4 **CAlN** **Aluminum isocyanide** **$C_{\infty v}$**
MW (effective symmetry class)
(large-amplitude bending vibration)
Al–N=C

r_0	Å [a])
Al–N	1.8548(49)
N=C	1.1626(76)

r_s	Å [b])
Al–N	1.874(5)
N=C	1.155(5)

$r_{I\varepsilon}$	Å [b]) [c])
Al–N	1.874(5)
N=C	1.155(5)

$r_m^{(2)}$	Å [b]) [d])
Al–N	1.883(5)
N=C	1.160(5)

Molecular geometries determined from rotational constants using a linear model have revealed unexpectedly short N=C bond length, and are interpreted in terms of a broadened potential well for the bending mode. This interpretation is confirmed with *ab initio* calculations. The centrifugal distortion constants are consistent with this picture. A new formulation of the rigid bender model has produced a plausible value for bond length and bending amplitude.

[a]) Estimated standard errors.
[b]) Uncertainties were not estimated in the original paper.
[c]) $\varepsilon_0 = -0.855$ u Å^2 assumed.
[d]) $c = -0.183$ u^{½} Å

Walker, K.A., Evans, C.J., Suh, S.-H. K., Gerry, M.C.L., Watson, J.K.G.: J. Mol. Spectrosc. **209** (2001) 178.