OP-16

HOST BEHAVIOUR OF *N*,*N'*-BIS(9-PHENYL-9-THIOXANTHENYL)ETHYLENEDIAMINE IN THE PRESENCE OF AROMATIC AND ALIPHATIC FIVE-MEMBERED HETEROCYCLIC GUEST COMPOUNDS

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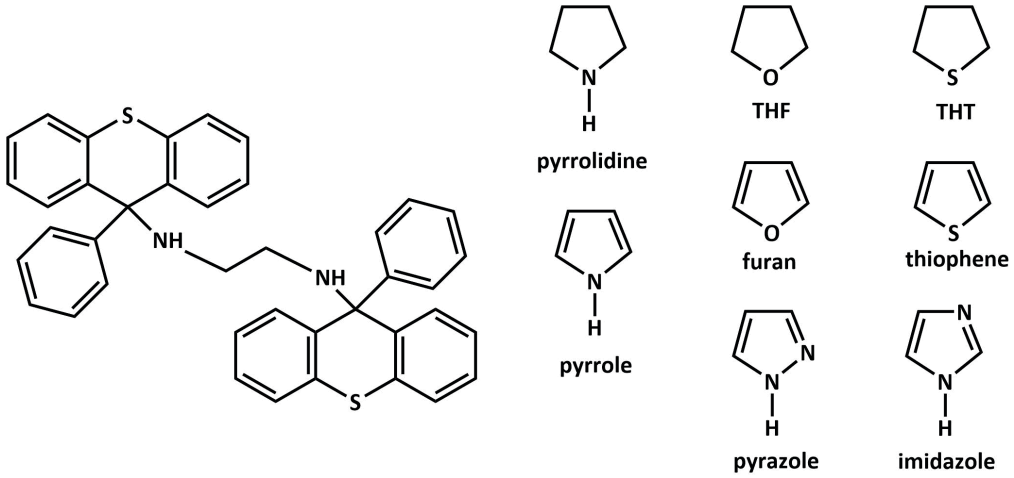
This work describes the host ability of the crystalline compound *N*,*N'*-bis(9-phenyl-9-thioxanthenyl)-ethylenediamine **1**[1] in the presence of eight five-membered ring heterocyclics, namely saturated tetrahydrofuran (THF), tetrahydrothiophene (THT) and pyrrolidine, and aromatic equivalents furan, thiophene and pyrrole and, additionally, imidazole and pyrazole (Scheme 1).



Scheme 1. Structures of host compound *N*,*N'*-bis(9-phenyl-9-thioxanthenyl)ethylenediamine **1** and the eight potential five-membered ring guest compounds

Host **1** clathrated all six mono-heteroatomic guests, while complexes were not formed with imidazole and pyrazole. Specifically designed guest/guest competition experiments revealed that **1** preferred the saturated heterocyclics relative to the aromatics, and also the sulfur-containing guests (in both saturated and aromatic series') followed by oxygen and nitrogen (S > O > N). The affinity of the host for the saturated guests was explained by means of a consideration of the applicable host–guest interactions (obtained from single crystal diffraction analyses), where these guests were observed to experience a greater variety and number of these interaction types relative to the aromatic guests. The host selectivity order for the various heteroatoms (S > O > N) was clarified unfailingly when investigating, quantitatively, the percentage of the guest heteroatom–host interactions in each complex by means of Hirshfeld surface analyses. Finally, thermal experiments carried out on all six inclusion compounds provided further illumination for some of the observations made from the competition experiments.

REFERENCE

[1] B. Barton, C.W. McCleland and B. Taljaard, *The South African Journal of Chemistry* **2002**, *55*, 144–148.