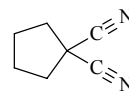


**804**      **C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>**ED, *ab initio* and DFT  
calculations**1,1-Cyclopentanedicarbonitrile**

1,1-Dicyanocyclopentane

**C<sub>s</sub>/C<sub>2</sub>** (pseudorotation)

$r_\alpha$	$\text{\AA}^a$	$\theta_\alpha$	$\text{deg}^a$
C $\equiv$ N	1.152(2)	C(5)–C(1)–C(2)	103.6(31)
C(1)–C(1',1'')	1.472(5)	$\Delta[\text{C}(5)\text{--C}(1)\text{--C}(2)]$	3.5 <sup>b)</sup>
C–H	1.068(4)	C(1')–C(1)–C(1'')	109.1(37)
C–C (ring) <sup>c)</sup>	1.549(3)	H–C–H	112.6(23)
$q^d$	0.434(51)	C–C $\equiv$ N <sup>e)</sup>	175.2(34)

The molecule was described by a pseudorotational model including the conformations of C<sub>s</sub> and C<sub>2</sub> symmetry. The potential function, estimated from MP2 and DFT calculations with various basis sets, gave the energy difference,  $\Delta E(\text{C}_2 - \text{C}_s)$ , of *ca.* 1 kcal mol<sup>−1</sup>. The nozzle temperature was 126 °C.

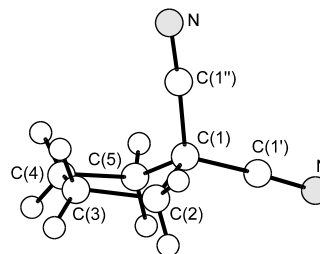
<sup>a)</sup> 2.45 times the estimated standard errors including a systematic error.

<sup>b)</sup> Difference between the C(5)–C(1)–C(2) angles in the conformations with C<sub>s</sub> and C<sub>2</sub> symmetry.

<sup>c)</sup> Average.

<sup>d)</sup> Puckering amplitude of the ring, defined as such that the displacement of the C<sub>*i*</sub> atom from the ring base plane,  $z_i$ , is given as a function of the phase angle  $\phi$  by  $z_i = (2/5)^{1/2} q \cos[\phi + 4\pi(i - 1)/5]$ , ( $i = 1 \dots 5$ ).

<sup>e)</sup> Bent outwards.



Dakkouri, M., Typke, V.: J. Mol. Struct. **612** (2002) 181.