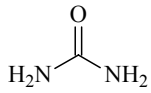
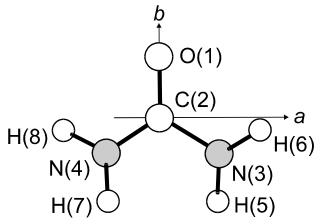
131 **CH_4N_2O** **Urea** **C_2**
MW (effective symmetry class)



r_s [a])	Å [b])
C(2)–O(1)	1.2211(30)
N(3)–C(2)	1.3779(30)
H(5)–N(3)	0.9978(20)
H(6)–N(3)	1.0212(20)

θ_s [a])	deg [b])
O(1)–C(2)–N(3)	122.64(30)
N(3)–C(2)–N(4)	114.71(30)
C(2)–N(3)–H(5)	119.21(30)
C(2)–N(3)–H(6)	112.78(30)
H(5)–N(3)–H(6)	118.61(20)
$\Sigma\alpha$(N) [c])	350.60(50)
N(4)–C(2)–N(3)…O(1) [d])	180.0(3)
H(5)–N(3)–C(2)–O(1) [d])	156.9(3)
H(5)–N(3)–C(2)–N(4) [d])	–23.2(3)
H(6)–N(3)–C(2)–O(1) [d])	10.8(3)
H(6)–N(3)–C(2)–N(4) [d])	–169.2(3)
H(7)–N(4)–C(2)–O(1) [d])	156.9(3)
H(7)–N(4)–C(2)–N(3) [d])	–23.2(3)
H(8)–N(4)–C(2)–O(1) [d])	10.8(3)
H(8)–N(4)–C(2)–N(3) [d])	–169.2(3)

Atom	$\|a_s\|$ [Å]	$\|b_s\|$ [Å]	$\|c_s\|$ [Å]
O(1)	0.0115	1.3049	0.0280i [e])
C(2)		0.0838 [f])	
N(3,4)	1.1603	0.6595	0.0
H(5,7)	1.1383	1.5964	0.3424
H(6,8)	1.9922	0.0940	0.1760



The conformer of lowest energy is predicted to be nearly planar with C_2 symmetry, a second minimum for a shape of C_s symmetry being higher in energy by 421 cm^{-1}. However, these are separated by a barrier estimated to be no higher than about 130 cm^{-1}. Thus the two shapes are likely to be parts of the potential energy surface domain that is associated with the most stable shape of urea, *i.e.*, one in which the zero-point vibration covers both C_2 and C_s geometries, the most probable geometry being C_2.

[a]) Almost all structural parameters are r_s, but, because the *b* coordinate of C(2) is determined by the first-moment equation, those involving the C(2) coordinate may be regarded as r_0.
[b]) Uncertainties were not estimated in the original paper.
[c]) Sum of pyramidal angles around N, *i.e.*, [C(2)–N(3)–H(5)] + [C(2)–N(3)–H(6)] + [H(5)–N(3)–H(6)].
[d]) Dihedral angle.
[e]) Imaginary value.
[f]) Derived from first-moment equation.

Godfrey, P.D., Brown, R.D., Hunter, A.N.: J. Mol. Struct. **413-414** (1997) 405.