Crystal structure of diazabicyclo[2.2.2]octanium-tri(thiocyanato)zinc(II) hydrate, (C₆H₁₃N₂)(SCN)₃Zn(H₂O)

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Source of material: Crystallization from an aqueous solution of zinc sulfate heptahydrate ($c = 0.05$ mol/l), potassium thiocyanate ($c = 0.1$ mol/l), and diazabicyclo[2.2.2]octane ($c = 0.05$ mol/l). H positions at C atoms were calculated assuming sp^2 hybridization and C–H distances 1.08 Å. H atoms at N42 of the diazabicyclooctane molecule and of the water molecule refined, all thermal parameters of H atoms fixed.

C₉H₁₅N₅OS₃Zn, monoclinic, $P12_1/c1$ (No. 14), $a = 7.886(2)$ Å, $b = 13.015(2)$ Å, $c = 15.636(3)$ Å, $\beta = 98.59(2)^\circ$, $V = 1586.9$ Å³, $Z = 4$, $R(F) = 0.038$, $R_w(F) = 0.039$.

Reference

1. Sheldrick, G. M.: SHELXL-76, Programs for Crystal Structures Determination. University of Cambridge, UK 1976.

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Zn	4e	0.43473(4)	0.12690(2)	0.69407(2)	0.0398(2)	0.0449(2)	0.0420(2)	−0.0025(1)	0.0036(1)	−0.0022(1)
S(11)	4e	0.2547(1)	0.38568(6)	0.49577(5)	0.0661(5)	0.0460(4)	0.0490(4)	0.0030(3)	0.0079(4)	0.0044(3)
S(21)	4e	0.8028(1)	−0.05823(7)	0.54383(6)	0.0695(6)	0.0672(5)	0.0627(5)	0.0210(4)	0.0156(4)	−0.0054(4)
C(11)	4e	0.3192(4)	0.3060(2)	0.5729(2)	0.044(1)	0.045(1)	0.042(1)	0.002(1)	0.004(1)	−0.011(1)
N(11)	4e	0.3617(4)	0.2491(2)	0.6279(2)	0.080(2)	0.057(1)	0.051(1)	0.008(1)	−0.007(1)	0.003(1)
C(21)	4e	0.6746(4)	−0.0025(2)	0.6003(2)	0.047(2)	0.036(1)	0.045(1)	−0.005(1)	−0.001(1)	−0.002(1)
N(21)	4e	0.5817(3)	0.0371(2)	0.6405(2)	0.054(1)	0.057(1)	0.061(2)	−0.002(1)	0.013(1)	−0.012(1)
S(31)	4e	0.0221(1)	−0.05338(7)	0.81902(6)	0.0712(6)	0.0580(5)	0.0748(6)	−0.0002(4)	0.0338(5)	0.0037(4)
N(41)	4e	0.5935(2)	0.1830(2)	0.8016(1)	0.035(1)	0.032(1)	0.035(1)	0.0011(8)	0.0060(9)	0.0023(8)
C(41)	4e	0.6327(4)	0.0993(2)	0.8671(2)	0.048(2)	0.035(1)	0.043(1)	−0.001(1)	0.004(1)	0.008(1)
C(42)	4e	0.7503(4)	0.1386(2)	0.9462(2)	0.062(2)	0.044(1)	0.046(2)	−0.006(1)	−0.005(1)	0.011(1)
C(43)	4e	0.5110(4)	0.2694(2)	0.8426(2)	0.063(2)	0.042(1)	0.050(2)	0.016(1)	−0.004(1)	−0.009(1)
C(45)	4e	0.7575(4)	0.2189(2)	0.7758(2)	0.046(2)	0.061(2)	0.049(2)	−0.018(1)	0.006(1)	0.005(1)
C(46)	4e	0.8792(4)	0.2566(3)	0.8545(2)	0.057(2)	0.079(2)	0.059(2)	−0.026(2)	−0.004(2)	0.013(2)
C(44)	4e	0.6309(5)	0.3108(3)	0.9205(2)	0.084(2)	0.058(2)	0.062(2)	0.025(2)	−0.018(2)	−0.023(2)
C(31)	4e	0.1538(4)	0.0095(2)	0.7705(2)	0.044(2)	0.053(2)	0.044(2)	0.003(1)	0.003(1)	−0.009(1)
N(31)	4e	0.2480(4)	0.0545(2)	0.7347(2)	0.055(2)	0.087(2)	0.069(2)	−0.025(2)	0.016(1)	−0.008(2)
N(42)	4e	0.7921(3)	0.2485(2)	0.9320(2)	0.060(2)	0.042(1)	0.045(1)	−0.004(1)	−0.013(1)	0.001(1)
O	4e	0.9522(3)	0.1836(2)	0.5886(2)	0.056(1)	0.082(2)	0.057(1)	−0.010(1)	−0.003(1)	0.015(1)

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless prism, size 0.5 x 0.4 x 0.35 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	19.60 cm ^{−1}
Diffractometer:	Siemens-Nicolet P2 ₁
Scan mode:	ω
T _{measurement} :	293 K
2 θ _{max} :	55°
N(hkl) _{unique} :	3467
Criterion for F _o :	$F_o > 4 \sigma(F_o)$
N(param) _{refined} :	181
Program:	SHELX-76

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U _{iso}
H(411)	4e	0.5144(4)	0.0723(2)	0.8863(2)	0.08
H(412)	4e	0.6949(4)	0.0367(2)	0.8387(2)	0.08
H(421)	4e	0.8671(4)	0.0940(2)	0.9560(2)	0.08
H(422)	4e	0.6867(4)	0.1322(2)	1.0026(2)	0.08
H(431)	4e	0.4801(4)	0.3304(2)	0.7960(2)	0.08
H(432)	4e	0.3949(4)	0.2417(2)	0.8635(2)	0.08
H(451)	4e	0.8172(4)	0.1556(2)	0.7470(2)	0.08
H(452)	4e	0.7319(4)	0.2804(2)	0.7292(2)	0.08
H(461)	4e	0.9115(4)	0.3360(3)	0.8449(2)	0.08
H(462)	4e	0.9947(4)	0.2109(3)	0.8635(2)	0.08
H(441)	4e	0.5704(5)	0.3046(3)	0.9779(2)	0.08
H(442)	4e	0.6605(5)	0.3904(3)	0.9098(2)	0.08
H(1)	4e	0.860(5)	0.269(3)	0.981(2)	0.08
H(2)	4e	1.032(5)	0.198(3)	0.615(3)	0.08
H(3)	4e	0.963(6)	0.124(3)	0.592(3)	0.08