On the formation of gold nanoparticles from $[Au^{III}Cl_4]^-$ and a non-classical reduced polyoxomolybdate as electron source: quantum mechanical modelling and experimental study

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Supporting Information

Methods

Experiments

$(NH_4)_{15}\{Na[(Mo_2O_4)_6(\mu_2\text{-}SO_3)_3(\mu_6\text{-}SO_3)]_2\}\cdot 5H_2O$ (Kabanos). Kabanos POM was synthesized according to the literature.[1] Briefly, $Na_2Mo^{VI}O_4\cdot 2H_2O$ (3.00 g, 12.6 mmol) was dissolved in HCl (37 %):H_2O (1:4 v/v, 25 mL, pH~0) under magnetic stirring. Hydrazine monohydrate (0.320 g, 6.3 mmol) was then added, whereupon the light yellow color of the solution turned into dark-blue. Solid $(NH_4)_2SO_3$ (9.00 g, 67 mmol) was then added and the dark-blue color of the solution almost instantly became olive-green. The solution was kept in an open beaker for 2-3 days, over which time an abundance of thin red crystals were produced. These were filtered, washed with ethanol and air-dried. The yield obtained was *ca.* 97 % based on Mo (2.72 g). The FTIR spectrum at room temperature was dominated by bands at 1414 (NH_4^+); 1073 (SO_3^{2-}); 980 and 961 (Mo=O) from terminal oxygen atoms; 921, 890, 840 and 816 (SO_3^{2-}); 718, 644 and 609 cm^{-1} (Mo-O-Mo or Mo-O-S) from vibrations involving edge and corner sharing oxygen atoms. The UV-Vis spectrum (in H_2O) was dominated by a broad absorption band from 200 to 600 nm.

1. M. J. Manos, J. D. Woollins, A. M. Z. Slawin and T. A. Kabanos, *Angew. Chem., Int. Ed.* 2002, **15**, 2801.

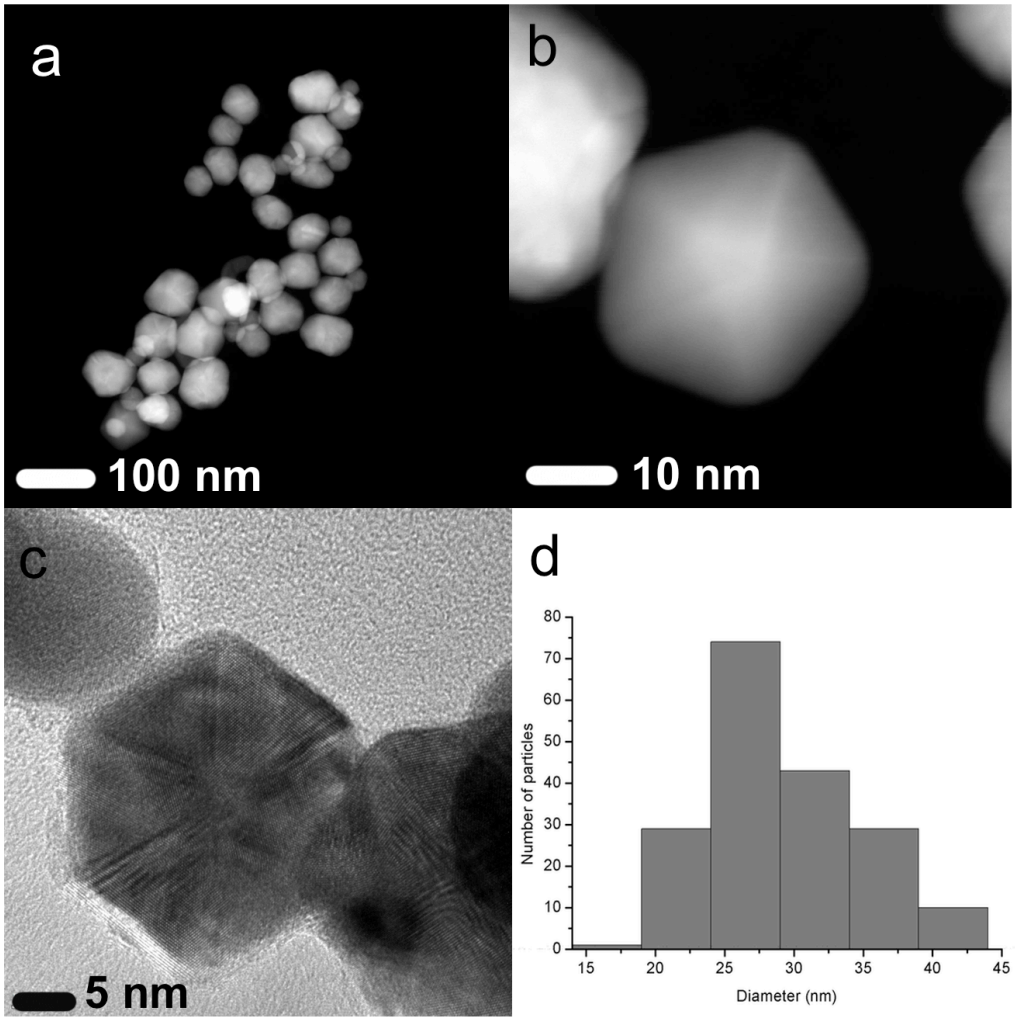

Figure S1. (a-b) STEM-HAADF and c) HR-TEM images of AuNPs@POM and (d) size-dispersion histogram of the number of particles found for different diameter ranges.

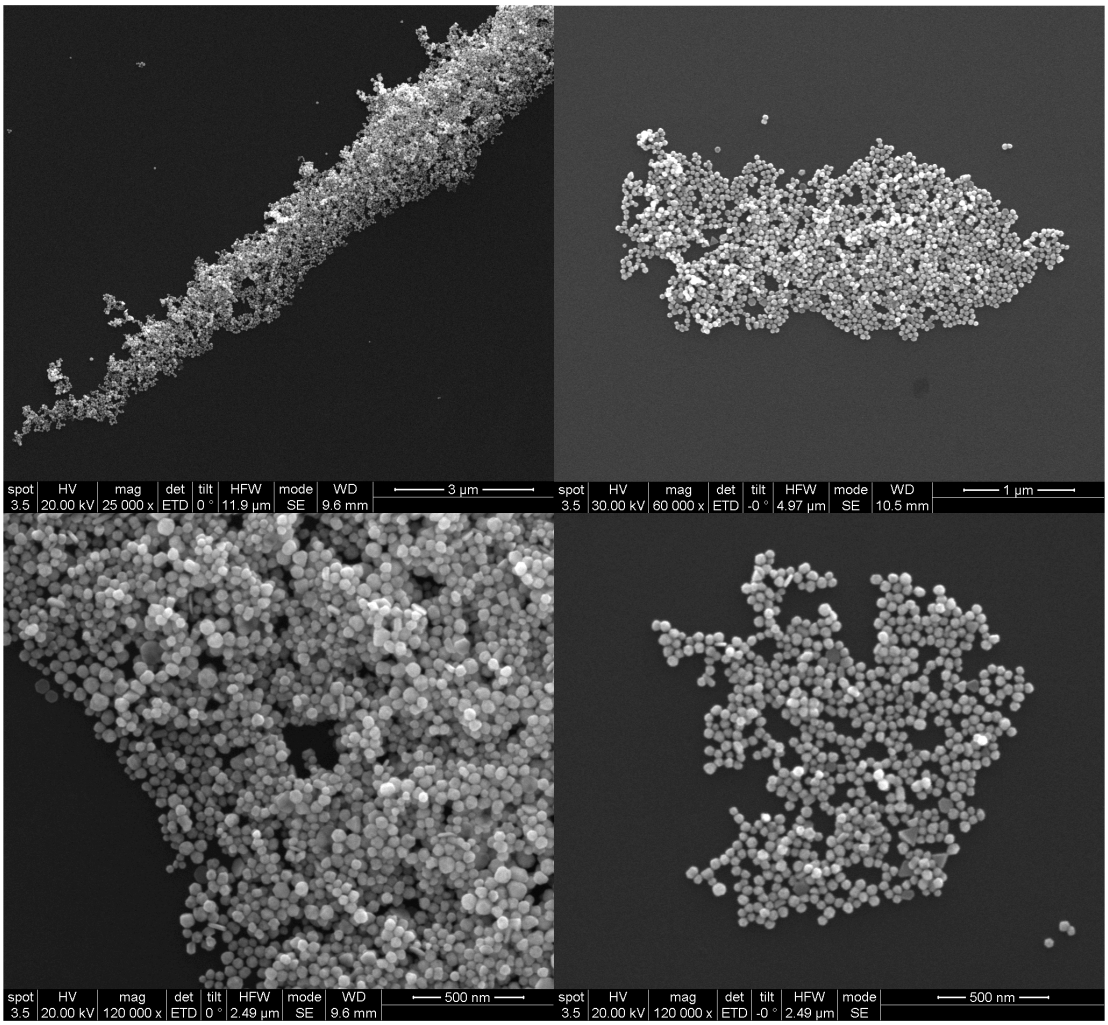

Figure S2. Scanning Electron Microscopy (SEM) images of polyhedral AuNPs@POM.

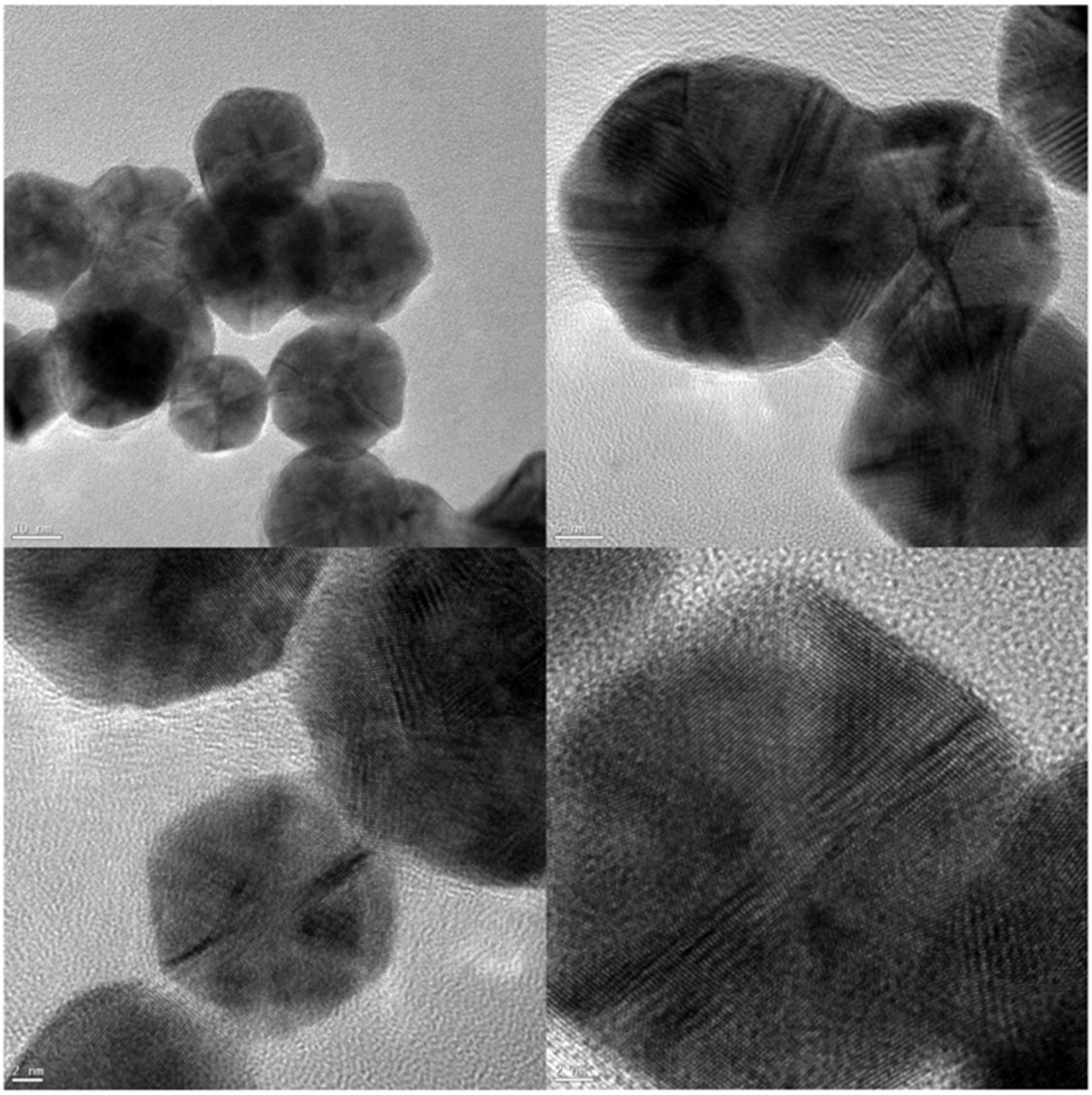

Figure S3. High-Resolution Transmission Electron Microscopy (HR-TEM) images of polyhedral AuNPs@POM.

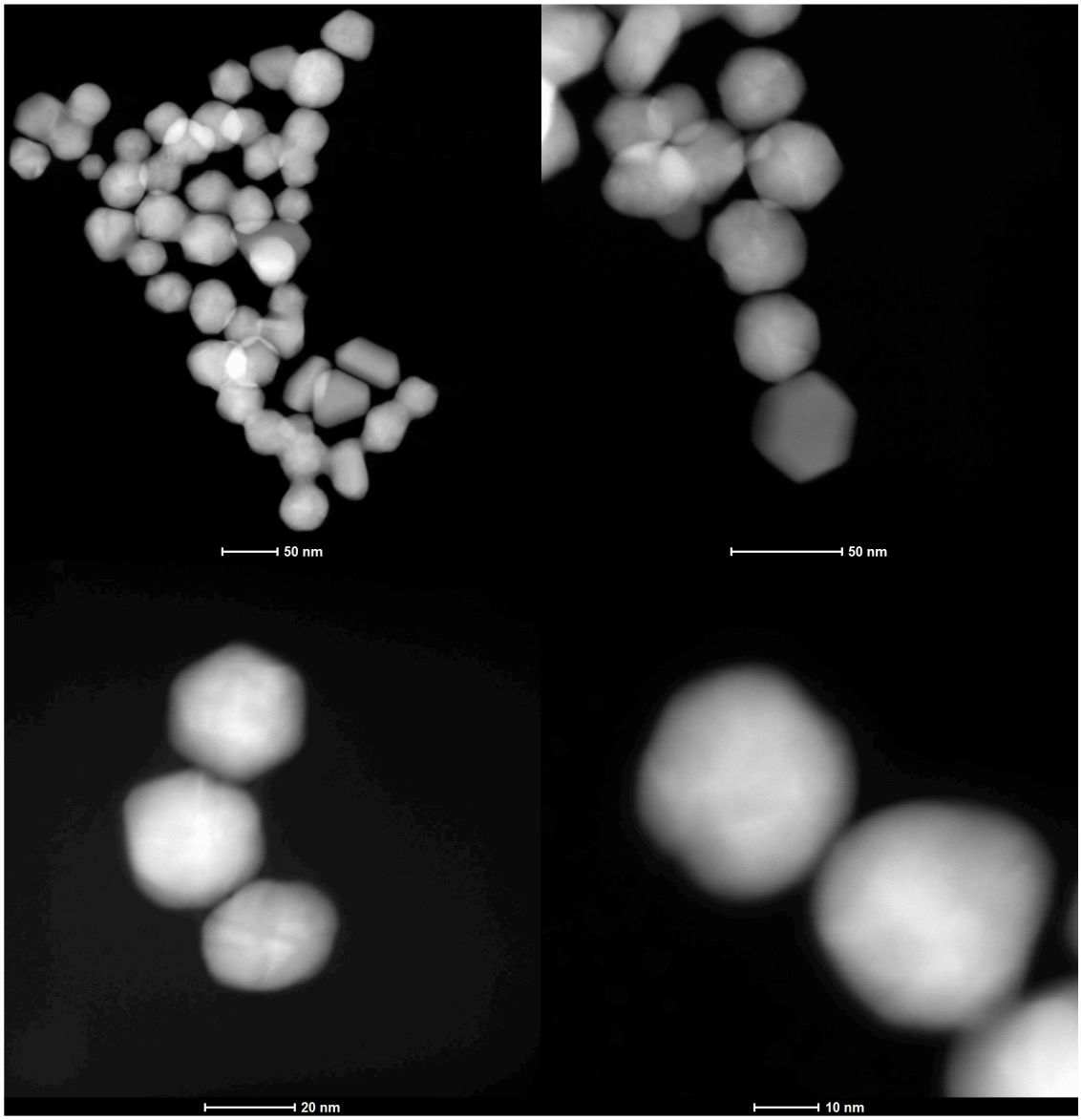

Figure S4. High-Angle Annular Dark Field Scanning Transmission Electron Microscopy (HAADF-STEM) images of polyhedral AuNPs@POM.

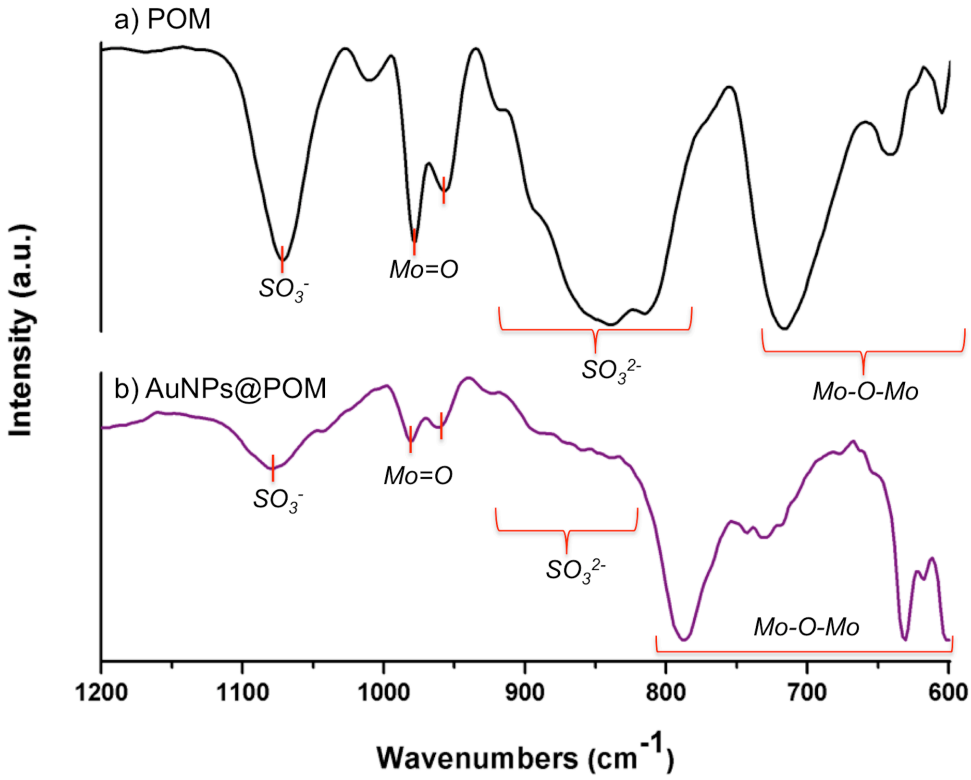

Figure S5. FTIR spectra of a) Kabanos POM single crystals and b) lyophilized AuNPs@POM. Both show prominent vibrational stretches for SO_3^- and terminal Mo=O bonds, along with Mo-O-Mo stretches.

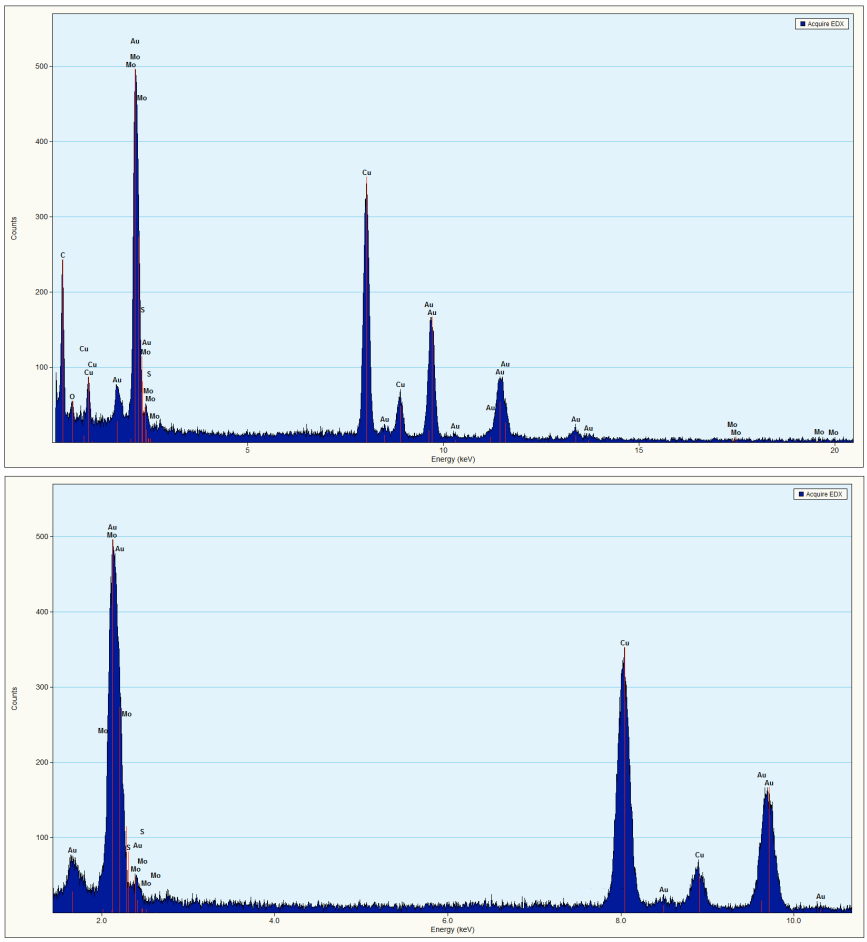

Figure S6. EDX spectra of AuNPs@POM showing the presence of Au and Mo. The Cu signal comes from TEM grid.

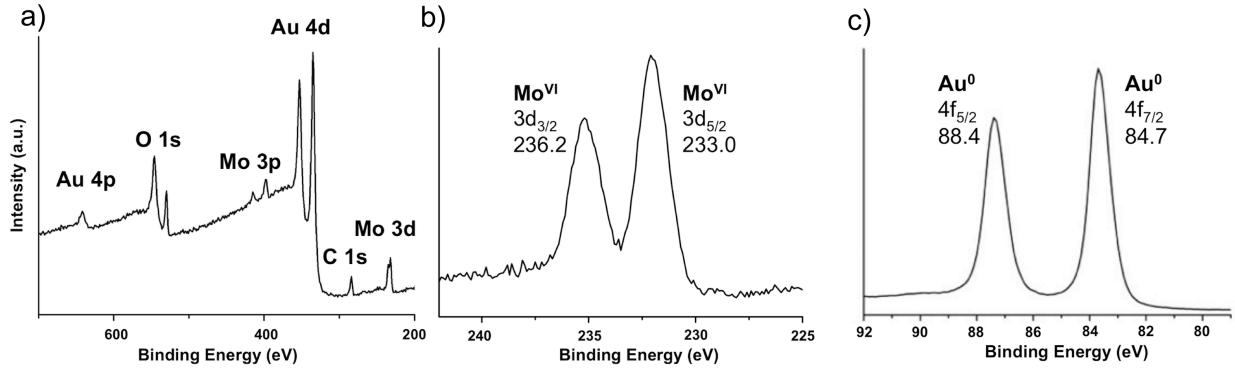

Figure S7. XPS spectra of AuNPs@POM showing a) general spectrum in the 200-700 eV range; b) the characteristic doublet for Mo^{VI} in the 230-235 eV region; c) the spin-orbit doublet of Au^0 at 88.4 and 84.7 eV (splitting of 3.7 eV) for $4f_{5/2}$ and $4f_{7/2}$, respectively. Note that there was no evidence of any Mo^V.

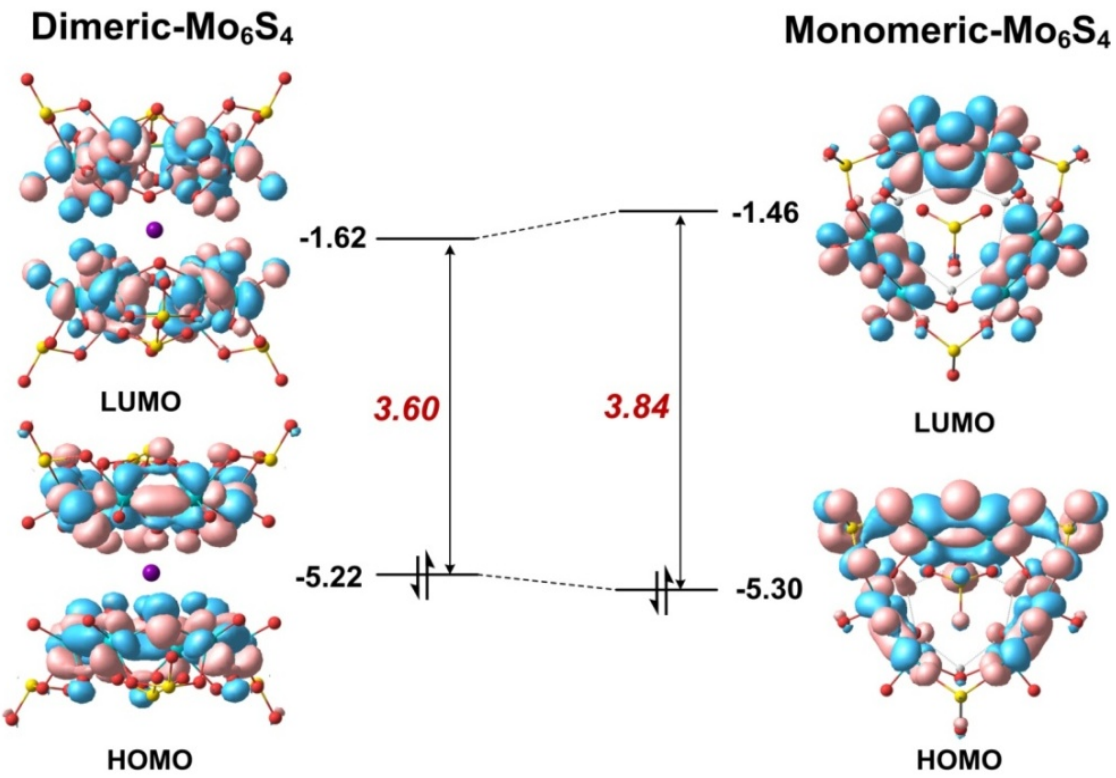

Figure S8. Energy (in eV) and composition of the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals for **{dimeric-$H_3S_4Mo_6$}** and **{ $H_3S_4Mo_6$}**.The HOMO-LUMO (H-L) gaps are 3.60 and 3.84 eV for the dimer and monomer structures, that is, the latter is only 0.24 eV (*ca.* 6%) larger. The three highest occupied orbitals (six for the dimer) have significant contributions from the $Mo^{V}_2O_4$ core and have Mo-Mo bonding character, where each couple of electrons occupying them are provided by two Mo^{V}.

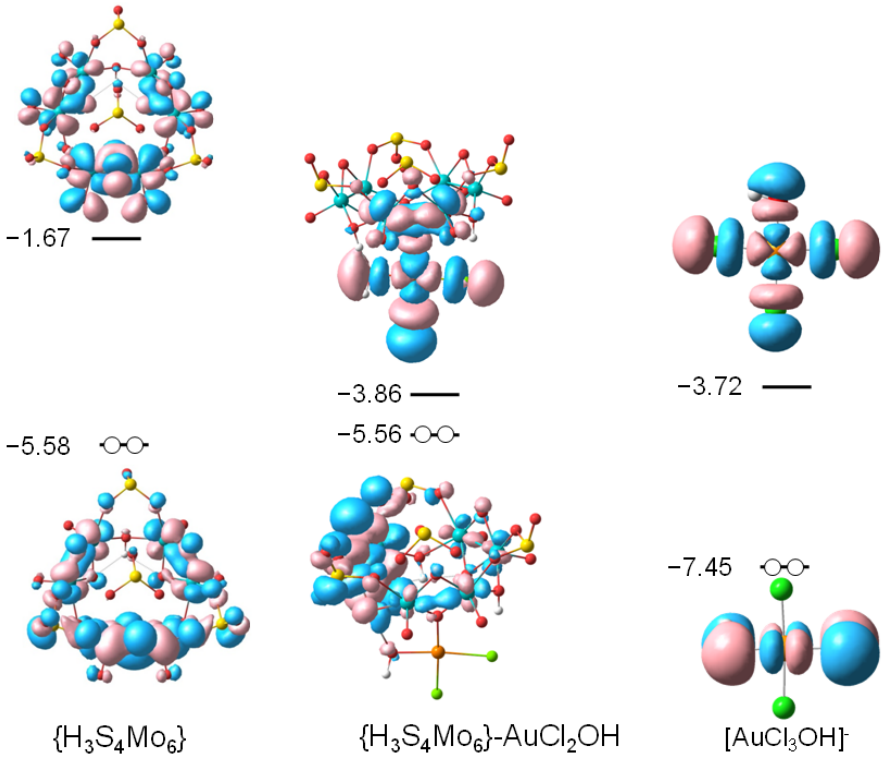

Figure S9. Schematic view of the frontier molecular orbitals of the **{$H_3S_4Mo_6$}**-$AuCl_3$ adduct (**A-1**), compared with the independent **{$H_3S_4Mo_6$}** and $[AuCl_3OH]^-$ units at B3LYP-D3(BJ)/6-311++G(d,p),def2-TZVPP level. The HOMO of the adduct resembles in energy and shape to that of **{ $H_3S_4Mo_6$}**, whereas the LUMO is $[AuCl_3OH]^-$ -like. Even though, there is some mixing of the orbitals leading to stabilization of the HOMO and destabilization of the LUMO.

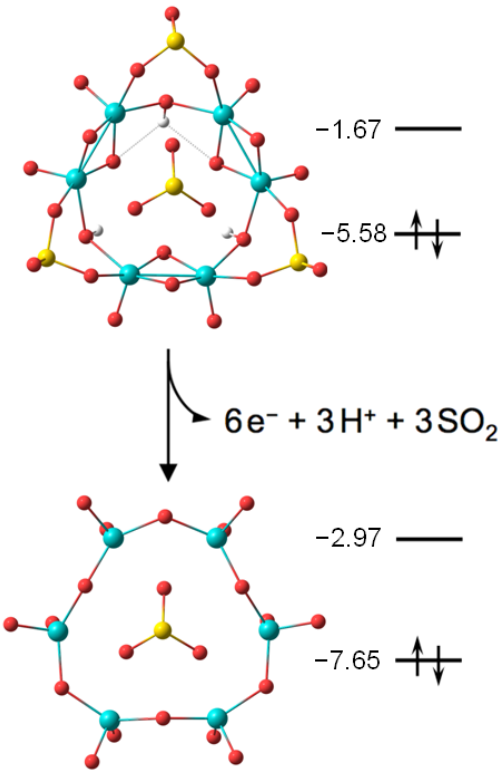

Figure S10. Evolution from the initial POM structure, $[(Mo_2{}^{V}O_4)_3(\mu_2\text{-}OH)_3(\mu_2\text{-}SO_3)_3(\mu_6\text{-}SO_3)]^{5-}$, to the proposed final one, $[SMo^{VI}{}_6O_{21}]^{2-}$, with the associated loss of electrons, protons and SO_2. Indicated are the corresponding HOMO and LUMO energies, in eV.

Optimized coordinates (xyz) for the **$\{H_3S_4Mo_6\}^{5-}$**, **$\{H_2S_4Mo_6\}^{4-}$, $\{HS_4Mo_6\}^{3-}$, A**, **B**, **C-1**, **C-2**, **D-1**, and **D-2** species as described in the manuscript which have been obtained in our work at B3LYP-D3(BJ)/6-311++G(d,p),def2-TZVPP level.

$\{H_3S_4Mo_6\}^{5-}$

40

Mo	0.33296573	0.32194773	3.10661442
O	1.11074463	0.73098958	4.55452751
Mo	0.27955905	2.54830596	1.82349876
O	1.03568349	3.62764128	2.88550035
Mo	0.41969048	-2.84574644	1.28413326
O	1.24807671	-4.27180768	1.66890757
O	1.49464209	1.04208071	1.73817581
O	-1.09862753	1.59683257	2.81402914
O	1.57496749	-1.97254048	0.00000000
O	-0.97047033	-3.28294051	0.00000000
S	-1.33907562	-0.04089164	0.00000000
O	-0.66109161	-0.73196485	1.23364446
O	-0.73468270	1.40120473	0.00000000
S	-1.02781197	-2.47732636	4.23887434
O	-1.10994293	-0.89598440	3.97646010
O	-1.04802231	-3.05167153	2.73886322
S	-1.48401991	4.80611372	0.00000000
O	-1.24656591	3.83887137	1.24852016
O	-2.37556504	-2.84028004	4.80295241
O	-0.38027735	5.83621386	0.00000000
O	1.34890191	-1.50354285	2.65875531
O	1.24587639	3.05259865	0.00000000
O	-0.66109161	-0.73196485	-1.23364446
O	-1.24656591	3.83887137	-1.24852016
Mo	0.33296573	0.32194773	-3.10661442
O	1.11074463	0.73098958	-4.55452751
Mo	0.27955905	2.54830596	-1.82349876
O	1.03568349	3.62764128	-2.88550035
Mo	0.41969048	-2.84574644	-1.28413326
O	1.24807671	-4.27180768	-1.66890757
O	1.49464209	1.04208071	-1.73817581
O	-1.09862753	1.59683257	-2.81402914
S	-1.02781197	-2.47732636	-4.23887434
O	-1.10994293	-0.89598440	-3.97646010
O	-1.04802231	-3.05167153	-2.73886322
O	-2.37556504	-2.84028004	-4.80295241
O	1.34890191	-1.50354285	-2.65875531
H	2.14359914	-1.21122269	2.19127377
H	2.14359914	-1.21122269	-2.19127377
H	2.01114290	2.45981906	0.00000000

$\{H_2S_4Mo_6\}^{4-}$

39

Mo	-2.74571400	1.70107300	-0.07022600
O	-4.26685800	2.28372300	-0.52163200
Mo	-3.04238700	-0.84852400	-0.13690000
O	-4.63161000	-1.03475200	-0.67651000
Mo	0.51133700	3.02781600	-0.97444200
O	0.95631200	4.51280200	-1.67929600
O	-2.27942000	0.39203500	-1.41354700
O	-3.00728900	0.40781500	1.34454600
O	0.54645000	1.98091000	-2.32464500
O	2.13876700	2.48792200	-0.09311900
S	0.13407500	0.13742000	1.18779400
O	-0.38045700	1.32027300	0.29411300
O	-0.72167500	-1.07004000	0.70671400
S	-1.53757200	4.41200800	1.40577800
O	-2.32445000	3.00723800	1.46444200
O	-0.14058300	3.97868200	0.75724400
S	-2.83115900	-3.88422300	1.29458800
O	-3.16909800	-2.32635600	1.31646300
O	-1.22688900	4.72913100	2.84097400
O	-3.56724800	-4.51201400	0.13887400
O	-1.59140100	3.06180400	-1.26659400
O	-1.91087900	-2.19608900	-1.32154500
O	1.57815100	-0.17554600	0.63301300
O	-1.27057100	-3.86663000	0.93048200
Mo	2.23034200	-2.02300800	-0.49929000
O	3.18728200	-3.11514800	-1.36657500
Mo	-0.12345200	-3.02258100	-0.55044800
O	0.05668100	-4.40069800	-1.50754000
Mo	3.48932800	1.21019700	-0.22081500
O	4.76651200	2.05328000	-0.96410000
O	0.74419500	-1.60970300	-1.61887200
O	1.28108400	-3.05169100	0.79720600
S	4.10788000	-1.04163200	2.30250000
O	3.79557400	-1.87265900	1.07901600
O	4.13076200	0.76980200	1.40043400
O	2.98420200	-0.91205100	3.23538400
O	3.34410600	-0.29819700	-1.16040500
H	-1.73633100	2.78013900	-2.17914300
H	-1.62319300	-1.62932300	-2.05259500

{HS_4Mo_6}$^-$

38

Mo	-2.83389500	2.40035700	-0.86478000
O	-3.85818800	3.33187800	-1.86471400
Mo	-3.81417900	-0.98844900	-0.09309400
O	-4.88069400	-1.72164100	-1.18270400
Mo	0.79624000	2.91623000	-0.72963500
O	0.73964000	4.48231600	-0.07853300
O	-3.22121900	0.60821100	-1.11947600
O	-4.78774200	-0.08631500	0.97655100
O	1.39144700	3.05190900	-2.32508200
O	2.54578600	2.40812500	0.04271800
S	0.74387000	0.32080200	1.49523100
O	0.14306300	1.42514000	0.47046900
O	-0.22035600	-0.82907300	1.39935600
S	-2.22942400	2.86884100	3.11386200
O	-3.16076900	2.83012400	0.77277300
O	-1.20706700	3.89978400	2.91430700
S	-2.73933900	-3.93845000	1.14510200
O	-3.37796100	-2.39306100	1.15855200
O	-1.73583900	1.49559600	3.23544700
O	-3.28577000	-4.59310700	-0.07733500
O	-1.10674000	2.81847600	-1.29339600
O	-1.88451600	-1.53675400	-0.92844200
O	2.06150600	-0.16483100	0.73942500
O	-1.21822100	-3.60777900	0.92783900
Mo	2.27445100	-1.86436400	-0.68585700
O	2.96638400	-2.83161500	-1.88767600
Mo	-0.15169300	-2.64720500	-0.59638500
O	-0.21703500	-3.84192100	-1.77534200
Mo	3.85857600	1.14045500	-0.20938500
O	5.10623100	2.03402700	-0.94205200
O	0.68136900	-1.10638400	-1.44846600
O	1.38722300	-3.02824800	0.53604000
S	4.62235200	-1.41371900	1.83897300
O	4.01722400	-2.08784100	0.60054200
O	4.69978600	0.33619000	1.23134000
O	3.67489100	-1.35032300	2.96711600
O	3.47636000	-0.14575300	-1.36222100
H	-1.62871900	-0.77160100	-1.46326300

A
46

Mo	-2.10167800	-1.73427000	-1.24790900
O	-3.65237600	-2.33402600	-0.92249600
Mo	-2.49277300	0.79652100	-1.47052400
O	-4.15891200	0.95225800	-1.19871800
Mo	1.09760200	-3.01885100	-0.12209300
O	1.42842900	-4.36455800	0.85170100
O	-1.85066400	-0.27647900	-0.00376600
O	-2.22952000	-0.58651700	-2.80726400
O	1.14792600	-1.53998800	1.13327100
O	2.75239600	-2.52636800	-1.02281400
S	0.91130400	-0.05205800	-2.04863900
O	0.21224000	-1.36409500	-1.55158900
O	-0.14918100	1.06913900	-1.80564000
S	-0.81923200	-4.60625700	-2.29747800
O	-1.56806200	-3.22470100	-2.60975600
O	0.63452300	-4.09349900	-1.83606000
S	-1.97209400	3.66125900	-3.23275200
O	-2.38970600	2.12946700	-3.07407800
O	-0.58495600	-5.22655200	-3.65123300
O	-2.94186900	4.49463700	-2.42771200
O	-1.00491500	-2.90537700	0.13998900
O	-1.79791100	2.40507900	-0.27885000
O	2.00716700	0.21259800	-0.95997300
O	-0.55065400	3.72458800	-2.50513500
Mo	2.40783200	2.23016200	0.21579300
O	2.95230600	3.46857600	1.23790400
Mo	0.15819700	3.13102100	-0.63945700
O	0.04113500	4.64949300	0.10404700
Mo	2.97358300	-1.36659000	0.52114300
O	3.85596700	-2.22017600	1.68770400
O	0.59310300	1.91850000	0.78820800
O	1.90638000	3.01362300	-1.48875400
S	5.37117500	0.80795400	-0.16295000
O	4.26273900	1.85491400	-0.65932300
O	4.63912300	-0.59084500	-0.45760200
O	6.46594700	0.89178100	-1.19465800
O	2.83762800	0.54171800	1.45452600
H	-1.16809900	-2.54744900	1.04425000
H	2.06543000	0.47770800	2.04278100
H	-1.77759000	2.06797300	0.62995200
Au	-1.69583100	-0.12450900	2.97237300
Cl	-2.55550600	2.06401500	3.12246200
Cl	0.39716100	0.56065800	3.79836100
Cl	-3.84019800	-0.96562400	2.52919200
O	-0.95596800	-1.96821900	2.74152500
H	-0.04689000	-1.77572300	2.42475300

B

45

Mo	0.82928100	3.08447400	-0.26360700
O	1.04867900	4.54224000	0.56816700
Mo	2.88292800	1.68897600	0.40478900
O	3.72987100	2.71316700	1.45090600
Mo	-2.27819600	1.42157300	-1.05534600
O	-3.87494100	1.83810700	-0.71609900
O	1.06626100	1.71113100	1.08324200
O	2.46168900	2.68114700	-1.21546900
O	-1.98629000	0.08032400	0.41717300
O	-2.41844400	0.09580300	-2.45658400
S	0.78238200	-0.03826000	-1.91766600
O	-0.02448300	1.21128400	-1.40382000
O	2.00664800	-0.10194400	-0.96668400
S	-1.33522900	4.22367900	-2.50120400
O	0.17448100	3.90237500	-2.07007800
O	-1.97958600	2.72943900	-2.59080400
S	5.47466700	-0.27652000	-0.55911500
O	4.54123600	1.01624400	-0.64817900
O	-1.23986900	4.65497100	-3.93688600
O	6.07198100	-0.32306700	0.82652300
O	-1.25922300	2.87744300	0.03537600
O	2.92833300	-0.14747400	1.45631100
O	-0.13419100	-1.22365700	-1.45857100
O	4.42027100	-1.46988200	-0.67727700
Mo	0.51344800	-3.15600800	-0.27258100
O	0.59468300	-4.61606500	0.58163200
Mo	2.70088400	-1.96981300	0.37666300
O	3.44226400	-3.06121700	1.43748400
Mo	-2.42715500	-1.22618000	-1.03805900
O	-4.06176900	-1.45391700	-0.69625200
O	0.89523300	-1.78806100	1.03872100
O	2.17933500	-2.92465900	-1.23476400
S	-1.76967500	-4.12714700	-2.44985700
O	-0.22759100	-3.93893500	-2.06188000
O	-2.27063100	-2.57954500	-2.54835100
O	-1.75500600	-4.58727800	-3.87959300
O	-1.52979000	-2.72287500	0.06026300
H	-1.49413200	2.79467800	0.97822400
H	-1.64701900	-2.49831800	1.03160200
H	2.10262400	-0.11538600	1.96218000
Au	-2.05695600	0.01278600	2.48846400
Cl	-2.50398700	2.31077800	2.69274600
Cl	-2.21110000	-0.16656700	4.82041700
O	-1.76999600	-1.97860200	2.47238700
H	-2.42201500	-2.34183300	3.08482700

C-1

45

Mo	0.07396300	3.15762100	-0.21245400
O	-0.19880100	4.59382300	0.63664500
Mo	2.34609000	2.37010600	0.66237200
O	2.75667900	3.55884500	1.79103200
Mo	-2.49319300	0.90106200	-1.42045200
O	-4.16017400	0.96320000	-1.13240000
O	0.52654800	1.86224800	1.13223100
O	1.83444700	3.25138100	-0.99197500
O	-1.97870800	-0.31787000	-0.03618400
O	-2.22394500	-0.51228800	-2.55881500
S	0.97997200	0.17101600	-1.86058600
O	-0.15471000	1.22207800	-1.54375000
O	2.06189200	0.43628600	-0.78047700
S	-2.00255500	3.96286300	-2.69215300
O	-0.55553100	3.92924100	-2.09781500
O	-2.35539600	2.30611700	-2.72763800
S	5.44168400	1.19623300	-0.03719200
O	4.20676700	2.19766000	-0.21765800
O	-1.87213500	4.31752500	-4.13275400
O	5.89132300	1.26967500	1.40016400
O	-1.92070500	2.42533900	-0.12968200
O	2.79129000	0.60326000	1.72417900
O	0.34652300	-1.20558500	-1.44130200
O	4.75231100	-0.22613400	-0.26607900
Mo	1.44086000	-2.92360300	-0.12225200
O	1.86382700	-4.30905500	0.74982500
Mo	3.16664100	-1.19220500	0.65901800
O	4.09536500	-2.05242000	1.78043500
Mo	-1.80111500	-2.00485000	-1.22624400
O	-3.30006200	-2.69000500	-0.89387700
O	1.33502500	-1.51118100	1.18650300
O	3.03775300	-2.23057200	-0.97432400
S	-0.19744700	-4.53537900	-2.52355000
O	1.13267900	-3.86781900	-1.96808100
O	-1.17519700	-3.21216400	-2.67777100
O	0.10494200	-4.91675800	-3.93957300
O	-0.65013700	-3.04306300	0.05802600
H	-2.27736800	2.28707500	0.77375400
H	-0.98443800	-2.81400700	1.03095200
H	1.94894600	0.39808000	2.15739700
Au	-2.38974800	-0.49236800	2.29977100
Cl	-3.35187100	1.71050200	2.43960800
Cl	-2.98319500	-0.96793300	4.70419900
O	-1.50001000	-2.37650000	2.26371600
H	-2.07856300	-2.97708200	2.74665400

C-2

45

Mo	1.69347800	2.83102000	-0.02535400
O	2.18401300	4.16063200	0.93499600
Mo	3.33772200	0.94375400	0.68133000
O	4.36100500	1.68564900	1.83361600
Mo	-1.69354700	2.03450400	-1.18667300
O	-3.19071100	2.82701900	-0.97200300
O	1.53266000	1.36694900	1.26510500
O	3.27737900	2.09605700	-0.89831000
O	-1.86753000	0.57351400	0.17771300
O	-1.95867700	0.85718600	-2.73269100
S	1.04206000	-0.18091900	-1.82695800
O	0.55322300	1.24707700	-1.39057200
O	2.10356600	-0.58543700	-0.75576600
S	0.02739700	4.63996300	-2.18329500
O	1.40795200	3.91290900	-1.78542100
O	-0.90544500	3.34960700	-2.54043100
S	5.43272300	-1.57290500	-0.24693100
O	4.84657500	-0.09620900	-0.36296100
O	0.29338600	5.27449200	-3.51458300
O	5.87783100	-1.81024000	1.16642700
O	-0.44068400	3.05945800	0.17001800
O	2.87788000	-0.88973400	1.70742400
O	-0.19609800	-1.08999400	-1.51053000
O	4.11064400	-2.50511400	-0.49818700
Mo	-0.47898600	-3.18029500	-0.25568300
O	-0.91348000	-4.64127800	0.54072000
Mo	2.38278900	-2.59583000	0.56656600
O	2.80748400	-3.83702700	1.65967000
Mo	-2.42291200	-0.49971300	-1.41931000
O	-4.12929800	-0.43076600	-1.24649400
O	0.44562000	-2.24634100	1.09341300
O	1.36507000	-3.46291600	-0.86977600
S	-2.41643400	-3.43371900	-2.84425700
O	-0.95133400	-3.74534200	-2.17657000
O	-2.38601900	-1.82797700	-3.01704400
O	-2.31002900	-3.96624700	-4.23718900
O	-2.09086000	-2.22457400	-0.27486400
H	-0.69297800	2.80144500	1.08215700
H	-3.15778500	-1.95383600	0.95872700
H	2.05292100	-0.65786700	2.16758400
Au	-2.52077500	0.33195300	2.28580800
Cl	-1.51913400	2.48518100	3.07009000
Cl	-3.28414300	-0.22265900	4.58369600
O	-3.79498100	-1.48122300	1.56209900
H	-4.42915500	-1.08119500	0.94217200

D-1

45

Mo	-2.42398500	-0.73146000	-1.69267700
O	-4.11112700	-0.80492200	-1.79024300
Mo	-1.94236200	1.78107700	-1.43830700
O	-3.48734100	2.46527900	-1.39887000
Mo	-0.25144800	-3.06381500	0.03497000
O	-0.54357900	-4.63828400	0.61506600
O	-2.03930400	0.35231000	-0.14397100
O	-1.80754200	0.58799600	-2.96425200
O	-0.32286200	-2.14288300	1.47010900
O	1.67477200	-3.05697900	-0.22523900
S	1.04992100	-0.18244100	-1.75304400
O	-0.07298400	-1.12679500	-1.21205300
O	0.48657200	1.23792400	-1.45854100
S	-1.62900100	-3.66122000	-3.04090600
O	-1.91181000	-2.07573000	-3.16499400
O	-0.45215400	-3.70907000	-1.96767000
S	-0.33900200	4.57123000	-2.45807900
O	-1.12789300	3.21135600	-2.71286300
O	-0.99068200	-4.02498300	-4.35456500
O	-1.18373100	5.45654300	-1.57758100
O	-2.19196900	-2.43139400	-0.40083500
O	-0.92668300	2.76705700	0.13008700
O	2.24674000	-0.34877900	-0.72655100
O	0.91231100	4.05999500	-1.59330500
Mo	2.98055700	1.22894500	0.73037800
O	3.89092000	1.99487500	1.93261300
Mo	1.16573000	2.91812200	0.09215400
O	1.43710900	4.18542100	1.17280800
Mo	3.09099200	-2.24621800	0.69055900
O	3.48855700	-3.41235700	1.86354500
O	1.15628200	1.33219000	1.27249200
O	2.87231400	2.46605700	-0.72311100
S	5.85906700	-0.50962400	-0.30054200
O	4.85000900	0.60170900	-0.37489500
O	4.52258200	-2.15157300	-0.36401000
O	6.55045300	-0.68245700	-1.57942700
O	3.14468100	-0.69781800	1.62498900
H	-2.67197700	-2.25296600	0.43258800
H	0.89575100	0.57161200	3.04768200
H	-1.17960300	2.34042000	0.97004100
Au	-2.88475600	0.04447300	2.63310400
Cl	-1.85760500	2.08812900	3.14469600
Cl	-3.97252000	-1.98890300	2.18250900
O	1.29542400	0.06125900	3.77403200
H	2.01705600	-0.39325400	3.31375800

D-2

45

Mo	-3.15840100	0.08679600	-0.35137800
O	-4.60807700	0.02060200	0.51343600
Mo	-2.24664300	2.40651800	0.22169100
O	-3.42056600	3.05204600	1.25054000
Mo	-1.00244100	-2.71929800	-1.21821300
O	-1.15924100	-4.33767400	-0.73964600
O	-1.84630100	0.65273700	0.94051600
O	-3.12809400	1.73329800	-1.36264500
O	0.23796000	-2.10622300	0.02785200
O	0.36853500	-2.67839200	-2.45167200
S	-0.08452200	0.65871000	-2.03680500
O	-1.21007600	-0.36968100	-1.64910600
O	-0.26884600	1.83661300	-1.02711900
S	-4.06661000	-2.24181100	-2.53913700
O	-3.95844600	-0.72836300	-2.12711900
O	-2.45312600	-2.66731300	-2.51213200
S	-0.90530500	5.30858000	-0.98243900
O	-1.94496300	4.11159300	-0.93597600
O	-4.41776600	-2.26376100	-3.98834400
O	-0.96873000	6.04405600	0.32679300
O	-2.48738000	-1.89415100	0.01701000
O	-0.49195600	2.92510600	1.30175300
O	1.23955800	-0.02994000	-1.56584100
O	0.51441400	4.51246700	-1.00496800
Mo	3.11172500	0.83943400	-0.26802600
O	4.54207000	1.21274300	0.56100900
Mo	1.28964500	3.12733100	0.23360500
O	2.14886300	4.14633300	1.26200100
Mo	1.87931300	-2.21819700	-1.16440700
O	2.47584100	-3.71987400	-0.70274400
O	1.78656300	1.30093700	0.94318900
O	2.56918300	2.48810000	-1.10907600
S	4.45270800	-0.91592800	-2.74688900
O	3.96019000	0.48208000	-2.12849000
O	3.07171300	-1.79854900	-2.72246000
O	4.68628500	-0.64588000	-4.19730300
O	3.02765000	-1.02342400	-0.08256200
H	-2.29443400	-2.03940000	0.96659500
H	3.77445400	-1.81462100	1.41743400
H	-0.35634500	2.18648900	1.91411100
Au	-0.06665400	-1.49832900	3.50800700
Cl	1.93487200	-0.49207200	4.16582600
Cl	-2.10235700	-2.55851700	3.04340600
O	4.05096300	-2.16500300	2.28267500
H	3.44481700	-1.72972300	2.90267400