.915150
H	-1.904005	-3.699088	0.717389
H	-3.321268	-0.490703	-0.967619
H	-2.451451	2.595141	2.854727
H	-2.057997	4.347923	2.935419
H	-0.768928	3.119869	3.172761
H	0.428132	4.359880	1.346436
H	-0.969420	5.442702	1.098672
H	-1.227824	4.633094	-1.249351
H	0.405148	5.305526	-0.991619
H	0.917698	2.268578	-2.975533
H	0.731265	4.052059	-3.061015
H	-0.727153	2.993788	-3.022247
H	3.498034	0.771196	2.860679
H	4.822072	-0.440946	2.929744
H	3.119669	-0.953356	3.174416
H	5.212392	-1.934549	1.090785
H	3.570635	-2.599991	1.317763
H	4.411856	-3.015574	-1.027239
H	4.659760	-1.261982	-1.246689
H	1.556240	-1.867915	-3.014067
H	3.199104	-2.585962	-3.104276
H	2.999455	-0.797269	-3.007759
H	-1.144152	-3.298864	2.915021
H	-2.852081	-3.855729	2.959183
H	-2.463570	-2.111030	3.154119
H	-4.084745	-1.781286	1.249938
H	-4.287348	-3.545284	1.046915
H	-3.364422	-3.426548	-1.266581
H	-4.779926	-2.351029	-1.106058
H	-2.334060	-0.440970	-3.051581
H	-3.769195	-1.514531	-3.162425
H	-2.118754	-2.225475	-3.023552
H	0.459327	0.512181	2.740226
H	0.360146	-0.573307	2.739428

1-H_2

E(UB-P86) = -2435.65909815 a. u.
Free energy = -2435.201913 a. u.
D3(BJ) dispersion correction = -0.26367570 a.u.
Cartesian

C	-1.726070	3.374288	2.551115

N	-1.442551	3.341568	1.089645
C	-0.566752	4.488962	0.703560
C	-0.323524	4.470529	-0.795571
N	0.255059	3.160583	-1.227243
C	0.285014	3.094042	-2.718220
Mo	-0.688180	1.417524	0.007997
S	1.134123	1.582224	1.609043
Mo	1.587083	-0.158510	0.020336
N	2.611005	-1.813410	-1.241210
C	2.567540	-1.744138	-2.732440
Mo	-0.971465	-1.254239	0.020777
N	-2.859976	-1.360058	-1.287351
C	-2.748798	-1.378699	-2.775856
Cl	-2.717047	1.976781	-1.357118
S	0.018741	-0.014608	-1.758254
S	-1.935196	0.195810	1.591919
Cl	3.111257	1.416077	-1.234255
S	0.789075	-1.771960	1.612466
N	3.619461	-0.505012	1.101397
C	4.153262	-1.842344	0.705486
C	4.026926	-2.008547	-0.798367
Cl	-0.333708	-3.386822	-1.189366
N	-2.295723	-2.831086	1.102800
C	-3.710592	-2.634146	0.670729
C	-3.756668	-2.472409	-0.838597
C	3.786253	-0.283516	2.565205
C	-2.217101	-3.051722	2.573597
H	-2.342798	3.460555	0.598052
H	1.244261	3.115058	-0.923611
H	4.183739	0.210294	0.613971
H	2.060955	-2.650165	-0.979473
H	-1.947371	-3.687949	0.642528
H	-3.298545	-0.454690	-1.037003
H	-2.458024	2.594140	2.799862
H	-2.125959	4.361998	2.841565
H	-0.796310	3.186986	3.109039
H	0.379252	4.390860	1.263352
H	-1.036070	5.446294	0.997182
H	-1.276076	4.596623	-1.338446
H	0.344537	5.300715	-1.087788
H	0.916774	2.251417	-3.027619
H	0.699106	4.030355	-3.133319
H	-0.740330	2.946533	-3.087897
H	3.509611	0.750369	2.813390
H	4.834860	-0.461126	2.862430
H	3.135461	-0.976652	3.119205
H	5.212276	-1.938966	1.008803
H	3.574781	-2.610378	1.246569
H	4.393869	-3.002578	-1.111296
H	4.634126	-1.246273	-1.316169

H	1.527935	-1.851414	-3.068416
H	3.175515	-2.556773	-3.168732
H	2.963199	-0.770356	-3.056031
H	-1.191676	-3.339163	2.844362
H	-2.912214	-3.853742	2.878896
H	-2.482072	-2.121053	3.096838
H	-4.095191	-1.736102	1.183348
H	-4.332249	-3.496546	0.975247
H	-3.397322	-3.391799	-1.332188
H	-4.791229	-2.287941	-1.178425
H	-2.301323	-0.436053	-3.116258
H	-3.749500	-1.491141	-3.229136
H	-2.109343	-2.222783	-3.073670
H	0.551717	0.916344	2.697641
H	0.390184	-0.982058	2.700972

TS-1

E(UB-P86) = -3008.40862723 a. u.

Imaginary Frequency = 534.62i cm^{-1}

Free energy = -3007.791632 a.u.

D3(BJ) dispersion correction = -0.33161125

Cartesian

C	4.657972	-2.779889	-0.817935
C	4.521144	-1.850337	0.240252
C	5.421226	-1.880603	1.335496
C	6.454443	-2.822808	1.343817
C	6.624723	-3.710034	0.262742
C	5.727923	-3.682775	-0.819679
N	3.350663	-1.048351	0.193758
N	3.254995	0.120816	0.670012
C	4.308524	0.979089	1.105180
C	5.488825	1.152104	0.343791
C	6.414453	2.125239	0.735535
C	6.187092	2.909231	1.883324
C	5.008754	2.738043	2.630140
C	4.052952	1.792899	2.231825
S	0.010193	-2.054713	-0.199184
Mo	-1.391551	-0.459340	0.960614
S	0.433611	1.095167	1.200144
Mo	-0.905334	1.698484	-0.720776
S	-2.944423	0.468345	-0.575449
Mo	-1.298217	-0.753603	-1.775105
Cl	-2.436175	-0.011819	-3.922632
N	0.507146	3.515977	-1.050588
C	0.257475	4.075072	-2.410891
C	-1.238804	4.203721	-2.638997
N	-1.932258	2.897982	-2.414762
C	-3.407826	3.112239	-2.413340
C	1.966366	3.439944	-0.774915
Cl	-1.991965	3.492482	0.741594

S	0.574130	0.640321	-2.199508
N	-0.394573	-2.236670	-3.334014
C	1.072185	-2.385666	-3.528516
N	-2.870148	-2.477758	-1.893347
C	-4.328240	-2.163858	-1.921241
C	-1.035628	-3.573504	-3.160801
C	-2.538806	-3.408804	-3.014643
N	-0.587168	-1.324319	2.967938
C	-0.890845	-0.363006	4.068138
C	-2.322562	0.125133	3.934529
N	-2.561613	0.721997	2.584613
C	-4.020620	0.982103	2.415031
Cl	-3.054176	-2.322232	1.446050
C	0.796864	-1.852563	3.103298
H	-0.782065	-1.814033	-4.193176
H	-2.701804	-2.961163	-0.993065
H	-1.236822	-2.122380	3.063070
H	-2.094071	1.643772	2.540289
H	0.092120	4.167808	-0.364658
H	-1.728386	2.264021	-3.209265
H	1.512980	-1.405224	-3.754680
H	1.283783	-3.088104	-4.354744
H	1.521289	-2.775642	-2.602562
H	-0.595340	-4.039953	-2.262682
H	-0.811351	-4.225044	-4.026302
H	-2.963733	-2.969421	-3.933661
H	-3.019767	-4.391390	-2.856746
H	-4.607306	-1.673173	-0.979762
H	-4.918645	-3.091032	-2.037208
H	-4.529506	-1.488859	-2.766246
H	0.961280	-2.644131	2.359509
H	0.956632	-2.263279	4.116481
H	1.515360	-1.038179	2.929311
H	-0.746513	-0.844671	5.053462
H	-0.175076	0.472976	3.987997
H	-2.555352	0.859014	4.727551
H	-3.023893	-0.720423	4.041646
H	-4.170924	1.631509	1.542852
H	-4.428459	1.480284	3.313498
H	-4.536943	0.023651	2.257251
H	2.123561	3.174641	0.279340
H	2.449810	4.411775	-0.981842
H	2.416127	2.665328	-1.413424
H	0.716763	3.388528	-3.142311
H	0.739640	5.065032	-2.517608
H	-1.671897	4.923406	-1.922872
H	-1.444210	4.576653	-3.658727
H	-3.912900	2.140679	-2.488354
H	-3.702342	3.742507	-3.271689
H	-3.692707	3.608163	-1.473619

H	1.289823	-1.495808	-0.299661
H	1.831477	0.557152	0.805605
H	5.660768	0.548589	-0.551074
H	6.923438	3.659358	2.186571
H	4.825554	3.348936	3.519038
H	3.125156	1.661061	2.796317
H	5.290147	-1.201317	2.180804
H	3.930577	-2.762459	-1.634550
H	7.134753	-2.865825	2.199664
H	5.848637	-4.380153	-1.653751
H	7.446422	-4.432390	0.275033
H	7.320308	2.274243	0.140207

TS-2A

E(UB-P86) = -3009.6348324 a.u.

Imaginary frequency = 682.61i cm^{-1}

Free energy = -3008.990592 a.u.

D3(BJ) dispersion correction = -0.33863220 a.u.

Cartesian

C	5.196868	1.336055	-0.356650
C	4.902694	0.698245	0.865987
C	5.684277	0.976510	2.006293
C	6.739792	1.896928	1.925014
C	7.040046	2.530737	0.707513
C	6.266866	2.241379	-0.429334
N	3.760924	-0.155283	1.006487
N	3.503109	-1.117206	-0.047557
C	4.555912	-2.086652	-0.315989
C	4.801205	-3.093328	0.636701
C	5.793368	-4.051919	0.383925
C	6.526518	-4.014583	-0.815699
C	6.268617	-3.011798	-1.764446
C	5.286529	-2.038490	-1.516732
S	0.901497	0.127367	-1.902930
Mo	-0.677837	-1.521595	-1.269926
S	-2.586166	-0.481843	-0.304846
Mo	-0.828570	1.093038	-0.597043
Cl	-2.284973	2.831159	0.570681
Mo	-0.955609	-0.819213	1.384665
Cl	-2.250298	-2.877179	2.139877
S	0.767111	-2.287379	0.507940
N	-2.427784	0.321350	2.779028
C	-3.898874	0.232065	2.544674
N	-0.106469	-1.185325	3.523755
C	1.341443	-1.403806	3.777739
S	0.549305	1.070578	1.398338
C	-2.139954	0.010763	4.212757
C	-0.647797	-0.144322	4.445778
N	-1.968804	1.786824	-2.488588

C	-3.455903	1.693012	-2.550387
N	0.225454	3.086292	-1.180241
C	1.658884	3.335194	-0.871473
C	-1.542236	3.164714	-2.884633
C	-0.063037	3.377395	-2.614282
N	0.506968	-3.042185	-2.588290
C	1.968889	-2.937720	-2.824229
N	-1.897701	-3.514395	-1.099216
C	-3.386994	-3.502188	-1.172393
Cl	-1.884916	-1.386090	-3.502653
C	0.144566	-4.430453	-2.178115
C	-1.363541	-4.544383	-2.040542
H	0.033748	-2.849705	-3.486577
H	-1.658357	-3.786200	-0.128493
H	-0.596373	-2.071522	3.730495
H	-2.168475	1.305698	2.590681
H	-0.335964	3.740789	-0.610930
H	-1.599133	1.108624	-3.178823
H	2.207401	-1.933217	-3.200091
H	2.298413	-3.693379	-3.560217
H	2.502925	-3.112175	-1.878798
H	0.651209	-4.638130	-1.220323
H	0.508650	-5.161276	-2.924667
H	-1.847358	-4.369369	-3.017114
H	-1.644105	-5.558703	-1.702689
H	-3.783927	-2.929926	-0.324201
H	-3.781479	-4.533750	-1.129927
H	-3.691922	-3.028593	-2.117380
H	1.697661	-2.241570	3.162363
H	1.519008	-1.630795	4.844382
H	1.895018	-0.490030	3.512919
H	-0.457282	-0.423271	5.499089
H	-0.109837	0.797365	4.240922
H	-2.553884	0.797597	4.869216
H	-2.660895	-0.933291	4.448482
H	-4.137796	0.692587	1.577169
H	-4.446962	0.762618	3.344438
H	-4.193388	-0.827729	2.533743
H	1.816650	3.259669	0.213325
H	1.960171	4.340984	-1.215664
H	2.273916	2.577063	-1.378016
H	0.556521	2.697116	-3.223286
H	0.219267	4.417710	-2.863511
H	-2.143123	3.871131	-2.286009
H	-1.771310	3.345574	-3.950391
H	-3.752771	0.637723	-2.497176
H	-3.827474	2.128347	-3.495563
H	-3.881015	2.242196	-1.697216
H	2.211826	-1.645709	0.254039
H	1.811945	0.588901	1.021276

H	4.596838	1.138859	-1.250451
H	7.870844	3.239661	0.643850
H	7.337926	2.105359	2.817726
H	5.465330	0.472415	2.954170
H	4.219927	-3.131383	1.563582
H	5.093307	-1.249283	-2.250131
H	5.987066	-4.834747	1.123425
H	6.838230	-2.976067	-2.697973
H	7.296733	-4.767111	-1.009578
H	6.490899	2.725916	-1.384903
H	3.229234	-0.579961	-0.889363
H	3.787375	-0.670258	1.892825

I-2

E(UB-P86) = -3009.64012052 a.u.
Free energy = -3008.994303 a.u.
D3(BJ) dispersion correction = -0.33472550 a.u.
Cartesian

C	4.660099	-1.288072	-1.212369
C	3.693927	-1.520257	-0.221449
C	3.661940	-2.708424	0.527134
C	4.627315	-3.692332	0.266188
C	5.603187	-3.480282	-0.723483
C	5.618348	-2.283957	-1.460004
N	2.691037	-0.484141	0.077042
N	3.000792	0.450586	1.192859
C	4.204399	1.213691	1.000146
C	4.259337	2.183117	-0.022650
C	5.405965	2.977201	-0.163695
C	6.484654	2.833680	0.727456
C	6.417681	1.880274	1.756009
C	5.288128	1.056523	1.885387
S	-0.220810	-1.662385	0.615541
Mo	-2.011218	-0.295889	1.440077
S	-0.550318	1.619601	1.442106
Mo	-1.925230	1.613592	-0.538766
N	-0.948760	3.648181	-1.123837
C	-1.196523	3.898649	-2.572521
C	-2.655408	3.618855	-2.889536
N	-3.038851	2.233263	-2.482327
C	-4.518176	2.082299	-2.582971
S	-0.114739	0.696825	-1.773166
Mo	-1.640237	-1.015388	-1.179218
Cl	-2.798190	-0.949547	-3.470869
S	-3.618247	-0.033010	-0.287256
N	-0.375604	-2.502566	-2.459133
C	-0.684680	-3.897293	-2.031185
C	-2.190133	-4.076145	-1.927672
N	-2.796212	-3.050156	-1.028216
C	-4.280483	-3.099462	-1.147087

Cl	-3.484335	3.314785	0.582921
Cl	-3.276662	-2.387838	2.209593
N	-3.542367	0.804028	2.815512
C	-3.250525	0.520720	4.252672
C	-1.754144	0.417582	4.494366
N	-1.170599	-0.614800	3.589383
C	0.283087	-0.777497	3.851229
C	-5.006204	0.661528	2.569734
C	0.455416	3.978525	-0.766676
C	1.080134	-2.339020	-2.691653
H	-0.853274	-2.339832	-3.361472
H	-2.572802	-3.284275	-0.044129
H	-1.631860	-1.514925	3.801125
H	-3.314656	1.793081	2.612533
H	-1.566809	4.279165	-0.587216
H	-2.624567	1.557857	-3.148451
H	1.278323	-1.325813	-3.068272
H	1.444849	-3.083050	-3.423193
H	1.616618	-2.489654	-1.743367
H	-0.193708	-4.063275	-1.057176
H	-0.271428	-4.625762	-2.754632
H	-2.654363	-3.946690	-2.920857
H	-2.433365	-5.094877	-1.573720
H	-4.725451	-2.519829	-0.328104
H	-4.637290	-4.144187	-1.088295
H	-4.573671	-2.663129	-2.113634
H	0.671920	-1.605842	3.242841
H	0.465792	-0.986206	4.921084
H	0.805144	0.150955	3.573693
H	-1.560483	0.160759	5.553131
H	-1.247456	1.374508	4.279638
H	-3.692869	1.299677	4.900661
H	-3.739738	-0.438070	4.497268
H	-5.247889	1.090344	1.588283
H	-5.581957	1.191803	3.350596
H	-5.265525	-0.407489	2.580090
H	0.582168	3.906791	0.322559
H	0.711918	5.000754	-1.099467
H	1.127558	3.257701	-1.255810
H	-0.528207	3.232214	-3.144520
H	-0.948203	4.944578	-2.835123
H	-3.303581	4.311078	-2.324175
H	-2.854567	3.774960	-3.965557
H	-4.776511	1.017854	-2.512622
H	-4.881505	2.482405	-3.547366
H	-4.987871	2.632878	-1.754203
H	1.709205	-0.902004	0.320656
H	0.682279	1.113795	1.009724
H	3.407004	2.327099	-0.694863
H	7.371661	3.465144	0.620430

H	7.252660	1.760962	2.453085
H	5.243950	0.298265	2.674460
H	2.893209	-2.867631	1.289773
H	4.667030	-0.353600	-1.780799
H	4.612251	-4.625802	0.835778
H	6.376663	-2.120313	-2.230829
H	6.352752	-4.251790	-0.922532
H	5.447490	3.724265	-0.962101
H	2.476069	0.111047	-0.747026
H	3.086301	-0.150934	2.022491

TS-2B

E(UB-P86) = -3009.63064595 a.u.

Imaginary frequency = 290.1024i cm^{-1}

Free energy = -3008.990202 a.u.

D3(BJ) dispersion correction = -0.33087970 a.u.

Cartesian

C	5.719201	-1.509037	-1.216327
C	4.700874	-1.840404	-0.294333
C	4.724228	-3.074422	0.397666
C	5.754118	-3.984191	0.136845
C	6.764664	-3.665934	-0.791540
C	6.745692	-2.431186	-1.462523
N	3.694676	-0.893983	0.010358
N	4.113096	0.355253	1.401447
C	5.401993	0.835328	1.198931
C	5.573260	1.982843	0.370579
C	6.839622	2.545429	0.204919
C	7.955977	1.984967	0.861032
C	7.803064	0.848339	1.676710
C	6.543137	0.260238	1.830479
S	0.632898	-2.141685	0.554313
Mo	-1.133431	-0.775860	1.382924
S	0.327280	1.146349	1.326681
Mo	-1.084367	1.111157	-0.633054
N	-0.114213	3.130041	-1.275285
C	-0.391203	3.353114	-2.723385
C	-1.855960	3.067120	-3.007324
N	-2.231461	1.688871	-2.568316
C	-3.712216	1.534592	-2.640211
S	0.691009	0.176609	-1.881505
Mo	-0.790964	-1.538900	-1.230816
Cl	-1.969121	-1.522703	-3.513718
S	-2.762509	-0.542103	-0.327550
N	0.492928	-3.026776	-2.480760
C	0.184831	-4.419926	-2.045129
C	-1.320347	-4.604842	-1.943879
N	-1.930748	-3.578235	-1.047940
C	-3.415429	-3.638903	-1.154689

Cl	-2.617072	2.828733	0.487647
Cl	-2.400508	-2.844428	2.202224
N	-2.633720	0.353854	2.770088
C	-2.316968	0.090087	4.205714
C	-0.816659	-0.017404	4.421086
N	-0.255153	-1.066101	3.520574
C	1.202817	-1.233985	3.756969
C	-4.102089	0.213791	2.550612
C	1.299521	3.459615	-0.952681
C	1.954393	-2.853521	-2.676632
H	0.035078	-2.877856	-3.395397
H	-1.697384	-3.802626	-0.064405
H	-0.716873	-1.960270	3.755231
H	-2.406353	1.339007	2.549259
H	-0.717547	3.775330	-0.739187
H	-1.828460	1.001748	-3.229117
H	2.153263	-1.846306	-3.068070
H	2.344522	-3.609911	-3.381829
H	2.463846	-2.971575	-1.709439
H	0.673331	-4.577901	-1.068491
H	0.603763	-5.151773	-2.761756
H	-1.784362	-4.480058	-2.937625
H	-1.559292	-5.623385	-1.586398
H	-3.857466	-3.049453	-0.341031
H	-3.764858	-4.684869	-1.077494
H	-3.718616	-3.218906	-2.125295
H	1.572267	-2.080308	3.161764
H	1.405242	-1.418268	4.827726
H	1.728029	-0.318247	3.445320
H	-0.604776	-0.260293	5.479630
H	-0.309113	0.933700	4.183857
H	-2.743337	0.880605	4.850360
H	-2.806270	-0.862547	4.473092
H	-4.357706	0.628227	1.566524
H	-4.662890	0.758706	3.332229
H	-4.365085	-0.853883	2.582041
H	1.441793	3.426898	0.136475
H	1.558191	4.467511	-1.325193
H	1.959929	2.716364	-1.424314
H	0.266235	2.677110	-3.296589
H	-0.149054	4.394082	-3.009933
H	-2.493861	3.769115	-2.442401
H	-2.075251	3.203710	-4.082114
H	-3.967540	0.471019	-2.548233
H	-4.093094	1.918543	-3.604325
H	-4.168569	2.097711	-1.812436
H	2.776223	-1.277570	0.349863
H	1.539662	0.631165	0.866847
H	4.693859	2.419661	-0.113103
H	8.944662	2.436769	0.735308

H	8.670988	0.416310	2.183987
H	6.417345	-0.626356	2.461557
H	3.933435	-3.312418	1.116302
H	5.692555	-0.550371	-1.743075
H	5.769618	-4.945814	0.657848
H	7.530459	-2.184563	-2.183306
H	7.566060	-4.383283	-0.991354
H	6.964463	3.431086	-0.425312
H	3.494706	-0.206379	-0.728573
H	4.150034	-0.387055	2.119342

TS for the elimination of HCl from 1

E(UB-P86) = -2434.437395 a.u.

Imaginary frequency = 335.3175i cm^{-1}

Free energy = -2434.005931 a.u.

D3(BJ) dispersion correction = -0.244247 a.u.

Cartesian

S	-1.08653600	-1.57007300	-1.58495500
Mo	0.78463800	-1.34244900	-0.06276400
S	1.88947200	0.17148300	-1.52943000
Mo	0.64738800	1.48217900	-0.07901200
S	-0.10147300	0.03254400	1.66824100
Mo	-1.70870200	0.04434700	-0.09190100
Cl	-3.08605300	1.67243900	1.36325100
N	1.64341800	3.29756500	-1.09462400
C	1.07191000	4.55273300	-0.51510600
C	1.07454700	4.44683400	0.99899200
N	0.36394200	3.20387400	1.44376700
C	0.59323900	2.98701200	2.90585400
C	1.71823000	3.38977500	-2.58376100
Cl	4.94206100	0.39863500	0.54727000
S	-1.14060400	1.94442100	-1.38392100
N	-3.73507400	-0.00201400	-1.17862000
C	-3.84334000	0.26579700	-2.64072800
N	-2.92358400	-1.47984700	1.13654500
C	-2.86897700	-1.47777000	2.62711000
C	-4.43779100	-1.27274500	-0.82162800
C	-4.34676000	-1.50071800	0.67803900
N	1.77022100	-3.03776000	-1.26450500
C	3.16231400	-3.18386300	-0.75767100
C	3.13302000	-3.03446100	0.75319200
N	2.32604500	-1.85839400	1.13170300
C	2.52075200	-1.58366900	2.55922500
Cl	-0.33622900	-3.46009400	1.02840500
C	1.72861900	-3.09236900	-2.75109700
H	-4.21289400	0.76663500	-0.68003400
H	-2.44346600	-2.35077900	0.83561900
H	1.21803900	-3.83232800	-0.90098100
H	3.75033100	-0.03585000	0.18825700
H	2.61762800	3.22943000	-0.75954900

H	-0.65319600	3.34872500	1.32141800
H	-3.42550500	1.25688300	-2.86416700
H	-4.90057500	0.23430400	-2.95809500
H	-3.27472600	-0.49727400	-3.19280700
H	-3.95323200	-2.08992700	-1.38192500
H	-5.49768200	-1.22439300	-1.13265500
H	-4.86956100	-0.69331000	1.21842200
H	-4.82243500	-2.45917900	0.95271100
H	-1.84166800	-1.69578400	2.94746800
H	-3.54560400	-2.25284600	3.02870000
H	-3.17555300	-0.48831100	2.99571900
H	0.68361000	-3.08946200	-3.08949400
H	2.23095400	-4.00613500	-3.11545400
H	2.24087200	-2.20903600	-3.16105300
H	3.59177600	-4.15730000	-1.05831800
H	3.76496000	-2.38277300	-1.21815000
H	4.16449900	-2.92942600	1.14127900
H	2.69862700	-3.94011900	1.23045600
H	2.05206300	-0.63530300	2.85015700
H	3.60128600	-1.53205000	2.79365100
H	2.08274000	-2.39813800	3.17315900
H	2.21402300	2.49317900	-2.97929900
H	2.28405400	4.28939300	-2.88120100
H	0.69857100	3.44736400	-2.99172600
H	0.04864900	4.66711700	-0.91058000
H	1.66193500	5.43113100	-0.83399100
H	2.10912700	4.38261000	1.37811300
H	0.60759800	5.33795800	1.45366000
H	-0.08813100	2.20872900	3.27161500
H	0.41071500	3.92392700	3.46009700
H	1.63322100	2.66714400	3.06829200

Complex between HCl and the cluster resulting from the HCl elimination

E(UB-P86) = -2434.439477 a.u.
Free energy = -2434.008829 a.u.
D3(BJ) dispersion correction = -0.243658 a.u.
Cartesian

S	-1.03862900	-1.56778100	-1.60029100
Mo	0.76594100	-1.36791800	0.01325600
S	1.95894600	0.14193900	-1.41646200
Mo	0.65599800	1.46738200	-0.00928100
S	-0.18799300	0.01954800	1.69575600
Mo	-1.70920000	0.05399600	-0.13884600
Cl	-3.12603300	1.70817300	1.25195900
N	1.69333000	3.28843100	-0.98746100
C	1.09778900	4.53755300	-0.41925700
C	1.05620000	4.42168100	1.09367800
N	0.33629500	3.17363300	1.51384900
C	0.54606500	2.94077700	2.97671300
C	1.81736600	3.38451300	-2.47281600

Cl	5.02071400	0.39307500	0.09957400
S	-1.05653100	1.94707800	-1.39831700
N	-3.68226900	0.04708200	-1.31919100
C	-3.71400400	0.32005200	-2.78389700
N	-3.00511100	-1.44570400	1.02915500
C	-3.01976800	-1.43945200	2.52113300
C	-4.42366300	-1.21112300	-0.99828300
C	-4.40589300	-1.44380100	0.50395000
N	1.78464800	-3.07356500	-1.14526400
C	3.15603900	-3.22654700	-0.58709700
C	3.07572800	-3.05224000	0.91947600
N	2.25914600	-1.86869800	1.24887400
C	2.48850600	-1.49806200	2.64801500
Cl	-0.42770100	-3.46054900	1.05003500
C	1.79996300	-3.12720900	-2.63302000
H	-4.16712700	0.82438600	-0.84133500
H	-2.52658500	-2.32519800	0.75308100
H	1.21442000	-3.86509700	-0.80478600
H	3.79776600	0.28133200	-0.47200200
H	2.65608600	3.22389900	-0.61989200
H	-0.67918000	3.32103800	1.37721200
H	-3.27437000	1.30721700	-2.98243700
H	-4.75407600	0.30209100	-3.15457500
H	-3.12622700	-0.44734200	-3.30923900
H	-3.92803100	-2.03599800	-1.53729300
H	-5.46720400	-1.14366200	-1.35682200
H	-4.94205200	-0.63064400	1.02235700
H	-4.90750400	-2.39611400	0.75260100
H	-2.01100000	-1.66825600	2.89008900
H	-3.72394900	-2.20465700	2.89302500
H	-3.33049800	-0.44462800	2.87136800
H	0.76911300	-3.11509400	-3.01223200
H	2.30891600	-4.04459500	-2.97858100
H	2.33466100	-2.24760500	-3.02154300
H	3.58556700	-4.20833100	-0.85880100
H	3.78330200	-2.43640900	-1.03251300
H	4.09300100	-2.94212800	1.34021600
H	2.62041300	-3.94660100	1.39819000
H	1.95344700	-0.57798000	2.91333400
H	3.57044900	-1.34471200	2.82552100
H	2.15215000	-2.31220000	3.32355100
H	2.31979000	2.48528000	-2.85377400
H	2.39758800	4.28148400	-2.74928300
H	0.81226000	3.44905700	-2.91468700
H	0.08649500	4.64995700	-0.84487200
H	1.69296300	5.42073000	-0.71438600
H	2.08009500	4.35723300	1.50113300
H	0.57394900	5.30820300	1.54083700
H	-0.14564300	2.16499700	3.32795300
H	0.36474300	3.87445700	3.53672900

H 1.58162600 2.61105200 3.14752300

Cluster resulting from the HCl elimination

E(UB-P86) = -1973.601391 a.u.
Free energy = -1973.173645 a.u.
D3(BJ) dispersion correction = -0.233736 a.u.
Cartesian

S	0.648930	-1.728146	-1.556907
Mo	1.551581	-0.218217	-0.022169
S	1.474340	1.706079	-1.361239
Mo	-0.507737	1.712494	-0.124088
S	-0.086461	0.133728	1.643801
Mo	-1.093211	-1.049944	-0.181056
Cl	-3.288816	-0.998037	1.070544
N	-0.873209	3.637858	-0.682586
C	-2.243785	4.125815	-0.452423
C	-2.633752	3.794156	0.975797
N	-2.298883	2.365996	1.255771
C	-2.300505	2.123184	2.727085
C	-0.202787	4.437715	-1.713867
S	-1.878127	0.687874	-1.613839
N	-2.330103	-2.569936	-1.394102
C	-2.478381	-2.444834	-2.871322
N	-0.854486	-3.006782	1.042607
C	-0.924526	-2.984858	2.532098
C	-1.898418	-3.950353	-1.014791
C	-1.772580	-4.056511	0.497991
N	3.616690	-0.584747	-1.020493
C	4.618030	0.389777	-0.488948
C	4.463924	0.531834	1.016732
N	3.067597	0.947147	1.353471
C	2.873257	0.988821	2.831138
Cl	2.437666	-2.148400	1.363689
C	3.744380	-0.706360	-2.500380
H	-3.258645	-2.410758	-0.970574
H	0.120289	-3.254643	0.801637
H	3.839148	-1.505905	-0.609874
H	2.948372	1.908512	1.005555
H	-3.043300	1.768200	0.860299
H	-2.921614	-1.468690	-3.111786
H	-3.127446	-3.247593	-3.263518
H	-1.487537	-2.514840	-3.344621
H	-0.934325	-4.147860	-1.513506
H	-2.628834	-4.695594	-1.380950
H	-2.756138	-3.898660	0.972116
H	-1.416171	-5.062772	0.782573
H	-0.100964	-2.369842	2.918412
H	-0.834116	-4.009607	2.934173
H	-1.887904	-2.550172	2.835573

H	3.095963	-1.517947	-2.857714
H	4.790767	-0.922766	-2.779963
H	3.431341	0.237417	-2.971399
H	5.643676	0.058210	-0.734266
H	4.445848	1.354929	-0.996105
H	5.187332	1.270980	1.406195
H	4.651100	-0.430420	1.521221
H	1.921180	1.487663	3.058516
H	3.699581	1.541471	3.312391
H	2.844489	-0.041324	3.214810
H	0.869191	4.198091	-1.759706
H	-0.314435	5.518734	-1.496793
H	-0.642794	4.251362	-2.716746
H	-2.949877	3.661973	-1.176857
H	-2.299700	5.221111	-0.601161
H	-2.032793	4.406040	1.669449
H	-3.703223	3.987298	1.174227
H	-2.272921	1.043183	2.921898
H	-3.215010	2.548295	3.178264
H	-1.418855	2.603785	3.176993

HCl

E(UB-P86) = -460.828362 a.u.
Free energy = -460.839817 a.u.
D3(BJ) dispersion correction = -0.000476 a.u.
Cartesian

H	0.000000	0.000000	0.102128
Cl	0.000000	0.000000	1.397872

TS for the hydrogenation of the Cluster resulting from the HCl elimination

E(UB-P86) = -1974.749595 a.u.
Imaginary frequency = 908.3501i cm^{-1}
Free energy = -1974.307682 a.u.
D3(BJ) dispersion correction = -0.241570 a.u.
Cartesian

S	-1.18330200	-1.93330900	-1.29728500
Mo	0.74342300	-1.57995600	-0.04243900
S	2.01125500	-0.37488400	-1.53870000
Mo	0.90758100	1.19856300	-0.17240700
S	0.04714400	-0.04249200	1.66710200
Mo	-1.59792500	-0.00693700	-0.04002700
Cl	-2.80153800	1.79774400	1.25815500
N	1.94688900	2.86329300	-1.39290100
C	1.33558500	4.17984000	-1.03463500
C	1.17048800	4.28310500	0.47319900
N	0.38038900	3.12963900	1.00698500
C	0.39829100	3.14398200	2.49952100
C	2.11766900	2.74685900	-2.86899600
Cl	3.06234400	1.46520400	1.14577900
S	-0.88257500	1.56782300	-1.60351800

N	-3.65325900	-0.00810300	-1.10431800
C	-3.74792600	0.05553000	-2.59137000
N	-2.94940100	-1.35119700	1.34351600
C	-2.82015300	-1.28134000	2.82771000
C	-4.49850700	-1.12325500	-0.57676800
C	-4.38104900	-1.19891300	0.93690800
N	1.57505500	-3.46271900	-0.76324600
C	3.00979600	-3.55778300	-0.50644400
C	3.25736100	-3.25829400	0.96477600
N	2.56613100	-1.98440000	1.35078700
C	2.43464800	-1.90325100	2.83517800
C	1.17042200	-4.10121800	-2.01248200
H	-4.04008900	0.87218400	-0.72818300
H	-2.65155000	-2.29599700	1.06148400
H	0.62391900	-3.47719900	0.51257700
H	3.15396700	-1.18182000	1.06545900
H	2.88688700	2.83254700	-0.96589000
H	-0.60848200	3.24992800	0.73116300
H	-3.22946400	0.95357300	-2.95406400
H	-4.80552800	0.09044300	-2.90686400
H	-3.27015500	-0.83572800	-3.02487900
H	-4.15086800	-2.05714500	-1.05092400
H	-5.55480700	-0.97194100	-0.86591700
H	-4.75377500	-0.27165600	1.40225800
H	-4.98078800	-2.04202300	1.32471100
H	-1.80804100	-1.59249900	3.11967400
H	-3.55922900	-1.94638400	3.30823500
H	-2.99129200	-0.24414400	3.14998300
H	0.07464400	-4.21486700	-2.04928000
H	1.62212900	-5.11099200	-2.08985500
H	1.47977800	-3.52209500	-2.91066800
H	3.37735800	-4.58105200	-0.72721700
H	3.59536700	-2.85852700	-1.14899300
H	4.33317300	-3.19065100	1.20368600
H	2.81634200	-4.05898900	1.58281100
H	2.13576100	-0.88715100	3.12376900
H	3.39952300	-2.14677800	3.31328400
H	1.67039400	-2.61968900	3.17231300
H	2.67556900	1.82931200	-3.10059900
H	2.66757000	3.62015700	-3.26179500
H	1.12759600	2.69467500	-3.34584700
H	0.36164000	4.24592000	-1.54881800
H	1.96846500	5.00943100	-1.40011300
H	2.15456000	4.25539400	0.97051400
H	0.68138500	5.23703300	0.73999100
H	-0.36155700	2.44492100	2.87308200
H	0.17098000	4.15894900	2.87072900
H	1.39440800	2.83543800	2.84824200
H	0.11048900	-3.07416700	1.13681700

$[Mo_3S_4Cl_2H(dmen)_3]^+$
E(UB-P86) = -1974.806915 a.u.
Free energy = -1974.357706 a.u.
D3(BJ) dispersion correction = -0.240960 a.u.
Cartesian

S	1.492148597734	1.473134903804	1.458395831302
Mo	1.550038996575	-0.430292468425	0.143317714166
S	0.538580539341	-2.085730907745	1.511871620141
Mo	-1.134296824125	-1.204169790369	0.137391860571
S	-0.002575527691	-0.046886903256	-1.609917567206
Mo	-0.442410805081	1.511376101394	0.132226169521
Cl	-2.365532537035	2.388692260206	-1.264631814566
N	-2.654951867643	-2.569868903165	1.210956137273
C	-4.041528287531	-2.175674000170	0.813975695233
C	-4.110166366368	-1.951319863301	-0.688693248515
N	-3.095971296321	-0.945589256804	-1.130640165700
C	-3.050321422863	-0.889187052110	-2.619662576099
C	-2.570586647624	-2.788655281334	2.682145946371
Cl	-1.016292007238	-3.288053509324	-1.306501690242
S	-1.939498169477	0.453007329797	1.575089866728
N	-0.910669278321	3.495284827288	1.225835655158
C	-1.071407560456	3.528984912733	2.707374356193
N	0.677265259166	3.138633305308	-1.147867891442
C	0.730412523747	3.036395660804	-2.633815905376
C	0.041900985890	4.558031256570	0.779346967161
C	0.223362948922	4.499751347148	-0.729256508244
N	3.540482588437	-0.932980286426	1.207789702554
C	4.001861737396	-2.282664835882	0.760068091705
C	3.832830627245	-2.412578834280	-0.743320068796
N	2.410666687732	-2.179961443824	-1.138349483319
C	2.298835132842	-2.141022832902	-2.623954049099
C	3.638269044097	-0.817442331769	2.691966192788
H	-1.828332597592	3.712559074966	0.805225092599
H	1.639901121075	3.015094160092	-0.804762982512
H	4.189536087898	-0.242685186901	0.807314655649
H	1.849802168856	-2.986031511520	-0.820040530949
H	-2.442614819221	-3.467105708038	0.745661933892
H	-3.397283816561	-0.008803894097	-0.814441623098
H	-1.870301330024	2.835697030421	3.004275775043
H	-1.326819659058	4.549499362270	3.043550558538
H	-0.129092696908	3.216216705652	3.181375754237
H	0.998555493021	4.387698230041	1.302691730774
H	-0.331695769472	5.555542782988	1.075839707113
H	-0.732312973406	4.695942731930	-1.242754091804
H	0.951731460081	5.264121318125	-1.055569449738
H	1.254720990815	2.112443677965	-2.913350630526
H	1.266140854967	3.903563332271	-3.059222086794
H	-0.296666609219	3.007916427999	-3.025603920435

H	3.409765176653	0.213599348030	2.994225309677
H	4.654584811947	-1.083885317102	3.032612380327
H	2.907209358153	-1.496611323794	3.155204724128
H	5.059806586526	-2.442121127839	1.039130151402
H	3.393417925132	-3.033031011354	1.293129809785
H	4.168542717458	-3.409607891779	-1.082519679360
H	4.442052245683	-1.654795078697	-1.266067691502
H	1.237561588852	-2.155365765542	-2.905456100249
H	2.805706441189	-3.016127522270	-3.068868998772
H	2.766270232321	-1.216293777675	-2.993358741441
H	-1.579224840866	-3.190307455786	2.933000160175
H	-3.350629673083	-3.497406303890	3.012296928091
H	-2.708560686047	-1.827271617330	3.199047702777
H	-4.296989235476	-1.255873174609	1.367210263804
H	-4.762823890534	-2.960214108834	1.108972861171
H	-3.886865692639	-2.889172128919	-1.224600052660
H	-5.125874739218	-1.627262691042	-0.979687607803
H	-2.459979744716	-0.015986960652	-2.927298795781
H	-4.071927694713	-0.799184430798	-3.030847229559
H	-2.580057003243	-1.808942908288	-2.996030861203
H	2.697092260059	0.230438330017	-0.991816633234

$[Mo_3S_4Cl_2(dmen)_3]^{2+}$
E(UB-P86) = -1974.057058 a.u.
Free energy = -1973.612998 a.u.
D3(BJ) dispersion correction = -0.235985 a.u.
Cartesian

C	0.085184	-0.452842	-0.038796
N	0.037323	-0.202551	1.435664
Mo	1.957206	-0.269442	2.692554
S	2.821188	1.259520	1.179055
Mo	4.520413	0.877194	2.744976
N	5.761159	2.338475	1.454512
C	5.987855	2.069266	0.003611
C	-0.999131	-1.063978	2.088553
C	-1.057773	-0.727987	3.566700
N	0.304394	-0.853045	4.188596
C	0.287591	-0.268050	5.567830
S	2.398159	-2.215534	1.647953
Mo	4.174356	-1.852182	3.175357
N	5.097233	-3.825195	2.419730
C	5.037033	-4.208286	0.978508
S	3.393265	-0.103835	4.594799
N	5.959687	-2.168375	4.603250
C	6.537929	-3.536699	4.402266
C	6.498959	-3.930776	2.935384
Cl	3.123003	-3.475330	4.771127
S	5.623128	-0.858746	1.652281
C	5.817313	-1.880312	6.062778

N	4.001953	2.989064	3.639423
C	4.983123	3.994649	3.122681
C	5.269150	3.739195	1.652343
Cl	6.492674	1.214764	4.239858
C	3.803796	3.157601	5.109313
H	-0.272824	0.776055	1.547096
H	0.515830	-1.859977	4.295480
H	4.526093	-4.505656	2.946727
H	6.630428	-1.472169	4.237594
H	6.675372	2.266944	1.928867
H	3.097272	3.191641	3.190956
H	0.814370	0.225838	-0.501079
H	-0.910538	-0.283926	-0.482038
H	0.392317	-1.492678	-0.219482
H	-0.716055	-2.116633	1.920471
H	-1.986812	-0.897741	1.622801
H	-1.386919	0.314633	3.715079
H	-1.773111	-1.383878	4.091497
H	1.201597	-0.556634	6.101636
H	-0.590317	-0.643216	6.120211
H	0.232713	0.827730	5.497551
H	3.988230	-4.271426	0.658275
H	5.523164	-5.187093	0.825025
H	5.553537	-3.447405	0.375202
H	6.871413	-4.964127	2.813887
H	7.133075	-3.268133	2.322552
H	7.573783	-3.567874	4.782912
H	5.931083	-4.232949	5.004594
H	5.608325	-0.811095	6.199099
H	6.754498	-2.136641	6.586361
H	4.989798	-2.480729	6.466060
H	6.467995	1.088955	-0.117366
H	6.635326	2.850386	-0.430691
H	5.021911	2.065026	-0.522385
H	4.356857	3.861134	1.043488
H	6.020308	4.459613	1.281440
H	5.900895	3.896665	3.724894
H	4.588888	5.016851	3.262281
H	2.947208	2.551166	5.433478
H	3.612302	4.218055	5.348472
H	4.710097	2.819726	5.632104

TS for hydrogenation of $[Mo_3S_4Cl_2(dmen)_3]^{2+}$
E(UB-P86) = -1975.203798 a.u.
Imaginary frequency = 1071.0529i cm^{-1}
Free energy = -1974.749634 a.u.
D3(BJ) dispersion correction = -0.247114 a.u.
Cartesian

C	2.123514	-3.507544	-2.255037

N	2.230092	-3.130611	-0.812551
C	3.662846	-2.922183	-0.427275
C	3.739527	-2.659099	1.064745
N	2.829882	-1.532321	1.455273
C	2.646667	-1.532514	2.941212
Mo	0.972135	-1.412325	0.081934
S	0.024829	-0.024737	1.769359
Mo	0.641573	1.315950	-0.107781
S	-1.112289	1.332719	-1.644181
Mo	-1.564534	-0.248123	0.004764
Cl	-3.061110	1.255575	1.289426
S	-0.723127	-1.965176	-1.448566
S	1.860915	-0.124527	-1.600696
N	-3.582577	-0.617349	-1.092263
C	-4.183051	-1.897975	-0.604411
C	-4.054567	-1.994553	0.905603
N	-2.615770	-1.893543	1.310400
C	-2.505328	-1.854638	2.799234
C	-3.702098	-0.525827	-2.576171
N	1.400282	3.102413	-1.373092
C	0.560253	4.296797	-1.052138
C	0.382132	4.400797	0.452199
N	-0.193733	3.133863	1.011608
C	-0.154164	3.178156	2.505304
Cl	2.767286	1.884734	1.100494
C	1.620904	2.993402	-2.844493
H	1.893287	-3.948092	-0.276237
H	3.289764	-0.634686	1.218295
H	2.323993	3.248538	-0.934155
H	-1.193009	3.083806	0.747600
H	-4.139915	0.153393	-0.690717
H	-2.157349	-2.762389	0.999968
H	1.082315	-3.763754	-2.492335
H	2.771503	-4.374559	-2.467503
H	2.442517	-2.658254	-2.876902
H	4.046569	-2.071237	-1.014140
H	4.262079	-3.813554	-0.686235
H	3.409987	-3.551662	1.624581
H	4.777083	-2.439469	1.370452
H	2.208596	-0.576304	3.254931
H	3.620873	-1.666326	3.442436
H	1.974656	-2.355138	3.227601
H	2.360275	2.206547	-3.047177
H	1.994231	3.951868	-3.244803
H	0.673095	2.736889	-3.339943
H	1.036477	5.215848	-1.439527
H	-0.408544	4.173802	-1.565258
H	-0.267629	5.255809	0.708162
H	1.356529	4.554335	0.945999
H	-0.784581	2.374314	2.906799

H	-0.534171	4.151401	2.861021
H	0.884921	3.041345	2.837820
H	-3.376674	0.467941	-2.911351
H	-4.749355	-0.691109	-2.883760
H	-3.065109	-1.291487	-3.043395
H	-3.651721	-2.727689	-1.102169
H	-5.246846	-1.955702	-0.898351
H	-4.591090	-1.166528	1.397969
H	-4.486466	-2.944774	1.266808
H	-1.455025	-1.976284	3.093925
H	-3.107198	-2.663398	3.249151
H	-2.871338	-0.880513	3.154895
H	0.704626	-0.373255	-2.679806
H	-0.199942	-1.024543	-2.620710

$[Mo_3S_2(SH)_2Cl_2(dmen)_3]^{2+}$
E(UB-P86) = -1975.209392 a.u.
Free energy = -1974.751312 a.u.
D3(BJ) dispersion correction = -0.246736 a.u.
Cartesian

C	2.107827	-3.008832	-2.752203
N	2.102542	-2.941486	-1.258253
C	3.505458	-2.930266	-0.732638
C	3.460452	-2.963774	0.781757
N	2.607431	-1.850575	1.312525
C	2.313302	-2.108492	2.758047
Mo	0.870207	-1.357368	-0.120026
S	-0.176436	-0.330554	1.753392
Mo	0.720361	1.346938	0.306548
S	-0.832112	1.855174	-1.375891
Mo	-1.571235	0.009199	-0.151881
Cl	-3.080394	1.303721	1.322234
S	-0.740944	-1.487631	-1.890067
S	2.074844	0.218762	-1.378687
N	-3.494614	0.118556	-1.470625
C	-4.257600	-1.163005	-1.354261
C	-4.277334	-1.633788	0.089088
N	-2.877398	-1.799790	0.595338
C	-2.895506	-2.154200	2.045991
C	-3.459644	0.563523	-2.893364
N	1.704253	3.325205	-0.408204
C	0.892404	4.465476	0.114905
C	0.559818	4.219828	1.575436
N	-0.132634	2.901267	1.753945
C	-0.240779	2.588059	3.211689
Cl	2.750424	1.456006	1.781154
C	2.084983	3.560657	-1.830552
H	1.670898	-3.823515	-0.933983
H	3.151248	-0.969314	1.285723
H	2.578494	3.291227	0.141433

H	-1.101933	2.987327	1.399409
H	-4.015676	0.833751	-0.938738
H	-2.481288	-2.610272	0.097235
H	1.081166	-3.140473	-3.119105
H	2.728078	-3.856436	-3.089728
H	2.524844	-2.074907	-3.156366
H	3.996651	-2.017436	-1.108394
H	4.064284	-3.802447	-1.116691
H	3.010793	-3.911544	1.126127
H	4.477156	-2.904774	1.206721
H	1.923545	-1.191804	3.218919
H	3.235260	-2.414008	3.282499
H	1.564249	-2.910061	2.841427
H	2.804786	2.794221	-2.149323
H	2.547382	4.556983	-1.940009
H	1.188131	3.504608	-2.464717
H	1.450648	5.413892	0.010858
H	-0.020373	4.537879	-0.500418
H	-0.071563	5.033568	1.972645
H	1.482574	4.180025	2.178785
H	-0.953368	1.765472	3.353084
H	-0.597468	3.476711	3.760596
H	0.750433	2.293480	3.585837
H	-3.009898	1.563277	-2.956106
H	-4.482804	0.595490	-3.306570
H	-2.857488	-0.142166	-3.484590
H	-3.764126	-1.904793	-2.005746
H	-5.290627	-1.026951	-1.722852
H	-4.774329	-0.893236	0.737264
H	-4.827933	-2.587570	0.173948
H	-1.888227	-2.454558	2.362887
H	-3.600841	-2.983545	2.229240
H	-3.207679	-1.270335	2.621266
H	1.289248	0.426683	-2.529493
H	-0.291924	-0.567061	-2.848476

TS for H transfer from $[Mo_3S_2(SH)_2Cl_2(dmen)_3]^{2+}$ to $[Mo_2(MoH)S_3(SH)Cl_2(dmen)_3]^{2+}$

E(UB-P86) = -1975.179058 a.u.
Imaginary frequency = 255.0191i cm^{-1}
Free energy = -1974.721506 a.u.
D3(BJ) dispersion correction = -0.245768 a.u.
Cartesian

C	0.108788	-0.078944	0.122941
N	0.087767	-0.020717	1.617441
C	1.478867	-0.055566	2.170032
C	1.398837	-0.069730	3.683540
N	0.574220	1.078738	4.192958

C	0.259590	0.838926	5.638039
Mo	-1.109162	1.580223	2.749326
S	-2.187118	2.607593	4.613535
Mo	-1.230573	4.238126	3.160593
S	-2.864461	4.745853	1.537460
Mo	-3.652485	2.954031	2.759013
Cl	-5.127861	4.124977	4.312122
S	-2.924702	1.364112	1.041796
S	0.334063	3.156630	1.609989
N	-5.591858	3.073523	1.486831
C	-6.314522	1.763390	1.547470
C	-6.294626	1.212703	2.963840
N	-4.884898	1.070430	3.450469
C	-4.873160	0.675378	4.891928
C	-5.570958	3.587486	0.085642
N	-0.256597	6.219817	2.426327
C	-1.070487	7.360566	2.946496
C	-1.408436	7.123607	4.406800
N	-2.127796	5.820264	4.587992
C	-2.256147	5.525970	6.047584
Cl	0.756394	4.386873	4.689172
C	0.105609	6.450936	0.998274
H	-0.375735	-0.891818	1.924922
H	1.152372	1.939244	4.171288
H	0.622818	6.197066	2.967836
H	-3.087586	5.932066	4.223004
H	-6.135582	3.745931	2.050666
H	-4.462260	0.286685	2.931665
H	-0.918551	-0.163452	-0.257542
H	0.691312	-0.953343	-0.212691
H	0.575572	0.834663	-0.273220
H	2.011696	0.833636	1.795261
H	2.012132	-0.953604	1.809890
H	0.910377	-0.997392	4.029033
H	2.407315	-0.037676	4.130114
H	-0.106996	1.769618	6.089551
H	1.169362	0.511915	6.170263
H	-0.511045	0.058130	5.719475
H	0.855832	5.712520	0.684220
H	0.527255	7.463252	0.871286
H	-0.791998	6.350837	0.370341
H	-0.512943	8.309030	2.838698
H	-1.981858	7.432085	2.328349
H	-2.024132	7.951692	4.799767
H	-0.486954	7.069090	5.010525
H	-2.976793	4.710852	6.192071
H	-2.612301	6.423496	6.582709
H	-1.271909	5.228471	6.436963
H	-5.195862	4.619558	0.080684
H	-6.588599	3.566364	-0.341329

H	-4.905380	2.959828	-0.524762
H	-5.817786	1.072526	0.843952
H	-7.358057	1.888581	1.206326
H	-6.810453	1.898880	3.655591
H	-6.811316	0.237400	3.002604
H	-3.852480	0.396958	5.185074
H	-5.548766	-0.181912	5.057083
H	-5.205886	1.529042	5.499823
H	-0.220516	3.364878	0.358249
H	-1.635688	1.970203	0.890051

$[Mo_2(MoH)S_3(SH)Cl_2(dmen)_3]^{2+}$
E(UB-P86) = -1975.188514 a.u.
Free energy = -1974.731178 a.u.
D3(BJ) dispersion correction = -0.243164a.u.
Cartesian

C	2.290352	-2.501283	-2.991728
N	2.084992	-2.786896	-1.539192
C	3.364779	-3.205122	-0.884707
C	3.127096	-3.388871	0.603677
N	2.592219	-2.121258	1.204922
C	2.231015	-2.347529	2.639045
Mo	0.990326	-1.246694	-0.223034
S	-0.062198	-0.254302	1.685777
Mo	0.787486	1.429757	0.238271
S	-0.882144	1.870725	-1.311553
Mo	-1.576807	-0.042873	-0.145083
Cl	-3.089135	1.321887	1.312816
S	-0.822171	-1.613184	-1.687132
S	2.906050	0.341826	-0.682412
N	-3.506203	-0.012918	-1.417778
C	-4.270486	-1.283446	-1.210609
C	-4.285638	-1.648718	0.264939
N	-2.886376	-1.753235	0.786255
C	-2.891172	-1.980580	2.261485
C	-3.458959	0.338889	-2.867286
N	1.669421	3.427491	-0.468637
C	0.780500	4.533767	0.009015
C	0.385349	4.290582	1.455554
N	-0.248009	2.940023	1.633167
C	-0.417097	2.657141	3.090658
Cl	2.575210	1.780651	1.996889
C	2.042274	3.632496	-1.898440
H	1.449117	-3.598146	-1.492892
H	3.361053	-1.434032	1.197178
H	2.536849	3.466360	0.091086
H	-1.203866	2.965240	1.237942
H	-4.025227	0.736514	-0.933341
H	-2.465655	-2.589023	0.357621

H	1.323504	-2.272270	-3.459969
H	2.745695	-3.373198	-3.491425
H	2.960950	-1.637148	-3.102521
H	4.113896	-2.418286	-1.073918
H	3.735794	-4.143874	-1.333171
H	2.382089	-4.182190	0.786322
H	4.061542	-3.683830	1.112199
H	2.042435	-1.380490	3.123188
H	3.058179	-2.861519	3.158408
H	1.325867	-2.969401	2.696566
H	2.787835	2.883507	-2.196387
H	2.468666	4.640646	-2.039803
H	1.147284	3.523942	-2.528301
H	1.301327	5.504560	-0.076975
H	-0.101603	4.561848	-0.651933
H	-0.312907	5.073548	1.799343
H	1.273938	4.315030	2.107232
H	-1.072083	1.785543	3.216095
H	-0.881516	3.529181	3.582281
H	0.568777	2.460711	3.533742
H	-3.022631	1.339813	-2.986673
H	-4.476824	0.329941	-3.294022
H	-2.833920	-0.391959	-3.400921
H	-3.781976	-2.069201	-1.812219
H	-5.304709	-1.169454	-1.582778
H	-4.797923	-0.870832	0.854347
H	-4.820776	-2.602725	0.418300
H	-1.879071	-2.250196	2.592383
H	-3.588098	-2.797101	2.518864
H	-3.206038	-1.055202	2.764849
H	2.807746	0.432907	-2.041664
H	0.891606	-0.177548	-1.503918

Cl^-
E(UB-P86) = -460.390584 a.u.
Free energy = -460.405234 a.u.
D3(BJ) dispersion correction = 0.000000 a.u.

TS for the partial decoordination of one of the dmen ligands of $[Mo_3S_4Cl_3(dmen)_3]^+$
E(UB-P86) = -2434.451719 a.u.
Imaginary frequency = 133.2590i cm^{-1}
Free energy = -2434.014223 a.u.
D3(BJ) dispersion correction = -0.246347 a.u.
Cartesian

C	-0.332852	3.657152	2.676514
N	-0.061746	3.595913	1.210880
Mo	-0.004700	1.587184	0.101632
S	-1.778919	0.817252	1.425455
Mo	-1.256414	-0.907115	-0.014388
N	-4.455375	-1.834562	1.234675

C	-4.449371	-1.726465	2.688870
C	1.163542	4.383316	0.864139
C	1.421781	4.309147	-0.632476
N	1.516957	2.886534	-1.091036
C	1.565455	2.830662	-2.582645
S	1.691120	1.062660	1.595972
Mo	1.516540	-0.777154	0.170308
N	3.236113	-1.758997	1.347423
C	3.316393	-1.632405	2.831988
Cl	-1.617439	2.874341	-1.345986
S	0.165324	-0.036515	-1.652432
N	1.971818	-2.724042	-1.053918
C	3.259149	-3.317122	-0.574781
C	3.369884	-3.192709	0.936339
Cl	3.498109	0.025768	-1.158349
S	0.110067	-2.052916	1.500717
C	1.923188	-2.710534	-2.545552
N	-3.085907	-0.184214	-1.325352
C	-4.460191	-0.706761	-0.985606
C	-4.851368	-0.643183	0.492021
Cl	-1.829187	-2.996115	-1.130417
C	-2.915049	-0.271563	-2.809567
H	-0.859397	4.040240	0.728261
H	2.412272	2.493013	-0.757931
H	4.039885	-1.249459	0.946442
H	1.208037	-3.341492	-0.740212
H	-3.702624	-2.392030	0.826212
H	-3.074519	0.826684	-1.102928
H	-1.301761	3.185036	2.888262
H	-0.354370	4.707402	3.015892
H	0.457716	3.116160	3.217058
H	2.005357	3.961265	1.438673
H	1.037714	5.437337	1.171940
H	0.589578	4.771366	-1.189274
H	2.347380	4.854540	-0.889099
H	1.859546	1.819656	-2.894737
H	2.304848	3.556318	-2.964542
H	0.569912	3.071262	-2.982129
H	3.345582	-0.569565	3.107411
H	4.225216	-2.133440	3.208173
H	2.429422	-2.098523	3.285765
H	4.339924	-3.596833	1.278447
H	2.570294	-3.759431	1.443210
H	3.326481	-4.377615	-0.876946
H	4.075452	-2.767314	-1.071542
H	0.901458	-2.471948	-2.871632
H	2.209277	-3.699462	-2.944442
H	2.618993	-1.945464	-2.918870
H	-3.822474	-0.892393	3.072276
H	-4.084760	-2.668570	3.126954

H	-5.480229	-1.560321	3.053029
H	-4.444008	0.290268	0.946028
H	-5.954123	-0.541437	0.544044
H	-4.510694	-1.748198	-1.347596
H	-5.186107	-0.118919	-1.576011
H	-2.749728	-1.320853	-3.093308
H	-2.052023	0.334717	-3.114357
H	-3.818505	0.108326	-3.318481

$[Mo_3S_4Cl_3(dmen)_3]^+$ with one of the dmen ligands partially decoordinated

E(UB-P86) = -2434.452153 a.u.
Free energy = -2434.014505 a.u.
D3(BJ) dispersion correction = -0.245135 a.u.
Cartesian

C	-0.196953	3.669091	2.645841
N	0.060067	3.593821	1.178224
Mo	0.088509	1.573923	0.087497
S	-1.679077	0.839307	1.432027
Mo	-1.175826	-0.919276	0.011805
N	-4.497575	-2.102883	1.162897
C	-4.635879	-2.038608	2.619971
C	1.288820	4.367779	0.814025
C	1.534439	4.277319	-0.683855
N	1.613974	2.849753	-1.129983
C	1.648771	2.779624	-2.621324
S	1.801164	1.055361	1.566476
Mo	1.595987	-0.801596	0.167108
N	3.319908	-1.787728	1.331159
C	3.421525	-1.644747	2.812945
Cl	-1.518507	2.861339	-1.359079
S	0.230775	-0.070636	-1.647729
N	2.010797	-2.765597	-1.041981
C	3.296652	-3.369883	-0.572241
C	3.430992	-3.227928	0.935511
Cl	3.565967	-0.033862	-1.195198
S	0.195320	-2.042912	1.535249
C	1.947012	-2.764979	-2.533304
N	-3.036308	-0.234391	-1.285640
C	-4.391592	-0.832744	-0.987158
C	-4.820429	-0.842368	0.484615
Cl	-1.713991	-3.012319	-1.109569
C	-2.843967	-0.261818	-2.769914
H	-0.738161	4.040746	0.698989
H	2.509033	2.452503	-0.800983
H	4.124276	-1.292465	0.913833
H	1.241944	-3.370828	-0.715943
H	-3.587571	-2.483682	0.883367
H	-3.076689	0.765946	-1.027083
H	-1.168652	3.208615	2.870072
H	-0.204611	4.722055	2.977219

H	0.592907	3.124074	3.183367
H	2.131736	3.944594	1.386073
H	1.173677	5.425576	1.112843
H	0.701891	4.741479	-1.238405
H	2.462646	4.812259	-0.952742
H	1.930314	1.762923	-2.926576
H	2.391749	3.494450	-3.016471
H	0.652128	3.026314	-3.014228
H	3.463226	-0.579129	3.075604
H	4.331161	-2.149292	3.182314
H	2.537157	-2.098299	3.284163
H	4.401269	-3.639034	1.268419
H	2.632652	-3.778798	1.461338
H	3.345662	-4.434908	-0.861614
H	4.113243	-2.837711	-1.087556
H	0.924548	-2.518451	-2.850978
H	2.217802	-3.760718	-2.925827
H	2.647547	-2.011361	-2.920749
H	-4.041451	-1.226419	3.094426
H	-4.331326	-3.000132	3.062954
H	-5.696215	-1.867249	2.878384
H	-4.395450	0.050085	1.003140
H	-5.918595	-0.712550	0.520785
H	-4.385591	-1.862015	-1.384189
H	-5.128778	-0.257559	-1.575948
H	-2.624336	-1.291755	-3.086299
H	-2.010083	0.397886	-3.042636
H	-3.759646	0.089807	-3.277431

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)_3Br_3(dmen)_3]^+$
E(UB-P86) = -8768.82269631 a.u.
Free energy = -8768.38574731 a.u.
D3(BJ) dispersion correction = -0.26606871 a.u.
Cartesian

C	-3.493067	-1.274071	2.859746
N	-3.485832	-1.067552	1.383364
C	-4.560528	-0.110089	0.976562
C	-4.543207	0.076074	-0.532342
N	-3.188213	0.499598	-1.006947
C	-3.139366	0.472299	-2.498950
Mo	-1.529922	-0.523296	0.276163
S	-1.528563	1.317588	1.686906
Mo	0.311885	1.586277	0.276404
N	2.026505	2.512470	-1.007250
C	1.978882	2.483481	-2.499271
Mo	1.218583	-1.062704	0.276558
N	1.163110	-3.010707	-1.006624
C	1.162028	-2.953846	-2.498630
S	0.000124	-0.000295	-1.471205

S	-0.378179	-1.985090	1.685402
S	1.907379	0.665793	1.686009
N	0.817253	3.552168	1.383923
C	2.183065	4.005618	0.976253
C	2.335990	3.897869	-0.532659
N	2.667838	-2.483337	1.384207
C	2.378105	-3.893172	0.976795
C	2.208162	-3.971544	-0.532107
C	0.644004	3.660416	2.860794
C	2.848902	-2.386653	2.860949
H	-3.700293	-1.976345	0.941087
H	-3.035449	1.487857	-0.737603
H	0.136210	4.192214	0.943382
H	2.806810	1.887326	-0.737454
H	3.562321	-2.213475	0.943214
H	0.231395	-3.373529	-0.736958
H	-2.780766	-2.068739	3.120560
H	-4.503283	-1.560302	3.201061
H	-3.190813	-0.341875	3.359566
H	-4.375403	0.842597	1.500984
H	-5.549385	-0.487055	1.296464
H	-4.778483	-0.875674	-1.038096
H	-5.302621	0.818615	-0.836027
H	-2.224011	0.975627	-2.838033
H	-4.017431	0.996873	-2.915079
H	-3.136261	-0.574030	-2.836889
H	-0.400447	3.442373	3.122379
H	0.903089	4.677671	3.202979
H	1.299416	2.931023	3.359379
H	2.349856	5.050657	1.296059
H	2.916383	3.369947	1.500662
H	3.358734	4.185087	-0.835994
H	1.629154	4.576984	-1.038715
H	1.961217	1.439018	-2.838270
H	2.870667	2.984802	-2.914860
H	1.069568	3.000804	-2.837709
H	3.182815	-1.373098	3.121760
H	3.600156	-3.119750	3.203316
H	1.889617	-2.588670	3.360061
H	1.461269	-4.211047	1.501473
H	3.200146	-4.559728	1.296380
H	3.149712	-3.698799	-1.038093
H	1.945652	-5.000813	-0.835545
H	0.266733	-2.415207	-2.837066
H	1.149629	-3.976270	-2.915556
H	2.065000	-2.425004	-2.836230
Br	3.466426	-0.685969	-1.155834
Br	-2.328052	-2.659425	-1.154998
Br	-1.140330	3.343784	-1.154916

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)(\mu\text{-}SH)_2Br_3(dmen)_3]^+$
E(UB-P86) = -8769.98125455 a.u.
Free energy = -8769.52839855 a.u.
D3(BJ) dispersion correction = -0.27569298 a.u.
Cartesian

C	-1.660477	3.342966	2.820025
N	-1.402428	3.335150	1.353380
C	-0.522397	4.480925	0.972522
C	-0.314761	4.492096	-0.532017
N	0.226595	3.180801	-1.005935
C	0.218973	3.146807	-2.498510
Mo	-0.675679	1.418609	0.230278
S	1.160094	1.559629	1.818478
Mo	1.599219	-0.161695	0.209479
N	2.631630	-1.791208	-1.079802
C	2.605795	-1.695479	-2.570189
Mo	-0.969906	-1.256741	0.219450
N	-2.860926	-1.375459	-1.080973
C	-2.763562	-1.417808	-2.570345
S	0.014328	-0.001910	-1.556598
S	-1.909747	0.184216	1.810736
S	0.802834	-1.790351	1.789420
N	3.631945	-0.539947	1.290188
C	4.151027	-1.879457	0.882632
C	4.038193	-2.022809	-0.624753
N	-2.300912	-2.825927	1.313416
C	-3.718438	-2.609339	0.900460
C	-3.781776	-2.458649	-0.609519
C	3.793806	-0.334010	2.756861
C	-2.203062	-3.048416	2.782896
H	-2.310947	3.475100	0.882384
H	1.225802	3.114317	-0.732423
H	4.211377	0.172289	0.815783
H	2.064182	-2.626320	-0.843102
H	-1.972679	-3.690052	0.851152
H	-3.280324	-0.453676	-0.846495
H	-2.395088	2.564716	3.067036
H	-2.046946	4.328392	3.135046
H	-0.723349	3.137947	3.358886
H	0.435038	4.360562	1.507939
H	-0.974111	5.436550	1.297512
H	-1.276765	4.651534	-1.049175
H	0.364345	5.314278	-0.821310
H	0.812417	2.289744	-2.842902
H	0.655929	4.077325	-2.902662
H	-0.819497	3.042610	-2.846007
H	3.532039	0.702056	3.012185
H	4.838015	-0.530055	3.057767
H	3.129859	-1.021617	3.301950

H	5.205394	-1.994460	1.195408
H	3.556535	-2.646652	1.407227
H	4.385798	-3.020863	-0.946899
H	4.669123	-1.268326	-1.125739
H	1.567182	-1.767322	-2.919240
H	3.194835	-2.517814	-3.014045
H	3.031438	-0.727628	-2.873426
H	-1.177186	-3.348940	3.037508
H	-2.903033	-3.842472	3.097519
H	-2.448746	-2.115512	3.311442
H	-4.081912	-1.702012	1.411943
H	-4.349058	-3.459875	1.219536
H	-3.456970	-3.392601	-1.100114
H	-4.815266	-2.247205	-0.936492
H	-2.283310	-0.497828	-2.928307
H	-3.772016	-1.497560	-3.012919
H	-2.158895	-2.289444	-2.862014
H	0.577582	0.885123	2.902789
H	0.419856	-1.004570	2.886778
Br	-0.287196	-3.519705	-1.054697
Br	-2.870100	2.009613	-1.160447
Br	3.205733	1.539029	-1.082743

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)_3Cl_3(dnbpy)_3]^+$
E(UB-P86) = -3113.21216469 a.u.
Free energy = -3112.82061069 a.u.
D3(BJ) dispersion correction = -0.3030287 a.u.
Cartesian

S	1.136802	-1.680840	1.456641
Mo	-0.728762	-1.470842	0.070271
S	-2.024738	-0.146149	1.455356
Mo	-0.910101	1.366684	0.071536
S	0.885266	1.824396	1.458613
Mo	1.638843	0.105070	0.072732
Cl	2.966194	1.738045	-1.295333
S	0.001121	0.001117	-1.668400
Cl	-2.986411	1.698973	-1.298895
Cl	0.022626	-3.435744	-1.298303
C	-0.929955	4.432852	-0.576474
C	0.205935	3.285679	-2.278563
C	0.421442	4.464899	-2.999689
C	-0.054653	5.671407	-2.473302
C	-0.736184	5.652133	-1.251389
C	-1.668544	4.337243	0.699418
C	-2.485926	2.947432	2.400229
C	-3.025603	4.030837	3.099555
C	-2.874210	5.318055	2.567994
C	-2.187307	5.467833	1.359813
H	0.564867	2.326637	-2.652516

H	0.954025	4.422332	-3.952539
H	0.094192	6.615386	-3.004380
H	-1.121365	6.583481	-0.833818
H	-2.577136	1.931384	2.788126
H	-3.548340	3.853958	4.042382
H	-3.277904	6.192868	3.084473
H	-2.052428	6.463485	0.935173
N	-0.447603	3.259577	-1.092578
N	-1.826799	3.081760	1.222978
C	4.306764	-1.405693	-0.577093
C	2.747396	-1.814413	-2.281348
C	3.665208	-2.580765	-3.007529
C	4.950535	-2.764496	-2.484347
C	5.271377	-2.170187	-1.258874
C	4.588231	-0.728426	0.705400
C	3.790651	0.669082	2.409311
C	4.994149	0.584036	3.115403
C	6.031132	-0.195782	2.587224
C	5.820858	-0.857753	1.374184
H	1.736115	-1.649516	-2.653619
H	3.364050	-3.017347	-3.962562
H	5.698004	-3.355180	-3.020694
H	6.272745	-2.294823	-0.844450
H	2.957217	1.258501	2.795506
H	5.100253	1.119800	4.061511
H	6.986055	-0.293905	3.110200
H	6.613113	-1.478263	0.953190
N	3.048811	-1.240272	-1.092305
N	3.580713	0.038300	1.227555
C	-2.924596	-3.610364	0.699566
C	-1.317571	-3.617345	2.405532
C	-1.991936	-4.619151	3.109616
C	-3.183596	-5.129621	2.578816
C	-3.651274	-4.616192	1.365705
C	-3.370225	-3.026352	-0.582244
C	-2.943376	-1.470204	-2.285071
C	-4.065918	-1.880759	-3.011901
C	-4.868694	-2.901592	-2.489446
C	-4.515176	-3.477777	-1.264274
H	-0.391701	-3.188998	2.793534
H	-1.581691	-4.978834	4.056059
H	-3.744607	-5.909821	3.099944
H	-4.582801	-4.994466	0.942463
H	-2.294785	-0.676606	-2.656535
H	-4.292883	-1.400648	-3.966551
H	-5.754374	-3.252166	-3.026057
H	-5.125081	-4.281868	-0.850031
N	-1.758250	-3.119918	1.223653
N	-2.597509	-2.019372	-1.096322

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)(\mu\text{-}SH)_2Cl_3(dnbpy)_3]^+$
E(UB-P86) = -3114.36769735 a.u.
Free energy = -3113.96016335 a.u.
D3(BJ) dispersion correction = -0.31253177 a.u.
Cartesian

N	0.548757	3.161629	-1.115530
C	0.488009	4.420863	-0.576318
C	1.120350	5.509271	-1.205278
C	1.799773	5.319428	-2.413988
C	1.829824	4.037924	-2.974550
C	1.201627	2.990936	-2.291639
C	-0.318628	4.579921	0.653342
C	-0.450562	5.819221	1.309907
C	-1.263425	5.929038	2.441878
C	-1.938895	4.789167	2.894521
C	-1.758138	3.584669	2.207552
N	-0.963636	3.464103	1.116175
Mo	-0.534488	1.509928	0.006758
Cl	-2.398473	2.377948	-1.370334
S	-1.912186	0.437154	1.578601
Mo	-1.127248	-1.154843	0.061870
N	-2.633891	-2.410673	1.208956
C	-3.887430	-2.499919	0.668254
C	-4.916867	-3.196664	1.330232
C	-4.662356	-3.820756	2.555100
C	-3.372261	-3.739286	3.093823
C	-2.394963	-3.026315	2.392422
C	-4.085590	-1.844637	-0.640692
C	-5.303381	-1.914680	-1.341375
C	-5.420261	-1.320212	-2.602426
C	-4.307208	-0.666893	-3.143272
C	-3.125854	-0.620844	-2.396351
N	-3.004425	-1.186004	-1.169388
S	1.325240	1.486618	1.571766
Mo	1.597004	-0.356783	0.046718
N	3.474665	-0.976405	1.176231
C	4.164419	-2.045313	0.673765
C	5.316774	-2.533982	1.320591
C	5.777305	-1.918980	2.487738
C	5.073729	-0.815222	2.987691
C	3.933919	-0.381796	2.305286
C	3.645212	-2.628831	-0.578510
C	4.296982	-3.686747	-1.238991
C	3.800615	-4.165444	-2.455438
C	2.653837	-3.565916	-2.988757
C	2.038459	-2.531489	-2.277622
N	2.503826	-2.061464	-1.090769
S	0.028278	-0.044375	-1.723549
S	0.600525	-1.838182	1.646418

Cl	3.341994	0.939721	-1.179167
Cl	-0.824093	-3.370802	-1.055341
H	1.138939	-2.053322	-2.663246
H	2.225662	-3.887316	-3.941175
H	4.307034	-4.982834	-2.975523
H	5.198658	-4.129281	-0.813359
H	3.363134	0.475186	2.665180
H	5.390658	-0.289983	3.891585
H	6.670648	-2.295317	2.993174
H	5.854784	-3.391385	0.914339
H	-2.237585	-0.123467	-2.785314
H	-4.337599	-0.194924	-4.127937
H	-6.363534	-1.377765	-3.152136
H	-6.156568	-2.442149	-0.912976
H	-1.380284	-2.943462	2.783339
H	-3.112744	-4.213263	4.043286
H	-5.458193	-4.361239	3.074264
H	-5.915196	-3.252231	0.894243
H	-2.260651	2.673621	2.536989
H	-2.595473	4.815992	3.767272
H	-1.367450	6.888922	2.954688
H	0.078321	6.698455	0.939926
H	1.204003	1.978960	-2.695786
H	2.331008	3.835476	-3.923905
H	2.284480	6.164299	-2.910602
H	1.070213	6.507201	-0.767940
H	0.313483	-0.997336	2.729607
H	0.685830	0.934942	2.686891

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)_3(tacn)_3]^{4+}$
E(UB-P86) = -1451.53546448 a.u.
Free energy = -1450.92221748 a.u.
D3(BJ) dispersion correction = -0.28965536 a.u.
Cartesian

C	3.605449	-1.910582	1.953745
C	2.329228	-2.657163	2.307906
N	1.512735	-2.913296	1.073453
C	1.979846	-4.040436	0.190704
C	3.133123	-3.608249	-0.707503
N	2.929430	-2.212395	-1.266042
C	4.221721	-1.440911	-1.307769
C	4.435952	-0.606237	-0.014599
N	3.311700	-0.801173	0.969672
Mo	1.297190	-1.012647	-0.193632
S	1.866813	0.757134	-1.592961
Mo	0.218095	1.596802	-0.198754
N	-1.035893	3.188768	0.968497
C	-1.597285	4.140468	-0.052220
C	-0.473352	4.668207	-0.941188

N	0.517247	3.578398	-1.308289
C	1.936022	4.029067	-1.098030
C	2.243747	4.064486	0.396253
N	1.676741	2.850848	1.111134
C	1.003010	3.216913	2.401730
C	-0.316417	3.909056	2.087513
Mo	-1.505761	-0.647837	-0.234013
N	-3.328154	-1.427414	-1.379465
C	-4.423509	-0.401356	-1.298089
C	-4.668920	-0.027242	0.161575
N	-3.367572	0.118362	0.929547
C	-3.425520	-0.540185	2.276090
C	-3.375154	-2.050575	2.078570
N	-2.343305	-2.409541	1.031560
C	-2.837451	-3.441828	0.056813
C	-3.807725	-2.796047	-0.929660
S	-0.020611	-0.028471	1.562576
S	-0.226084	-2.008523	-1.625433
S	-1.557380	1.193742	-1.646178
H	1.110378	-4.341460	-0.413123
H	2.283784	-4.905600	0.805613
H	4.084716	-3.617616	-0.159333
H	3.241886	-4.321282	-1.539967
H	4.176209	-0.768592	-2.176602
H	5.055977	-2.140753	-1.477071
H	5.390743	-0.860717	0.473491
H	4.472958	0.462687	-0.269353
H	-3.333345	-4.271541	0.590694
H	-1.955265	-3.846930	-0.459874
H	-3.938280	-3.447444	-1.807232
H	-4.802365	-2.674508	-0.473939
H	-5.352173	-0.792479	-1.749823
H	-4.103813	0.471465	-1.885113
H	-5.238692	0.912631	0.218809
H	-5.273582	-0.795249	0.665930
H	-4.343947	-0.250556	2.815928
H	-2.560003	-0.184152	2.853723
H	-3.136701	-2.555456	3.027034
H	-4.348523	-2.440151	1.744660
H	2.091075	5.028279	-1.541587
H	2.591289	3.319598	-1.623423
H	3.331469	4.112378	0.557009
H	1.813676	4.963649	0.862217
H	1.651569	3.875281	3.005986
H	0.838627	2.285832	2.962772
H	-0.954926	3.943446	2.983186
H	-0.151941	4.950183	1.771822
H	-2.113610	4.979052	0.447061
H	-2.340828	3.590970	-0.646958
H	-0.897132	5.103420	-1.859097

H	0.081199	5.472054	-0.433999
H	0.594117	-3.210519	1.421787
H	3.246145	0.060195	1.523052
H	2.617880	-2.317109	-2.239061
H	-3.057802	-1.501397	-2.367838
H	-3.237823	1.121427	1.096395
H	-1.556982	-2.828433	1.538054
H	-1.830882	2.704558	1.400268
H	0.408860	3.383646	-2.311009
H	2.476329	2.261364	1.366741
H	1.699461	-2.051503	2.977748
H	2.564834	-3.607066	2.818304
H	4.065279	-1.490816	2.862683
H	4.349266	-2.580451	1.502613

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)(\mu\text{-}SH)_2(tacn)_3]^{4+}$
E(UB-P86) = -1452.69708429 a.u.
Free energy = -1452.06603629 a.u.
D3(BJ) dispersion correction = -0.2987101 a.u.
Cartesian

C	0.695314	3.283188	2.345130
C	2.200690	3.136862	2.148654
N	2.502882	2.114603	1.072203
C	3.569346	2.575608	0.116509
C	2.988789	3.622267	-0.830080
N	1.599267	3.233384	-1.293775
C	0.633754	4.379375	-1.194006
C	0.265806	4.613018	0.268816
N	0.035106	3.302782	0.997619
Mo	0.717209	1.417841	-0.191174
S	-1.098120	1.569577	-1.786922
Mo	-1.628785	-0.128297	-0.183836
N	-2.904884	-1.628977	1.006948
C	-3.726973	-2.407255	0.018261
C	-4.506283	-1.436750	-0.865228
N	-3.643893	-0.262621	-1.283058
C	-4.358101	1.050225	-1.125642
C	-4.432397	1.414772	0.353371
N	-3.123531	1.116563	1.060736
C	-3.344335	0.421447	2.374935
C	-3.749296	-1.024951	2.111960
Mo	0.945200	-1.280623	-0.187997
N	2.150403	-2.897580	-1.293036
C	1.398319	-4.196209	-1.238997
C	1.043798	-4.524056	0.209022
N	0.573163	-3.291290	0.957299
C	1.193013	-3.184689	2.320254
C	2.654280	-2.781563	2.160632
N	2.793858	-1.692828	1.117788

C	3.943949	-1.931053	0.178583
C	3.576698	-3.043958	-0.799802
S	-0.038720	-0.000280	1.603999
S	1.924028	0.159377	-1.751572
S	-0.830481	-1.725773	-1.787915
H	0.281848	2.430333	2.902764
H	0.470898	4.206704	2.907480
H	2.654527	4.091955	1.845142
H	2.683736	2.839101	3.091654
H	3.912091	1.692066	-0.440598
H	4.430280	2.990348	0.669529
H	2.922886	4.603743	-0.336324
H	3.649515	3.747787	-1.701399
H	-0.253076	4.117412	-1.788662
H	1.075239	5.294531	-1.626640
H	1.066898	5.155653	0.792930
H	-0.636863	5.239390	0.335701
H	4.854638	-2.198756	0.742646
H	4.132926	-0.987530	-0.353502
H	4.267896	-3.033856	-1.656216
H	3.673471	-4.031257	-0.323309
H	2.001662	-5.011298	-1.676434
H	0.493593	-4.077855	-1.852245
H	0.260491	-5.296976	0.239812
H	1.914173	-4.935469	0.741938
H	1.117056	-4.142575	2.864751
H	0.628154	-2.423981	2.879703
H	3.064992	-2.433610	3.120583
H	3.269273	-3.636420	1.841770
H	-5.373101	0.991041	-1.556236
H	-3.792412	1.803740	-1.692201
H	-4.683923	2.480058	0.468486
H	-5.226974	0.845181	0.857769
H	-4.124734	0.937271	2.962066
H	-2.400324	0.472399	2.936667
H	-3.641457	-1.622721	3.029797
H	-4.806038	-1.092493	1.812067
H	-4.419836	-3.090440	0.540572
H	-3.037381	-3.018695	-0.582499
H	-4.880964	-1.956997	-1.759697
H	-5.385706	-1.042502	-0.333839
H	2.874521	1.288477	1.552762
H	-0.974430	3.230366	1.161346
H	1.662415	2.974474	-2.285433
H	2.192310	-2.611971	-2.278465
H	-0.433291	-3.412990	1.105332
H	2.995525	-0.826792	1.628933
H	-2.274380	-2.295680	1.462167
H	-3.437392	-0.373765	-2.282783
H	-2.695841	2.021813	1.278999

H	-0.401157	-0.948298	-2.878393
H	-0.546069	0.872033	-2.876916

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)_3Cl_3(edpp)_3]^+$
E(UB-P86) = -3440.4020224 a.u.
Free energy = -3439.7220634 a.u.
D3(BJ) dispersion correction = -0.43355585 a.u.
Cartesian

Mo	-1.593336	-0.259226	-1.075320
Cl	-2.667036	-1.994962	-2.561177
Mo	0.571396	1.504985	-1.076113
Cl	-0.400106	3.299472	-2.564171
Mo	1.018691	-1.253541	-1.078881
Cl	3.056230	-1.313038	-2.568046
S	-0.725088	-1.918967	0.323016
S	-0.002432	-0.002572	-2.838264
S	-1.293407	1.584149	0.325907
S	2.020225	0.323400	0.322668
P	2.256837	-3.137318	0.183575
P	-3.843419	-0.375741	0.189013
P	1.591825	3.514686	0.184409
N	0.580356	-3.094411	-2.397891
N	2.379490	2.044515	-2.401717
N	-2.964637	1.040177	-2.398335
C	-4.868466	-1.920416	0.079454
C	-3.961986	0.062097	1.990589
C	-4.792991	0.981181	-0.695098
C	-4.445083	0.969789	-2.185198
C	4.109135	-3.233063	0.084426
C	1.574910	-4.643795	-0.706778
C	1.396158	-4.333382	-2.194444
C	2.036632	3.397417	1.984341
C	1.931321	-3.466644	1.982841
C	3.238905	3.667011	-0.704377
C	3.055543	3.364415	-2.193270
C	0.758567	5.171356	0.080081
H	3.902826	2.924484	-0.228983
H	3.694834	4.659946	-0.563021
H	4.033139	3.367257	-2.705777
H	2.419589	4.126286	-2.671065
H	0.603214	-4.857249	-0.228891
H	2.216069	-5.529034	-0.568965
H	2.370128	-4.154783	-2.676378
H	0.914387	-5.184977	-2.705539
H	-4.936012	1.814975	-2.698070
H	-4.790741	0.037790	-2.659513
H	-2.619296	2.009907	-2.299135
H	-2.765455	0.779406	-3.372465
H	0.691213	-2.791140	-3.373817

H	-0.428493	-3.290509	-2.286236
H	-4.471501	1.924898	-0.221741
H	-5.880943	0.888799	-0.548309
H	3.048460	1.262418	-2.301576
H	2.053044	1.998950	-3.375333
C	4.786578	-4.203201	-0.681012
C	6.191790	-4.217097	-0.717365
C	6.928493	-3.266440	0.006415
C	6.256845	-2.297390	0.772565
C	4.854662	-2.277417	0.810399
H	4.236309	-4.956265	-1.251979
H	6.707138	-4.977223	-1.313017
H	8.022481	-3.281169	-0.023114
H	6.824222	-1.555777	1.343874
H	4.342110	-1.518109	1.410982
C	1.604427	-2.406186	2.853508
C	1.408262	-2.652599	4.223294
C	1.526379	-3.957562	4.729151
C	1.850068	-5.017743	3.864686
C	2.058994	-4.775816	2.497577
H	1.500501	-1.388179	2.463469
H	1.158950	-1.822980	4.892157
H	1.367764	-4.149008	5.795048
H	1.944539	-6.036471	4.253602
H	2.324271	-5.610859	1.841517
C	-0.450598	5.342484	0.790717
C	-1.124127	6.572394	0.753953
C	-0.602030	7.640840	0.003524
C	0.598119	7.474776	-0.705205
C	1.279190	6.245463	-0.668923
H	-0.867213	4.516800	1.377828
H	-2.056992	6.695556	1.313348
H	-1.128518	8.599945	-0.025549
H	1.012969	8.302668	-1.288871
H	2.213810	6.143067	-1.227524
C	3.096616	4.172868	2.503869
C	3.407817	4.112459	3.871603
C	2.658637	3.290804	4.731691
C	1.597459	2.525446	4.220854
C	1.288689	2.572902	2.850490
H	3.680347	4.829234	1.850983
H	4.234823	4.712240	4.264433
H	2.901473	3.248801	5.798099
H	1.009342	1.885754	4.886234
H	0.467092	1.965476	2.456295
C	-2.875668	-0.184159	2.856015
C	-2.987306	0.102103	4.227511
C	-4.177376	0.644030	4.740332
C	-5.261875	0.892316	3.881102
C	-5.160356	0.597347	2.512165

H	-1.941642	-0.597090	2.460509
H	-2.140746	-0.095751	4.892357
H	-4.261063	0.871499	5.807664
H	-6.192184	1.313082	4.275409
H	-6.019530	0.782723	1.859898
C	-6.064457	-1.996696	-0.661620
C	-6.792812	-3.198534	-0.701802
C	-6.335522	-4.327563	-0.004384
C	-5.143725	-4.255097	0.738463
C	-4.411222	-3.059492	0.779065
H	-6.444005	-1.130358	-1.210679
H	-7.721436	-3.245803	-1.279385
H	-6.906435	-5.260817	-0.036174
H	-4.783084	-5.129901	1.288896
H	-3.483236	-3.014435	1.359558

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)(\mu\text{-}SH)_2Cl_3(edpp)_3]^+$
E(UB-P86) = -3441.55261545 a.u.
Free energy = -3440.85362745 a.u.
D3(BJ) dispersion correction = -0.44226055 a.u.
Cartesian

C	4.232274	-3.202893	0.172436
C	3.193876	-4.147143	0.017456
C	3.516370	-5.509064	-0.154979
C	4.860558	-5.918170	-0.176249
C	5.889577	-4.976311	-0.014243
C	5.572891	-3.618539	0.163738
P	1.437693	-3.546320	0.148117
C	0.357799	-4.818525	-0.710442
C	0.284205	-4.491210	-2.202357
N	-0.216366	-3.097206	-2.411869
Mo	0.685715	-1.402572	-1.141863
S	-1.143064	-1.623866	0.463967
Mo	-1.639729	0.104852	-1.115579
N	-2.670477	1.661245	-2.433868
C	-4.105590	2.003639	-2.180920
C	-4.360775	2.185281	-0.683793
P	-3.863686	0.607532	0.193353
C	-5.312756	-0.552511	0.084975
C	-5.080055	-1.930727	0.287285
C	-6.152903	-2.835429	0.295962
C	-7.464475	-2.376297	0.085849
C	-7.700246	-1.008258	-0.125744
C	-6.631231	-0.096252	-0.121030
Cl	2.640403	-1.903838	-2.609374
Mo	0.882203	1.282821	-1.131720
N	2.677382	1.406789	-2.520930
C	3.699038	2.478896	-2.301177
C	4.041330	2.601032	-0.815776

P	2.461257	2.934627	0.133427
C	2.892070	2.689392	1.926657
C	1.865403	2.816195	2.888579
C	2.148099	2.653956	4.253421
C	3.457630	2.360140	4.672718
C	4.483093	2.237865	3.721558
C	4.205791	2.403215	2.352945
S	1.913961	-0.148572	0.432154
S	-0.079703	0.010354	-2.919234
Cl	-3.081241	-1.453974	-2.453120
S	-0.879178	1.754096	0.469384
Cl	0.202407	3.327765	-2.434357
C	2.168962	4.772021	0.050966
C	3.202643	5.692153	-0.220544
C	2.941360	7.072975	-0.205282
C	1.653216	7.546383	0.091427
C	0.620333	6.634117	0.367723
C	0.873196	5.253997	0.339915
C	1.076719	-3.763299	1.962300
C	1.589128	-2.814948	2.875466
C	1.362766	-2.963639	4.253061
C	0.621072	-4.056829	4.733361
C	0.112174	-5.004537	3.830544
C	0.339285	-4.863272	2.450498
C	-3.817574	1.027504	2.005599
C	-4.142104	2.311847	2.491134
C	-4.091700	2.577722	3.870884
C	-3.721263	1.569019	4.774625
C	-3.405249	0.285121	4.296750
C	-3.451561	0.014795	2.920465
H	-3.720022	2.989179	-0.282579
H	-5.407815	2.465017	-0.488996
H	-4.374665	2.922913	-2.729519
H	-4.714993	1.177913	-2.582810
H	4.438383	1.644201	-0.435564
H	4.807674	3.374042	-0.650401
H	3.271054	3.419965	-2.683378
H	4.606364	2.254303	-2.888111
H	-0.376162	-5.209842	-2.718375
H	1.282058	-4.553182	-2.666090
H	-1.244828	-3.044848	-2.292460
H	-0.054724	-2.834973	-3.392250
H	2.312307	1.492556	-3.477913
H	3.110366	0.464863	-2.478315
H	-0.643224	-4.737872	-0.251977
H	0.713537	-5.848726	-0.554018
H	-2.074391	2.508384	-2.402270
H	-2.588654	1.309964	-3.396704
H	4.217893	5.350198	-0.440714
H	3.751270	7.776730	-0.422084

H	1.453807	8.622557	0.105543
H	-0.387851	6.995335	0.594865
H	0.057475	4.549507	0.530454
H	0.841708	3.049652	2.577434
H	1.343748	2.757429	4.988577
H	3.677717	2.232435	5.737204
H	5.507150	2.018348	4.039972
H	5.024060	2.313298	1.633263
H	-4.058713	-2.299003	0.424426
H	-5.960839	-3.901220	0.455789
H	-8.299989	-3.083400	0.084853
H	-8.718859	-0.643162	-0.290836
H	-6.842564	0.965842	-0.274243
H	-4.443603	3.111400	1.809137
H	-4.349472	3.577156	4.235444
H	-3.684571	1.779690	5.847960
H	-3.123489	-0.509450	4.994787
H	-3.211559	-0.992632	2.563911
H	2.160935	-1.954714	2.512692
H	1.765867	-2.222134	4.950129
H	0.443759	-4.171085	5.807355
H	-0.460823	-5.862520	4.196335
H	-0.057915	-5.620891	1.769451
H	2.732518	-6.263510	-0.268710
H	5.099329	-6.977312	-0.315682
H	6.935470	-5.298942	-0.028147
H	6.370168	-2.878300	0.285970
H	3.989995	-2.141051	0.286467
H	-0.470598	0.977237	1.563182
H	-0.570123	-0.956851	1.556538

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)_3Cl_3(dmpe)_3]^+$
E(UB-P86) = -2381.3685054 a.u.
Free energy = -2380.8390884 a.u.
D3(BJ) dispersion correction = -0.36356697 a.u.
Cartesian

C	-1.289233	3.535959	3.208314
C	-1.197367	5.094277	0.718270
C	-0.941509	5.039760	-0.795094
C	0.331387	3.606951	-3.054677
Mo	-0.675837	1.487220	0.043208
S	1.161691	1.687935	1.442565
Mo	1.626480	-0.158347	0.044375
C	2.956670	-2.086599	-3.056074
Mo	-0.950117	-1.329338	0.043272
C	-3.287188	-1.516093	-3.055492
Cl	-2.544934	2.125030	-1.557578
S	0.000858	-0.000163	-1.713147
S	-2.042393	0.163536	1.441158

Cl	3.113670	1.143412	-1.555245
S	0.879293	-1.852274	1.441245
C	5.009977	-1.513038	0.717432
C	4.835090	-1.704022	-0.796448
Cl	-0.567915	-3.267538	-1.557231
C	-3.814896	-3.581596	0.717970
C	-3.894449	-3.334188	-0.795684
C	3.708053	-0.654400	3.208603
C	-2.418721	-2.882824	3.208159
H	-1.653456	2.632142	3.721329
H	-1.760777	4.426943	3.653114
H	-0.196368	3.595468	3.322134
H	-0.281303	5.381680	1.263115
H	-1.974930	5.835189	0.971277
H	-1.874007	4.861964	-1.354102
H	-0.492594	5.981275	-1.156788
H	1.132562	2.909858	-3.344630
H	0.558688	4.616158	-3.433860
H	-0.628266	3.255402	-3.460563
H	3.109546	0.114192	3.722278
H	4.715699	-0.694009	3.652486
H	3.211131	-1.629593	3.322428
H	6.040581	-1.211566	0.971497
H	4.799930	-2.451067	1.260206
H	5.425784	-2.562768	-1.160206
H	5.147312	-0.806331	-1.353492
H	1.952701	-2.433023	-3.345866
H	3.717877	-2.786547	-3.436454
H	3.130419	-1.078943	-3.460709
H	-1.453651	-2.746402	3.720774
H	-2.954797	-3.736082	3.653679
H	-3.016178	-1.965732	3.321559
H	-4.520907	-2.930245	1.261924
H	-4.069547	-4.624805	0.971854
H	-3.274485	-4.053896	-1.353658
H	-4.934040	-3.415511	-1.158142
H	-3.086786	-0.473031	-3.344886
H	-4.273720	-1.826458	-3.435508
H	-2.500632	-2.169092	-3.460716
P	-1.721260	3.418660	1.403967
P	0.227394	3.626409	-1.202744
P	-3.253585	-1.616103	-1.203596
P	3.026647	-2.008488	-1.204134
P	-2.101595	-3.199329	1.403982
P	3.822037	-0.220957	1.404482
C	4.821393	1.345935	1.435497
H	5.066920	1.641231	0.405779
H	4.221266	2.141551	1.903487
H	5.742035	1.182449	2.018203
C	2.815138	-3.783970	-0.688648

H	3.021041	-3.886764	0.387397
H	1.776064	-4.086614	-0.886288
H	3.512284	-4.416469	-1.262137
C	-4.685174	-0.545545	-0.686657
H	-4.428061	0.505870	-0.883204
H	-5.581486	-0.832643	-1.260353
H	-4.876963	-0.674008	0.389384
C	-1.244070	-4.847969	1.435519
H	-1.845838	-5.563069	2.018842
H	-1.111258	-5.208776	0.405963
H	-0.254873	-4.725583	1.903217
C	1.870161	4.330754	-0.685156
H	2.069272	5.251652	-1.257218
H	1.855529	4.558925	0.391226
H	2.652190	3.582836	-0.883524
C	-3.577917	3.498389	1.435441
H	-3.965533	2.581221	1.905361
H	-3.897303	4.378001	2.016832
H	-3.956928	3.561050	0.405783

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)(\mu\text{-}SH)_2Cl_3(dmpe)_3]^+$
E(UB-P86) = -2382.5181725 a.u.
Free energy = -2381.9729075 a.u.
D3(BJ) dispersion correction = -0.37539172 a.u.
Cartesian

C	-1.397736	3.481908	3.157222
C	-1.098972	5.058491	0.708155
C	-0.696702	5.015669	-0.772968
C	0.738119	3.616261	-2.934332
Mo	-0.681659	1.434954	-0.026491
S	1.144023	1.569869	1.577697
Mo	1.610310	-0.210970	0.006418
C	2.726946	-2.229418	-3.050853
Mo	-0.976418	-1.268465	0.006928
C	-3.262126	-1.306502	-3.119134
Cl	-2.389991	2.223850	-1.666386
S	0.042540	-0.031387	-1.790458
S	-1.943227	0.206200	1.556744
Cl	3.166563	1.132455	-1.502612
S	0.804279	-1.795768	1.606620
C	5.019093	-1.627058	0.566093
C	4.734534	-1.825427	-0.929141
Cl	-0.654574	-3.291831	-1.487121
C	-3.973668	-3.361820	0.625067
C	-3.993108	-3.099281	-0.887784
C	3.808011	-0.894414	3.129733
C	-2.657956	-2.744461	3.167554
H	-1.811250	2.584094	3.642334
H	-1.876818	4.380881	3.577052

H	-0.313219	3.522909	3.339558
H	-0.233426	5.320049	1.341430
H	-1.879075	5.816530	0.893789
H	-1.574948	4.877657	-1.423433
H	-0.186399	5.948115	-1.071907
H	1.535030	2.897467	-3.177507
H	1.031415	4.629548	-3.253061
H	-0.195280	3.317181	-3.434004
H	3.235632	-0.158475	3.715795
H	4.832248	-0.961113	3.530694
H	3.316237	-1.875918	3.206728
H	6.059800	-1.305946	0.742737
H	4.868766	-2.568585	1.122268
H	5.285912	-2.695491	-1.326613
H	5.016402	-0.934551	-1.512324
H	1.692338	-2.526322	-3.280579
H	3.431184	-2.977487	-3.449062
H	2.932747	-1.241930	-3.490332
H	-1.716822	-2.667928	3.734155
H	-3.260193	-3.573904	3.571811
H	-3.211337	-1.798649	3.264726
H	-4.667048	-2.682427	1.150761
H	-4.286350	-4.393682	0.860307
H	-3.393438	-3.845839	-1.432370
H	-5.024271	-3.125589	-1.281599
H	-2.986680	-0.280243	-3.406257
H	-4.261126	-1.551220	-3.514219
H	-2.515248	-2.011248	-3.513805
H	0.566582	0.874374	2.655064
H	0.390365	-1.000017	2.695191
P	-1.723752	3.388622	1.327670
P	0.467129	3.573221	-1.099288
P	-3.254614	-1.411909	-1.267481
P	2.895946	-2.100142	-1.208043
P	-2.269237	-3.064373	1.376122
P	3.859901	-0.358307	1.347329
C	4.872838	1.198004	1.449847
H	5.095578	1.553664	0.434617
H	4.290618	1.966724	1.981257
H	5.804735	0.992042	2.000305
C	2.692149	-3.854590	-0.617424
H	2.906702	-3.911589	0.460864
H	1.653313	-4.169844	-0.793522
H	3.386144	-4.511234	-1.167066
C	-4.639561	-0.284655	-0.744547
H	-4.814855	-0.397464	0.335831
H	-4.353469	0.756131	-0.952844
H	-5.554078	-0.547073	-1.300955
C	-1.508587	-4.761122	1.460544
H	-2.167607	-5.428258	2.039055

H	-1.366183	-5.150208	0.443101
H	-0.528547	-4.687037	1.956942
C	2.060287	4.235405	-0.396302
H	2.321678	5.171790	-0.915655
H	1.940274	4.434121	0.679457
H	2.852653	3.487267	-0.542939
C	-3.576194	3.540411	1.264184
H	-4.019630	2.624986	1.685788
H	-3.893734	4.414423	1.855136
H	-3.899667	3.647788	0.219605

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)_3H_3(dmpe)_3]^+$
E(UB-P86) = -1002.32401324 a.u.
Free energy = -1002.64513354a.u.
D3(BJ) dispersion correction = -0.3211203 a.u.
Cartesian

C	-3.343252	-2.168257	-3.042288
C	-3.776115	-3.528548	-0.474785
C	-3.579042	-3.498229	1.047357
C	-2.042354	-2.457342	3.308509
Mo	-1.410116	-0.804201	-0.075929
S	0.011993	-2.213157	-1.377823
Mo	1.402596	-0.818786	-0.075998
C	3.152214	-0.540046	3.309240
Mo	0.009183	1.621831	-0.075128
C	-1.112992	2.994837	3.309223
H	-2.696980	-0.543659	1.073429
S	0.000059	-0.001689	1.690590
S	-1.919540	1.096199	-1.380853
H	1.821853	-2.063988	1.072375
S	1.912018	1.117707	-1.376218
C	4.946017	-1.498398	-0.475803
C	4.821960	-1.343559	1.046398
H	0.877220	2.605241	1.075485
C	-1.174738	5.030362	-0.474724
C	-1.249530	4.844552	1.047341
C	3.552890	-1.811175	-3.042380
C	-0.202977	3.979271	-3.040383
H	-3.250092	-1.207596	-3.572643
H	-4.254453	-2.688869	-3.378703
H	-2.456382	-2.782682	-3.260683
H	-3.074258	-4.236058	-0.950861
H	-4.800084	-3.838200	-0.747358
H	-4.329913	-2.849033	1.530942
H	-3.672986	-4.504835	1.490195
H	-1.057287	-2.161331	3.701075
H	-2.394466	-3.358458	3.836033
H	-2.751320	-1.629758	3.462956
H	2.675659	-2.214176	-3.572407

H	4.460922	-2.338493	-3.377138
H	3.638983	-0.736200	-3.263202
H	5.727522	-2.228477	-0.749606
H	5.205088	-0.536067	-0.951781
H	5.739879	-0.919157	1.488630
H	4.638252	-2.319100	1.529808
H	2.402725	0.162922	3.704352
H	4.109313	-0.393601	3.835389
H	2.792436	-1.568840	3.462506
H	0.584088	3.418089	-3.568128
H	-0.197509	5.028482	-3.377424
H	-1.177663	3.517997	-3.261802
H	-2.136667	4.773180	-0.952532
H	-0.933501	6.072647	-0.747003
H	-0.314332	5.174257	1.532864
H	-2.077694	5.426099	1.488010
H	-1.349337	1.994171	3.702723
H	-1.718527	3.750716	3.834850
H	-0.042177	3.195877	3.464967
P	-3.415056	-1.837217	-1.213534
P	-1.891236	-2.790261	1.486695
P	-1.474815	3.028291	1.487029
P	3.362170	-0.239879	1.487570
P	0.114560	3.875898	-1.210610
P	3.301730	-2.035612	-1.213131
C	3.326368	-3.887036	-1.024452
H	3.353246	-4.142661	0.045742
H	2.402379	-4.297673	-1.460398
H	4.203117	-4.316501	-1.535512
C	4.096226	1.473946	1.447350
H	4.425123	1.707806	0.423407
H	3.315390	2.195233	1.734251
H	4.949049	1.541052	2.142117
C	-3.325854	2.805668	1.444640
H	-3.559800	1.769190	1.733473
H	-3.811280	3.511732	2.137724
H	-3.691875	2.971284	0.420010
C	1.704878	4.824225	-1.020706
H	1.638419	5.797902	-1.532588
H	1.911756	4.976364	0.049542
H	2.523266	4.229596	-1.455488
C	-0.777361	-4.285367	1.446156
H	-1.147915	-5.056725	2.140631
H	-0.739564	-4.686807	0.422141
H	0.238311	-3.972557	1.734086
C	-5.028994	-0.928927	-1.028295
H	-4.918958	0.076212	-1.464238
H	-5.839611	-1.471517	-1.541062
H	-5.266078	-0.823601	0.041328

$[Mo_3(\mu_3\text{-}S)(\mu\text{-}S)(\mu\text{-}SH)_2H_3(dmpe)_3]^+$
E(UB-P86) = -1003.46410096 a.u.
Free energy = -1002.90126696 a.u.
D3(BJ) dispersion correction = -0.33184763 a.u.
Cartesian

C	2.007130	-3.479175	-2.974097
P	1.619579	-3.483291	-1.153795
C	0.591807	-5.028271	-0.980901
C	3.262623	-3.966916	-0.372275
C	3.234995	-3.716756	1.142216
P	2.668308	-1.960249	1.516690
C	4.246295	-0.978602	1.353064
Mo	0.697905	-1.418832	-0.006438
S	-1.128951	-1.649024	-1.678689
Mo	-1.608714	0.074537	-0.006970
P	-3.876169	0.419834	-1.136937
C	-4.631630	2.109114	-0.933670
S	2.053431	-0.142097	-1.528777
Mo	0.936267	1.277961	0.014008
P	2.385452	3.036099	-1.090121
C	4.216698	2.865022	-0.804175
S	-0.054451	0.001481	1.795977
S	-0.895143	1.848669	-1.547704
P	0.312191	3.368169	1.391317
C	-1.257289	4.302122	1.011280
P	-3.106946	-1.356848	1.439645
C	-3.116356	-3.207240	1.188160
C	2.413550	-2.000975	3.357352
C	-2.978173	-1.217605	3.290175
C	-4.905406	-0.894589	1.123631
C	-5.160030	-0.729089	-0.380409
C	0.259842	3.236139	3.243883
C	1.642982	4.665491	1.094176
C	1.990325	4.744243	-0.399561
C	-4.068201	0.120901	-2.964598
C	2.294868	3.303567	-2.929695
H	0.336283	-2.753128	1.082673
H	2.140613	1.725184	1.187486
H	-2.476985	1.225486	0.994859
H	1.069719	-3.344806	-3.536568
H	2.479676	-4.429618	-3.270740
H	2.679685	-2.637284	-3.198159
H	4.034701	-3.345152	-0.859717
H	3.487147	-5.021925	-0.607763
H	2.518288	-4.391665	1.642177
H	4.226516	-3.881898	1.598647
H	2.196313	-0.981526	3.711390
H	3.314494	-2.384695	3.863042
H	1.551545	-2.647102	3.583087

H	2.609369	2.378469	-3.437498
H	2.952714	4.134604	-3.231697
H	1.255262	3.529908	-3.212747
H	2.842037	5.421401	-0.585933
H	1.131908	5.124287	-0.981722
H	1.294114	5.639272	1.479930
H	2.520928	4.361488	1.690719
H	-0.578238	2.582608	3.530683
H	0.126287	4.231494	3.697707
H	1.200108	2.784763	3.595489
H	-3.436462	0.837562	-3.512800
H	-5.119255	0.252248	-3.268678
H	-3.735193	-0.901122	-3.201676
H	-5.065837	-1.696315	-0.905144
H	-6.171088	-0.336500	-0.586108
H	-5.086235	0.051789	1.662710
H	-5.561940	-1.664941	1.564498
H	-1.990412	-1.583324	3.609836
H	-3.768657	-1.812782	3.775485
H	-3.075099	-0.159167	3.575971
H	4.417153	2.875524	0.277970
H	4.546160	1.898002	-1.214987
H	4.764007	3.685507	-1.295889
H	-1.274412	4.583558	-0.053191
H	-2.111440	3.637405	1.212059
H	-1.324024	5.208158	1.635327
H	-2.117488	-3.592688	1.445399
H	-3.882680	-3.685312	1.820580
H	-3.315074	-3.433160	0.128828
H	-5.606733	2.160439	-1.444779
H	-4.755747	2.321846	0.138791
H	-3.947362	2.856833	-1.363917
H	5.043235	-1.417842	1.975097
H	4.556705	-0.961605	0.297100
H	4.044047	0.056365	1.669706
H	-0.400532	-4.842744	-1.421185
H	1.072607	-5.875962	-1.495949
H	0.464729	-5.260742	0.087274
H	-0.465831	1.126050	-2.665177
H	-0.577458	-0.925703	-2.749966

X3LYP-optimized structures

Acetic acid
E_{gas}(X3LYP/ def2-TZVP) = -229.088243171 a. u.
G_{gas}(X3LYP/ def2-TZVP) = -229.0538772 a. u.

$E_{methanol}$(X3LYP/ def2-TZVP(SMD)) = -229.104834074 a. u.
Cartesian

C	-1.368922	-0.051875	-0.000139
C	0.130157	0.140890	-0.000605
O	0.862516	-1.005541	0.000213
H	-1.857189	0.917870	-0.017106
H	-1.681763	-0.629132	-0.873076
H	-1.681686	-0.597006	0.893314
O	0.683142	1.199915	0.000053
H	0.287964	-1.780819	-0.000790

Acetate anion
E_{gas}(X3LYP/ def2-TZVP) = -228.529399799 a. u.
G_{gas}(X3LYP/ def2-TZVP) = -228.5093038 a. u.
$E_{methanol}$(X3LYP/ def2-TZVP(SMD)) = -228.640519306 a. u.
Cartesian

C	-1.348380	-0.047837	-0.001044
C	0.212827	0.001235	-0.002364
O	0.701225	1.153686	0.000448
H	-1.722081	-1.071419	-0.073585
H	-1.724287	0.408679	0.920015
H	-1.737778	0.545688	-0.833550
O	0.798458	-1.104104	0.000497

1-H_2
E_{gas}(X3LYP/ def2-TZVP) = -3986.78583754 a. u.
G_{gas}(X3LYP/ def2-TZVP) = -3986.301549 a. u.
$E_{methanol}$(X3LYP/ def2-TZVP(SMD)) = -3986.87413571 a. u.
Cartesian

C	-1.911277	3.313042	2.584171
N	-1.602526	3.281840	1.140482
C	-0.786302	4.454156	0.753794
C	-0.513523	4.439983	-0.731691
N	0.135334	3.177317	-1.155292
C	0.186809	3.116764	-2.636544
Mo	-0.744356	1.366927	0.073827
S	1.088319	1.630011	1.649616
Mo	1.584858	-0.085988	0.074715
N	2.700240	-1.693510	-1.213784
C	2.630945	-1.625057	-2.694048
Mo	-0.900227	-1.287673	0.079495
N	-2.790835	-1.479351	-1.242455
C	-2.680982	-1.480343	-2.721554
Cl	-2.751099	1.844265	-1.297027

S	0.025992	-0.010578	-1.659453
S	-1.918819	0.101548	1.622696
Cl	3.028602	1.549916	-1.157652
S	0.888626	-1.746751	1.646521
N	3.673881	-0.350257	1.125318
C	4.265711	-1.635963	0.698284
C	4.117801	-1.796733	-0.795163
Cl	-0.186651	-3.361277	-1.122769
N	-2.174130	-2.946311	1.144750
C	-3.575118	-2.812611	0.693024
C	-3.616694	-2.632236	-0.805855
C	3.862572	-0.135584	2.573583
C	-2.103902	-3.181003	2.601047
H	-2.484181	3.332041	0.631462
H	1.108651	3.176691	-0.843612
H	4.157310	0.399315	0.630622
H	2.210856	-2.548463	-0.947332
H	-1.768666	-3.756815	0.677637
H	-3.265897	-0.610690	-0.987879
H	-2.598568	2.509051	2.829753
H	-2.362189	4.269843	2.859998
H	-0.995469	3.182279	3.157295
H	0.143357	4.414816	1.323459
H	-1.298268	5.382909	1.024404
H	-1.450200	4.520312	-1.284741
H	0.105825	5.298183	-1.007074
H	0.857564	2.320408	-2.940208
H	0.559129	4.062051	-3.039341
H	-0.812314	2.927153	-3.020708
H	3.537863	0.866283	2.840515
H	4.914519	-0.251894	2.846585
H	3.276938	-0.862796	3.133010
H	5.324588	-1.680572	0.971754
H	3.754331	-2.436759	1.235070
H	4.542334	-2.751919	-1.116341
H	4.663107	-1.004558	-1.309883
H	1.609586	-1.799381	-3.015589
H	3.273910	-2.389534	-3.137573
H	2.957817	-0.641466	-3.022285
H	-1.079922	-3.411524	2.882188
H	-2.747070	-4.017277	2.886967
H	-2.426988	-2.288316	3.131813
H	-4.010805	-1.954192	1.205973
H	-4.156536	-3.696987	0.972202
H	-3.214238	-3.517513	-1.300114
H	-4.648732	-2.506398	-1.143454
H	-2.294019	-0.523781	-3.055427
H	-3.664376	-1.638915	-3.170362
H	-2.008822	-2.278176	-3.028084
H	0.565424	1.011900	2.755833

H	0.492239	-1.044074	2.755047

1-H_2 after deprotonation of a S-H moiety

E_{gas}(X3LYP/ def2-TZVP) = -3986.38615225 a. u.

G_{gas}(X3LYP/ def2-TZVP) = -3985.912398 a. u.

$E_{methanol}$(X3LYP/ def2-TZVP(SMD)) = -3986.87413571 a. u.

Cartesian

C	-1.129194	-3.664225	2.558597
N	-1.348704	-3.404033	1.127863
Mo	-0.544530	-1.452679	0.085088
S	1.247060	-1.448850	1.591928
Mo	1.556773	0.293669	0.105999
N	3.616770	0.547201	1.191382
C	3.688279	0.821862	2.636179
C	-2.762130	-3.590486	0.756993
C	-2.939513	-3.396084	-0.732318
N	-2.445862	-2.077080	-1.171088
C	-2.395471	-2.021816	-2.647255
S	-1.869543	-0.327951	1.742219
Mo	-1.025298	1.180403	0.079553
N	-2.273274	2.892883	1.129957
C	-2.544345	2.877945	2.576048
Cl	0.550775	-3.347183	-1.277835
S	0.009684	0.001816	-1.657173
N	-0.587243	3.114079	-1.211467
C	-1.490020	4.203013	-0.789988
C	-1.728213	4.193843	0.703345
Cl	-3.241809	1.173829	-1.201304
S	0.646514	1.828642	1.577527
C	-0.549122	3.038676	-2.685708
N	3.052298	-1.065466	-1.139866
C	4.432569	-0.833669	-0.673807
C	4.492221	-0.580374	0.817598
Cl	2.699319	2.098939	-1.294055
C	3.006026	-1.090295	-2.615438
H	-0.779611	-4.054885	0.585880
H	-3.096994	-1.347501	-0.877941
H	-3.146491	2.726678	0.630450
H	0.360664	3.312858	-0.893179
H	3.924426	1.376531	0.684554
H	2.721868	-1.974990	-0.815754
H	-0.066083	-3.616294	2.776227
H	-1.515540	-4.649535	2.840688
H	-1.639163	-2.904712	3.148710
H	-3.351889	-2.864231	1.319743
H	-3.110995	-4.591071	1.039799
H	-2.361222	-4.148685	-1.270915
H	-3.991935	-3.529649	-1.005587
H	-2.253711	-0.992251	-2.959085
H	-3.330558	-2.395852	-3.077378

H	-1.563293	-2.628779	-2.996569
H	-3.072563	1.964370	2.834779
H	-3.151285	3.741136	2.869739
H	-1.602564	2.903436	3.121221
H	-2.414021	5.007890	0.967525
H	-0.795384	4.355681	1.245909
H	-1.091774	5.176648	-1.096312
H	-2.435481	4.054811	-1.314565
H	0.277533	2.405695	-2.990242
H	-0.409650	4.035073	-3.118290
H	-1.485341	2.615599	-3.044136
H	3.130046	1.726563	2.859200
H	4.727988	0.944168	2.957945
H	3.237376	-0.003767	3.182770
H	4.155323	-1.456050	1.373782
H	5.529404	-0.377150	1.109789
H	4.807574	0.038711	-1.211250
H	5.076709	-1.681809	-0.930828
H	2.041740	-1.472840	-2.933168
H	3.792217	-1.740803	-3.012633
H	3.144544	-0.079534	-2.992708
H	-0.978257	-0.170808	2.784289