Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

10-Formyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazatetracyclo-[5.5.0.0^{5,9}.0^{3,11}]dodecane acetone solvate

Huaxiong Chen,[a,b] Lijie Li,[a] Sufen Liu,[a] Shusen Chen[a] and Shaohua Jin[a]*

[a]School of Materials Science and Engineering, Beijing Institute of Technology, Beijing 100081, People's Republic of China, and [b]Gansu Yinguang Chemical Industry Group Co. Ltd, Gansu 730900, People's Republic of China
Correspondence e-mail: nanfei314@126.com

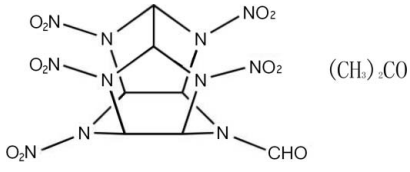
Received 10 January 2010; accepted 22 January 2010

Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.066; data-to-parameter ratio = 7.5.

The title compound, $C_7H_7N_{11}O_{11}\cdot C_3H_6O$, consisting of one molecule of 10-formyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.0^{5,9}.0^{3,11}]dodecane (pentanitromonoformylhexaazaisowurtzitane, PNMFIW) and one acetone solvent molecule, is a member of the caged hexaazaisowurtzitane family. PNMFIW has a cage structure which is constructed from one six-membered and two five-membered rings which are linked by a C—C bond, thus creating two seven-membered rings. In the PNMFIW molecule, one formyl group is bonded to the N heteroatom of the six-membered cycle, and five nitro groups are appended to other five N heteroatom of the caged structure. The acetone solvent molecule is arranged beside a five-membered plane of PNMFIW with an O atom and an H atom close (with respect to the sum of the van der Waals radii) to the neighbouring nitro O atom [O$\cdots$O = 2.957 (3) and 2.852 (3) Å; O$\cdots$H = 2.692 (2), 2.526 (3) and 2.432 (3) Å].

Related literature

For the synthesis see: Golfier *et al.* (1998); Liu *et al.* (2006); Ou *et al.* (2000). For structures with similar properties, see: Chen *et al.* (2010); Jin *et al.* (2009); Lu *et al.* (2004).



Experimental

Crystal data

$C_7H_7N_{11}O_{11}\cdot C_3H_6O$
M_r = 479.31
Monoclinic, $P2_1$
a = 10.432 (3) Å
b = 7.9230 (19) Å
c = 12.191 (3) Å
β = 113.493 (2)°
V = 924.1 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 93 K
0.60 × 0.27 × 0.17 mm

Data collection

Rigaku Saturn724+ diffractometer
7388 measured reflections
2257 independent reflections
2056 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.066
S = 1.00
2257 reflections
301 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *CrystalClear*; program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2324).

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