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Ab initio Calculations on Ethylene and Fluoroethylene. A Comparative Study

S. MEZA* and U. WAHLGREN
Institute of Theoretical Physics, University of Stockholm, Stockholm, Sweden

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Self-consistent-field calculations are reported on the ethylene and fluoroethylene molecules. A comparative analysis of the two molecules shows that the effects of substituting a hydrogen atom with a fluorine atom in ethylene are fairly local. Ionization potentials in the ethylene molecule are calculated. The effects of hydrogen *p*-functions are studied in both molecules, and these effects are found to be rather small, particularly in fluoroethylene. A number of molecular properties are reported for both molecules.

Für Äthylen und Fluoroäthylen werden SCF-Rechnungen durchgeführt. Eine vergleichende Analyse der beiden Moleküle zeigt, daß die Effekte der Substitution eines Wasserstoffatoms durch Fluor in Äthylen ziemlich lokal begrenzt sind. Die Ionisationspotentiale für Äthylen werden berechnet. Die Auswirkung von Funktionen am Wasserstoffatom werden in beiden Molekülen untersucht; sie sind relativ gering, besonders im Fluoroäthylen. Eine Reihe von molekularen Eigenschaften wird für beide Moleküle angegeben.

Calculs SCF sur l'éthylène et le fluoroéthylène. Une analyse comparée des deux molécules montre que les effets de la substitution d'un atome d'hydrogène par un atome de fluor dans l'éthylène sont pratiquement locaux. Les potentiels d'ionisation de la molécule d'éthylène sont calculés. L'effet de l'introduction de fonctions *p* sur l'hydrogène est étudié dans les deux molécules; on le trouve faible, en particulier dans le fluoroéthylène. Etude de quelques autres propriétés moléculaires.

1. Introduction

The main purpose of this paper is to make a comparative study of the ethylene and the fluoroethylene molecules. The approach to the problem is to regard fluoroethylene as an ethylene molecule with one hydrogen substituted by a fluorine atom. In order to get a clear picture of the effects of this substitution, a rather detailed study was done on orbital energies and populations.

Several non-empirical LCAO-SCF calculations have been performed on the ethylene [1 – 8] molecule during the last ten years. As is well known, LCAO-SCF *ab initio* calculations are sensitive to the choice of basis functions, thus making it necessary to use the same basis set, that is, basis sets optimized in the same way on the two molecules. Our choice of basis sets made it necessary to make a new calculation on the ethylene molecule.

Furthermore, we considered it to be of interest to study the influence on energies, populations and, for fluoroethylene, dipole moment, of polarizing *p*-type functions on hydrogen. The inclusion of these functions greatly increases

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* Present address: Department of Chemistry, University of Mexico, Mexico 20 D. F.

the number of basis orbitals, and it is desirable to find out in which types of compounds their effect is small or negligible.

A series of open shell calculations on the positive ethylene ion were performed in order to compute ionization potentials for ethylene.

We also report calculations of a number of molecular properties other than populations and dipole moment (quadrupole moments, magnetic susceptibility etc.). As there are at the present time no experimental values reported for these properties in ethylene and fluoroethylene, we publish, whithout discussion, the values obtained.

2. Method

Linear combinations of simple Gaussians were used as basis functions. The notation throughout this paper will be $(A/N_s, N_p)$ to denote the number of uncontracted Gaussians centered on atom A, and $[A/N_s, N_p]$ to denote the corresponding contracted basis set. N_s and N_p are the number of s and p-type functions respectively.

The calculations were performed with two basis sets, one [C/4, 2] [F/4, 2] [H/2, 1] and one [C/4, 2] [F/4, 2] [H/2]. In what follows these two basis sets will be referred to as the [H/2, 1] and the [H/2] basis sets respectively. Both basis sets were obtained by contracting the first 4 single Gaussians centered on carbon and fluorine (C/7, 3) and (F/7, 3) sets and by contracting the first three in a (H/4) set and, for the [H/2, 1] basis, adding a p-type function to the hydrogen. The orbital exponents and contraction coefficients for the (C/7, 3) and (F/7, 3)-sets are the optimized atomic exponents and the corresponding atomic orbital coefficients calculated by Roos and Siegbahn [9]. The (H/4) set is taken from a report by Huzinaga [10], with the orbital exponents multiplied with a scaling factor of 1.25. The orbital exponents on the hydrogen p-functions are set equal to 0.875.

The geometrics were taken from Allen and Plyler [11] and from Laurie [12] for ethylene and fluoroethylene respectively. The coordinates are listed in Table 1. Both molecules were placed in the xz-plane, the y-axis being perpendicular to the molecular plane, and the z-axis being along the carbon-carbon bond. Planar ethylene belongs to the symmetry group D_{2h}, and its electron configuration in the ground state is $(1a_g)^2$ $(1b_{1u})^2$ $(2a_g)^2$ $(2b_{1u})^2$ $(1b_{3u})^2$ $(3a_g)^2$ $(1b_{2g})^2$ $(1b_{2u})^2$. The first seven orbitals, being symmetrical on reflection in the molecular plane, constitutes the σ-core, while the eight orbital is the binding carbon-carbon π orbital.

The fluoroethylene molecule has only one symmetry element, reflection in the molecular plane. In the ground state, ten of its twelve occupied molecular orbitals are of σ type and two are of π type, the two latter being one binding carbon-carbon orbital and one fluorine lone pair orbital.

Open shell calculations were done on five different electron configurations of $C_2H_4^+$, keeping the geometry of the neutral molecule. The singly occupied orbital was taken to be the highest MO in each of the five irreducible representations in turn, i.e. the $1b_{2u}$, $1b_{2g}$, $3a_g$, $1b_{3u}$, $2b_{1u}$ orbitals. The vertical ionization potentials were simply found as the difference between the total energy of the respective ions and the total energy of the molecule in its ground state.

Table 1. *Geometries*[a] *used in the present calculations on ethylene and fluoroethylene*

	X	Y	Z
Ethylene			
C(1)	0.0	0.0	−1.263305
C(2)	0.0	0.0	1.263305
H(1)	−1.752667	0.0	−2.331023
H(2)	−1.752667	0.0	2.331023
H(3)	1.752667	0.0	2.331023
H(4)	1.752667	0.0	−2.331023
Fluoroethylene			
C(1)	0.0	0.0	0.0
C(2)	0.0	0.0	2.517160
F(3)	2.182406	0.0	−1.313922
H(4)	−1.733944	0.0	−1.043924
H(5)	1.781789	0.0	3.535543
H(6)	−1.770304	0.0	3.528978

[a] Distances are in atomic units (1 a.u. = 0.529168 Å).

Population analysis was carried out following the method of Mulliken [13]. A number of conclusions are drawn from these figures concerning the qualitative classification of the molecular orbitals, and, as already mentioned, the effects of the fluorine substitution in ethylene and the effect of polarizing functions on hydrogen. Contour maps showing the total electron density are also presented, in order to illustrate the populations in a more pictorial form. Figs. 1 and 2.

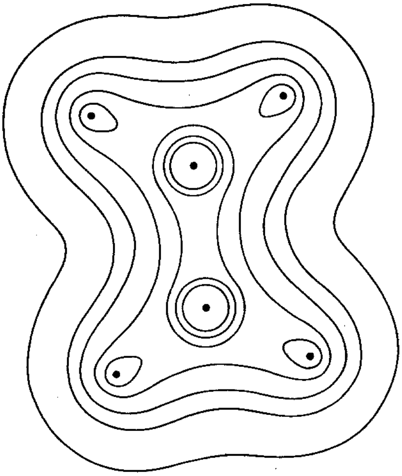

Fig. 1

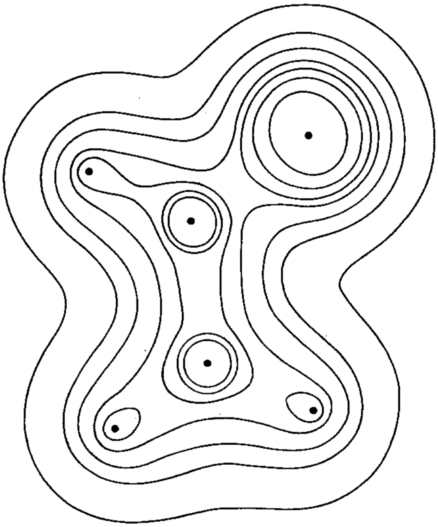

Fig. 2

Fig. 1. Total electrons density contours for ethylene. Plotted contours are: 0.01, 0.05, 0.10, 0.20, 0.30, 0.50 and 1.00

Fig. 2. Total electron density contours for fluoroethylene. Plotted contours are: 0.01, 0.05, 0.10, 0.20, 0.30, 0.50 and 1.00

The one electron properties were all calculated using both the [H/2, 1] and the [H/2] basis sets, but only the results from the [H/2, 1] basis set are shown in the tables, although some comments are made concerning the effect of including the hydrogen p-functions.

The program used for the SCF-calculation is the IBMOL program version 4 [14].

The calculations were carried out on the IBM 360/75 computer at Stockholm's Datacentral.

3. Results and Discussion

Ionization Potentials for Ethylene

The results of the open-shell calculations on $C_2H_4^+$ are presented in Table 2, together with the orbital energies of the ground state of the neutral molecule. The values of the ionization potentials obtained from the ion in the manner described earlier, are all seen to be considerably smaller than the corresponding values given by Koopmans' theorem. They are also in much better agreement with experiment as far as the σ-type orbitals are concerned, but for the loosely bound π electron Koopmans' theorem yields a better agreement. For the latter orbital, the ionization potential given by Koopmans' theorem is 4% below the experimental value, while the value calculated from the ion is as much as 15% below. For the remainder of the calculated ionization potentials which could be compared with experiment this difference is smaller than 5%. As is well known, two main errors are obtained in the ionization potentials obtained from Koopmans' theorem. The first one is the neglect of the change in SCF energy due to electron reorganization and the second one is the neglect of correlation energy changes. If these two effects are of opposite sign and of the same order they cancel out yielding good experimental agreement. This is often the case for the ionization potential obtained when a loosely bound electron is removed from a molecule. In ethylene these two effects are of the same sign for the $1b_{3u}$ and the $1b_{2g}$ and of opposite sign for the $3a_g$ and $1b_{2u}$ orbitals. They are of the same order and opposite sign only for the $1b_{2u}$ orbital, which is the highest occupied MO in the molecule.

It could be noted that the figures here presented indicates a larger correlation energy change when an electron is removed from the π orbital than when it is removed from the σ core.

Good agreement with experimental data for ionization potentials given by Koopmans' theorem for π orbitals is found for other small carbon-containing compounds, e.g. formaldehyde in a calculation reported by Winter [15] *et al.*

Effects of Fluorine Substitution

The main concern of this section is to compare the orbitals on fluoroethylene with the orbitals on ethylene. Furthermore, the change in population resulting from the fluorine substitution is studied.

A number of conclusions can be drawn from a comparison of the orbital energies (Tables 2 and 3) for the two molecules. Orbitals $2a_1$ and $3a_1$ in fluoro-

Table 2. *Orbital energies and calculated ionization potentials for ethylene (energy in atomic units*[b]*)*

Molecular orbital	[H/2, 1] $-\varepsilon_i$	[H/2, 1] Calculated IP	[H/2] $-\varepsilon_i$	[H/2] Calculated IP	Experimental IP[a]
$1a_g$	11.2467		11.2479		
$1b_{1u}$	11.2451		11.2463		
$2a_g$	1.0377		1.0397		
$2b_{1u}$	0.7861	0.7614	0.7895	0.7655	
$1b_{3u}$	0.6388	0.6134	0.6412	0.6163	0.5847
$3a_g$	0.5790	0.5305	0.5809	0.5325	0.5413
$1b_{2g}$	0.4998	0.4786	0.4999	0.4796	0.4697
$1b_{2u}$	0.3702	0.3296	0.3728	0.3323	0.3862

[a] See Ref. [17].

[b] 1 a.u. = 27.2107 eV. Total energies: $E_{[H/2,1]} = -77.9685$, $E_{[H/2]} = -77.9464$.

Table 3. *Orbital energies and total energies for fluoroethylene (energy in atomic units*[b]*)*

Molecular orbital	$-\varepsilon_i$ [H/2, 1]	$-\varepsilon_i$ [H/2]	Experimental IP[a]
$1a_1$	26.3348	26.3346	
$2a_1$	11.3434	11.3440	
$3a_1$	11.2545	11.2531	
$4a_1$	1.6242	1.6241	
$5a_1$	1.0594	1.0607	
$6a_1$	0.8202	0.8223	
$7a_1$	0.7232	0.7243	
$8a_1$	0.6664	0.6676	0.6604
$1a_2$	0.6650	0.6649	0.6163
$9a_1$	0.5770	0.5773	0.5332
$10a_1$	0.5463	0.5459	0.5068
$2a_2$	0.3756	0.3773	0.3888
Total energy	−176.6543	−176.6367	

[a] See Ref. [16].

[b] 1 a.u. = 27.2107 eV.

ethylene correspond to the ethylene orbitals $1a_g$ and $1b_{1u}$. Orbitals $5a_1$ and $6a_1$ in fluoroethylene would thus correspond to the $2a_g$ and the $2b_{1u}$ orbitals in ethylene, shifted 0.6 and 0.9 eV respectively. Orbital $8a_1$ can be identified as the shifted $1b_{3u}$ orbital in ethylene. This identification can be done, since the other orbital in fluoroethylene with its energy close to that of the orbital $8a_1$ is of π symmetry. Orbitals $9a_1$ and $10a_1$ in fluoroethylene correspond to the $3a_g$ and $1b_{2g}$ orbitals, shifted 0.05 and 1.3 eV respectively, and finally the 2π orbital in fluoroethylene corresponds to the binding C–Cπ orbital in ethylene. The shift for the latter orbital is seen to be very small.

From the orbital populations (Tables 4 and 5) and from the results discussed above, some further characteristics of the orbitals follow. The orbital $1a_1$ is essentially a fluorine $1s$ orbital, while orbitals $2a_1$ and $3a_1$ are mainly of carbon

Table 4. *Orbital atomic and overlap populations for ethylene* [H/2, 1] *basis set*

Molecular orbital[a]	q(C)	q(H)	O(C–C)	O(C–H)
$1a_g$	0.9994	0.0003	−0.0008	0.0004
$1b_{1u}$	0.9996	0.0002	0.0086	0.0004
$2a_g$	0.8481	0.0760	0.5246	0.0776
$2b_{1u}$	0.5818	0.2091	−0.0498	0.2206
$1b_{3u}$	0.5870	0.2065	0.1674	0.1674
$3a_g$	0.7048	0.1476	0.2984	0.1128
$1b_{2g}$	0.4159	0.2920	−0.1846	0.2458
$1b_{2u}$	0.9939	0.0030	0.5128	0.0052

[a] The molecular orbitals are ordered according to the orbitals energies. See Table 2.

1*s* character. Orbitals $4a_1$ and $1a_2$ are the fluorine lone pairs of σ and π type respectively. Thus only orbital $7a_1$ is not identified, and following the above arguments this would lead us to the conclusion that it corresponds to the second σ lone pair orbital on fluorine. It is seen, from the population analysis, that most of the fluoroethylene orbitals above the $4a_1$ are delocalized to a large extent, i.e. almost all these orbitals take part in the C–F bond.

From the results obtained here some conclusion can be drawn regarding the identification of the peaks in the fluoroethylene photoelectron spectra [16]. It seems reasonable to assume that the 16.8 eV peak should correspond to the ionization energy needed to remove an electron from the fluorine lone pair π orbital. The remaining ionization potentials are then easily identified as shown in Table 3.

The change in total populations resulting from the fluorine substitution is shown in Table 6. It is of interest to note, that the gross atomic population on the β-carbon (the carbon not neighbouring the fluorine atom), is almost the same as that of one of the carbon atoms in ethylene, while the absolute change in net population resulting from the substitution is rather similar in both carbon atoms. All the hydrogens are seen to loose electrons to the heavier atoms. A comparision of the contour maps of both molecules shown in Fig. 1 and 2, shows little difference in electron distribution in the region around the β-carbon, in spite of the difference of net change on the β-carbon in fluoroethylene and a carbon in ethylene and the changes of population on the hydrogens.

Effects of p-Type Functions on Hydrogen

All calculations have been done using both, the [H/2, 1] and the [H/2], basis sets.

The difference between the results thus obtained are fairly small as far as the energies and one-electron properties are concerned. For the ethylene molecule, one result of including hydrogen *p*-functions, is that all orbital energies are increased (Table 2). Better agreement between experimental values of the ionization potentials and the values given by Koopmans' theorem is obtained for the σ orbitals, while for the π orbital the agreement becomes less good. The

Table 5. *Orbital atomic and overlap populations for fluoroethylene* [H/2, 1] *basis set*

Molecular orbital[a]	q(C1)	q(C2)	q(F3)	q(H4)	q(H5)	q(H6)	O(C1-C2)	O(C1-F3)	O(C1-H4)	O(C2-H5)	O(C2-H6)
$1a_1$	0.0013	0.0000	1.9987	0.0000	0.0000	0.0000	0.0000	0.0024	0.0000	0.0000	0.0000
$2a_1$	1.9976	0.0022	−0.0004	0.0006	0.0000	0.0000	0.0036	−0.0008	0.0012	0.0000	0.0000
$3a_1$	0.0022	1.9967	0.0000	0.0000	0.0005	0.0005	0.0038	0.0000	0.0000	0.0008	0.0010
$4a_1$	0.1385	0.0101	1.8486	0.0026	0.0001	0.0002	0.0056	0.1796	0.0020	0.0000	0.0000
$5a_1$	0.8073	0.8446	0.1311	0.0718	0.0634	0.0818	0.5472	−0.0166	0.0758	0.0672	0.0814
$6a_1$	0.5685	0.3807	0.5319	0.2361	0.1685	0.1143	0.0026	0.1132	0.2592	0.1526	0.1224
$7a_1$	0.4677	0.2621	0.9783	0.1726	0.0081	0.1112	0.0508	0.1748	0.1510	0.0048	0.1224
$8a_1$	0.3220	0.5044	0.8691	0.0280	0.1938	0.0828	−0.0230	0.1026	0.0298	0.2284	0.1070
$1a_2$	0.2430	0.0226	1.7346	−0.0004	0.0001	0.0000	0.0214	0.1818	−0.0008	0.0002	0.0002
$9a_1$	0.0533	0.6946	0.5939	0.0028	0.1536	0.5017	0.0460	0.0028	−0.0020	0.1696	0.3136
$10a_1$	0.3259	0.4376	0.5030	0.3976	0.3145	0.0214	0.0194	−0.0918	0.3054	0.1748	0.0406
$2a_2$	0.7563	1.0366	0.1966	0.0042	0.0030	0.0034	0.4754	−0.1594	0.0070	0.0052	0.0060

[a] The molecular orbitals are ordered according to the orbitals energies. See Table 3.

negative of the calculated ionization potentials underwent the same changes as the orbital energies. In all cases they decreased, and the magnitude of the changes are about the same, except for the $1b_{2g}$ orbital.

In all cases the difference between energies obtained from the calculation with different basis sets are smaller than the difference between calculated and experimental values.

In the case of fluoroethylene, the effect on the energies of including hydrogen p-functions is much smaller than in ethylene. This is of course expected as the relative amount of added functions is smaller in fluoroethylene than in ethylene. Furthermore, the effect is negligible on the two lone pairs on fluorine, orbitals $4a_1$ and $1a_2$. The ordering of the orbitals is not changed by the inclusion of hydrogen p-functions. It could also be mentioned that the change of the orbital energies are irregular with respect to the sign of the change in fluoroethylene, while they all increased in ethylene. The effect of including the polarization functions on the population is more pronounced. In ethylene 0.24 electrons are transferred from each carbon to the hydrogens when the hydrogen p-functions are included, as is seen in Table 6. In fluoroethylene, where the corresponding values are shown in the same table, the electron flow is different for the different carbons. The carbon bound to the fluorine atom (C 1) is loosing only 0.11 electrons, while the carbon neighbouring two hydrogens looses almost the same amount of electrons as one carbon in ethylene. The electron loss at the carbons when going from the [H/2] to the [H/2, 1] basis set are evenly distributed among the hydrogens, each gaining about 0.1 electron. The effect on fluorine is negligible.

Table 6. *Total atomic populations*

Ethylene					Fluoroethylene				
	[H/2, 1]		[H/2]			[H/2, 1]		[H/2]	
	Net	Gross	Net	Gross		Net	Gross	Net	Gross
C	4.7358	6.1305	5.0474	6.3699	C1	4.5067	5.6836	4.6580	5.7882
H	0.5914	0.9347	0.4726	0.8150	C2	4.9320	6.1921	5.2355	6.4438
					F3	9.2147	9.3852	9.2159	9.3830
					H4	0.5910	0.9158	0.4739	0.7964
					H5	0.5497	0.9055	0.4410	0.7888
					H6	0.5668	0.9174	0.4559	0.7997

Table 7. *Total overlap population*

Ethylene			Fluoroethylene		
	[H/2, 1]	[H/2]		[H/2, 1]	[H/2]
C-C	1.2764	1.1850	C1-C2	1.1530	1.1010
C-H	0.8304	0.7942	C1-F3	0.4888	0.4666
C-H (on C2)	−0.0738	−0.0642	C1-H4	0.8290	0.7912
			C2-H5	0.8038	0.7666
			C2-H6	0.7946	0.7546
			F3-C2	−0.1005	−0.0955

The total overlap populations (Table 7) indicate that all bonds get stronger when the hydrogen *p*-functions are included. The C–C bond in ethylene is more affected by the change than the C–C bond in fluoroethylene, but the effects on the C–H bonds are the same in both molecules.

In comparing these results with the corresponding results for H_2O and NH_3 [18], it is seen that the loss of electrons from the heavy atoms is somewhat larger for these compounds than for ethylene and fluoroethylene when the hydrogen *p*-functions are included. The oxygen looses 0.41 electrons to two hydrogens, the nitrogen looses 0.56 electrons to three hydrogens and the carbon looses 0.58 electrons to four hydrogens.

Roos and Siegbahn [18] also found considerable changes in dipole moments for H_2O and NH_3, while we found that the dipole moment in fluoroethylene did not change at all, being 1.85 D with both basis sets (experimental [19] 1.427 D).

The one-electron properties calculated for the two molecules are shown in Tables 8-14. As we mentioned before the difference between the results obtained with the two basis sets are very small, and we present only the results obtained with the [H/2, 1] basis set.

4. Conclusions

The comparison of the wave functions of ethylene and fluoroethylene showed some peculiar effects resulting from the substitution of a hydrogen atom by a fluorine atom in the ethylene molecule. The changes in gross atomic populations on the β-carbon and on the two hydrogen atoms neighbouring it were very small, but the corresponding changes in net atomic populations indicated an eventual electron reorganization in this region of the molecule. A comparison of the electron density contour map of the two molecules shows almost no difference between the electron distribution in the region around the β carbon in fluoroethylene and in the region around one of the carbons in ethylene.

In order to be able to discuss these results, we believe it to be of importance to point out that the electronic population are related to the way the wave function is constructed in the LCAO-approximation, and does not correspond directly to any physically measurable quantities, while the electron density is a physical concept. We therefore believe, that the conclusion to be drawn from the above mentioned results, and from the fact that the orbital energy shifts resulting from the fluorine substitutions are reasonably small, is that the effects of substituting a hydrogen atom by a fluorine atom in ethylene are fairly local. The change in net population seems to result from a change in the MO's not affecting the electron density in the region concerned, and therefore also not affecting the physical properties of this part of the molecule.

The effect of the polarizing functions on the hydrogens is not negligible as far as the populations are concerned, but it seems reasonable to believe that they can be excluded in many cases where the compound contains more than one heavy atom. This problem needs to be studied further.

The supposition that contributions from the correlation energy change and the reorganization energy change to the ionization potentials are of different sign is not always correct according to the above presented results. Our wave

Table 8. *Quadrupole moment tensor (a.u.)*

	Ethylene	Fluoroethylene
θ_{xx}	0.4838	2.5018
θ_{yy}	−4.0312	−1.7179
θ_{zz}	3.5474	−0.7839

Table 9. *Diamagnetic susceptibility tensor (a.u.)*

	Ethylene	Fluoroethylene
χ_{xx}	−58.6245	−70.6533
χ_{yy}	−67.9018	−107.7779
χ_{zz}	−32.0683	−32.7383
χ_{xz}		−154.0935

Table 10. *Potential at nucleus (a.u.)*

	Ethylene		Fluoroethylene
Φ(C)	−14.1398	Φ(C1)	−14.6117
Φ(H)	−0.7677	Φ(C2)	−14.6997
		Φ(F3)	−26.5226
		Φ(H4)	−1.0713
		Φ(H5)	−1.0906
		Φ(H6)	−1.0860

Table 11. *Electric field at nucleus (a.u.)*

	Ethylene			Fluoroethylene	
	Ex	*Ez*		*Ex*	*Ez*
C		−0.3221	C1	−0.0588	0.0074
H	−0.0363	−0.0820	C2	0.0037	0.0417
			F3	0.2211	−0.1326
			H4	−0.0031	−0.0195
			H5	−0.0009	0.0049
			H6	−0.0032	0.0050

Table 12. *Charge densities at nucleus (a.u.)*

	Ethylene		Fluoroethylene
δ(C)	114.9699	δ(C1)	114.9710
δ(H)	0.4164	δ(C2)	114.9208
		δ(F3)	410.7207
		δ(H4)	0.4291
		δ(H5)	0.4063
		δ(H6)	0.4122

Table 13. *Electric field gradient at nucleus (a.u.)*

	Ethylene				Fluoroethylene		
	q_{xx}	q_{yy}	q_{zz}		q_{xx}	q_{yy}	q_{zz}
C	0.1936	−0.1618	−0.0318	C1	0.4229	−0.1028	−0.3200
H	0.1531	0.1894	−0.3425	C2	0.1301	−0.1977	0.0676
				F3	1.5920	1.3842	−2.9762
				H4	0.1491	0.1824	−0.3315
				H5	0.1448	0.1687	−0.3135
				H6	0.1489	0.1768	−0.3258

Table 14. *Magnetic shielding tensor (a.u.)*

	Ethylene						Fluoroethylene				
	σ_{xx}	σ_{yy}	σ_{zz}	σ_{xz}	σ_{av}		σ_{xx}	σ_{yy}	σ_{zz}	σ_{xz}	σ_{av}
C	−4.9520	−5.2091	−3.9788		−14.1398	C1	−4.7581	−5.3398	−4.5138	−0.1984	−14.6117
H	0.1252	−0.8290	−0.0640	0.6815	− 0.7677	C2	−4.9791	−5.2768	−4.4437	−0.0264	−14.6997
						F3	−8.4525	−9.2196	−8.8504	−0.4724	−26.5226
						H4	0.1722	−0.8676	−0.3759	0.5607	− 1.0713
						H5	0.0705	−0.8461	−0.3150	0.5473	− 1.0906
						H6	0.0931	−0.8417	−0.3373	−0.5521	− 1.0859

functions are not at the Hartree-Fock limit, but considering the size of the different energy changes and the fact that the same basis set have been used both for the ionic wave functions and the wave function of the neutral ethylene molecule, we believe this result to be correct.

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Dr. Ulf Wahlgren
Institute of Theoretical Physics
University of Stockholm
Vanadisvägen 9
Stockholm VA, Sweden