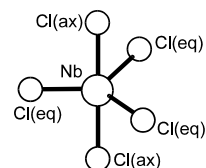


163 **Cl₅Nb**ED, *ab initio* and DFT
calculations**Niobium pentachloride**

Niobium(V) chloride

D_{3h} assumedNbCl₅

r_a	Å ^{a)}
Nb–Cl (average)	2.287(3)
Nb–Cl(ax)	2.306(5)
Nb–Cl(eq)	2.274(4)



The barrier to Berry pseudorotation was estimated as the difference between the energies of optimized models of C_{4v} and D_{3h} symmetry. According to VWNBP86 calculations, this energy difference is equal to 14 kJ mol⁻¹.

The nozzle temperature was 112(5) °C.

^{a)} Twice the estimated standard errors including a systematic error.

Gove, S.K., Gropen, O., Fægri, K., Haaland, A., Martinsen, K.-G., Strand, T.G., Volden, H.V., Swang, O.: J. Mol. Struct. **485-486** (1999) 115.

Replaces [II/25A\(2, 412\)](#)