

14 MW	CBrNO		Bromine fulminate		$C_{\infty v}$ (effective symmetry class) Br–C≡N–O
	$r_0$ <sup>a)</sup>	Å	$\theta_0$ <sup>a)</sup>	deg	
	Br–C	1.80548(25)	C≡N–O	173.04 <sup>b)</sup>	
	C≡N	1.1732 <sup>b)</sup>	Br–C≡N <sup>c)</sup>	27.430(42)	
	N–O	1.2037 <sup>b)</sup>			

The irregular sequence of satellite spectra indicates that the Br–C≡N mode is highly anharmonic; *i.e.*, BrCNO exhibits truly quasilinear behavior.

<sup>a)</sup> Structural parameters derived by a semirigid bender analysis, which yields the barrier to linearity of 130.82(56) cm<sup>−1</sup> and the force constant for bending of 0.08116(53) aJ rad<sup>−2</sup>.

<sup>b)</sup> Assumed.

<sup>c)</sup> Complement.

Lichau, H., Gillies, C.W., Gillies, J.Z., Ross, S.C., Winnewisser, B.P., Winnewisser, M.: J. Phys. Chem. A **105** (2001) 10065.