

## Supporting Information

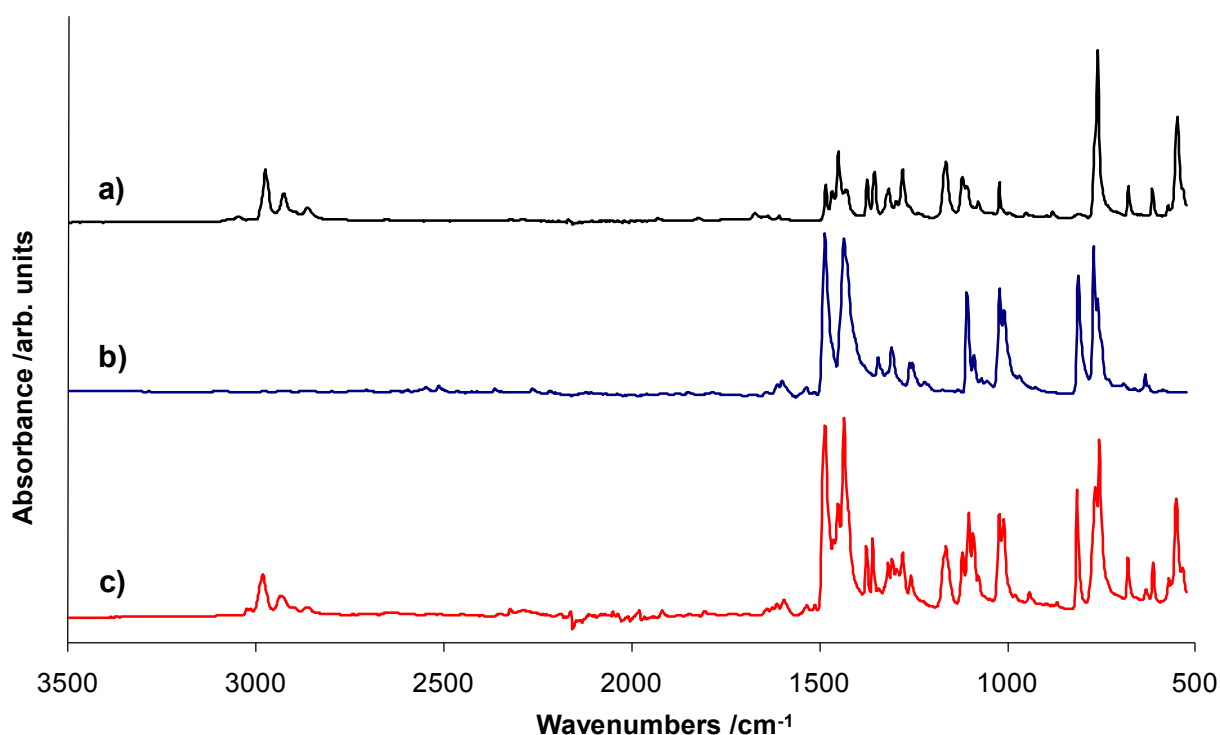
### Vapour Phase Assembly of a Halogen Bonded Complex of an Isoindoline Nitroxide and 1,2-Diiodotetrafluorobenzene

Karl J. P. Davy,<sup>a,b</sup> John McMurtrie,<sup>c</sup> Llew Rintoul,<sup>c</sup> Paul V. Bernhardt<sup>b</sup> and Aaron S. Micallef<sup>\*a,b</sup>

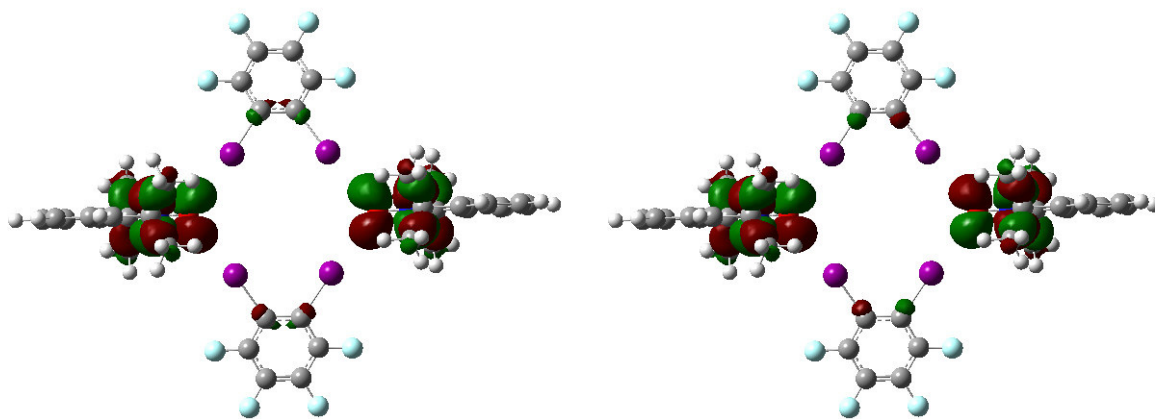
<sup>a</sup> Australian Institute for Bioengineering and Nanotechnology, University of Queensland, Brisbane, Queensland 4072, Australia. Fax: (+61) (0)7 3346 3973; Tel: (+61) (0)7 3346 3864; E-mail: [karl.davy@uqconnect.edu.au](mailto:karl.davy@uqconnect.edu.au); [a.micallef1@uq.edu.au](mailto:a.micallef1@uq.edu.au)

<sup>b</sup> School of Chemistry and Molecular Biosciences, University of Queensland, Brisbane, Queensland 4072, Australia. Fax: (+61) (0)7 3365 4273; Tel: (+61) (0)7 3365 4266; E-mail: [p.bernhardt@uq.edu.au](mailto:p.bernhardt@uq.edu.au)

<sup>c</sup> Chemistry, Queensland University of Technology, Brisbane, Queensland 4001, Australia. Fax: (+61) (0)7 3138 1804; Tel: (+61) (0)7 3138 1220; E-mail: [j.mcmurtrie@qut.edu.au](mailto:j.mcmurtrie@qut.edu.au); [l.rintoul@qut.edu.au](mailto:l.rintoul@qut.edu.au)



**Figure S1.** The IR spectra (ATR; diamond cell) of crystalline TMIO (a; black), 1,2-DITFB (b; blue) and (TMIO)<sub>2</sub>.(1,2-DITFB)<sub>2</sub> co-crystal (c; red).



**Figure S2.** Illustration of electron density in the (TMIO)<sub>2</sub>·(1,2-DITFB)<sub>2</sub> SOMOs. The lowest energy SOMO is on the left.