X-Ray Structure of 6(*E*)-[2(*Z*)-(Hydroxyimino)-2-phenylethylidene]-7,7,8,8,9,9-hexamethyl-3-phenyl-1,2-oxazaspiro[4.4]non-2-ene

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1,3-Dipolar Cycloaddition Product, Oxime, Isoxazoline

The X-ray crystallographic structure of the title compound, a product of a 1,3-dipolar cycloaddition reaction of benzonitrile oxide to 3,3,4,4,5,5-hexamethyl-1,2-bis(methylene)cyclopentane, has been determined. Colourless plates crystallize in the orthorhombic space group Pbca with cell dimensions a = 13.698(2), b = 11.836(2), c = 29.157(4) Å, V = 4727.2(1.2)Å^3, Z = 8, 3736 reflections, final $R(F)$ = 0.063 and $wR(F^2)$ = 0.166. The crystals are racemic, the molecules of opposite chirality form centrosymmetric dimers via intermolecular hydrogen bonds O-H···N between their oxime groups. The molecules are highly strained and the geometrical consequences of the steric strain are discussed.