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Aqua(hexacyanoferrato-*N*)bis(μ-glycine)-glycinecerium(III) Monohydrate

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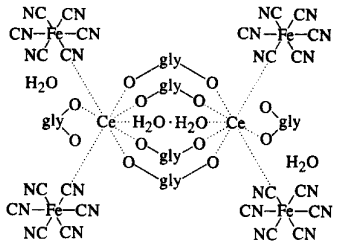
Abstract

The structure of the title compound, $[Ce\{Fe(CN)_6\}(C_2H_5NO_2)_3(H_2O)].H_2O$, consists of FeC_6 octahedra linked to an eight-coordinate cerium ion *via* two cyanide bridging Ce—N—C—Fe groups. The rest of the coordination polyhedron of the cerium is formed by six O atoms: one from a molecule of water and five from glycine molecules. The three-dimensional framework is formed through N—H···N and O—H···N hydrogen-bonding interactions. Two glycine molecules form bifurcated hydrogen bonds. An additional uncoordinated molecule of water is within hydrogen-bonding distance of two glycine molecules.

Comment

In a previous paper, we reported the synthesis and the characterization, by X-ray powder diffraction, thermal analysis and Mössbauer and IR spectroscopy, of the hexacyanocobaltate(III) and the hexacyanoferrate(III) of lanthanum and glycine (Fernández-Bertrán, Reguera, Dago & López, 1996). We found that glycine takes the neutral zwitterion form. As a continuation of our studies of the metal–ligand bond interactions in this type of complex, the crystal structure of the isotypic cerium analogue, (I), was determined.



(I)

The low spin Fe^{3+} ion is octahedrally coordinated to six cyano groups. The average Fe—C and C—N bond distances are 1.941 (3) and 1.143 (4) Å, respectively, which compare well with literature values (Mullica, Herbert, Sappenfield & David, 1988). The Ce^{3+} ion is eight-coordinate. This is fairly common in molecular complexes of the lanthanide series (Hulliger, Landolt & Vetsch, 1976). Only two cyano groups are coordinated to cerium (Ce—N1 and Ce—N2), which is in accordance with IR and Mössbauer results (Fernández-Bertrán *et al.*, 1996), with an average Ce—N bond length of 2.623 (3) Å. The rest of the coordination polyhedron is formed by six O atoms, one from water (O7) and five from glycine moieties. The average Ce—O bond length is 2.502 (2) Å. The structure consists of FeC_6 octahedra linked to cerium *via* two cyanide bridging Ce—N—C—Fe linkages. The three-dimensional framework is completed through hydrogen-bonding interactions (Table 3). Among these, the most significant are the N—H···N interactions that link glycine NH_3 groups with the N atoms of the cyano groups not bonded to the Ce ion. The uncoordinated O atom of the glycine (O6) forms three hydrogen bonds, of which two are strong (to the water molecule coordinated to the cerium ion, O7—

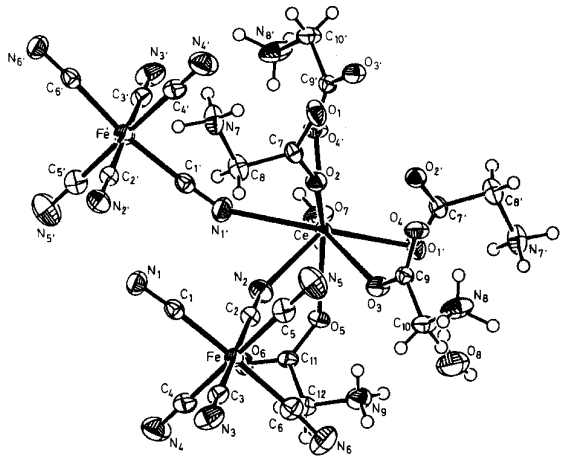


Fig. 1. *EUCLID* (Spek, 1982) plot, showing the atomic numbering scheme. Displacement ellipsoids are shown at the 50% probability level for non-H atoms; H atoms are represented by spheres of arbitrary radii.