

Crystal structure 2-[[2-(3-phenylallylidene)hydrazin-1-yl]thiocarbonylsulfanylmethyl]pyridinium chloride

ABSTRACT

In the title salt of an S-substituted dithiocarbazate, C₁₆H₁₆N₃S₂⁺·Cl⁻, the dihedral angles between the almost planar (r.m.s deviation = 0.005 Å) central CN₂S₂ residue and the terminal pyridinium and phenyl rings are 80.09 (11) and 3.82 (11)°, respectively, indicating the cation has an L-shape; the amine H and thione S atoms are syn. The conformation about each of the imine [1.376 (3) Å] and ethene [1.333 (4) Å] bonds is E. The shortened C-C bond [1.444 (4) Å] linking the double bonds is consistent with conjugation in this part of the molecule. In the crystal, supramolecular layers with a jagged topology are formed by charged-assisted amine-H...Cl⁻ and pyridinium-N⁺-H...Cl⁻ hydrogen bonds. The layers stack along the a axis with no specific directional interactions between them.

Keyword: Crystal structure; Hydrogen bonding; S-substituted dithiocarbazates; Salt