Crystal structure of 6-methylnicotinamide, C₇H₈N₂O

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Abstract

C₇H₈N₂O, monoclinic, *P*12₁/*n*1 (No. 14), *a* = 8.8355(9) Å, *b* = 7.4643(7) Å, *c* = 10.428(1) Å, β = 99.202(2)°, *V* = 678.9 Å³, *Z* = 4, *R*_g(*F*) = 0.058, *wR*_{ref}(*F*²) = 0.141, *T* = 213 K.

Source of material

The title compound was crystallized as received from Aldrich using CH₂Cl₂ solution layered with hexane.

Discussion

6-Methylnicotinamide was structured as part of a developing project. The related nicotinamide has been used as a ligand for various studies. The studies range from crystal engineering [1], photochemical properties [2], and biological properties [3] of the organometallic complexes derived with nicotinamide as a ligand to the electrostatic potential of nicotinamide [4]. The structure of nicotinamide has been studied thoroughly at various temperatures and by neutron diffraction [4]. The structure of 6-methyl reported here shows no significant differences in the structural parameters. The lack of any disconcertable differences between nicotinamide and 6-methylnicotinamide in the distances and angles may reflect a low electronic effect and therefore may provide more steric ef-

fects in the coordination chemistry. Studies are continuing to synthesize various metal coordination complexes with 6-methylnicotinamide. The hydrogen bonding between molecules shows that the amide of one molecule interacts with the carboxylate of an adjacent molecule in a pairwise fashion with a long the O...N-H distance of 2.91(2) Å. With this weak interaction we hope that we can break this hydrogen bonding by the presence of a H-bonding solvent. Crystallization in H-bonding solvents are under way.

Table 1. Data collection and handling.

Crystal:	colorless needle, size 0.08 × 0.08 × 0.20 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.93 cm ⁻¹
Diffractometer, scan mode:	Bruker CCD, 1271 frames, $\Delta\omega$ = 0.3°
2 θ _{max} :	56.56°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	4041, 1630
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 1010
<i>N</i> (<i>param</i>) _{refined} :	92
Programs:	SHELXS-97 [5], SHELXL-97 [6], SHELXLTL-PC [7]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2A)	4e	0.9732	0.0359	0.6209	0.037
H(2B)	4e	0.8533	0.1023	0.6971	0.037
H(2)	4e	0.3870	0.2847	0.7106	0.038
H(3)	4e	0.6341	0.1752	0.7163	0.038
H(4)	4e	0.5773	0.2227	0.3303	0.034
H(6A)	4e	0.1645	0.4839	0.4408	0.057
H(6B)	4e	0.1684	0.4417	0.5902	0.057
H(6C)	4e	0.1084	0.2951	0.4843	0.057

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
O(1)	4e	0.8254(2)	0.0828(2)	0.4055(1)	0.0279(8)	0.053(1)	0.0257(7)	0.0093(7)	0.0087(6)	0.0021(7)
N(1)	4e	0.3967(2)	0.3026(2)	0.4028(2)	0.0241(9)	0.037(1)	0.0287(9)	0.0021(7)	0.0051(7)	0.0035(7)
N(2)	4e	0.8825(2)	0.0799(2)	0.6229(1)	0.0222(9)	0.045(1)	0.0256(9)	0.0080(8)	0.0045(7)	−0.0013(8)
C(1)	4e	0.3418(2)	0.3193(3)	0.5152(2)	0.022(1)	0.023(1)	0.037(1)	−0.0035(8)	0.0068(8)	−0.0052(8)
C(2)	4e	0.4281(2)	0.2720(3)	0.6333(2)	0.029(1)	0.042(1)	0.027(1)	0.0015(9)	0.0107(8)	−0.0048(9)
C(3)	4e	0.5743(2)	0.2063(3)	0.6366(2)	0.029(1)	0.043(1)	0.024(1)	0.0027(9)	0.0046(8)	0.0003(9)
C(4)	4e	0.6329(2)	0.1860(3)	0.5215(2)	0.021(1)	0.023(1)	0.0240(9)	−0.0030(8)	0.0041(7)	−0.0005(8)
C(5)	4e	0.5390(2)	0.2361(3)	0.4088(2)	0.025(1)	0.037(1)	0.026(1)	0.0014(9)	0.0078(8)	0.0001(9)
C(6)	4e	0.1815(2)	0.3914(3)	0.5069(2)	0.028(1)	0.041(2)	0.048(1)	0.003(1)	0.009(1)	−0.004(1)
C(7)	4e	0.7883(2)	0.1127(2)	0.5127(2)	0.022(1)	0.024(1)	0.026(1)	−0.0018(8)	0.0062(8)	0.0024(8)

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