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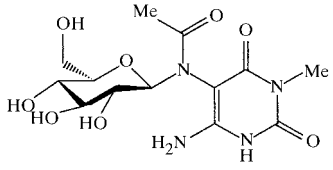
The title compound, $C_{13}H_{20}N_4O_8\cdot 2H_2O$, *i.e.* (I)·$2H_2O$, shows no unusual features. The structure contains two molecules of water of crystallization. The absolute configuration was not determined but was known from the starting materials.



(I)

Experimental

For preparation details, see Melgarejo *et al.* (1982). Suitable crystals (m.p. 543–545 K) for X-ray diffraction was obtained from the crude reaction (MeOH, NaOMe) after neutralization with acetic acid.

Crystal data

$C_{13}H_{20}N_4O_8\cdot 2H_2O$
M_r = 396.36
Orthorhombic, $P2_12_12_1$
a = 7.0911 (1) Å
b = 12.2566 (2) Å
c = 20.5272 (4) Å
V = 1784.08 (5) Å^3
Z = 4
D_x = 1.476 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2711 reflections
θ = 3.03–30.39°
μ = 0.127 mm^{-1}
T = 150 (2) K
Lath, colourless
0.33 × 0.15 × 0.13 mm

Data collection

KappaCCD diffractometer
φ and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.960, T_{max} = 0.984
12 217 measured reflections
2711 independent reflections
2482 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 29.0°
$h = -8 \rightarrow 9$
$k = -16 \rightarrow 17$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.100
S = 1.057
2711 reflections
251 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.5011P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Compound (I)·$2H_2O$ crystallized in the orthorhombic system; space group $P2_12_12_1$ was assumed from the systematic absences. H atoms were treated as riding atoms with C—H = 0.98–1.00 Å, N—H = 0.88 Å and O—H = 0.84 Å (except for those attached to the water O atoms). All H atoms were located initially by means of a difference Fourier synthesis, except for those attached to the methyl groups which were given a site-occupancy factor of 0.5 and placed at appropriate distances at the vertices of a regular hexagon. The water H atoms were fixed at the positions obtained from difference Fourier synthesis. Friedel pairs were merged since the the molecule contained no atom with $Z > 8$. Examination of the structure with *PLATON* (Spek, 2000) showed that there were no solvent-accessible voids in the crystal lattice.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97 and WordPerfect macro *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC, X-ray Crystallographic Service, University of Southampton, using an Enraf–Nonius KappaCCD diffractometer. The authors thank the staff for all their help and advice.

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