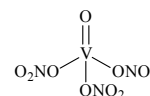


**311**     **N<sub>3</sub>O<sub>10</sub>V**ED, DFT  
calculations**Tris(nitrato- $\kappa$ O)oxovanadium**

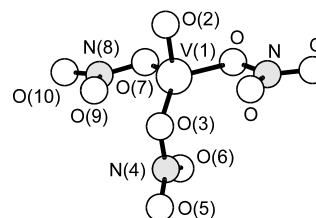
Vanadium(V) trinitrate oxide

**C<sub>s</sub>**, assumed

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
V(1)=O(2)	1.607(7)	O(2)=V(1)–O(3)	94.5(13)
V(1)–O(3)	1.915(7)	O(2)=V(1)–O(7)	96.3(9)
V(1)–O(7)	1.971(5)	V(1)–O(3)–N(4)	99.5(8)
V(1)...O(6)	2.258(20)	V(1)–O(7)–N(8)	96.9(4)
V(1)...O(9)	2.154(9)	O(3)–N(4)=O(5)	123.3(3)
N(4)–O(3)	1.310(6)	O(3)–N(4)=O(6)	113.8(8)
N(4)=O(5)	1.167(8)	O(5)=N(4)=O(6)	122.8(14)
N(4)=O(6)	1.251(5)	O(7)–N(8)=O(9)	112.5(5)
N(8)–O(7)	1.283(4)	O(7)–N(8)=O(10)	126.5(9)
N(8)=O(9)	1.271(4)	O(9)–N(8)=O(10)	121.0(13)
N(8)=O(10)	1.161(7)	twist(NO <sub>3</sub> ) <sup>b)</sup>	2.0(14)
		N(4)...V(1)=O(2)...N(8)	113.2(3)



According to the results of B3LYP/TZP calculations, the molecule exists as a single conformer. In this conformer one nitrate group lies in the mirror plane, while the two others are on either side of that plane and almost perpendicular to it. Differences in the similar parameters were restrained at the values from B3LYP/TZP calculations. Local C<sub>s</sub> symmetry was assumed for each VONO<sub>2</sub> group. The nozzle temperature was 360 K.



<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> Twist angle of the equivalent nitrate groups away from a structure in which the plane of the nitrate group is perpendicular to the O(2)V(1)N(8) plane, positive value for clockwise rotation.

Smart, B.A., Robertson, H.E., Rankin, D.W.H., Hope, E.G., Marsden, C.J.: J. Chem. Soc. Dalton Trans. (1999) 473.