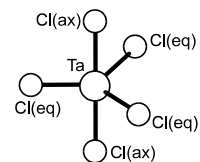


**165**      **Cl<sub>5</sub>Ta**ED, DFT  
calculations**Tantalum pentachloride**Tantalum(V) chloride  
Pentachlorotantalum(V)**D<sub>3h</sub>**  
**TaCl<sub>5</sub>**

$r_a$	$\text{\AA}^a$
Ta–Cl (mean)	2.285(2)
Ta–Cl(eq)	2.266(4)
Ta–Cl(ax)	2.313(5)
$\Delta(\text{Ta–Cl})^b$	0.047(7)



Molecular models with C<sub>2v</sub> and D<sub>3h</sub> symmetry were tested in the ED analysis, and the latter was preferred. WVN88P86 calculations of the molecular force field and vibrational frequencies showed that the optimized structure with D<sub>3h</sub> symmetry corresponds to a minimum on the full potential energy surface.

The nozzle temperature was 131(2) °C.

<sup>a</sup>) Twice the estimated standard errors including a systematic error.

<sup>b</sup>) [Ta–Cl(ax)] – [Ta–Cl(eq)].

Faegri, K., Haaland, A., Martinsen, K.-G., Strand, T.G., Volden, H.V., Swang, O., Anderson, C., Persson, C., Bogdanovic, S., Herrmann, W.A.: J. Chem. Soc., Dalton. Trans. (1997) 1013.

Replaces [II/25A\(2, 415\)](#)