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Crystal structure analysis of 4,5-diphenyl-3,5-dihydroisochromeno[8,1-ab]phenazine

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Abstract : The title compound, $C_{30}H_{18}N_2O$, crystalized with two independent molecules (A and B) in the asymmetric unit. In the molecule A, the plane of the central chromene ring forms dihedral angles of $66.4(2)$ and $41.7(2)^\circ$, with that of the terminal two benzene rings, and the dihedral angle between planes of the terminal phenazine and chromene rings is $1.04(11)^\circ$. The corresponding values for molecules B are $65.9(2)$, $41.6(2)$ and $0.30(13)^\circ$, respectively. The layers stack with interactions of the type (benzene) $C...H...π$ (outer-C8 ring of the fused the system) connections them. The crystal packing also features $π...π$ interactions. There are no classical hydrogen atoms present. Crystal data were collected using BRUKER SMART APEX II CCD X-ray diffractometer. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares procedures to the final R_1 of 0.065 using SHELXL programs.

Key Words : Isochromene, phenazine and crystal structure.

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