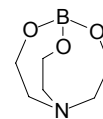


748 **C₆H₁₂BNO₃**ED, *ab initio* and DFT
calculations**2,8,9-Trioxa-5-aza-1-borabicyclo[3.3.3]undecane****C₃ assumed**

r_g	Å ^{a)}	θ_α	deg ^{a)}
N...B	1.846(42)	N...B-O	98.7(21)
C-N	1.466(18)	B-O-C	106.8(27)
B-O	1.415(27)	B...N-C	102.0(14)
C-O	1.422 ^{b)}	C-C-N	104.0 ^{c)}
C-C	1.507(27)	O-C-C	108.9 ^{c)}
		O-B-O	117.7 ^{c)}
		C-N-C	115.8 ^{c)}
		H-C-H	109 ^{d)}
		$\tau(\text{B-O})$ ^{c)}	33.9(40)
		$\tau(\text{N...B})$ ^{c)}	-11.5(26)
		$\tau(\text{C-O})$ ^{c)}	-48.7 ^{c)}
		$\tau(\text{C-C})$ ^{c)}	37.8 ^{c)}
		$\tau(\text{C-N})$ ^{c)}	-14.0 ^{c)}

The molecule was found to have distorted C(3)-envelope conformations of the five-membered rings. According to the results of HF/6-311++G(d,p) calculations, the conformer with C(3)-envelope conformations of the rings is *ca.* 4 kcal mol⁻¹ more stable than that with O-envelope rings, and *ca.* 6 kcal mol⁻¹ more stable than the conformers with N-, B- and C(4)-envelope rings.

The nozzle temperature was *ca.* 100 °C.

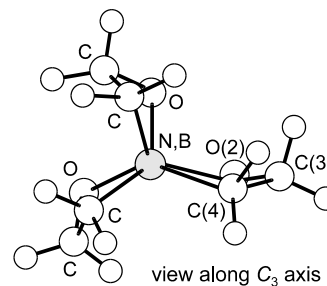
^{a)} Estimated standard errors.

^{b)} Assumed at the value for B(OCH₃)₃ molecule.

^{c)} Dependent parameter.

^{d)} Assumed.

^{e)} Torsional angle around the given bond.



Shishkov, I.F., Khristenko, L.V., Rudakov, F.M., Vilkov, L.V., Karlov, S.S., Zaitseva, G.S., Samdal, S.: J. Mol. Struct. **641** (2002) 199.