Cyclic Triindoles and Tetraindoles: Substituent and Symmetry Effects on their Structural and Electronic Characteristics

M. Carmen Ruiz Delgado,[a] Constanza Ruiz,[b] Juan T. López Navarrete[a] and Berta Gómez-Lor[a]

a, Department of Physical Chemistry, University of Málaga, 29071 Málaga, Spain
b, Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco 28049, Madrid, Spain

During the last decade heptacyclic 10,15-dihydro-5*H*-diindolo[3,2-a:3',2'-c]carbazole (triindole) has been extensively studied as a new π-conjugated platform in the construction of self-assembling materials for optoelectronics. Specially remarkably is the record hole mobility values determined on triindole liquid crystals.[1] In order to facilitate the design of new materials on a molecular basis and establish clear guidelines to fine tuning electronic parameters, we have recently synthesized new triindole and tetraindole-based systems.[2-3] Our joint experimental and theoretical investigation shows that *N*-substitution, symmetry lowering of the platform, and insertion of π-spacers in extended dimers strongly impact on the fundamental electronic properties of triindoles.[2] In addition, saddle-shaped tetraindoles are found to be an interesting 3D rigid scaffold to obtain electroactive molecules with increased dimensionality.[3] We hope that this study can not only advance useful structure-property relationships of conjugated indole-based systems but also guide the design of new materials with potential applications in organic electronics.

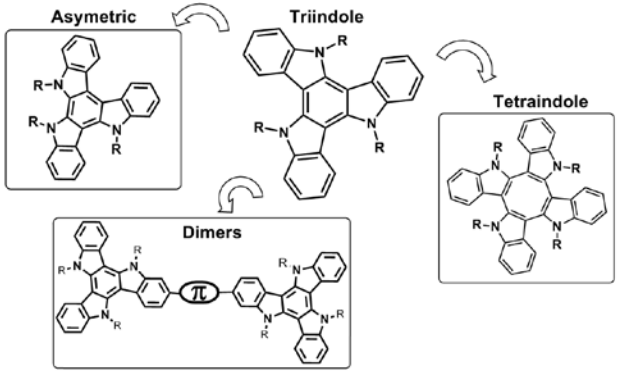

Figure 1. Cyclic triindoles and tetraindoles under study.

References

1. E.M. García-Frutos, U.K. Pandey, R. Termine, A. Omenat, J. Barberá, J.L. Serrano, A. Golemme, B. Gómez-Lor, *Angew. Chem. Int. Ed.* 2011, **50**, 7399
2. a) C. Ruiz, J.T. López Navarrete, M.C.Ruiz Delgado, B. Gómez-Lor, *Org. Lett.* 2015, **17**, 2258−2261. b) C. Ruiz, E.M. García-Frutos, D.A. da Silva Filho, J.T. López Navarrete, M.C. Ruiz Delgado, and B. Gómez-Lor, *J. Phys. Chem. C* 2014, **118**, 5470−5477
3. C. Ruiz, A. Monge, E. Gutiérrez-Puebla, I. Alkorta, J. Elguero, J. T. López Navarrete, M.C. Ruiz Delgado and B. Gómez-Lor, *submitted*