

X-ray and DFT structural study of some carbazole substituted imines

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The first x-ray structures of eight carbazole substituted imines (N-benzylidene-A, N-(4-methoxybenzylidene)-A, N-(3-methoxybenzylidene)-A, N-(3-chlorobenzylidene)-A, N-(3-nitrobenzylidene)-9-ethyl-A, N-(2-nitrobenzylidene)-A, N-(2-bromobenzylidene)-A and N-(4-fluorobenzylidene)-A; where A=9-ethyl-9H-carbazol-3-amine) have been performed. The addition of substituents imposes strong changes in the planarity between the substituted phenyl ring and the carbazole moiety, with dihedral angles ranging between 1 and 37°.

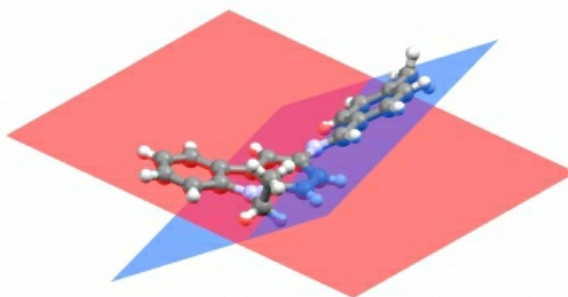
The DFT calculations using several different functional groups (B3LYP, CAM-B3LYP, B3PW91, PBEPBE and WB97XD) and the 6-31g (d,p) basis set were done to calculate the molecular geometry, bond length, bond angles and to evaluate the dihedral angle between the moieties linked by the imine group.

The X-ray structures, solved through Direct Methods procedure of SIR2008 [1] and refined by a full-matrix least-squares technique based on F2, SHELXL-97 [2], were superimposed with the theoretical calculated ones in order to evaluate the RMSD and to compare the used functional performance in the description of the studied molecule geometries.

Complete crystallographic data are available upon request from the Cambridge Crystallographic Data Centre (12 Union Road, Cambridge, CB2 1EZ, UK; email: deposit@ccdc.cam.ac.uk), by quoting the depository numbers CCDC 1530108-15.

[1] M.-C. Burla, R.-Caliandro, M.-Camalli, B.-Carrozzini, G. L.-Casarano, L. De-Caro, -C. Giacovazzo, G. Polidori, D. Siliqi, R. Spagna (2007) J. Appl.-Crystallogr. 40, 609–613.

[2] G. M. Sheldrick (1997) University-Of Gottingen, Germany.



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