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E)--2--acetyl--4--(4--methoxyphenyldiazenyl) phenol: X--ray and DFT--calculated structure

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Abstract: The crystal structure of the title compound, (E)-2-acetyl-4-(4-methoxyphenyldiazenyl) phenol, displays a trans configuration of the azo moiety as found for other azo (diazene) derivatives. The aromatic mean planes are nearly coplanar and the dihedral angle between the 2 aromatic rings is 3.04 (8)°. The molecules, with strong intramolecular O--H...O hydrogen bonding, are linked by weak van der Waals interactions in the 3-dimensional network. The molecular geometry, determined using X-ray diffraction techniques, was also calculated with the density functional theory (DFT), employing the hybrid exchange-correlation functional B3LYP. Experimental and theoretical IR spectra of the compound were also calculated for comparison. The results of the experimental and theoretical calculations are compared in this study.

Key Words: Diazenyl, X-ray, IR, DFT

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