Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

## Insight into Structure and Energy of $Mo_{27}S_xO_y$ clusters

Xingchen Liu[a], Dongbo Cao[a], Tao Yang[b], Hao Li[b], Hui Ge[a], Manuel Ramos[c], Qing Peng[d], Albert K. Dearden[e], Zhi Cao[f], Yong Yang[a,g], Yong-Wang Li[a,g], Xiao-Dong Wen[a,g*]

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[a.] *State Key laboratory of Coal Conversion, Institute of Coal Chemistry Chinese Academy of Sciences,Taiyuan, Shanxi, 03001 China*

[b.] *State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing 102249, China*

[c.] *Department of Physics and Mathematics, Universidad Autónoma de Cd. Juárez, 450 del Charro Ave. Cd. Juárez, México. 32310*

[d.] *Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, MI 48109-2104*

[e.] *Department of Physics, Berea College, Berea, KY 40403, USA*

[f.] *Department of Chemistry, University of California, Berkeley, California 94720, USA*

[g.] *Synfuels China Co. Ltd., Huairou, Beijing 100195*

**To whom correspondence should be addressed: wxd@sxicc.ac.cn*

**Cartesian coordinates of selected clusters in .xyz format.**

**Structure 27**

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| | | | |
|---|---|---|---|
| Mo | 5.68100 | 0.03000 | -0.06600 |
| Mo | 5.55800 | 3.16100 | -0.00600 |
| Mo | 5.67100 | 6.29300 | 0.04100 |
| Mo | 8.18900 | -1.70800 | -0.10100 |
| Mo | 8.19600 | 1.57900 | -0.01600 |
| Mo | 8.19200 | 4.74900 | 0.01500 |
| Mo | 8.17100 | 8.04700 | 0.04600 |
| Mo | 10.92200 | -3.27400 | 0.12400 |
| Mo | 10.96000 | -0.01700 | -0.03000 |
| Mo | 10.96600 | 3.17100 | -0.01300 |
| Mo | 10.95000 | 6.36000 | 0.02200 |
| Mo | 10.88800 | 9.60900 | 0.05500 |
| Mo | 13.71700 | -4.51600 | 0.10900 |
| Mo | 13.74700 | -1.58300 | -0.03800 |
| Mo | 13.70500 | 1.59900 | -0.04100 |
| Mo | 13.70400 | 4.75800 | -0.00600 |
| Mo | 13.72800 | 7.94300 | 0.02600 |
| Mo | 13.66100 | 10.91200 | 0.04700 |
| Mo | 16.42300 | -3.00800 | -0.01600 |
| Mo | 16.44300 | -0.01000 | -0.06900 |
| Mo | 16.46900 | 3.16900 | -0.01800 |
| Mo | 16.46900 | 6.35600 | -0.00200 |
| Mo | 16.42200 | 9.43100 | 0.00600 |
| Mo | 18.94000 | -1.46100 | 0.15600 |
| Mo | 19.26500 | 1.56000 | 0.09000 |
| Mo | 19.30700 | 4.71200 | -0.10000 |
| Mo | 19.07600 | 7.76200 | -0.06600 |
| S | 6.34400 | -1.53300 | -1.67200 |
| S | 6.32400 | -1.61200 | 1.45800 |
| S | 6.37800 | 1.65400 | -1.66200 |
| S | 6.35400 | 1.59200 | 1.60700 |
| S | 6.36100 | 4.72700 | -1.61800 |
| S | 6.36400 | 4.67700 | 1.65100 |
| S | 6.31200 | 7.91500 | -1.51100 |
| S | 6.32300 | 7.87900 | 1.62000 |
| S | 9.07400 | -3.31700 | -1.51000 |
| S | 9.11400 | -3.27900 | 1.56400 |
| S | 9.11300 | -0.02100 | -1.58700 |
| S | 9.09600 | -0.08700 | 1.50800 |

| | | | |
|---|---|---|---|
| S | 9.13300 | 3.18300 | -1.57500 |
| S | 9.14100 | 3.14900 | 1.56500 |
| S | 9.08900 | 6.40200 | -1.51700 |
| S | 9.09800 | 6.37200 | 1.57400 |
| S | 9.07500 | 9.61500 | -1.49900 |
| S | 9.09000 | 9.59000 | 1.61700 |
| S | 11.96800 | -4.86100 | -1.38900 |
| S | 12.04000 | -4.71000 | 1.73200 |
| S | 11.83700 | -1.70000 | -1.53500 |
| S | 11.91300 | -1.58100 | 1.54500 |
| S | 11.86300 | 1.58100 | -1.61500 |
| S | 11.87900 | 1.56900 | 1.55400 |
| S | 11.86300 | 4.78800 | -1.58200 |
| S | 11.87300 | 4.75600 | 1.58400 |
| S | 11.85200 | 7.99600 | -1.51200 |
| S | 11.86900 | 7.96600 | 1.58000 |
| S | 11.93800 | 11.14500 | -1.50800 |
| S | 11.95200 | 11.12700 | 1.62100 |
| S | 14.71300 | -3.22200 | -1.63900 |
| S | 14.75100 | -3.03300 | 1.67100 |
| S | 14.61600 | 0.02200 | -1.63600 |
| S | 14.63400 | 0.02900 | 1.52800 |
| S | 14.63600 | 3.19300 | -1.60600 |
| S | 14.63200 | 3.16700 | 1.56000 |
| S | 14.61700 | 6.35000 | -1.56600 |
| S | 14.63600 | 6.32300 | 1.57800 |
| S | 14.66500 | 9.52100 | -1.60500 |
| S | 14.69800 | 9.49700 | 1.65800 |
| O | 17.30300 | -1.49200 | -1.11200 |
| O | 17.19200 | -1.50800 | 1.13700 |
| S | 17.46600 | 1.59700 | -1.56800 |
| S | 17.33800 | 1.54500 | 1.55300 |
| S | 17.38700 | 4.76800 | -1.58000 |
| S | 17.46000 | 4.74400 | 1.52400 |
| S | 17.31700 | 7.96600 | -1.65000 |
| S | 17.38800 | 7.95700 | 1.61400 |
| S | 20.16900 | -0.15600 | -1.36100 |
| S | 19.87800 | -0.16900 | 1.78600 |
| S | 20.23500 | 3.14400 | -1.53500 |
| S | 20.21000 | 3.09600 | 1.53700 |
| S | 20.07000 | 6.39800 | -1.67900 |
| S | 20.18500 | 6.36800 | 1.44100 |

**Structure 11**

81

| | | | |
|---|---|---|---|
| Mo | 5.66200 | 0.03400 | 0.00500 |
| Mo | 5.55600 | 3.16700 | 0.00500 |
| Mo | 5.66300 | 6.30000 | 0.00600 |
| Mo | 8.17800 | -1.70100 | 0.00500 |
| Mo | 8.19500 | 1.58200 | 0.00500 |
| Mo | 8.19600 | 4.75100 | 0.00600 |
| Mo | 8.17900 | 8.03500 | 0.00600 |
| Mo | 10.88700 | -3.26600 | 0.00500 |
| Mo | 10.95300 | -0.02300 | 0.00500 |
| Mo | 10.96900 | 3.16600 | 0.00600 |
| Mo | 10.95400 | 6.35600 | 0.00600 |
| Mo | 10.88900 | 9.59900 | 0.00700 |
| Mo | 13.64700 | -4.57800 | 0.00500 |
| Mo | 13.72200 | -1.61000 | 0.00500 |
| Mo | 13.70800 | 1.58400 | 0.00600 |
| Mo | 13.70900 | 4.74800 | 0.00600 |
| Mo | 13.72400 | 7.94200 | 0.00700 |
| Mo | 13.65000 | 10.91000 | 0.00700 |
| Mo | 16.41400 | -3.10400 | 0.00500 |
| Mo | 16.46700 | -0.02600 | 0.00500 |
| Mo | 16.47800 | 3.16500 | 0.00600 |
| Mo | 16.46800 | 6.35700 | 0.00700 |
| Mo | 16.41600 | 9.43500 | 0.00700 |
| Mo | 19.07400 | -1.44600 | 0.00500 |
| Mo | 19.31900 | 1.60100 | 0.00600 |
| Mo | 19.32000 | 4.72900 | 0.00600 |
| Mo | 19.07600 | 7.77600 | 0.00700 |
| S | 6.32300 | -1.55800 | -1.56200 |
| S | 6.32200 | -1.55800 | 1.57100 |
| S | 6.36100 | 1.62600 | -1.62600 |
| S | 6.36100 | 1.62500 | 1.63600 |
| S | 6.36200 | 4.70900 | -1.62600 |
| S | 6.36200 | 4.70800 | 1.63700 |
| O | 6.44900 | 7.65600 | -1.13000 |
| O | 6.47100 | 7.63900 | 1.13900 |
| S | 9.08500 | -3.25800 | -1.55500 |
| S | 9.08500 | -3.25800 | 1.56400 |
| S | 9.09900 | -0.04700 | -1.54600 |
| S | 9.09800 | -0.04800 | 1.55600 |
| S | 9.13800 | 3.16700 | -1.56500 |
| S | 9.13800 | 3.16600 | 1.57600 |

| | | | |
|---|---|---|---|
| S | 9.10000 | 6.38100 | -1.54500 |
| S | 9.09900 | 6.38000 | 1.55700 |
| S | 9.22300 | 9.44100 | 1.67900 |
| S | 11.93800 | -4.80100 | -1.56300 |
| S | 11.93800 | -4.80200 | 1.57100 |
| S | 11.85900 | -1.64200 | -1.54600 |
| S | 11.85900 | -1.64200 | 1.55600 |
| S | 11.87200 | 1.56800 | -1.57700 |
| S | 11.87200 | 1.56700 | 1.58800 |
| S | 11.87300 | 4.76500 | -1.57600 |
| S | 11.87200 | 4.76400 | 1.58800 |
| S | 11.86100 | 7.97500 | -1.54500 |
| S | 11.86100 | 7.97400 | 1.55700 |
| S | 11.94100 | 11.13400 | -1.56000 |
| S | 11.94000 | 11.13300 | 1.57400 |
| S | 14.67600 | -3.17600 | -1.62700 |
| S | 14.67600 | -3.17700 | 1.63600 |
| S | 14.62300 | -0.00100 | -1.56500 |
| S | 14.62300 | -0.00200 | 1.57600 |
| S | 14.64100 | 3.16600 | -1.57600 |
| S | 14.64100 | 3.16500 | 1.58800 |
| S | 14.62400 | 6.33300 | -1.56400 |
| S | 14.62400 | 6.33300 | 1.57700 |
| S | 14.67800 | 9.50800 | -1.62500 |
| S | 14.67800 | 9.50800 | 1.63800 |
| S | 17.34600 | -1.63600 | -1.62600 |
| S | 17.34600 | -1.63600 | 1.63700 |
| S | 17.42700 | 1.57100 | -1.54500 |
| S | 17.42600 | 1.57100 | 1.55700 |
| S | 17.42700 | 4.76000 | -1.54500 |
| S | 17.42700 | 4.75900 | 1.55700 |
| S | 17.34800 | 7.96700 | -1.62500 |
| S | 17.34800 | 7.96600 | 1.63800 |
| S | 20.12300 | -0.07700 | -1.56100 |
| S | 20.12300 | -0.07800 | 1.57300 |
| S | 20.21400 | 3.16500 | -1.55300 |
| S | 20.21400 | 3.16500 | 1.56600 |
| S | 20.12400 | 6.40700 | -1.56000 |
| S | 20.12400 | 6.40700 | 1.57400 |
| O | 9.30300 | 9.26000 | -1.06100 |

**Example DMol3 Input file**

```
# Task parameters
Calculate                       optimize
Opt_energy_convergence          2.0000e-005
Opt_gradient_convergence        4.0000e-003 A
Opt_displacement_convergence    5.0000e-003 A
Opt_iterations                  500
Opt_max_displacement            0.3000 A


# Electronic parameters
Spin_polarization               restricted
Charge                          0.0000
Basis                           dnp
Atom_rcut                       5.5000 angstrom
Pseudopotential                 ecp
Functional                      gga(p91)
Aux_density                     octupole
Integration_grid                medium
Scf_density_convergence         1.0000e-005
Scf_charge_mixing               0.2000
Scf_iterations                  5000
Scf_diis                        6 pulay
Occupation                      thermal 0.00050

# Print options
Print                           eigval_last_it

# Calculated properties
Plot                            density
Plot                            potential
Mulliken_analysis               charge
Hirshfeld_analysis              charge
Grid                            msbox    3 0.2500 0.2500 0.2500 3.0000
```