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Crystallographic report

Crystal structure of the first alkaline earth metal compound with the antibacterial drug sulfasalazine: [Sr(H-Sulf)(H_2O)$_6$](H-Sulf)·3H_2O

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The structure of [Sr(H-Sulf)(H_2O)$_6$](H-Sulf)·3H_2O features a seven-coordinated distorted capped octahedral geometry around strontium(II) with Sr–O distances ranging from 2.445(5) to 2.606(5) Å.

KEYWORDS: sulfasalazine; strontium(II); crystal structure

COMMENT

Sulfasalazine (H_2-Sulf, 2-hydroxy-5-[[4-[(2-pyridinylamino) sulfonyl]phenyl]azo]benzoic acid) has been widely used to prevent and treat inflammatory bowel disease, such as ulcerative colitis,[1] and rheumatoid arthritis.[2] Thus far, metal complexes with this molecule have not yet been characterized by X-ray crystallography. Strontium has been known as an antagonist for calcium[3] and drugs based on complexing agents including amino acids have been developed for treatment of strontium ''poisoning''.[4] Therefore, it is important to investigate the coordination behavior of the drug sulfasalazine. Figure 1 shows the asymmetric unit of the first alkaline earth metal compound containing the antibacterial drug sulfasalazine [Sr(H-Sulf)(H_2O)$_6$](H-Sulf)·3H_2O (**1**). **1** is an ionic compound that comprises discrete [Sr(H-Sulf)(H_2O)$_6$]$^+$ cations, H-Sulf$^-$ anions and lattice H_2O molecules in the ratio 1 : 1 : 3. In the cation, the strontium(II) is coordinated in a distorted capped octahedral coordination environment by seven oxygen atoms from one deprotonated sulfasalazine (H-Sulf$^-$) and six aqua ligands. Sulfasalazine interacts with strontium(II) through its carboxylate group operating in a monodentate mode, while both the 2-hydroxyl groups and pyridine nitrogen remain uncoordinated. The Sr–O distances vary over a range from 2.445(5) to 2.606(5) Å and are comparable to those found in Sr(L-Asp)·3H_2O.[3]

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EXPERIMENTAL

To a solution of sulfasalazine (0.4 mmol, 0.159 g) and triethylamine (0.2 ml) in a mixed solvent comprising distilled water and tetrahydrofuran (20 ml) was added $Sr(NO_3)_2$ (0.2 mmol, 0.042 g). The mixture was stirred for 12 h. The resulting solution was allowed to stand in air and yellow rod-like crystals were obtained within a week. Yield 50%. Anal. Found: C, 41.47; H, 4.29; N, 10.79. Calc. for $C_{36}H_{44}N_8O_{19}S_2Sr$: C, 41.40; H, 4.25; N, 10.73. X-ray diffraction data were collected at 296 K on a Siemens P4 four-circle diffractometer using graphite-monochromated Mo Kα radiation on a block $0.20 \times 0.30 \times 0.52$ mm^3. Crystallographic data: $C_{36}H_{44}N_8O_{19}S_2Sr$, $M = 1044.53$, triclinic, space group $P\bar{1}$, $a = 11.583(2)$, $b = 15.128(3)$, $c = 15.518(4)$ Å, $\alpha = 113.19(1)$, $\beta = 109.18(1)$, $\gamma = 93.30(1)°$, $V = 2305.4(8)$ Å^3, $Z = 2$, $D_c = 1.505$ g cm^{-3}, 8520 reflections collected, 7811 unique and 3313 with $I > 2\sigma(I)$. R (obs. data on F^2) 0.059, wR (all data) 0.148, $\rho_{max} = 0.60$ e$^-$ Å^{-3}. Programs used: SHELXTL97, ORTEP. CCDC deposition number: CCDC197131.

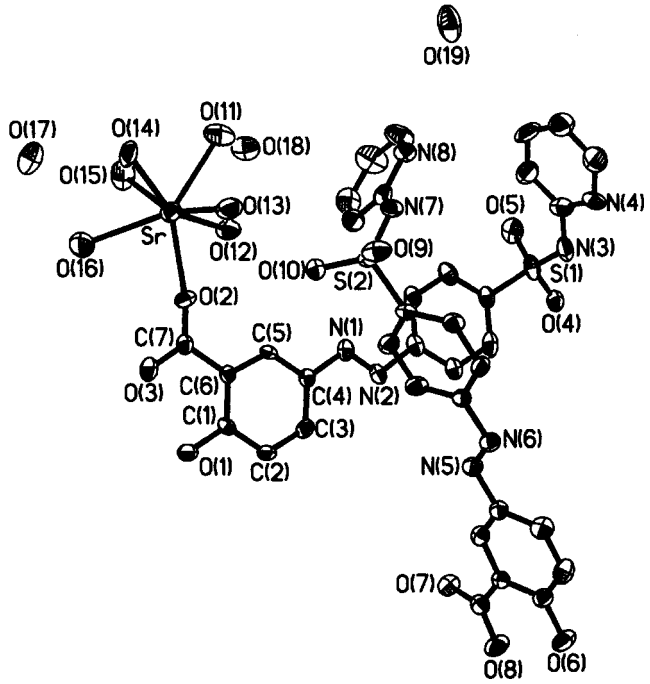

Figure 1. Asymmetric unit of $[Sr(H\text{-}Sulf)(H_2O)_6](H\text{-}Sulf)\cdot 3H_2O$. Key geometric parameters: Sr–O(2) 2.445(5), Sr–O(11) 2.535(6), Sr–O(12) 2.542(5), Sr–O(13), 2.506(6), Sr–O(14) 2.606(5), Sr–O(15) 2.563(6), Sr–O(16) 2.557(6) Å; O(2)–Sr–O(12) 83.84(18), O(2)–Sr–O(16) 79.37(18), O(11)–Sr–O(13) 77.5(2), O(12)–Sr–O(13) 102.3(2), O(11)–Sr–O(12) 72.5(2), O(11)–Sr–O(15) 79.0(2), O(15)–Sr–O(16) 68.2(2), O(13)–Sr–O(14) 71.3(2), O(11)–Sr–O(14) 81.8(2), O(12)–Sr–O(14) 154.3(2), O(14)–Sr–O(16) 81.0(2), O(14)–Sr–O(15) 94.7(20)°.

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