Liu TianLi, Wang Jianlong, Chen Lizhen, Cao DuanLin*, Lu ZhiYan and Wu NaNa

The crystal structure of hexaquamagnesium(II) bis (3,4-dinitropyrazol-1-ide), C₆H₁₄MgN₈O₁₄

Abstract
C₆H₁₄MgN₈O₁₄, monoclinic, P¯1 (no. 2), a = 6.1154(3) Å, b = 7.9529(4) Å, c = 9.0459(5) Å, α = 77.744(2)°, β = 82.589(2)°, γ = 81.134(3)°, V = 422.67(4) Å³, Z = 1, Rgt(F) = 0.0454, wRref(F²) = 0.1112, T = 150 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material
An amount of 0.80 g (0.02 mol) of NaOH was dissolved in 20 mL of water and added to a 100 mL stirred four-necked flask, and the temperature was raised to 323 K; then 3.22 g of 3,4-dinitro-1H-pyrazole (0.02 mol) was added, and the solution turned yellow. After 15 minutes of reaction at 323 K, a 1 mol/L aqueous solution of magnesium chloride hexahydrate (2.03 g, 0.01 L) was added dropwise, and the reaction was carried out for 2 h at 323 K. The solution turned dark yellow, and the reaction solution was slowly evaporated.
at room temperature in a quiet environment to obtain a transparent block crystal.

**Experimental details**

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms. All the non-hydrogen atoms were refined anisotropically.

**Comment**

The nitrogen heterocyclic compound in general has a high formation enthalpy due to a large amount of N–N, C–N, N=N, C=N bonds in the structure. Pyrazoles are one of the important classes of compounds [4–7]. These compounds can be widely used in medicine, pesticides, photosensitive materials, fine chemicals [8–10].

As shown in the figure, the crystal structure of the title compound consists of a hexaqua complex and two organic counter cations. Compared with potassium 3,4-dinitropyrazolatedihydrate and sodium 3,4-dinitropyrazolate dihydrate [11], potassium and sodium do not form a coordination with water. It was owing to potassium and sodium cannot provide lone pair electrons. The ring of the organic anion is planar. The least-squares has angles to the plane through the five atoms (C1, C2, C3, N3, N4) and angles to the two nitro groups of 14.2° (O1, N2, O2) and 9.2° (O3, N1, O4). These findings are in total accord with the literature [12].

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**References**