Theor Chem Account (2008) 121:181–186
DOI 10.1007/s00214-008-0462-3

REGULAR ARTICLE

Inverse hydrogen bonds between XeH_2 and hydride and fluoride derivatives of Li, Be, Na and Mg

Fernando Blanco · Mohammad Solimannejad · Ibon Alkorta · Jose Elguero

Received: 28 April 2008 / Accepted: 24 June 2008 / Published online: 23 July 2008

Abstract A theoretical study of the inverse hydrogen bonds complexes formed by the XeH_2 molecule and hydride and fluoride derivatives of Li, Be, Na and Mg has been carried out by means of DFT (B3LYP/DGDZVP) and ab initio [MP2/DGDZVP and MP2/LJ18/6-311++G(2d,2p)] calculations. The complexes obtained present interaction energies up to −81 kJ/mol. The analysis of the electron density shows electron transfer from the XeH_2 to the electron acceptor molecules. The calculated absolute chemical shieldings show the high sensitivity of the xenon atom upon complexation.

Keywords Inverse hydrogen bonds · XeH_2 · Metal hydride

1 Introduction

Classical hydrogen bonds (HB) are formed between two electronegative atoms with a hydrogen atom bonded to one of them. In the last years, an important number of new chemical groups have been added to those suitable to form HB [1,2]. One of the most interesting cases corresponds to those HB where the interaction is between two hydrogens, one hydric with partial negative charge and another protic with positive charge [3–12]. This special case of HB has been named dihydrogen bond (DHB) [13].

In a subsequent evolution of the possible interactions, it has been proposed to substitute in the DHB complex, the protic hydrogen by a more general electropositive moiety yielding what has been named an inverse hydrogen bond (IHB) or hydride bond [14–16].

Among the rare gas isolated derivatives, XeH_2 has been detected in the photolysis of hydrogen halides or in the electron irradiation of benzene, in both cases, in solid Xe [17–21]. Several theoretical works have been devoted to this compound due to its interesting properties as electron donor in DHB interactions [22–25].

In this article, we have studied the possible IHB formed between XeH_2 and the monomeric and dimeric hydride and fluoride derivatives of Li, Na, Be and Mg. The systems have been optimized with a full electron basis set and an effective core potential for the xenon atom using DFT (B3LYP), and MP2 computational methods. The electronic properties of the complexes have been analyzed by means of the atoms in molecules (AIM) methodology and the chemical shielding of the systems has been calculated to evaluate the effect of the complexation.

2 Methods

The geometry of the systems has been fully optimized with the full electron basis set, DGDZVP [26], at the B3LYP [27,28] and MP2 [29] computational levels. In addition, for xenon the relativistic effective core potential (ECP) by

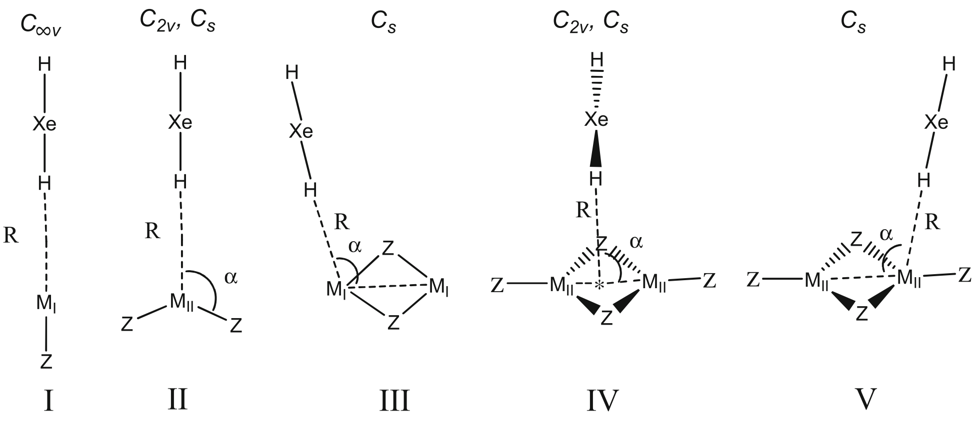
---

Electronic supplementary material The online version of this article (doi:10.1007/s00214-008-0462-3) contains supplementary material, which is available to authorized users.

F. Blanco · I. Alkorta (✉) · J. Elguero
Instituto de Química Médica (CSIC),
Juan de la Cierva, 3, 28006 Madrid, Spain
e-mail: ibon@iqm.csic.es

M. Solimannejad
Quantum Chemistry Group, Department of Chemistry,
Arak University, 38156-879 Arak, Iran

M. Solimannejad (✉)
Centre for Theoretical and Computational Chemistry,
Department of Chemistry, University of Oslo,
P.O. Box 1033, Blindern, 0315 Oslo, Norway
e-mail: mohammad.solimannejad@kjemi.uio.no;
m-solimannejad@araku.ac.ir



M_I = Li and Na M_{II} = Be and Mg Z = H and F

Fig. 1 Schematic representation of the minima configurations. The symmetries founds for each motif are indicated. The *R* and *α* parameters have been tabulated in Table 2

LaJohn et al. [30] and the standard 6-311++G(2d,2p)[31] for the rest of the atoms at the MP2 level have been used. In all cases, frequency calculations have been carried out to evaluate if the structures obtained correspond to an energetic minima or not. All these calculations have been carried out within the Gaussian-03 package [32].

The interaction energy has been corrected from the inherent basis set superposition error (BSSE) using the full counterpoise method [33].

The electron density of the complexes has been analyzed using the AIM methodology [34] and the PROAIMV [35] and MORPHY98 programs [36]. The evaluation of the atomic properties has been carried out by integration within the atomic basins. Default parameters have been used for the integration except in those cases where the absolute value of the integrated Laplacian was larger than 0.001, where more strict conditions have been used [37].

The absolute chemical shieldings have been evaluated with the GIAO method [38,39] at the B3LYP/DGDZP computational level, since previous results have provided good linear correlations between experimental and calculated results [25].

3 Results and discussions

The xenon dihydride, XeH_2, is a linear centrosymmetric molecule which presents a negative region of the electrostatic potential close to the hydrogen atoms along the symmetric axis of the molecule [25]. Thus, it is expected that the interaction of the hydrogen atoms of XeH_2 with electron deficient atoms should provide stable complexes. The systems chosen to interact with XeH_2 are hydride and fluoride derivatives of lithium, sodium, beryllium and magnesium in their monomeric and dimeric forms.

Considering the simplicity and high symmetry of the interacting molecules, a large number of different configurations have been found as energetic minima (Fig. 1). The reduction of the maximum symmetry expected for some of the complexes is an indication of the presence of secondary interactions.

The energetic results have been gathered in Table 1. In general, similar results are obtained for the three computational methods considered, especially between the B3LYP/DGDZVP and the MP2/DGDZVP one, being the interaction energy obtained with the latter methods always slightly larger than with the former. The most important difference was observed in the complexes between XeH_2 and Be_2Z_4 (Z = H and F). While the calculations with the DGDZVP basis set predict that the fluorinated complex is more stable, the opposite is obtained for the MP2/LJ18. Another interesting feature is the higher symmetry in some of the B3LYP calculations versus the ones obtained at MP2 level with the two basis sets. This could indicate the inability of the B3LYP method to properly consider weak interactions, as has already been described in the literature [40–42].

The interaction energies range between −18.9 and −81.1 kJ/mol indicating the high stability of the complexes formed. A systematic trend observed in those systems is the increment of the interaction energy when the hydrogen atoms of the electron acceptor molecule are replaced by fluorine, except in the cases previously mentioned at the MP2/LJ18 level.

The interaction energies obtained for these complexes are stronger than those obtained for the XeH_2:H_2O complex [22], −10.6 kJ/mol, and other neutral XeH_2:HX dihydrogen bonded complexes [25]. Only in the case of charged dihydogen bonded complexes as XeH_2:$HCNLi^+$ and XeH_2:$HCNNa^+$ interaction energies (−44.1 and −36.6 kJ/mol, respectively) in the range of those described here have been found [25].

Table 1 Symmetry group, PG, and corrected interaction energy (kJ/mol) for the minima found at the different computational levels considered

	Type	B3LYP/DGDZVP		MP2/DGDZVP		MP2/LJ18	
		PG	Ei + BSSE	PG	Ei + BSSE	PG	Ei + BSSE
LiH	I	$C_{\infty v}$	−43.55	$C_{\infty v}$	−40.41	$C_{\infty v}$	−44.13
LiF	I	$C_{\infty v}$	−47.29	$C_{\infty v}$	−44.32	$C_{\infty v}$	−43.67
NaH	I	$C_{\infty v}$	−30.48	$C_{\infty v}$	−26.59	$C_{\infty v}$	−28.03
NaF	I	$C_{\infty v}$	−36.34	$C_{\infty v}$	−31.90	$C_{\infty v}$	−31.82
BeH_2	II	C_s	−25.43	C_s	−18.88	C_s	−39.95
BeF_2	II	C_s	−53.74	C_s	−52.01	C_s	−47.83
MgH_2	II	C_{2V}	−29.99	C_s	−26.37	C_s	−36.89
MgF_2	II	C_s	−65.58	C_s	−63.38	C_s	−68.15
Li_2H_2	III	C_s	−30.97	C_s	−30.71	C_s	−33.99
Li_2F_2	III	C_s	−33.73	C_s	−32.86	C_s	−33.56
Na_2H_2	III	C_s	−23.09	C_s	−22.03	C_s	−26.19
Na_2F_2	III	C_s	−29.93	C_s	−27.25	C_s	−29.47
Be_2H_4	IV	C_{2V}	−49.48	C_s	−47.20	C_s	−81.13
Be_2F_4	V	C_s	−69.16	C_s	−74.95	C_s	−60.20
Mg_2H_4	IV	C_{2V}	−35.93	C_{2V}	−35.73	C_s	−44.41
Mg_2F_4	IV	–	–	C_s	−44.02	C_s	−49.07
Mg_2F_4	V	C_s	−66.69	C_s	−66.87	C_s	−71.23

Table 2 Geometrial properties (Å, ∘) of the complexes obtained (R and α are defined in the Fig. 1)

	Type	B3LYP/DGDZVP		MP2/DGDZVP		MP2/LJ18	
		R	α	R	α	R	α
LiH	I	1.926	180.0	1.931	180.0	1.866	180.0
LiF	I	1.918	180.0	1.921	180.0	1.869	180.0
NaH	I	2.240	180.0	2.280	180.0	2.295	180.0
NaF	I	2.222	180.0	2.253	180.0	2.257	180.0
BeH_2	II	1.734	102.2	1.747	102.9	1.565	108.3
BeF_2	II	1.639	103.6	1.594	105.1	1.543	107.6
MgH_2	II	2.058	101.5	2.090	97.1	2.027	97.3
MgF_2	II	1.935	92.7	1.925	93.1	1.908	94.3
Li_2H_2	III	1.957	155.0	1.953	153.3	1.904	156.5
Li_2F_2	III	1.968	147.8	1.959	148.9	1.923	152.0
Na_2H_2	III	2.291	143.6	2.308	141.7	2.313	141.3
Na_2F_2	III	2.268	135.2	2.307	133.7	2.320	133.5
Be_2H_4	IV	1.511	90.0	1.452	90.0	1.314	89.9
Be_2F_4	V	1.600	114.2	1.554	117.4	1.520	114.3
Mg_2H_4	IV	1.829	90.0	1.782	90.0	1.749	89.5
Mg_2F_4	IV	–	–	1.686	88.6	1.708	88.1
Mg_2F_4	V	1.936	116.9	1.923	117.6	1.908	118.0

Some of the geometrical characteristics of the complexes have been gathered in Table 2. In the complexes formed between the XeH_2 molecule with the hydride and fluoride monomers, shorter distances are observed for the fluoride complexes than for the corresponding hydride ones. In the case of the complexes with the dimeric units, the tendency is not so clear. The comparison of the distances obtained for the three computational methods presents linear relationship among them with high correlation coefficients (R^2 larger than 0.98). The distances obtained between the interacting hydrogen and the metallic atoms can be as short as 1.31 Å in the complex with Be_2H_4. The complex formation results in an elongation of the XeH bond involved in the interaction while the other XeH bond shortens, up to 0.1 Å in both cases.

Table 3 Dipole moment enhancement (Debye) and charge transfer (e) from the XeH_2 molecule to the metallic moiety at the B3LYP/DGDZVP computational level

Complexes with	Complex type	Dipole moment enhancement	Charge transfer Mulliken	Charge transfer NBO	Charge transfer AIM
LiH	I	3.79	0.427	0.046	−0.007
LiF	I	4.15	0.444	0.031	0.023
NaH	I	2.93	0.101	0.020	−0.009
NaF	I	3.68	0.133	0.020	0.036
BeH_2	II	4.87	0.358	0.007	−0.018
BeF_2	II	7.94	0.511	0.078	0.036
MgH_2	II	5.45	0.139	0.018	0.001
MgF_2	II	7.90	0.527	0.061	0.073
Li_2H_2	III	3.28	0.400	0.051	0.004
Li_2F_2	III	2.97	0.401	0.031	0.019
Na_2H_2	III	2.57	0.115	0.036	0.013
Na_2F_2	III	2.49	0.122	0.022	0.030
Be_2H_4	IV	5.84	0.468	0.005	0.040
Be_2F_4	V	9.45	0.564	0.105	0.046
Mg_2H_4	IV	4.67	0.182	0.010	0.012
Mg_2F_4	V	8.22	0.534	0.065	0.076

Table 4 Properties at the hydrogen–metal bcp (a.u.) and integrated volume (au) at the B3LYP/DGDZVP computational level

Complexes with	Complex type	Rho	Lap	H	Δ volume of XeH_2	Δ volume total
LiH	I	0.013	0.070	0.0035	6.2	5.9
LiF	I	0.013	0.071	0.0036	1.1	5.7
NaH	I	0.014	0.046	0.0004	3.7	2.1
NaF	I	0.014	0.050	0.0007	−2.9	0.3
BeH_2	II	0.026	0.098	−0.0028	−20.9	−38.9
BeF_2	II	0.031	0.159	−0.0002	−31.6	−52.3
MgH_2	II	0.020	0.064	−0.0005	−8.9	−23.6
MgF_2	II	0.027	0.094	−0.0011	−21.1	−31.6
Li_2H_2	III	0.012	0.065	0.0033	2.3	1.5
Li_2F_2	III	0.012	0.065	0.0034	−6.6	−9.7
Na_2H_2	III	0.012	0.043	0.0008	0.7	0.5
Na_2F_2	III	0.013	0.047	0.0009	−8.8	−12.2
Be_2H_4	IV	0.039	0.014	−0.0127	−41.8	−59.7
Be_2F_4	V	0.035	0.188	0.0006	−38.9	−62.6
Mg_2H_4	IV	0.017	0.017	−0.0022	−17.0	−36.5
Mg_2F_4	V	0.027	0.095	−0.0010	−22.9	−33.7

Among the observed electronic effect associated to complex formation, we noted a charge transfer from the XeH_2 and a subsequent increment of the total dipole moment versus the sum of those of the corresponding monomers (Table 3). The amount of charge transferred is highly dependent on the charge partition method and, in contrast to the expected tendency, the AIM partition provides negative charge transfer for some of the complexes. The individual effects on the atoms show a charge flow from the non-interacting hydrogen atom to the interacting one. Thus, the former atom loses charge while the latter gains it. A similar tendency has already been described for dihydrogen bonded complexes of XeH_2 [25]. The main contribution to the dipole moment enhancement comes from the distortion of the XeH_2 molecule that lacks its symmetry, and thus presents dipole moment itself.

The analysis of the electron density of the complexes, shows the presence of bond critical points (bcp) between the interacting hydrogen and the metallic atoms (Table 4) and in

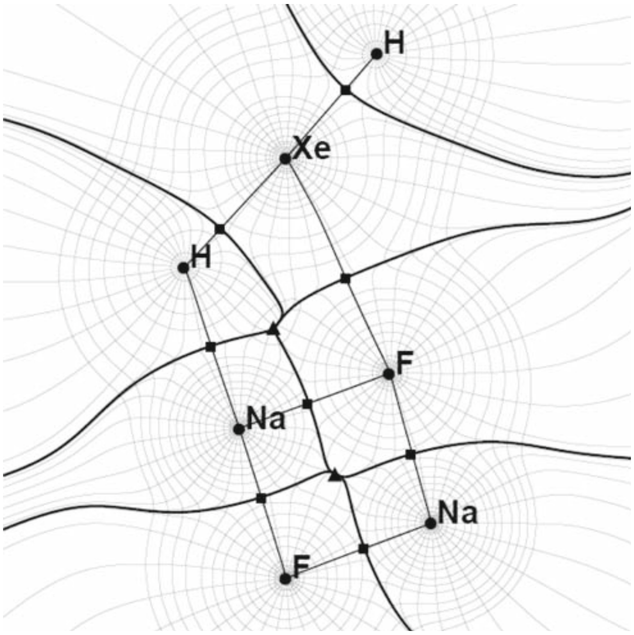


Fig. 2 Electron density map of the XeH_2:Na_2F_2 complex. *Squares*, *triangles* and *dots* indicate the position of the bond, ring and atomic critical points

most of the fluoro derivatives, between the xenon atom and the fluorine ones. As an example, the electron density map obtained for the XeH_2:Na_2F_2 complex is shown in Fig. 2. Similar interactions of electrostatic nature have been described in the literature between electron deficient and electron rich atoms [41,43]. These interactions are able to explain the extra stabilization observed in the fluoride derivatives versus the hydride ones. The characteristics of the bcps between the hydrogen atom of XeH_2 and the metal atom present small values of ρ and positive values of the Laplacian, as indication of closed shell interaction. However, in some of the cases with the larger values of rho a negative value of the total energy density, H, is obtained as indication of the partly covalent nature of those contacts [44,45].

The calculated variation of the molecular volume of XeH_2, present variable results depending on the complex formed. The variation of the total volume follows a similar tendency to the ones observed for the XeH_2 moiety, especially if the systems are divided in hydride and fluoride ones (Fig. 3).

The calculated chemical shieldings of the XeH_2 molecule within the complexes confirms the charge flow from the non-interacting hydrogen atom to the interacting one. Thus, the non-interacting hydrogen and the xenon atom present chemical shielding variations towards lower fields while the interacting hydrogen atom is shifted towards higher fields, in good agreement with the charge variation tendency previously described. The high sensitivity of the xenon atom is shown by the variation range observed upon complexation (between −20 and −269 ppm) (Table 5).

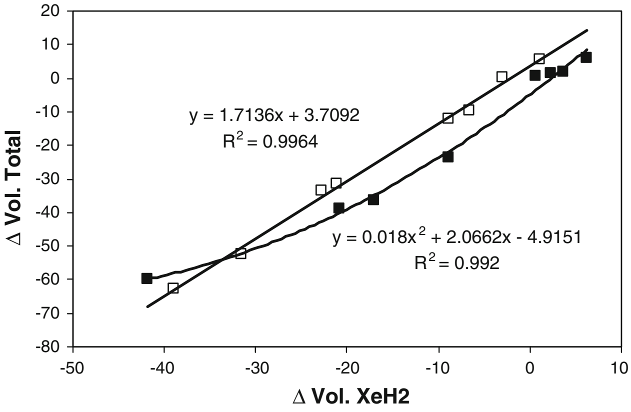


Fig. 3 ΔVol of XeH_2 versus ΔVol total (au.) *Black* and *white squares* represents the hydride and fluoride complexes

Table 5 Variation of the chemical shifts (ppm) of the XeH_2 molecule upon complexation at the B3LYP/DGDZVP computational level

	Type	H^a	Xe	H^b
LiH	I	−0.7	−69.2	1.0
LiF	I	−0.6	−22.5	1.3
NaH	I	−0.8	−72.6	0.3
NaF	I	−0.7	−20.1	0.7
BeH_2	II	−0.6	−138.1	0.6
BeF_2	II	0.2	−269.2	1.7
MgH_2	II	−0.6	−116.3	0.7
MgF_2	II	0.1	−231.5	1.5
Li_2H_2	III	−0.7	−132.6	0.5
Li_2F_2	III	−0.5	−145.9	0.7
Na_2H_2	III	−0.6	−142.9	0.3
Na_2F_2	III	−0.5	−126.3	0.4
Be_2H_4	IV	−0.5	−98.3	4.2
Be_2F_4	V	0.5	−278.5	2.3
Mg_2H_4	IV	−0.7	−75.4	1.6
Mg_2F_4	V	0.1	−224.4	1.6

The absolute chemical shielding of the isolated XeH_2 are 4,846.8 and 24.55 ppm for the Xe and H atoms, respectively

[a] Hydrogen atom non involved in the interaction

[b] Hydrogen atom involved in the interaction

4 Conclusions

A theoretical study of the inverse hydrogen bonds formed by XeH_2 and hydride and fluoride derivatives of Li, Be, Na and Mg has been carried out by means of DFT and ab initio methods, B3LYP and MP2. The results obtained conclude that very stable complexes are formed where a significant amount of electronic charge is transferred from the XeH_2 system to the metallic moieties, with concomitant important dipole moment enhancements.

The analysis of the electron density shows bcp between the interacting hydrogen and the metallic atoms as well as the interaction between the xenon and the fluorine atoms.

The calculated absolute chemical shieldings show the high sensitivity of the xenon atom and reflect the charge flow in this molecule upon complexation, making it a suitable probe for NMR studies [46].

Acknowledgments This work was carried out with financial support from the Ministerio de Educación y Ciencia (Project No. CTQ2007-61901/BQU) and Comunidad Autónoma de Madrid (Project MADRISOLAR, ref. S-0505/PPQ/0225). Thanks are given to the CTI (CSIC) and CESGA for allocation of computer time.

References

1. Alkorta I, Rozas I, Elguero J (1998) Chem Soc Rev 27:163. doi:10.1039/a827163z
2. Desiraju GR, Steiner T (1999) The weak hydrogen bond. Oxford University Press, Oxford
3. Klooster WT, Koetzle TF, Siegbahn PEM, Richardson TB, Crabtree RH (1999) J Am Chem Soc 121:6337. doi:10.1021/ja9825332
4. Alkorta I, Elguero J, FocesFoces C (1996) Chem Commun 1633
5. Rozas I, Alkorta I, Elguero J (1997) Chem Phys Lett 275:423. doi:10.1016/S0009-2614(97)00767-7
6. Alkorta I, Elguero J, Mo O, Yanez M, Del Bene JE (2002) J Phys Chem A 106:9325. doi:10.1021/jp021159w
7. Alkorta I, Elguero J, Grabowski SJ (2008) J Phys Chem A 112:2721. doi:10.1021/jp711387g
8. Alkorta I, Zborowski K, Elguero J, Solimannejad M (2006) J Phys Chem A 110:10279. doi:10.1021/jp061481x
9. Solimannejad M, Boutalib A (2006) Chem Phys 320:275. doi:10.1016/j.chemphys.2005.07.028
10. Solimannejad M, Alkorta I (2006) Chem Phys 324:459. doi:10.1016/j.chemphys.2005.11.007
11. Solimannejad M, Scheiner S (2005) J Phys Chem A 109:11933 doi:10.1021/jp0563383
12. Solimannejad M, Scheiner S (2005) J Phys Chem A 109:6137 doi:10.1021/jp052534y
13. Custelcean R, Jackson JE (2001) Chem Rev 101:1963 doi:10.1021/cr000021b
14. Rozas I, Alkorta I, Elguero J (1997) J Phys Chem A 101:4236. doi:10.1021/jp963943k
15. Lipkowski P, Grabowski SJ, Leszczynski J (2006) J Phys Chem A 110:10296 doi:10.1021/jp062289y
16. Grabowski SJ, Sokalski WA, Leszczynski J (2006) Chem Phys Lett 422:334. doi:10.1016/j.cplett.2006.01.120
17. Pettersson M, Lundell J, Räsänen M (1995) J Chem Phys 103:205. doi:10.1063/1.469632
18. Feldman VI, Sukhov FF (1996) Chem Phys Lett 255:425. doi:10.1016/0009-2614(96)00346-6
19. Feldman VI, Sukhov FF, Orlov AY (1997) Chem Phys Lett 280:507. doi:10.1016/S0009-2614(97)01208-6
20. Berghof V, Gudipati MS, Schwentner N (2004) J Chem Phys 120:1414. doi:10.1063/1.1631816
21. Feldman VI, Sukhov FF, Logacheva EA, Orlov AY, Tyulpina IV, Tyurin DA (2007) Chem Phys Lett 437:207. doi:10.1016/j.cplett.2007.02.039
22. Lundell J, Pettersson M (1999) PCCP 1:1691
23. Berski S, Lundell J, Latajka Z (2000) J Mol Struct 552:223. doi:10.1016/S0022-2860(00)00486-5
24. Lundell J, Berski S, Latajka Z (2000) PCCP 2:5521
25. Solimannejad M, Amlashi LM, Alkorta I, Elguero J (2006) Chem Phys Lett 422:226. doi:10.1016/j.cplett.2006.02.070
26. Godbout N, Salahub DR, Andzelm J, Wimmer E (1992) Can J Chem 70:560. doi:10.1139/v92-079
27. Becke AD (1993) J Chem Phys 98:5648. doi:10.1063/1.464913
28. Lee CT, Yang WT, Parr RG (1988) Phys Rev B 37:785. doi:10.1103/PhysRevB.37.785
29. Møller C, Plesset MS (1934) Phys Rev 46:618. doi:10.1103/PhysRev.46.618
30. LaJohn LA, Christiansen PA, Ross RB, Atashroo T, Ermler WC (1987) J Chem Phys 87:2812. doi:10.1063/1.453069
31. Frisch MJ, Pople JA, Binkley JS (1984) J Chem Phys 80:3265. doi:10.1063/1.447079
32. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Vreven T, Kudin KN, Burant JC, Millam JM, Iyengar SS, Tomasi J, Barone V, Mennucci B, Cossi M, Scalmani G, Rega N, Petersson GA, Nakatsuji H, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Klene M, Li X, Knox JE, Hratchian HP, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Ayala PY, Morokuma K, Voth GA, Salvador P, Dannenberg JJ, Zakrzewski VG, Dapprich S, Daniels AD, Strain MC, Farkas O, Malick DK, Rabuck AD, Raghavachari K, Foresman JB, Ortiz JV, Cui Q, Baboul AG, Clifford S, Cioslowski J, Stefanov BB, Liu G, Liashenko A, Piskorz P, Komaromi I, Martin RL, Fox DJ, Keith T, Al-Laham MA, Peng CY, Nanayakkara A, Challacombe M, Gill PMW, Johnson B, Chen W, Wong MW, Gonzalez C, Pople JA (2003) Gaussian-03. Gaussian, Inc., Wallingford, CT
33. Boys SF, Bernardi F (1970) Mol Phys 19:553. doi:10.1080/00268977000101561
34. Bader RFW (1990) Atoms in molecules: a quantum theory. The international series of monographs of chemistry. Clarendon Press, Oxford
35. Biegler-König FW, Bader RFW, Tang TH (1982) J Comput Chem 3:317. doi:10.1002/jcc.540030306
36. Popelier PLA (1999) With a contribution from R.G.A. Bone (UMIST,Engl,EU) MORPHY98, a topological analysis program
37. Alkorta I, Picazo O (2005) Arkivoc ix:305
38. Ditchfie R (1974) Mol Phys 27:789. doi:10.1080/00268977400100711
39. London F (1937) J Phys Radium 8:397 doi:10.1051/jphysrad:01937008010039700
40. Rozas I, Alkorta I, Elguero J (1997) J Phys Chem A 101:9457. doi:10.1021/jp971893t
41. Alkorta I, Rozas I, Elguero J (1998) J Phys Chem A 102:9278. doi:10.1021/jp982251o
42. Zhao Y, Truhlar DG (2008) Acc Chem Res 41:157 doi:10.1021/ar700111a
43. Alkorta I, Rozas I, Elguero J (2001) J Phys Chem A 105:743. doi:10.1021/jp002808b
44. Cremer D (1984) Croat Chem Acta 57:1259
45. Rozas I, Alkorta I, Elguero J (2000) J Am Chem Soc 122:11154. doi:10.1021/ja0017864
46. Raftery D, Webb GA (2006) Annual reports on NMR spectroscopy. Academic Press, 205