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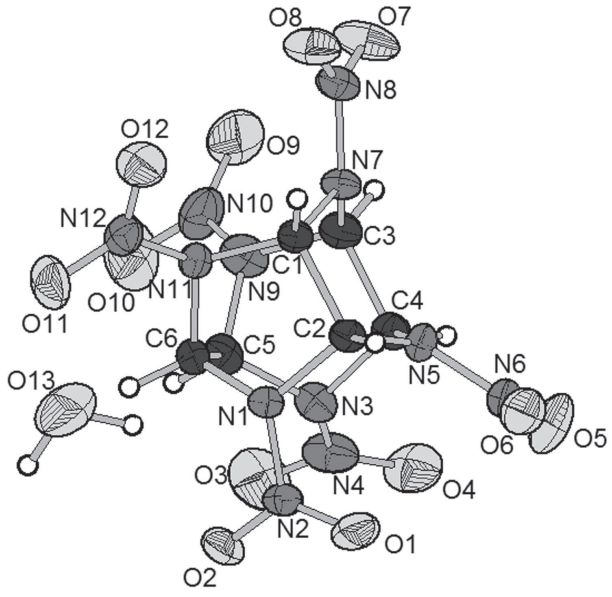
Yuehai Yu, Shaohua Jin, Jiaping Zhu, Lijie Li, Shusen Chen and Qinghai Shu*

Crystal structure of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5·5·0·$0_{5.9}$·$0_{3.11}$]dodecane 1/3 hydrate, $C_6H_8N_{12}O_{13}$



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Abstract

$C_6H_6N_{12}O_{12} \cdot 0.33\ H_2O$, orthorhombic, *Pbca* (no. 61), $a = 9.5152(7)$ Å, $b = 13.2551(11)$ Å, $c = 23.6736(18)$ Å, $V = 2985.8(7)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0727$, $wR_{ref}(F^2) = 0.1268$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

***Corresponding author: Qinghai Shu,** School of Materials Science and Engineering, Beijing Institute of Technology, P. R. China, e-mail: qhshu121@bit.edu.cn
Yuehai Yu, Shaohua Jin, Jiaping Zhu, Lijie Li and Shusen Chen: School of Materials Science and Engineering, Beijing Institute of Technology, P. R. China

Table 1: Data collection and handling.

Crystal:	Yellow, block, size 0.20×0.21×0.22 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.96 cm^{-1}
Diffractometer, scan mode:	CCD, φ and ω scans
$2\theta_{max}$:	50.1°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	17728, 2637
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2196
$N(param)_{refined}$:	299
Programs:	SHELX [6], Diamond [7]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1)	8*c*	1.2643	0.1508	0.1380	0.027
H(2)	8*c*	1.1511	0.2272	0.2110	0.027
H(3)	8*c*	0.9646	0.2484	0.0317	0.034
H(4)	8*c*	0.8489	0.3200	0.1056	0.034
H(5)	8*c*	0.7784	0.0349	0.1134	0.035
H(6)	8*c*	0.9519	−0.0223	0.1736	0.030
H(13A)	8*c*	1.0640	0.3958	0.0586	0.142
H(13B)	8*c*	1.0087	0.5057	0.0483	0.142

Source of material

The title compound was obtained as follows: HNIW (hexanitrohexaazaisowurtzitane, CL-20) was dissolved in the mixed solution of water and acetone with heating. The colorless transparent cocrystal compound was formed by slow evaporation of solvent.

Experimental details

Single-crystal X-ray diffraction data were collected using a Bruker-AXS SMART APEX2 CCD diffractometer. The coordinates of the H atoms were idealized and refined using the AFIX 13 or the AFIX 3 option respectively of the SHELX program [6]).

Discussion

HNIW is a novel high energetic explosive. ε-CL-20 is the most stable in the known four polymorphs at normal temperatures and pressures, unfortunately, which had

Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	8*c*	0.9171(2)	0.2056(1)	0.27540(7)	0.055(1)	0.049(1)	0.0358(8)	−0.0096(8)	0.0168(8)	−0.0159(8)
N(1)	8*c*	1.0027(2)	0.1165(1)	0.20449(6)	0.0227(8)	0.0268(8)	0.0202(8)	−0.0006(7)	0.0024(6)	0.0007(7)
C(1)	8*c*	1.1627(2)	0.1509(1)	0.13189(7)	0.0222(9)	0.026(1)	0.0194(9)	−0.0004(8)	−0.0004(7)	0.0010(8)
O(2)	8*c*	0.8063(2)	0.0715(1)	0.24738(7)	0.0311(8)	0.0354(8)	0.0455(9)	−0.0047(7)	0.0116(7)	0.0070(7)
N(2)	8*c*	0.9015(2)	0.1326(1)	0.24494(7)	0.0282(9)	0.0339(9)	0.0234(8)	0.0020(8)	0.0048(7)	0.0030(8)
C(2)	8*c*	1.0844(2)	0.2027(1)	0.18262(8)	0.0226(9)	0.026(1)	0.0197(9)	−0.0028(8)	−0.0011(7)	−0.0003(8)
O(3)	8*c*	0.5820(2)	0.1288(2)	0.1218(1)	0.0260(9)	0.080(2)	0.096(2)	−0.013(1)	−0.010(1)	0.008(1)
N(3)	8*c*	0.8023(2)	0.1813(1)	0.13822(7)	0.0190(8)	0.0345(9)	0.0342(9)	0.0008(7)	−0.0036(7)	0.0067(8)
C(3)	8*c*	0.9798(2)	0.2101(2)	0.06674(8)	0.028(1)	0.035(1)	0.0229(9)	−0.0003(9)	−0.0022(8)	0.0038(9)
O(4)	8*c*	0.6221(2)	0.2884(2)	0.12955(8)	0.038(1)	0.066(1)	0.063(1)	0.0227(9)	0.0062(9)	0.010(1)
N(4)	8*c*	0.6560(2)	0.2013(2)	0.12776(8)	0.025(1)	0.062(1)	0.037(1)	0.006(1)	0.0003(8)	0.010(1)
C(4)	8*c*	0.8999(2)	0.2596(2)	0.11779(8)	0.026(1)	0.029(1)	0.030(1)	0.0036(8)	−0.0001(8)	0.0064(8)
O(5)	8*c*	0.8764(2)	0.4209(1)	0.1830(1)	0.077(1)	0.038(1)	0.088(2)	0.026(1)	0.014(1)	−0.011(1)
N(5)	8*c*	1.0002(2)	0.2840(1)	0.16099(7)	0.0307(9)	0.0212(8)	0.0293(9)	0.0003(7)	0.0016(7)	−0.0047(7)
C(5)	8*c*	0.8542(2)	0.0844(2)	0.11757(9)	0.027(1)	0.031(1)	0.031(1)	−0.0073(9)	−0.0031(8)	−0.0003(9)
O(6)	8*c*	1.0570(2)	0.3816(1)	0.23404(7)	0.072(1)	0.045(1)	0.043(1)	−0.0206(9)	0.0123(9)	−0.0211(8)
N(6)	8*c*	0.9744(2)	0.3680(1)	0.19602(9)	0.053(1)	0.0251(9)	0.044(1)	−0.0064(9)	0.018(1)	−0.0077(9)
C(6)	8*c*	0.9732(2)	0.0452(1)	0.15888(8)	0.028(1)	0.0221(9)	0.025(1)	−0.0011(8)	0.0012(8)	0.0008(8)
O(7)	8*c*	1.1848(2)	0.2392(2)	−0.00816(6)	0.044(1)	0.086(1)	0.0242(8)	−0.0065(9)	0.0011(7)	0.0202(8)
N(7)	8*c*	1.1268(2)	0.2053(1)	0.08092(7)	0.0242(8)	0.0318(9)	0.0187(8)	0.0001(7)	0.0024(7)	0.0034(7)
O(8)	8*c*	1.3401(2)	0.1734(1)	0.04730(7)	0.0293(9)	0.065(1)	0.0398(9)	0.0043(8)	0.0088(7)	0.0090(8)
N(8)	8*c*	1.2240(2)	0.2044(1)	0.03673(7)	0.033(1)	0.039(1)	0.0237(9)	−0.0065(8)	0.0040(7)	0.0029(8)
N(9)	8*c*	0.9169(2)	0.1100(2)	0.06323(7)	0.037(1)	0.049(1)	0.0213(8)	−0.0121(9)	−0.0089(7)	−0.0011(8)
O(9)	8*c*	0.9079(3)	0.1106(2)	−0.02962(8)	0.109(2)	0.066(1)	0.0290(9)	−0.002(1)	0.002(1)	−0.0107(9)
N(10)	8*c*	0.8675(2)	0.0714(2)	0.01389(9)	0.063(1)	0.042(1)	0.038(1)	0.003(1)	−0.006(1)	−0.013(1)
O(10)	8*c*	0.7895(3)	−0.0008(2)	0.01781(9)	0.125(2)	0.064(1)	0.063(1)	−0.039(2)	−0.015(1)	−0.018(1)
O(11)	8*c*	1.1563(2)	−0.1088(1)	0.16057(8)	0.051(1)	0.0287(8)	0.064(1)	0.0057(7)	0.0011(9)	0.0129(8)
N(11)	8*c*	1.1072(2)	0.0475(1)	0.12995(7)	0.0269(9)	0.0220(8)	0.0273(8)	0.0033(7)	0.0027(7)	0.0017(7)
O(12)	8*c*	1.3239(2)	−0.0144(1)	0.12873(8)	0.0325(9)	0.048(1)	0.061(1)	0.0137(8)	0.0092(8)	0.0115(8)
N(12)	8*c*	1.2037(2)	−0.0313(1)	0.14178(7)	0.038(1)	0.029(1)	0.0288(9)	0.0086(8)	−0.0011(8)	0.0023(8)
O(13)	8*c*	0.9918(9)	0.4354(6)	0.0411(3)	0.111(6)	0.071(4)	0.102(6)	−0.038(4)	−0.051(5)	0.004(4)

high sensitivity and high production cost. Based on the cocrystallization [1–5], we therefore present a cocrystal of CL-20/H_2O to synthesize a new cocrysal explosive. We provide a method for the security of energetic materials. The crystal structure reveals that the cocrystal is made up of 0.33 H_2O and two 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5·5·0·$0_{5\cdot9}$·$0_{3\cdot11}$]dodecane molecules. In crystal structure CL-20 builds up intermolecular hydrogen bonds to water molecules. Hydrogen bonds between all molecules form a two-dimensional cocrystal.

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