55 **CGaN** **Gallium(I) isocyanide** $C_{\infty v}$
MW Ga–N=C

r_0	Å [a])
Ga–N	1.9382(29)
N=C	1.1494(46)

r_s	Å [a])
Ga–N	1.9422(42)
N=C	1.1419(80)

$r_{I\varepsilon}$	Å [a]) [b])
Ga–N	1.9510(35)
N=C	1.1441(25)

$r_m^{(1)}$	Å [a]) [c])
Ga–N	1.9580(52)
N=C	1.1482(21)

$r_m^{(2)}$	Å [a]) [d])
Ga–N	1.9443(1)
N=C	1.1629(1)

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]) $\varepsilon_0 = -0.91(23)$ u Å^2 assumed.
[c]) $c = -0.161(40)$ u$^{1/2}$ Å assumed.
[d]) $c = -0.4534(17)$ u$^{1/2}$ Å and $d = 1.1109(63)$ u$^{1/2}$ Å^2 assumed.

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