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Coupled cluster and density functional investigation of the hydrogen bond between halides, paraffines, olefins, and alkynes

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Abstract By means of coupled cluster and density functional M06-2X calculations we have studied the directionality and energetics of the hydrogen bond (HB) between halides and the following H donors: methane, ethylene, and acetylene. The largest interaction energy was obtained for acetylene, the molecule in which the hydrogen atoms present the largest positive charge. For the complex $[X\cdots HCCH]^-$, fluoride presented a different behavior since acetylene donates a hydrogen to fluoride and the $[HF\cdots CCH]^-$ complex was formed. We found that for ethylene there is a strong competition between the monodentate- and bidentate-like structures. Because of its small size, fluoride leads to a monodentate complex with C_2H_4 . However, as we move down in the periodic table, the bidentate-like structure becomes more stable. In effect, for chloride and bromide they are nearly isoenergetic, while for iodide the bidentate-like complex is formed. These present results question previous investigations about the directionality of the HB in halide–ethylene complexes.

Keywords Hydrogen bond · Density functional theory · Coupled clusters · Correlation consistent basis sets

Introduction

Hydrogen bond (HB) is ubiquitous [1], its relevance is so fundamental that life would not exist without it, since the high boiling point of water for instance, is due to the presence of this fascinating force. Of particular interest are hydrogen-bonded complexes in which one of the interacting molecules is an anion. Said type of interaction is one of the strongest HBs that can be found. Indeed, Larson and McMahon [2] showed that the HB energy between fluoride and HF is 39 ± 1 kcal/mol. Although the HB interaction between halide ions and olefins and aromatic compounds is much weaker [3], there is renewed interest because the interaction between halides and CH groups can be used to construct better halide receptors [4–13]. For example, the recently synthesized receptor bambus[6]jeryl hosts iodide selectively over the rest of the halide anions. This molecule interacts with halides with its six pairs of methine hydrogens. It is a bit surprising that this host preferentially binds iodide because fluoride forms stronger HBs with CH groups than chloride, bromide or iodide [3]. Indeed, the recent work by Hiraoka et al. [3] showed that the HB energies between X^- and ethane are 8.8, 5.4, 4.7, and 3.7 kcal/mol, for F^- , Cl^- , Br^- , and I^- , respectively. Quantum chemical optimizations at the MP4SDQ/6-31+G* and B3LYP/LANL2DZ(*,+) levels indicated that the halide ions interact via H-bond with one CH group instead of adopting a bidentate-like structure with two H atoms. This situation is different than that observed for the complex between iodide and benzene [3], which has a bidentate structure, i.e., I^- interacts with two CH groups. Considering the size of this halide ion, it is quite unexpected that iodide interacts with ethylene in a monodentate fashion. The recent advances in computer science have made possible the study of compounds containing 10–20

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atoms at the CCSD(T) level, in conjunction with correlation consistent basis set. Herein, we have performed a coupled cluster and density functional investigation of the interaction between halide and paraffins, olefins, and alkynes. We discuss the strength and directionality of this type of HB. Our results indicated that in contrast with the results obtained by Hiraoka et al. [3], for iodide the directionality of the HB is lost forming a bidentate complex with ethylene. In the case of chloride and bromide the monodentate- and bidentate-like structure have nearly the same energy. We expect that this work can help to understand the HB in halide-containing systems and to design better receptors for halide ions.

Methods

Theoretical calculations were carried out employing the M06-2X [14] and B3LYP [15, 16] functionals as implemented in Gaussian 2009 [17]. These results were compared with those obtained at the CCSD(T) levels. The coupled cluster calculations were performed with CFOUR [18, 19]. The basis sets employed for all atoms were Dunning's augmented correlation consistent basis sets, i.e., aug-cc-pVXZ, X = D, T, Q [20]. For comparative purposes the 6-311G and 6-311+G [21] basis sets were employed for the DFT calculations.

Results and discussion

$[X\cdots\text{CH}_4]^-$ complexes, X = F[−], Cl[−], Br[−], and I[−]

We analyzed the hydrogen bonding of methane to halides in the gas-phase. These systems are small enough to be studied at the CCSD(T) level. The results were used to benchmark the performance of M06-2X. The interaction energies at different levels are presented in Table 1 and the structures in Fig. 1. The optimized geometries and the most relevant structural parameters are shown in Table 2. The complexes have C_{3v} symmetry in all cases. The H-bond distance is strongly dependent on the halide considered. Indeed, at the CCSD(T)/aug-cc-pVQZ level, for fluoride it is 0.7987 Å shorter than for chloride and 1.0318 and 1.157 Å smaller than those computed for bromide and iodide, respectively. The complexes have two different types of C–H bond distances, one corresponds to the H which interacts with the halide (dubbed C–H1) and the other distance (dubbed C–H2) corresponds to the remaining three H atoms that are far away. As we move down in the periodic table, CH1 and CH2 become similar. In the case of fluoride, the difference between both bond lengths is 0.0168 Å, but for bromide and iodide it decreases to just

0.0003 Å. Regarding the performance of M06-2X for energetics, the results presented in Table 1 indicate that it is excellent. In the case of fluoride and iodide the CCSD(T)/aug-cc-pVQZ and M06-2X/aug-cc-pVQZ results are identical, whereas for chloride and bromide the M06-2X/aug-cc-pVTZ values are only 0.3 kcal/mol lower than the CCSD(T) ones. The HB energies follow the expected trend F[−] ≫ Cl[−] > Br[−] > I[−]. At the CCSD(T)/aug-cc-pVQZ level the interaction energies are: −7.1, −3.2, −2.6, and −1.8 kcal/mol, respectively. For the sake of completeness, we evaluated the effect of core correlation in the interaction energies. At the CCSD(T)/aug-cc-pwCVTZ level, core correlation increases the interaction energy by 0.06 and 0.01 kcal/mol, chloride and fluoride, respectively.

It is important to study the basis set effect for M06-2X because the aug-cc-pVXZ are too large to be used for larger complexes. The H-bond energies calculated at the M06-2X/aug-cc-pVQZ level are very close to those calculated using the 6-311+G basis set. The agreement occurs because of fortuitous error cancellation, which can be attributed to the lack of BSSE in the 6-311+G values. Comparison with the results obtained employing the 6-311G basis set reveals that the diffuse function is important for fluoride but not for chloride,

Table 1 Interaction energies (kcal/mol) determined for the C_{3v} complexes $[X\cdots\text{CH}_4]^-$, X = F[−], Cl[−], Br[−], and I[−] at different levels of theory

	F [−]	Cl [−]	Br [−]	I [−]
CCSD(T)				
aug-cc-pVDZ	−7.3	−3.5	−3.1	−2.5
aug-cc-pVDZ + BSSE	−6.2	−2.5	−2.1	−1.5
aug-cc-pVTZ	−7.0	−3.1	−2.8	−2.2
aug-cc-pVQZ	−7.1	−3.2	−2.6	−1.8
M06-2X				
aug-cc-pVDZ	−7.6	−3.2	−2.6	−1.9
aug-cc-pVDZ+BSSE	−7.4	−3.0	−2.4	−1.7
aug-cc-pVTZ	−7.2	−2.9	−2.4	−1.8
aug-cc-pVQZ	−7.1	−2.9	−2.3	−1.8
6-311G	−16.2	−2.9	−2.8	−2.3
6-311G+BSSE	−7.7	−2.6	−2.2	−1.5
6-311+G	−7.1	−2.7	−2.1	
6-311+G+BSSE	−6.5	−2.5	−1.9	
B3LYP				
aug-cc-pVTZ	−6.4	−2.3	−1.7	−1.1
B97D				
aug-cc-pVTZ	−6.6	−2.9	−2.6	−2.1
B97D				
aug-cc-pVQZ	−6.5	−2.9	−2.5	−2.1
MP2				
aug-cc-pVTZ	−6.7	−3.3	−2.8	−2.2
aug-cc-pVQZ	−6.6	−3.2	−2.6	−1.9

Best values are in bold

bromide, or iodide. The BSSE decreases in going from F^- to I^- , being extremely important only for fluoride. By inclusion of BSSE in the calculations performed with the 6-311G basis set the interaction energy is reduced by 8.5 kcal/mol for the system $[F \cdots CH_4]^-$. The complexation energy becomes 0.6 kcal/mol larger, than the one computed using the much more expensive aug-cc-pVQZ basis set. Interestingly, when the 6-311+G results are corrected by BSSE, they deviate from the ones calculated with the aug-cc-pVQZ basis sets.

$[X \cdots C_2H_2]^-$ complexes ($X^- = F^-, Cl^-, Br^-, I^-$)

The next H-donor that we analyzed was acetylene. In Table 3 we present the interaction energies computed at the

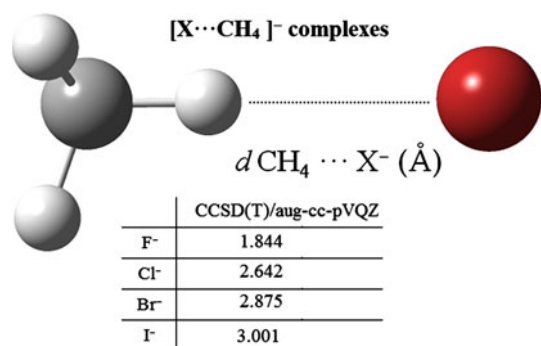


Fig. 1 Optimized structures for the complexes between methane and halide ions, at the CCSD(T)/aug-cc-pVQZ level

CCSD(T) and M06-2X levels of theory and the structures in Fig. 2. The most important difference with respect to the $[X \cdots CH_4]^-$ is that with acetylene, fluoride forms a different structure. In effect, instead of finding a $F^- \cdots HCCH$ interaction, we observed that the hydrogen atom becomes attached to fluoride and a $[FH \cdots CCH]^-$ complex was obtained. The interaction energy is quite large, -24.1 kcal/mol, at the CCSD(T)/aug-cc-pVTZ level of theory, the HB distance being 1.4931 \AA , extremely short for a $H \cdots C$ H-bond. The carbon atom which donates hydrogen to fluoride supports a negative charge of $-0.58 e^-$, close to that of fluoride ($-0.74 e^-$), as indicated by natural population analysis (NPA), at the CCSD(T)/aug-cc-pVTZ level. The interaction energies determined for the complexes of chloride, bromide and iodide are -10.9 , -9.1 , and -7.2 kcal/mol, at the CCSD(T)/aug-cc-pVQZ level of theory, respectively. These values are nearly identical to those obtained at

Table 3 Interaction energies (kcal/mol) of the complexes $[X \cdots C_2H_2]^-$, $X = F^-, Cl^-, Br^-$, and I^- , at different levels of theory

		F^-	Cl^-	Br^-	I^-
CCSD(T)	aug-cc-pVTZ	-23.6^a	-11.3	-9.5	-7.7
	aug-cc-pVQZ	-24.1^a	-10.9	-9.1	-7.2
M06-2X	aug-cc-pVTZ	-27.5	-10.9	-9.1	-7.3

Best values are in bold

^a In the case of fluoride, the complex optimization converged to the $[FH \cdots CCH]^-$ complex

Table 2 Bond distances (\AA) determined for the complexes $[X \cdots CH_4]^-$, $[X \cdots C_2H_2]^-$, $[X \cdots C_2H_4]^-$, $X = F^-, Cl^-, Br^-$, and I^- , at the CCSD(T) level with different basis sets unless otherwise is noted^{a,b}

		F [−]	Cl [−]	Br [−]	I [−]
CH ₄ ⋯X [−]					
aug-cc-pVDZ	dX⋯H1	1.8542	2.6446	2.8272	3.0198
	dC-H1	1.1227	1.1060	1.0149	1.1042
	dC-H2	1.1083	1.1055	1.1052	1.1049
aug-cc-pVTZ	dX⋯H1	1.8517	2.6288	2.8309	2.9679
	dC-H1	1.1115	1.0949	1.0934	1.093
	dC-H2	1.0953	1.0927	1.0923	1.092
aug-cc-pVQZ	dX⋯H1	1.8435	2.6422	2.8753	3.0005
	dC-H1	1.1105	1.0930	1.0909	1.0907
	dC-H2	1.0937	1.0910	1.0906	1.0904
C ₂ H ₂ ⋯X [−]					
aug-cc-pVTZ	dX⋯H ^b	1.4931	2.2405	2.4587	2.7440
aug-cc-pVQZ	dX⋯H ^b	1.5021	2.2517	2.4767	2.7903
C ₂ H ₄ ⋯X [−]					
aug-cc-pVTZ	dX⋯H _{monodentate}	1.7220	2.4774	2.6877	2.9553
aug-cc-pVTZ	dX⋯H _{bidentate-A}		2.8159	2.9802	3.2503
C ₂ H ₄ ⋯X [−]					
aug-cc-pVTZ-M06-2X	dX⋯H _{monodentate}	1.7089	2.5043	2.7165	
aug-cc-pVTZ-M06-2X	dX⋯H _{bidentate-A}	2.1954	2.8050	2.9775	3.2020
aug-cc-pVTZ-M06-2X	dX⋯H _{bidentate-B}	2.3448	2.9822	3.1924	3.3896

^a The C-H distance in methane is: 1.1027, 1.0900, and 1.0882 \AA at the CCSD(T)/aug-cc-pVDZ, CCSD(T)/aug-cc-pVTZ and CCSD(T)/aug-cc-pVQZ levels, respectively

^b For fluoride it is a $[FH \cdots CCH]^-$ complex

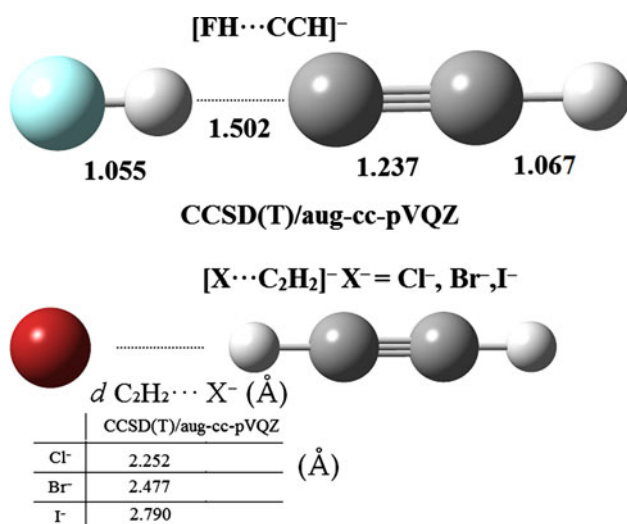


Fig. 2 Optimized structures for the complexes between acetylene and halide ions, at the CCSD(T)/aug-cc-pVQZ level

the M06-2X/aug-cc-pVTZ level of theory. A comparison between the interaction energies of the complexes formed with the halides by methane and acetylene reveals that the interaction in the $\text{X}^- \cdots \text{HCCH}$ complexes is roughly 3–4 times larger. This difference may be related to the charges of the hydrogen atoms in both free molecules: it is much larger in C_2H_2 . In effect, at the CCSD(T)/aug-cc-pVTZ level NPA indicated that the charges of the H atoms are +0.23 and +0.18 e , for C_2H_2 and CH_4 , respectively. It is interesting to compare the charges of the halide and that of the hydrogen atom that participates in the H-bond. In the case of acetylene the charges of Cl^- and H are -0.958 and $+0.296 e^-$, respectively. These values can be compared with those obtained for methane, namely -0.992 and $+0.263$, for Cl^- and H, respectively. If we consider Coulomb law, and the H-bond distances determined at the CCSD(T)/aug-cc-pVTZ level, we find that the attracting force in the methane complex is 68 % of the value computed in $\text{Cl}^- \cdots \text{HCCH}$. Thus, the interaction energies are consistent with an electrostatic-based interaction. Finally, and as expected, because the interaction energies are larger than those computed for the complexes with methane, we found that the $\text{X}^- \cdots \text{H}$ distances are shorter than those calculated for $[\text{X} \cdots \text{CH}_4]^-$, namely, 2.2517, 2.4767, and 2.7903 Å, for Cl^- , Br^- , and I^- , at the CCSD(T)/aug-cc-pVQZ level, respectively.

$[\text{X} \cdots \text{C}_2\text{H}_4]^-$ complexes ($\text{X}^- = \text{F}^-, \text{Cl}^-, \text{Br}^-, \text{I}^-$)

The complexes between halides and ethylene present a more complex potential energy surface than the two cases studied in previous sections. Because of the good agreement observed between CCSD(T) and M06-2X results for the complexes formed by the halides and methane/

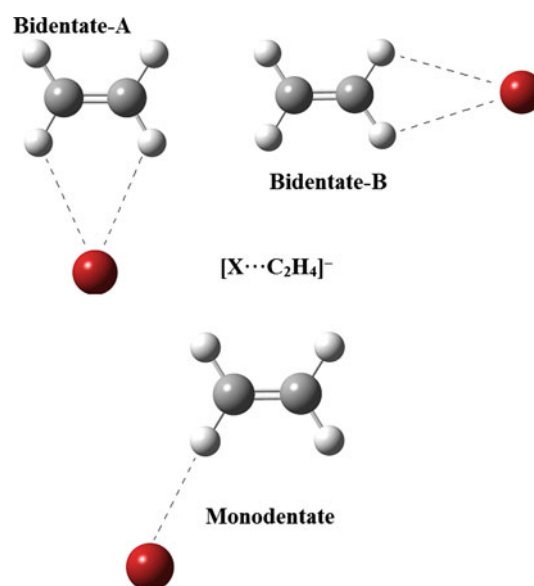


Fig. 3 Optimized structures for the complexes between ethylene and halide ions. Bond distances are presented in Table 2

acetylene, we performed an initial investigation of the PES, at the M06-2X/aug-cc-pVTZ level of theory. Three structures were considered (Fig. 3): (a) the monodentate-like structure in which the halide interacts with one hydrogen atom, (b) a bidentate-like structure (bidentate-A) in which the halide interacts with two hydrogen atoms which are bonded to different carbon atoms and (c) another bidentate-like structure (bidentate-B) where the halide forms HBs with two hydrogen atoms which are bonded to the same carbon atom. Structures A and B present C_{2v} symmetry whereas the monodentate one has C_s symmetry. In agreement with Hiraoka et al. [3], we found that the bidentate-B structure is a first-order transition state, at the M06-2X/aug-cc-pVTZ level. These bidentate-B complexes present very long $\text{X}^- \cdots \text{H}$ HB distances, i.e., 2.345, 2.982, 3.182, and 3.390 Å, for F^- , Cl^- , Br^- , and I^- , respectively. Analysis of the M06-2X/aug-cc-pVTZ interaction energies displayed in Table 4 revealed that the bidentate-A structure is the global minima for chloride, bromide, and iodide. This structure resulted 1.1, 1.1, and 1.2 kcal/mol more stable than bidentate B, for Cl^- , Br^- , and I^- , respectively. However, the bidentate-A structure is only slightly more stable than the monodentate-like structure. Indeed, A is more stable than the monodentate-like complex by 0.2 and 0.3 kcal/mol, for Cl^- and Br^- , respectively, while for iodide the monodentate structure was not found. Fluoride presents a different case due to its small size. The bidentate structure A is a first order transition state and only the monodentate structure is a local minimum. These findings are in disagreement with the work by Hiraoka et al. [3], which proposed that the monodentate structure is the most stable structure for all halides. In order to shed light into

Table 4 Interaction energies (kcal/mol) of the complexes $[X \cdots C_2H_4]^-$, $X = F^-$, Cl^- , Br^- , and I^- , at different levels of theory

		Monodentate	F^-	Cl^-	Br^-	I^-
CCSD(T)	aug-cc-pVTZ		-11.3	-5.6	-4.7	3.8
	aug-cc-pVQZ		-11.1	-5.4	-4.5	-3.5
M06-2X	aug-cc-pVTZ		-11.3	-5.1	-4.3	
		Bidentate A	F^-	Cl^-	Br^-	I^-
CCSD(T)	aug-cc-pVTZ			-5.2	-4.6	-3.9
	aug-cc-pVQZ			-5.2	-4.5	-3.7
M06-2X	aug-cc-pVTZ			-5.3	-4.6	-3.7
		Bidentate B	F^-	Cl^-	Br^-	I^-
M06-2X	aug-cc-pVTZ		-7.7	-4.2	-3.5	-2.9

these discordances we performed CCSD(T) calculations for the monodentate and bidentate-A structures. In the case of fluoride, CCSD(T) and M06-2X indicated that the monodentate-like structure is preferred. The interaction energy computed at the CCSD(T)/aug-cc-pVQZ level is only 0.2 kcal/mol larger than the M06-2X/aug-cc-pVTZ value. In contrast with the DFT results, we found that the monodentate-like structure is the most stable conformation for chloride. Yet, the relative energy is extremely small. At the CCSD(T)/aug-cc-pVQZ level the monodentate-like complex of chloride is more stable by just 0.2 kcal/mol. For bromide the two structures under consideration display similar interaction energy, 4.5 kcal/mol. This value is nicely bracketed by the interaction energies computed at the M06-2X/aug-cc-pVTZ level for both bromide containing complexes. Finally, some problems arose when trying to obtain the monodentate-like structure of iodide. Nevertheless, the bidentate-A structure was found to be the global minima as confirmed by CCSD(T)/aug-cc-pVTZ optimizations and single point CCSD(T)/aug-cc-pVQZ calculation. On the basis of the coupled cluster results, we conclude that fluoride presents a strong preference for the monodentate structure, but for chloride and bromide the monodentate and bidentate structures are nearly isoenergetic, whereas the bidentate structure being preferred for iodide. Thus, as the size of the halide increases, the preference for a monodentate-like complexation decreases and that for bidentate-like complexation increases. Hiraoka et al [3] proposed that the charge of the hydrogen atoms in benzene is larger than those of the hydrogen atoms in ethylene, the bidentate form is preferred for benzene-iodide complex and the monodentate one for ethylene-iodide. The strength of the H-bond in the $[X \cdots H_2CCH_2]^-$ complexes is

Table 5 Reaction energies (kcal/mol), enthalpies (kcal/mol), free energy (kcal/mol), and entropy changes (e.u.) determined for $[X \cdots C_2H_4]^-$, $X = F^-$, Cl^- , Br^- , and I^- at the CCSD(T) level of theory

	F^-	Cl^-	Br^-	I^-
ΔE	-11.1	-5.4	-4.5	-3.7
$\Delta E^\circ + ZPE$	-10.9	-4.8	-4.3	-3.5
ΔH_{298}°	-11.5	-5.0	-3.8	-3.6
$\Delta G_{f,298}^\circ$	-5.9	-0.6	-0.2	0.5
ΔS_{298}°	19	15	12	13
ΔH_{exp}° (ref. 3)	-8.8	-5.4	-4.7	-3.7
ΔS_{exp}° (ref. 3)	14	18	15	14

Computed using CCSD(T)/aug-cc-pVQZ reaction energies and M06-2X/aug-cc-pVTZ thermodynamic corrections

intermediate between those computed for methane and acetylene. This finding is not line with the charges of the hydrogen atoms in CH_4 , C_2H_4 , and C_2H_2 . NPA indicated that the charges are +0.18, +0.17, and +0.23 e , respectively, at the CCSD(T)/aug-cc-pVTZ level. However, if we consider the charge in the $[Cl \cdots H_2CCH_2]^-$ complex and use Coulomb law as we did in the previous section for methane and ethylene, we found that the attraction in $[Cl \cdots H_2CCH_2]^-$ is a 73 % of the value found in the complex between chloride and acetylene. This value is larger than that computed for the complex between chloride and methane. Thus, a simple analysis by means of Coulomb law, using the charges and distances determined at the CCSD(T)/aug-cc-pVTZ level, explains the qualitative order observed for the H-bond energies: $X^- \cdots C_2H_2 \gg X^- \cdots C_2H_4 > X^- \cdots CH_4$. Finally, because thermodynamic experimental values are available, it is interesting to assess the performance of the methodologies employed. The theoretical and experimental values are gathered in Table 5. In the case of Cl^- , Br^- , and I^- there is a superb agreement between experiment and theory. However, fluoride presents a much larger deviation between the experimental and theoretical values. We considered the possibility of problems associated with core correlation correction but this possibility alters reaction energies by less than 0.1 kcal/mol for all halides.

Conclusions

We have studied the halide HB with the H-donors: methane, ethane, and acetylene, at the CCSD(T) and M06-2X levels of theory. The following are considered to be the most important findings of the work:

- (1) The calculated interaction energies follow the same trend as the Coulomb forces computed using charges

and distances determined at the CCSD(T) level. The largest interaction energy was obtained for acetylene, the molecule in which the hydrogen atoms present the largest charge and shortest H-bond distance.

- (2) For the complex between acetylene and fluoride we observed a particular different behavior: acetylene donates a hydrogen to fluoride with the concomitant formation of the $[\text{FH}\cdots\text{CCH}]^-$ complex.
- (3) In the case of ethylene, there is a strong competition between the monodentate and bidentate structures. Because of its small size fluoride leads to a monodentate complex with C_2H_4 . However, as we move down in the periodic table, the bidentate structure becomes the preferred conformation. In effect, for chloride and bromide they are nearly isoenergetic, while for iodide the bidentate complex is formed. These results question recent results about the directionality of the HB in halide–ethylene complexes.
- (4) For chloride, bromide and iodide we observed an excellent agreement between the experimental and CCSD(T)/CBS enthalpy changes. However, in the case of fluoride the difference was significantly higher, close to 2 kcal/mol.

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18. CFOUR, a quantum chemical program package written by J.F. Stanton, J. Gauss, M.E. Harding, P.G. Szalay with contributions from A.A. Auer, R.J. Bartlett, U. Benedikt, C. Berger, D.E. Bernholdt, Y.J. Bomble, O. Christiansen, M. Heckert, O. Heun, C. Huber, T.-C. Jagau, D. Jonsson, J. Jusélius, K. Klein, W.J. Lauderdale, D.A. Matthews, T. Metzroth, D.P. O'Neill, D.R. Price, E. Prochnow, K. Ruud, F. Schiffmann, S. Stopkowitz, J. Vázquez, F. Wang, J.D. Watts and the integral packages MOL-ECULE (J. Almlöf and P.R. Taylor), PROPS (P.R. Taylor), ABACUS (T. Helgaker, H.J. Aa. Jensen, P. Jørgensen, and J. Olsen), and ECP routines by A. V. Mitin and C. van Wüllen. For the current version, see <http://www.cfour.de>
19. Basis sets were obtained from the Extensible Computational Chemistry Environment Basis Set Database, Version 7/30/02, as developed and distributed by the Molecular Science Computing Facility, Environmental and Molecular Sciences Laboratory which is part of the Pacific Northwest Laboratory, P.O. Box 999, Richland, Washington 99352, USA, and funded by the U.S. Department of Energy. The Pacific Northwest Laboratory is a multi-program laboratory operated by Battelle Memorial Institute for the U.S. Department of Energy under contract DE-AC06-76RLO 1830. Contact David Feller or Karen Schuchardt for further information
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