326 **C_2N_2O** **Cyanogen fulminate** **$C_{\infty v}$**
MW, IR Ethanedinitrile *N*-oxide (large-amplitude motion)
Cyanogen *N*-oxide (effective symmetry class)
N≡C–C≡N–O

r [a])	Å	θ [a])	deg
N≡C	1.16161(70)	C–C≡N	1.3075(22)
C–C	1.3669(16)		
C≡N	1.1652(17)		
N–O	1.19467(75)		

[a]) Parameters derived from a general semirigid bender analysis of rotational and rovibrational transitions.

Lichau, H., Ross, S.C., Lock, M., Albert, S., Winnewisser, B.P., Winnewisser, M., De Lucia, F.C.:J. Phys. Chem. A **105** (2001) 10080.

$C_{\infty v}$ [a])

r_0	Å [b])
N≡C	1.1602(20)
C–C	1.3639(20)
C≡N	1.1586(20)
N–O	1.1925(20)

r_s	Å [b])
N≡C	1.1606(20)
C–C	1.3633(30)
C≡N	1.1574(30)
N–O	1.1933(20)

$r_{I\varepsilon}$	Å [b])
N≡C	1.1606(20)
C–C	1.3633(20)
C≡N	1.1574(20)
N–O	1.1933(20)

[a]) Though the present data strongly indicate that the molecule is linear, they are insufficient to completely rule out quasilinear behavior.
[b]) Uncertainties were not estimated in the original paper.

Brupbacher, T., Bohn, R.K., Jäger, W., Gerry, M.C.L., Pasinszki, T., Westwood, N.P.C.: J. Mol. Spectrosc. **181** (1997) 316.