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Crystal structure and Hirshfeld surface analysis of [S-(–)(C_6H_5)CH(CH_3)NP(S)NH(S)-(–)CH(CH_3)(C_6H_5)]$_2$,H_2O

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Abstract:

The cyclic compound [S-(–)-(C_6H_5)CH(CH_3)NP(S)NH(S)-(–)-CH(CH_3)(C_6H_5)]$_2$,H_2O, or $C_{32}H_{38}N_4P_2S_2$,H_2O is a member of a class of molecules that may be used for extraction of metals. The literature shows many studies of the bidentate phosphorus ligands HN[P(E)R_2]$_2$ (E: O, S) [1] and RN[P(E)R_2]$_2$ [2]. The title compound was characterized in the solid state by IR and X-ray crystallography and in the solution with calculation of the specific optical rotation. The compound crystallizes in the chiral space group $P2_12_12_1$ and the asymmetric unit of the structure consists of four symmetry-independent cyclodiphosphazanes and four water (H_2O) molecules. In the molecular structure, each phosphorus atom is bonded to one sulfur and three nitrogen atoms. The P–N bond distances in the ring are longer than the P–N_H distances, and the P–S distances are in the range of 1.9376 (9) to 1.9434 (9) Å. These geometric parameters are in agreement with those observed in related compounds [3]. In the crystal structure, molecules are linked through N–H…O_W hydrogen bonds in a tape arrangement along the *c* axis (O_W is the oxygen of H_2O molecule). This pattern includes an $R_2^1(8)$ graph-set motif, formed through (NH…)(NH…)O_W grouping. The prevalence of these interactions is illustrated by an analysis of the three-dimensional Hirshfeld surface (HS) and by two-dimensional fingerprint plots (FP) for one of the cyclodiphosphazane molecules in the asymmetric unit. The relative contributions of different interactions in the HS are: H…H 69.0%, C…H/H…C 17.4% and S…H/H…S 10.6%.

References:

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