



STRUCTURAL
CHEMISTRY

Volume 77 (2021)

Supporting information for article:

A 35-year-old mystery solved: a facile synthetic route and structural confirmation of tetrachlorobis(diethyl ether)tungsten(IV)

Thomas E. Shaw, Alfred P. Sattelberger and Titel Jurca

Figure S1 ^1H spectrum of $\text{WCl}_4(\text{Et}_2\text{O})_2$. The gold highlighted portions are the peaks corresponding to the title complex. The peaks highlighted in red belong to toluene- d_8 and the peaks highlighted in blue indicate the presence of uncoordinated diethyl ether.

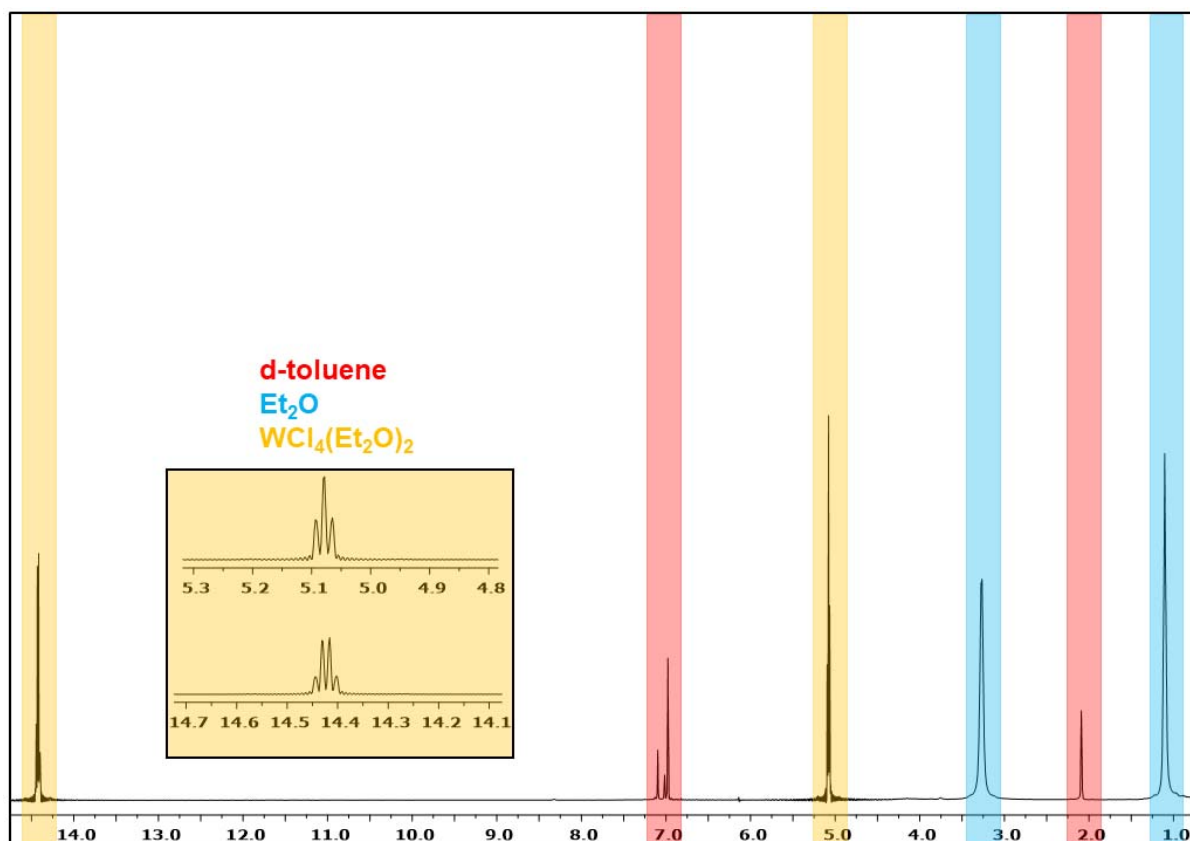
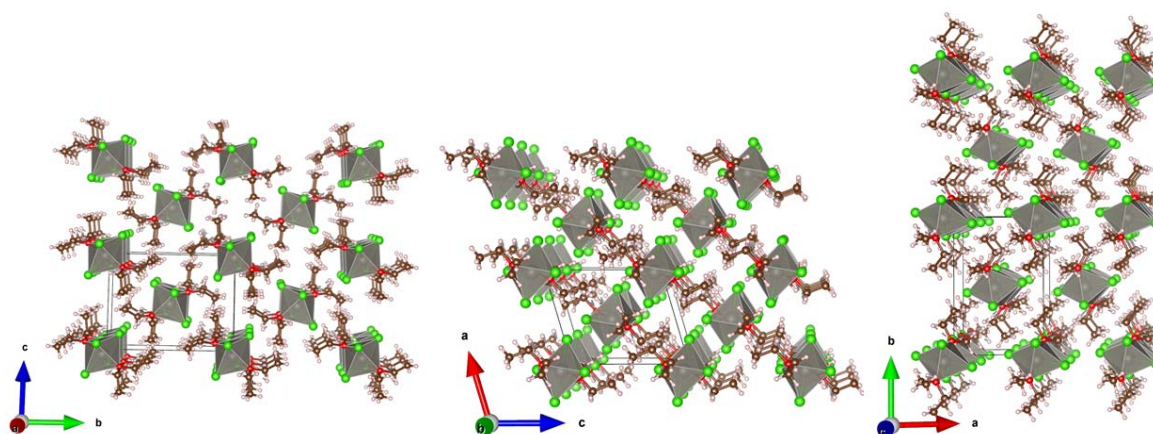
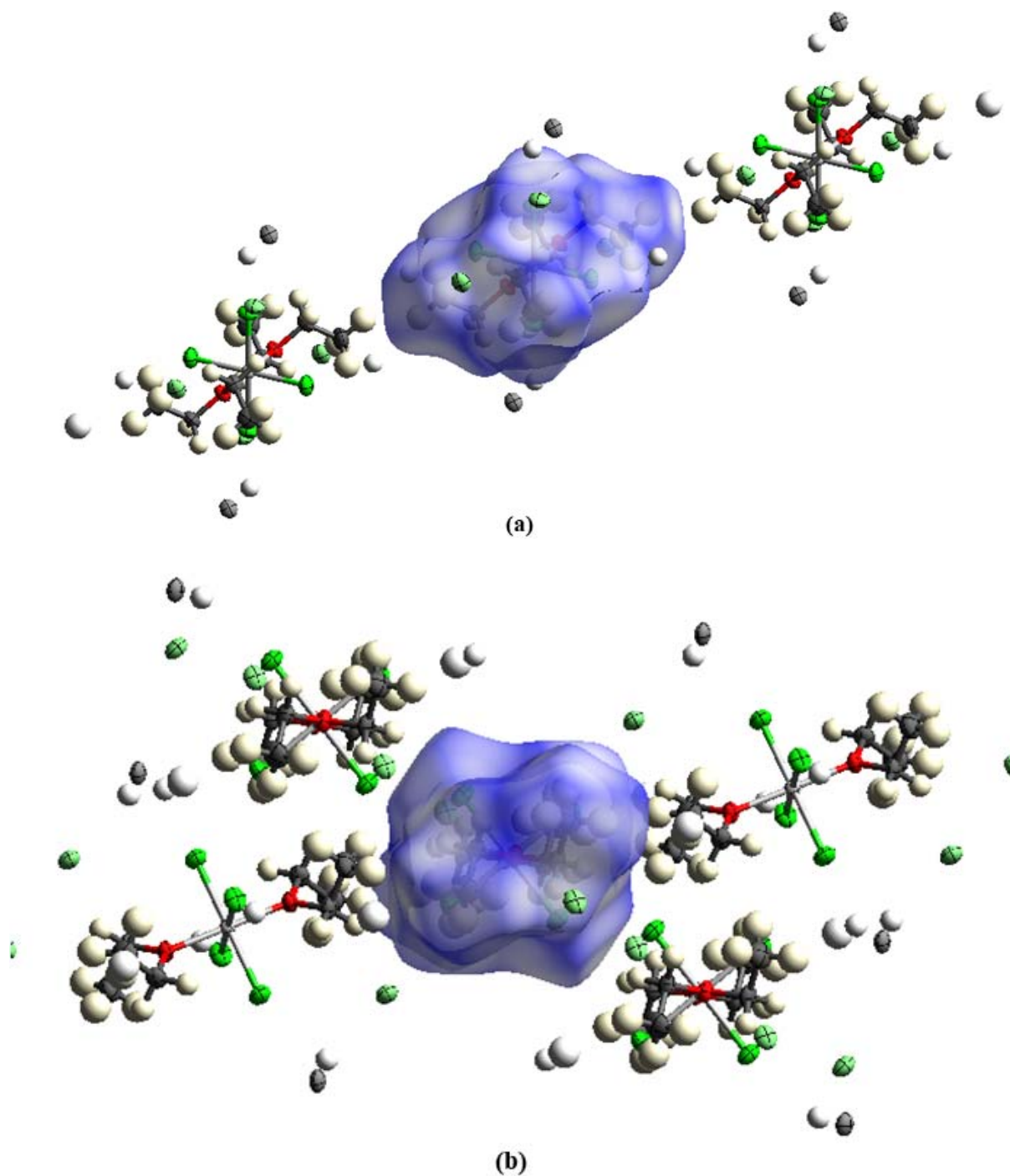


Figure S2 Expanded packing ($2 \times 2 \times 2$ unit) of $\text{WCl}_4(\text{Et}_2\text{O})_2$.



Images generated using VESTA 3.5.6 (2020) (Momma *et al.*, 2011).

Figure S3 Hirshfeld surface highlighting adjacent molecules responsible for surface generation.

D_{norm} Hirshfeld surfaces of *trans*-WCl₄(Et₂O)₂ highlighting (a) H-H interactions between interior and exterior CH₃ hydrogens from the diethyl ether ligands, and (b) H-Cl and Cl-H interactions between interior and exterior chlorine and hydrogen atoms. Images generated using Crystal Explorer17 (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).

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>
<https://hirshfeldsurface.net>.