

Accepted Manuscript

Research paper

Hydrogen-Bonded Complexes with Carbenes as Electron-Pair Donors

Janet E. Del Bene, Ibon Alkorta, José Elguero

PII: S0009-2614(17)30118-5

DOI: <http://dx.doi.org/10.1016/j.cplett.2017.02.012>

Reference: CPLETT 34525

To appear in: *Chemical Physics Letters*

Received Date: 23 January 2017

Accepted Date: 7 February 2017

Please cite this article as: J.E. Del Bene, I. Alkorta, J. Elguero, Hydrogen-Bonded Complexes with Carbenes as Electron-Pair Donors, *Chemical Physics Letters* (2017), doi: <http://dx.doi.org/10.1016/j.cplett.2017.02.012>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Research paper

Hydrogen-Bonded Complexes with Carbenes as Electron-Pair Donors

Janet E. Del Bene,^{*,‡} Ibon Alkorta,^{*,§} José Elguero[§]

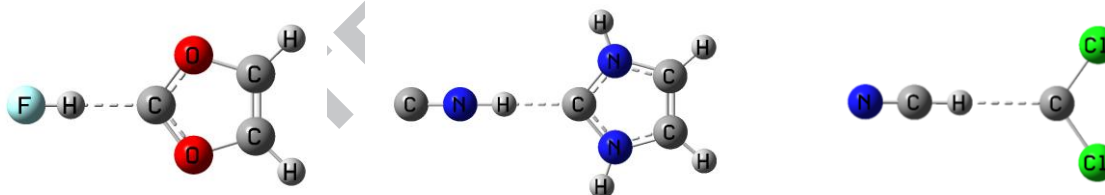
[‡] Department of Chemistry, Youngstown State University, Youngstown, Ohio 44555 USA

[§] Instituto de Química Médica (IQM-CSIC), Juan de la Cierva, 3, E-28006 Madrid, Spain

* Corresponding authors: J.E.D.B., jedelbene@ysu.edu (+1 330-609-5593)

I.A., ibon@iqm.csic.es (+34 915622900)

Graphical Abstract



Highlights:

- ▶ FH, NCH, and CNH form stable X-H...C hydrogen-bonded complexes with carbenes.
- ▶ The X-H...C bonds in 33 complexes are traditional hydrogen bonds, with no proton transfer.
- ▶ Binding energies and charge-transfer energies correlate with X-C and H-C distances.
- ▶ Coupling constants $^{2h}J(X-C)$ increase as the corresponding X-C distances decrease.

Download English Version:

<https://daneshyari.com/en/article/5377977>

Download Persian Version:

<https://daneshyari.com/article/5377977>

[Daneshyari.com](https://daneshyari.com)