



STRUCTURAL  
CHEMISTRY

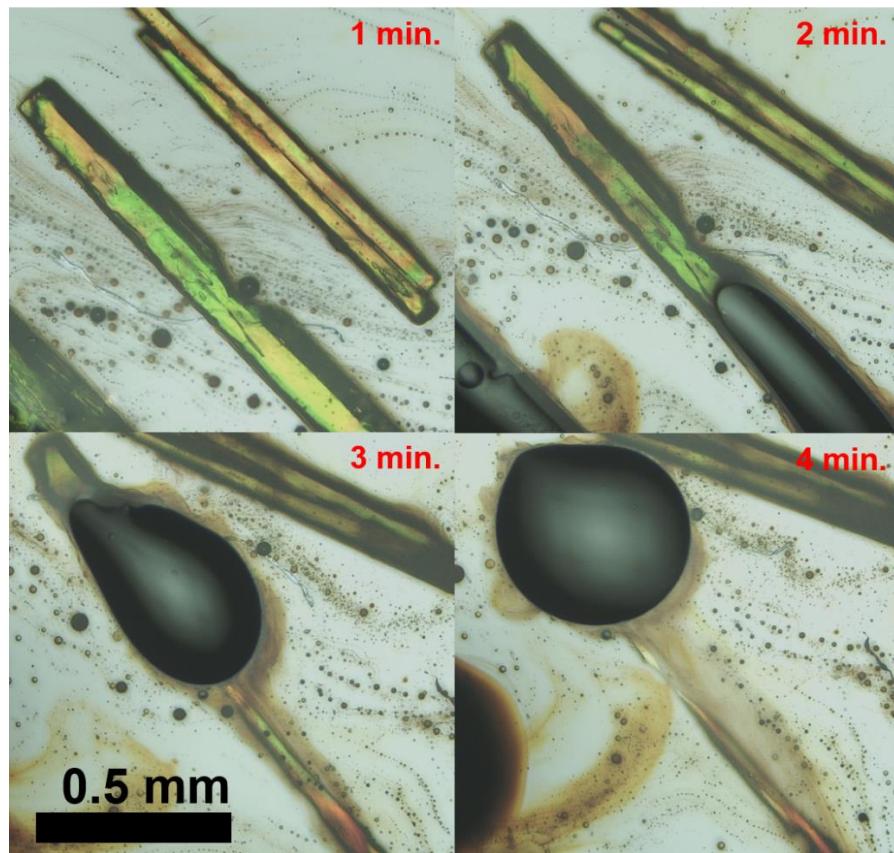
**Volume 76 (2020)**

**Supporting information for article:**

**Crystal structure and Hirshfeld surface analysis of the elusive tri-chloridobis(diethyl ether)oxidomolybdenum(V)**

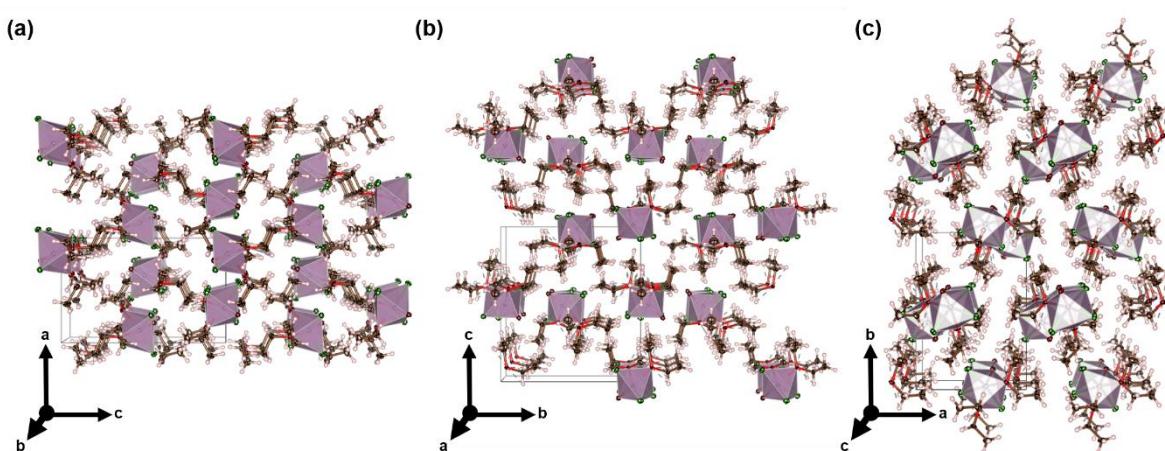
**Thomas E. Shaw, Pierre LeMagueres, Alfred P. Sattelberger and Titel Jurca**

Figure S1 Degradation of **2** in Paratone under ambient conditions.



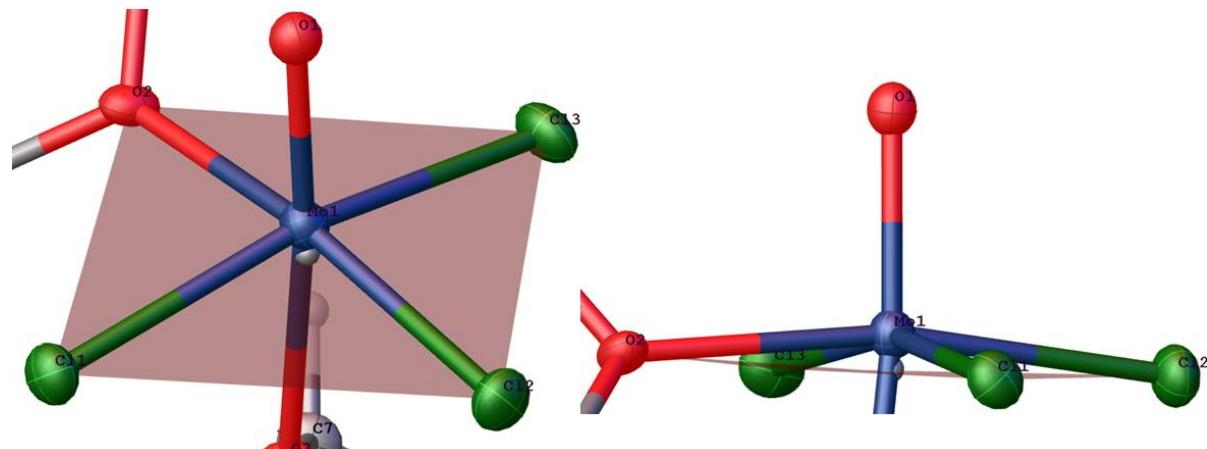
Time-lapse reflective optical microscope (Leica DM2500m) images of **2** suspended in Paratone oil on Si wafer under ambient conditions.

Figure S2 Expanded packing ( $2 \times 2 \times 2$  unit cells) of **2**.



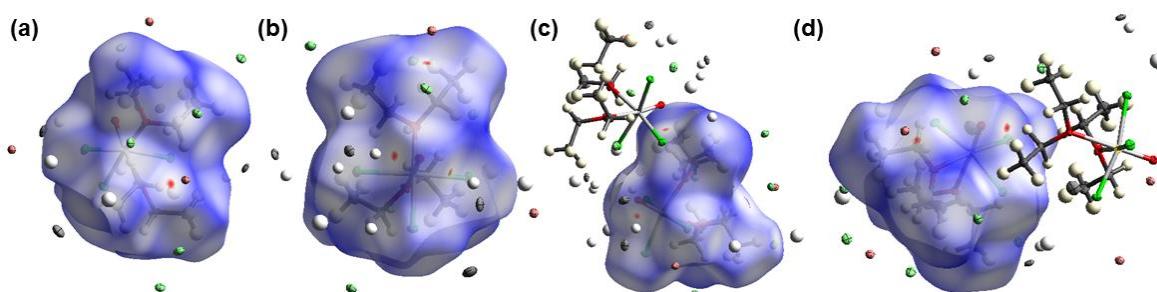
Images generated using VESTA 3.5.2 (2020) (Momma, *et al.* 2011)

**Figure S3** Basal plane measurements.



Basal plane generated with the equation  $-0.272x + 0.709y - 0.650z - 0.536 = 0$ . Images generated with Olex (Dolomanov, *et. al.*, 2009).

Figure S4 Hirshfeld surface showcasing adjacent molecule fragments and whole neighbouring molecules.



$d_{\text{norm}}$  Hirshfeld surfaces of  $\text{MoOCl}_3(\text{Et}_2\text{O})$  from various viewpoints highlighting the areas of intimate contact. (a) and (b) highlight the areas of interactions that are shorter than vdW radii, (c) an exterior Mo=O oxygen interacting with the CH<sub>2</sub> hydrogens of an Et<sub>2</sub>O ligand on an adjacent complex, (d) an exterior CH<sub>2</sub> from an Et<sub>2</sub>O ligand interacting with the Mo=O oxygen of the interior complex. Images generated using CrystalExplorer17 (Turner, *et. al.*, 2017).

## References

- K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data," *J. Appl. Crystallogr.*, 44, 1272-1276 (2011).  
 Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, J. D., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). University of Western Australia. <https://hirshfeldsurface.net>"  
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