CORA Cork Open Research Archive
Cartlann Taighde Oscailte Chorcaí

Title	Tuning the strength of the resonance-assisted hydrogen bond in acenes and phenacenes with two o-hydroxyaldehyde groups - The importance of topology
Authors	Pareras, Gerard;Szczepanik, Dariusz Wojciech;Duran, Miquel;Solà, Miquel;Simon, Silvia
Publication date	2019-11-06
Original Citation	Pareras, G., Szczepanik, D. W., Duran, M., Solà, M. and Simon, S. (2019) 'Tuning the strength of the resonance-assisted hydrogen bond in acenes and phenacenes with two o-hydroxyaldehyde groups - The importance of topology', Journal of Organic Chemistry, 84(23), pp. 15538-15548. doi: 10.1021/acs.joc.9b02526
Type of publication	Article (peer-reviewed)
Link to publisher's version	10.1021/acs.joc.9b02526
Rights	© 2019, American Chemical Society. This document is the Accepted Manuscript version of a Published Work that appeared in final form in Journal of Organic Chemistry, copyright © American Chemical Society, after peer review and technical editing by the publisher. To access the final edited and published work see https://pubs.acs.org/doi/abs/10.1021/acs.joc.9b02526
Download date	2026-11-04 04:59:51
Item downloaded from	https://hdl.handle.net/10468/9436

UCC
University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

SUPPORTING INFORMATION

Tuning the strength of the resonance-assisted hydrogen bond in acenes and phenacenes with two *o*-hydroxyaldehyde groups. The importance of topology

Gerard Pareras[a,‡], Dariusz W. Szczepanik[b,‡], Miquel Duran[b], Miquel Solà[b,*] and Sílvia Simon[b,*]

[a] *Department of Chemistry, University College Cork, College Rd, Cork, Ireland*

[b] *Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, C/ Maria Aurèlia Capmany 69, 17003 Girona, Catalonia, Spain*

‡ These two authors contributed equally to this work.

Corresponding authors: silvia.simon@udg.edu, miquel.sola@udg.edu

Fig. S1 – Linear correlation between PDI for the *ipso* and *quasi*-rings for triphenylene-like compound. Grey for **KM-Ln A'** *quasi*-ring, yellow for **KM-Ln B'** *quasi*-ring, red for **KP-Lnb** and blue for **KP-Lna**, being n the number of added benzene rings (see Fig. 6 in text) **S2**

Fig. S2 – Linear correlation between aromaticity of the *ipso*-ring and RAHB bond length for the triphenylene-like compound. Grey for **KM-Ln A'** *quasi*-ring, yellow for **KM-Ln B'** *quasi*-ring, red for **KP-Lnb** and blue for **KP-Lna**, being n the number of added benzene rings (see Fig. 6 in text). **S2**

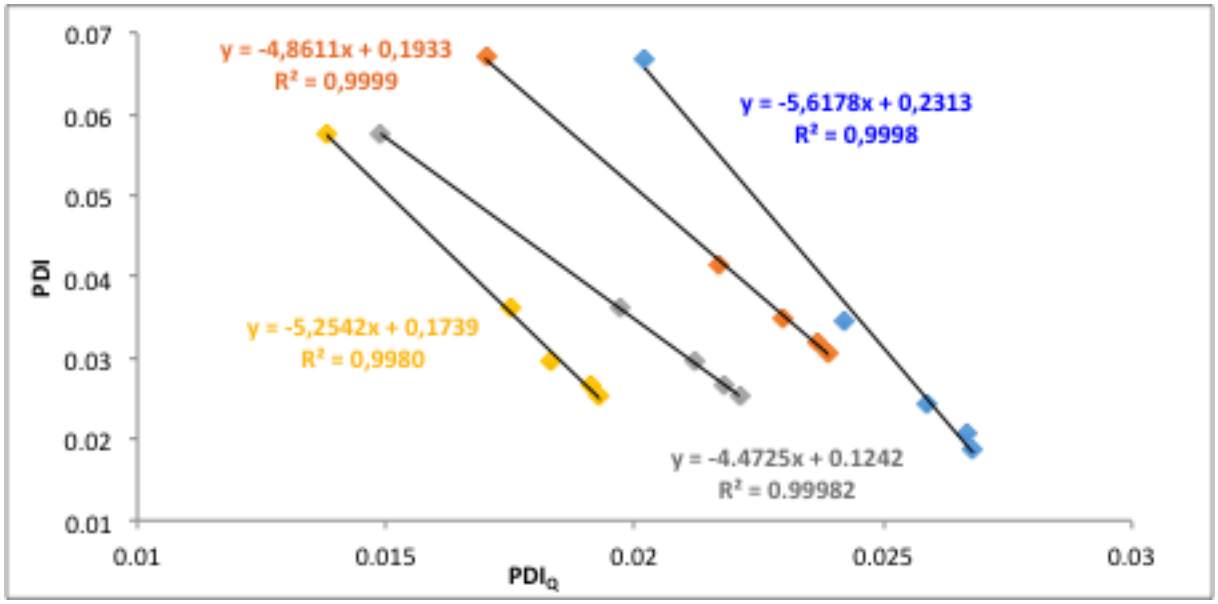


Fig. S1 – Linear correlation between PDI for the *ipso* and *quasi*-rings for triphenylene-like compound. Grey for **KM-Ln A'** *quasi*-ring, yellow for **KM-Ln B'** *quasi*-ring, red for **KP-Lnb** and blue for **KP-Lna**, being n the number of added benzene rings (see Fig. 6 in text).

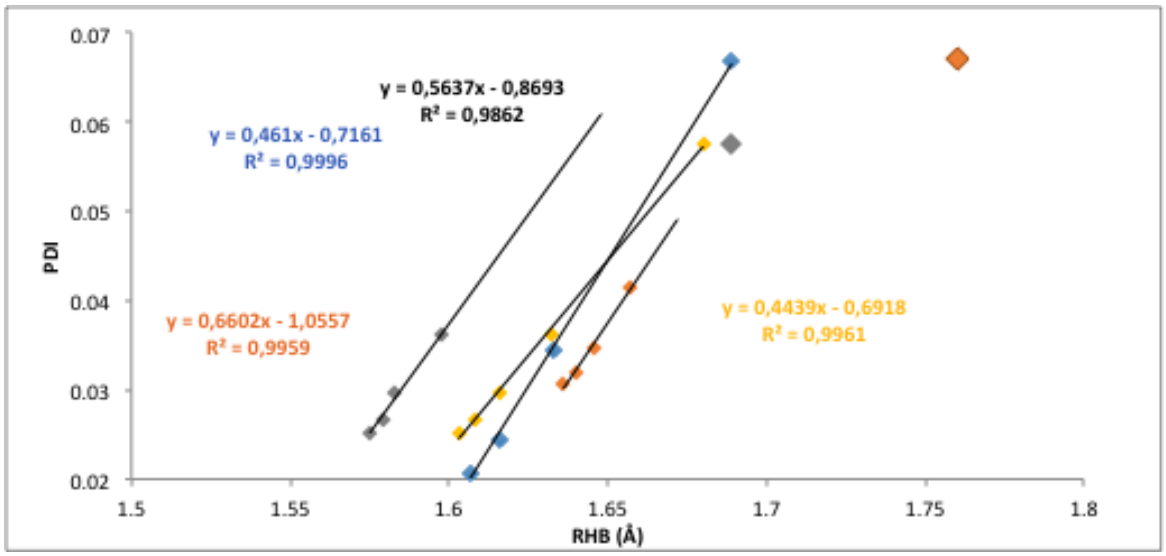


Fig. S2 – Linear correlation between aromaticity of the *ipso*-ring and RAHB bond length for the triphenylene-like compound. Grey for **KM-Ln A'** *quasi*-ring, yellow for **KM-Ln B'** *quasi*-ring, red for **KP-Lnb** and blue for **KP-Lna**, being n the number of added benzene rings (see Fig. 6 in text).