2,2',6',2"-Terpyridine 1,1"-dioxide dihydrate

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The title compound, C_{15}H_{11}N_{3}O_{3}·2H_{2}O, crystallizes with terpyridine dioxide molecules positioned on mirror planes in the space group Pnma. Catemeric assemblages of terpyridine molecules [C—H⋯O—N = 3.386 (4) Å] are linked by bridging water molecules [C—H⋯O = 3.288 (4) and 3.386 (4) Å; O—H⋯O—N = 2.837 (3) and 2.878 (4) Å], giving stacks of two-dimensional undulating motifs.

Comment

Our recent report of the structure of terpyridine trioxide described the contribution of weak C—H⋯O acceptor interactions to molecular organization (McKay et al., 2004). Inspection of the structure revealed that each terpyridine trioxide molecule participates in ten C—H⋯O—N contacts with neighboring molecules, creating a three-dimensional network of hydrogen bonds. As a means to further explore the crystal chemistry of the terpyridine chemical framework, we recently prepared and crystallographically determined the structure of terpyridine dioxide dihydrate, (I).

The asymmetric unit of (I) contains one half-molecule of terpyridine dioxide and a water molecule (Fig. 1). Each terpyridine dioxide molecule is positioned on a mirror plane,
dimethyldioxirane, was prepared (Murray & Jeyaraman, 1985) by undertaking to exclude water from the hygroscopic dimethyl-

The OH and ary H atoms were located in a difference density map and refined isotropically. The H-atom positions and \( U_{	ext{iso}} \) values were refined and no constraints to the H atoms were applied during the refinement process \[ C—H = 0.87 (3)–0.91 (3) \AA \]. After refinement, the C—H bonds were adjusted to 1.08 \AA \ for subsequent hydrogen-bond analysis (Fig. 2).
Data collection: XSCANS (Bruker, 1999); cell refinement: XSCANS; data reduction: XSCANS; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: X-SEED.

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References