

Poster Presentations

[MS25-P20] Heteropentalenes as donors in charge-transfer complexes

Demetrius C. Levendis and David H. Reid

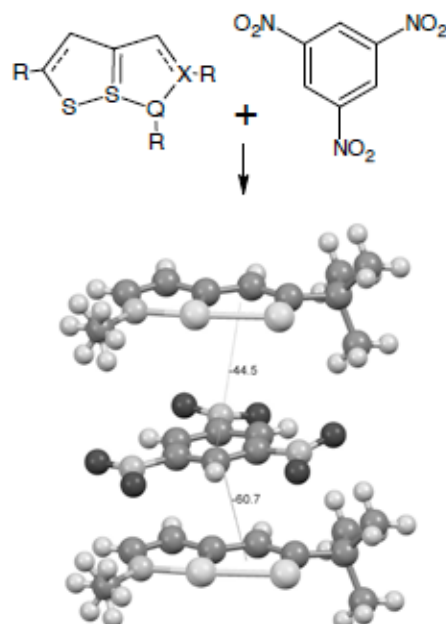
Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, PO WITS, Johannesburg, 2050, South Africa

Email: demetrius.levendis@wits.ac.za

Charge-transfer complexes (CTs) have been known for decades, as expertly documented by Herbstein [1]. One of the archetypal CTs involving heterocycles is tetrathiofulvalinium tetracyanoquinodimethane (TTFTCNQ), renowned for the observation of its high electrical conductivity [2]. Subtle structural features, such as modulation, obviously play an essential part in understanding structure-property relationships in such CTs [3]. The recent observation of room-temperature ferroelectricity in a different class of CTs demonstrates the topical interest in materials of this type [4], as well as the ongoing discussion about the nature of the CT interactions and the role of dispersive forces [5-6].

In this work we investigate the use of substituted heteropentalenes, such as dithia-6-azapentalene, together with strong aromatic donors, such as trinitrobenzene, to generate a new class of charge-transfer complexes. The heteropentalenes investigated, shown schematically in Fig.1, include those with Q = S, N; X = C, N and R = H, Me, iBu, Ph. They can be prepared by methods reported previously [7]. Only donors with Q = N, X = C have thus far yielded CT complexes. Their preparation, structures and solid-state properties will be discussed in this paper.

Fig. 1 Stacking of 2-*tert*-butyl-6-methyl-dithia-6azapentalene and TNB molecules in the 1:1 CT crystal showing the two strongest intermolecular interactions (-60.7 and -44.5 kJ/mol).



[1] Herbstein, F. H., Crystalline molecular complexes and compounds : structures and principles. (2005); New York : Oxford University Press.

[2] Coleman, L.; Cohen, M.; Sandman, D. J.; Yamagishi, F.; Garito, A. F.; Heeger, A. (1973). *Solid State Communications*, **12**, 1125.

[3] Coppens, P.; Petricek, V.; Levendis, D.; Larsen, F. K.; Paturle, A.; Yan, G.; Legrand, A. D. (1987). *Physical Review Letters* **59**, (15), 1695-1697.

[4] Tayi, A. S.; Shveyd, A. K.; Sue, A. C. H.; Szarko, J. M.; Rolczynski, B. S.; Cao, D.; Kennedy, T. J.; Sarjeant, A. A.; Stern, C. L.; Paxton, W. F.; Wu, W.; Dey, S. K.; Fahrenbach, A. C.; Guest, J. R.; Mohseni, H.; Chen, L. X.; Wang, K. L.; Stoddart, J. F.; Stupp, S. (2012). *Nature* **488**, 485.

[5] Schneider, H.-J. (2012). *Accounts of Chemical Research* **46**, 1010.

[6] Bertolasi, V.; Gilli, P.; Gilli, G. (2012). *Crystal growth & design* **12**, 4758.

[7] Dingwall, J. G., Ingram, A. S., Reid, D. H. & Svmon, J. D. (1973). *J. Chem. Soc. Perkin Trans. 1*, 2351-2358.

Keywords: charge-transfer complex, heteropentalene