

1555 **C₄H₄N₂O₂**
ED, *ab initio*
calculations (HF/4-21)

2,4(1*H*,3*H*)-Pyrimidinedione
Uracil

essentially C_s

r_g	Å ^{a)}	θ_α	deg ^{a)}
N–C (average)	1.399(6) ^{b)}	C(2)–N(1)–C(6)	123.2(12)
C=O (average)	1.212(3) ^{b)}	N(3)–C(4)–C(5)	115.5(18)
C(4)–C(5)	1.462(8)	C(4)–C(5)=C(6)	119.7(21)
C(5)=C(6)	1.343(24)	C(5)=C(6)–N(1)	122.1(22)
C–H	1.072 ^{c)}	N(1)–C(2)=O	123.8(14)
N–H	1.002 ^{c)}	C(5)–C(4)=O	124.3(20)
		C(6)–N(1)–H	121.0 ^{c)}
		C(4)–N(3)–H	116.1 ^{c)}
		C(6)=C(5)–H	122.5 ^{c)}
		C(5)=C(6)–H	122.8 ^{c)}

Planar or nearly planar models fit the experimental data.
The nozzle temperature was 201 °C.

^{a)} Estimated total errors.

^{b)} The difference between the N–C and C=O distances derived
from *ab initio* calculations was assumed.

^{c)} Assumed.

Ferenczy, G., Harsányi, L., Rozsondai, B., Hargittai, I.: J. Mol. Struct. **140** (1986) 71.

See also: Harsányi, L., Vajda, E., Ferenczy, G., Rozsondai, B., Császár, P., Császár, A.:
Kem. Kozl. **66** (1986) 277.

