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# A Conformational Study of Some 1,2-Disubstituted Ethanes by an *ab initio* Method

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The conformational energy differences in 1,2-difluoro-, 1,2-dichloro- and 1,2-dicyano-ethane have been estimated from *ab initio* calculations with Gaussian type basis functions and a limited geometry variation. The *anti* conformer is found to have the lowest energy for all three molecules, revealing a discrepancy in the relative energy up to 2 kcal mol$^{-1}$ when compared to the experimental values (1 kcal = 4.184 kJ). It is suggested that an incomplete cancelling of the correlation energy, possibly due to dispersion forces between the *gauche* halogens, may explain the apparent discrepancy for the dihaloethanes.

It has been extensively reported in the literature[1-3] that standard SCF-LCAO-MO procedures usually are able to reproduce torsional potentials in reasonably good agreement with available experimental data. Especially if care is taken in applying an adequately chosen basis set and optimizing, at least partially, the geometry during the internal rotation, the calculated conformational energy differences agree reasonably well with experimental results.

1,2-disubstituted ethanes have two conformers, *gauche* and *anti*. Usually *anti* is the most stable, but with substituents that can have some kind of favourable interactions, *gauche* has the lowest energy. Also 1,2-difluoroethane is most stable in *gauche*.[4-9,42] The relative stability of *gauche* to *anti* cannot be rationalized simply on the basis of steric effects. It has therefore been proposed that interactions between lone pairs or between unsaturated bonds can be attractive. Provided this effect is due to a bond established between the two substituents it should be detectable within the Hartree-Fock limit of calculations *ab initio*. However, if the stabilization of *gauche* is due to dispersion forces (arising from the interpair correlated electron motions) it should not be detectable with this method.

In a similar study of 1,2-difluoroethane Pople *et al.*[3] estimated the energy difference between *gauche* and *anti* to be +1.0 kcal mol$^{-1}$. This result is in obvious disagreement with the experimental data,[4-9,42] which give a *gauche* contribution of about 90 % at room temperature. In Ref. 3 standard geometry parameters were used,[10] only optimizing the torsional angle. Polarization functions are not included in the 4 – 31 G[11] basis set used. These could be the reasons for the apparent discrepancy. In a recent *ab initio* study of 1,2-difluoroethene Binkley and Pople[12] found, in agreement with experiments, the *cis* configuration to be the most stable one, provided the basis set applied was large enough (6 – 311 G*)[12] and polarization functions were included for both carbon and fluorine.

The scope of this work is to evaluate further these effects on the conformational predictions as obtained from *ab initio* calculations, as part of a conformational study of some disubstituted ethanes.[13-15] Thereby it is hoped to get some understanding of the factors determining the torsional potentials and the conformational mixtures in the gas phase. The *gauche-anti* energy differences in these molecules are rather small, and a careful analysis of the calculated energy differences is of importance, since, in these cases, even small contributions to the total energy might affect rather strongly the equilibrium parameters.

## METHOD

The program MOLECULE,[16] which solves the Roothaan-Hall equations for a Gaussian type basis set, was used in the calculations, carried out with (7,3) primitive basis[17] for C, N and F, and (10,6) for Cl. For hydrogen a 4 s primitive basis[18,19] was used. A double zeta contraction was employed for all atoms.

The polarization effects in the carbon–halogen bonds were studied in a limited number of runs by including *d*-orbitals in the basis set of the halogens, with exponents equal to 1.0[20] for F and 0.68[21] for Cl. The torsional angle in *gauche* was varied in all cases to minimum energy with rigid, experimental geometry[4,5,13–15] (Tables 1 and 4). Keeping this angle at the optimized value, the other most important structural parameters were optimized for both conformers (Table 5–7). Finally, energy differences between conformers with optimal geometry were calculated, and these are compared to the experimental values in Table 8.

*Table 1.* Structural parameters (distances in Å, angles in °) as determined from electron diffraction (ED), reported standard deviations in parentheses, and optimal values from *ab initio* calculations.

| | ED | *ab initio* *anti* | *gauche* |
|---|---|---|---|
| $C_2H_4F_2$[4,5] | | | |
| C–C | 1.505(10)[a] | 1.513 | 1.504 |
| C–F | 1.389(7) | 1.404 | 1.404 |
| C–H | 1.095(10) | – | – |
| ∠CCF | 110.3 (20) | 107.4 | 109.6 |
| ∠CCH | 110.6 (30) | – | – |
| $\phi$ | 69.4 (70)[a] | 180.0 | 75.0 |
| $C_2H_4Cl_2$[13,14] | | | |
| C–C | 1.531(3) | – | – |
| C–Cl | 1.790(2) | 1.815 | 1.811 |
| C–H | 1.112(5) | – | – |
| ∠CCCl | 109.0 (2) | – | – |
| ∠CCH | 113.2 (13) | – | – |
| $\phi$ | 75.3(9) | 180.0 | 70.5 |
| $C_2H_4(CN)_2$[15] | | | |
| C–C | 1.534(3) | 1.554 | 1.550 |
| C–CN | 1.471(1) | 1.464 | 1.465 |
| C≡N | 1.156(1) | – | – |
| C–H | 1.110(4) | – | – |
| ∠CCC | 111.8 (2) | 111.0 | 111.9 |
| ∠CCH | 109.5 (11) | – | – |
| $\phi$ | 70 (–) | 180.0 | 670 |

[a] Mijlhoff[6] reports C–C = 1.535 Å and $\phi_g$ = 74.5°, and Butcher[31] $\phi_g$ = 73°, when C–C = 1.51 Å.

All calculations have been carried out on the CYBER 74 computer at the University of Oslo.

## RESULTS

*Equilibrium structure.* An inspection of Table 1 reveals a general good agreement between the calculated and experimental geometries, most of the deviations being smaller than 0.02 Å and 1.0°. Compared with the C–C distance in ethane (1.538

*Table 2.* Atomic net charge.[36]

| | | *anti* | *gauche* |
|---|---|---|---|
| $C_2H_4F_2$ | C | –0.004 | +0.002 |
| | F | –0.409 | –0.404 |
| | H | +0.207 | +0.189 |
| | H′ | +0.207 | +0.213 |
| $C_2H_4Cl_2$ | C | –0.390 | –0.394 |
| | Cl | –0.142 | –0.128 |
| | H | +0.266 | +0.252 |
| | H′ | +0.266 | +0.269 |
| $C_2H_4(CN)_2$ | C | –0.297 | –0.306 |
| | C(N) | –0.027 | –0.009 |
| | N | –0.258 | –0.261 |
| | H | +0.291 | +0.284 |
| | H′ | +0.291 | +0.292 |

*Table 3.* Estimated force constants (stretch in mdyn $Å^{-1}$, bend and torsion in mdyn Å $rad^{-2}$) as obtained from normal coordinate analysis (Exp) and minimizing the *ab initio* energy as a function of the geometry (Calc).

| | | Exp. | Calc. |
|---|---|---|---|
| $C_2H_4F_2$ | $f_{C-C}$ | 4.0[9] | 4.62 |
| | $f_{C-F}$ | 5.15 | 7.11 |
| | $f_{CCF}$ | 1.21 | a:1.82<br>g:1.57 |
| | $f_{CCH}$ | 0.70 | a:1.57<br>g:1.48 |
| | $f_{\tau,g}$ | 0.13 | 0.12 |
| $C_2H_4Cl_2$ | $f_{C-Cl}$ | 3.18[35] | a:2.35<br>g:4.70 |
| | $f_{\tau,g}$ | 0.253[13] | 0.17 |
| $C_2H_4(CN)_2$ | $f_{C-C}$ | 4.62[15] | 4.79 |
| | $f_{C-CN}$ | 5.47 | 5.27 |
| | $f_{CCC}$ | 1.09 | 1.72 |
| | $f_{\tau,g}$ | 0.12 | 0.17 |

Å[22]) the experimentally observed trend is reproduced in these calculations, giving a shorter C−C bond upon fluorination, a longer upon substitution with larger groups (*e.g.* CN).

Because of the large number of basis functions used for dichloroethane, only the C−Cl distance has been varied in addition to the torsional angle ($\phi_g$). The optimal geometries have been obtained from the minima in the assumed parabolic potential surfaces (Tables 5−7). The energies were recalculated for these optimized sets to confirm the minima.

Comparison between the parameters in *anti* and *gauche* reveals no important structural changes, although a slight shortening in the C−C distance together with an opening of the CCF angle when going from *anti* to *gauche* is seen for difluoroethane.

Also the atomic net charges (Table 2) show only minor changes between the conformers, although there is a small flow of electrons to the hydrogen opposing the substituent as going from *anti* to *gauche*, most prominently in difluoroethane.

The obtained force constants are given in Table 3. Except for $f_{C-F}$ the agreement with those obtained from normal coordinate analysis is remarkable, especially when considering the rather limited geometry optimization that has been done.

*1,2-Difluoroethane.* Inclusion of *d*-orbitals (Tables 4 and 8) leads to an even larger discrepancy between calculated and observed conformational energy difference (*i.e.* favouring *anti* even more). Only a (7,3) primitive set has been used, and *d*-orbitals have only been added for fluorine, since previous experience[23−26] indicates that an enlargement of the primitive set does not change the results significantly, and that polarization functions are of importance mainly for atoms with lone pairs.

This is in contradiction of the results for 1,2-difluoroethene, which may be explained by a superposition error in the basis set used by Binkley and

*Table 4.* Energies (kcal mol$^{-1}$) for different torsional angles $\phi$ (°), given relatively to *anti* ($\phi$ = 180°), rigid rotation. Parameters as given in Table 1, ED.

| | $E_{anti}$ (a.u.) | | | | | | |
|---|---|---|---|---|---|---|---|
| $C_2H_4F_2$ | | $\phi_g$ | 60 | 65 | 69.4 | 75 | 90 |
| | −276.51045 | $E$ | 1.27 | 0.92 | 0.75 | 0.69 | 1.32 |
| | −276.55289 | $E^d$ | | | | 0.95 | |
| $C_2H_4Cl_2$ | | $\phi_g$ | 70 | 71.8 | 70.5$^d$ | 75.5 | 80 |
| | −996.56618 | $E$ | 2.40 | 2.38 | | 2.44 | 2.65 |
| | −996.62067 | $E^d$ | 2.32 | | 2.31 | 2.41 | 2.66 |
| $C_2H_4(CN)_2$ | | $\phi_g$ | 60 | 65 | 67 | 70 | 80 |
| | −262.35204 | $E$ | 0.64 | 0.48 | 0.47 | 0.50 | 1.00 |

[d] including *d*-orbitals on halogen.

*Table 5.* $C_2H_4F_2$. Energies (kcal mol$^{-1}$) given relatively to the energy of the corresponding experimental model (Table 1) in *anti* and *gauche* respectively, $\phi_g$ = 75.0°.

| C−C/∠CCF | $E_{anti}$ | $E_{gauche}$ | C−F | $E_{anti}$ | $E_{gauche}$ | ∠CCH | $E_{anti}$ | $E_{gauche}$ |
|---|---|---|---|---|---|---|---|---|
| 1.465/110.3 | 0.671 | 0.445 | 1.349 | 2.698 | 2.900 | 106.6 | 1.951 | 1.405 |
| 1.505/110.3 | 0 | 0 | 1.389 | 0 | 0 | 110.6 | 0 | 0 |
| 1.545/110.3 | 0.439 | 0.621 | 1.429 | 0.577 | 0.370 | 114.6 | 2.459 | 2.748 |
| 1.505/106.0 | −0.514 | | | | | | | |
| 1.505/114.0 | 2.811 | | | | | | | |
| 1.545/106.0 | −0.238 | | | | | | | |
| 1.505/106.3 | | 0.696 | | | | | | |
| 1.505/114.3 | | 1.500 | | | | | | |
| 1.465/106.3 | | 1.430 | | | | | | |

*Table 6.* $C_2H_4Cl_2$. Energies (kcal mol$^{-1}$) given relatively to the energy of the corresponding experimental model (Table 1) in *anti* and *gauche* respectively, $\phi_g = 70.5°$.

| C−Cl | $E_{anti}$ | $E_{gauche}$ |
|---|---|---|
| 1.79 | 0 | 0 |
| 1.83 | −0.122 | −0.038 |
| 1.813 | −0.199 | |
| 1.811 | | −0.286 |

Pople.[12] The superposition error in the present investigation has been estimated. HF and $F^-$ have been used as test molecules, adding an empty basis set identical to that of fluorine, but with no charge on the nucleus, at an F···F distance corresponding to that in *gauche* and *anti* difluoroethane, respectively. The *gauche*-like form was favoured with 0.08 and 0.2 kcal mol$^{-1}$, respectively. This indicates that with the basis used here, the superposition effect is negligible. The effect may, however, be of greater importance when the core electrons are less well described, and may therefore explain why Binkley and Pople[12] obtained a result for difluoroethene in better agreement with the experiment.

The reasons for the apparent discrepancies have therefore to be sought in the Hartree-Fock theory itself. As experienced by Roos[27,28] and others the neglect of correlation energy in different isomers may introduce an error in the calculated energy difference of as much as 3 kcal mol$^{-1}$, disfavouring the form where correlated electron motion (*i.e.* dispersion forces) seems to be of some importance. Although in general the correlation energy is believed to cancel out when conformational energy differences are calculated,[29,30] in the case of difluoroethane *gauche* seems to be favoured by ~2 kcal mol$^{-1}$ due to this difference (see Table 8). This is the same amount that Roos *et al.*[27] found stabilized the $F-H_2O^-$ system, which may be considered as an upper limit.

The calculated torsional angle $\phi_g = 75.0°$ is somewhat larger than the observed values, and may also indicate that the repulsion between the F atoms in *gauche* is overemphasized.

*1,2-Dichloroethane.* Even for this more electron-rich compound inclusion of *d*-orbitals only leads to a minor shift in the estimated torsional angle (Table 4) and the energy difference remains essentially unchanged.

A graphical plot of the calculated energies as a function of $\phi_g$, indicates that inclusion of *d*-orbitals makes the potential curve sharper, but does not change the minimum position. It was felt appropriate, therefore, to include *d*-orbitals on the Cl

*Table 7.* $C_2H_4(CN)_2$. Energies (kcal mol$^{-1}$) given relatively to the energy of the corresponding experimental model (Table 1) in *anti* and *gauche* respectively, $\phi_g = 67.0°$.

| C−C/∠CCC | $E_{anti}$ | $E_{gauche}$ | C−CN | $E_{anti}$ | $E_{gauche}$ |
|---|---|---|---|---|---|
| 1.491/111.0 | 1.157 | 1.162 | 1.434 | 0.618 | 0.683 |
| 1.531/111.0 | 0 | 0 | 1.474 | | 0 |
| 1.571/111.0 | −0.053 | −0.042 | 1.514 | [illegible] | 1.746 |
| 1.531/107.0 | 1.241 | 1.769 | | | |
| 1.531/115.0 | 1.168 | 0.601 | | | |
| 1.571/115.0 | 1.428 | 0.920 | | | |

*Table 8.* Conformational energy differences $\Delta E = E_g - E_a$ (kcal mol$^{-1}$), optimal geometries as given in Table 1, calculated and observed dipole moments, $\mu$(D), and bond moments, $\mu_{C-X}$(D).

| | $E_{anti}$ | $\phi_g$ | $\Delta E$ | $\Delta E^{exp\,b}$ | $\mu_g$ | $\mu^{exp\,c}$ | $\mu_{C-X}$ | $\mu_{C-X}^{exp}$ |
|---|---|---|---|---|---|---|---|---|
| $C_2H_4F_2$ | −276.51187 | 75.0 | 1.32 | −0.59−1.42 | 3.35 | 2.67[32] | 2.24 | 1.86[34] |
| $C_2H_4Cl_2$ | −996.62099 | 70.5 | 2.32[a] | 1.05 | 3.14 | 1.18[33] | 2.03 | 2.03[33] |
| $C_2H_4(CN)_2$ | −262.35246 | 67.0 | 0.48 | ~2.5 | 5.77 | 3.48[33] | 3.73 | 4.03[33] |

[a] With *d*-orbitals on Cl. [b] The difference in zero point vibrational energy between the two conformers is approximately 0.2 kcal mol$^{-1}$, therefore $\Delta E \approx \Delta E^{exp}$. [c] Given at appropriate temperatures, that is 25(?), 35 and 170 °C, respectively.

atoms in the remaining calculations.

Table 8 reveals a discrepancy between the observed and calculated conformational energy differences, the *ab initio* method again favouring *anti* too much. If contributed to the difference in correlation energy, it means that this difference must be $\sim 1.3$ kcal mol$^{-1}$ in favour of *gauche*.

The calculated torsional angle $\phi_g = 70.5°$ is somewhat smaller than the observed value.

*1,2-Dicyanoethane.* These calculations agree with the energy difference and torsional angle estimated from the previously reported torsional potential.[43] The energy difference between *gauche* and *anti* remains unchanged when essential parts of the geometry are optimized (Tables 4 and 8). But, contrary to the results for difluoro and dichloroethane the calculated energy difference is too small. The experimental value is very uncertain, but is definitely not smaller than 1.5 kcal mol$^{-1}$.[15] Although *d*-orbitals have not been included in this case, the previous results of this investigation indicate that inclusion of polarization functions may improve the results by about 0.3 kcal mol$^{-1}$.

## DISCUSSION

Although a general trend is hard to find, the present calculations on 1,2-disubstituted ethanes seem consistent with the assumption that the neglect of correlation energy may cause errors in calculated conformational energy differences, especially when the substituents are easily polarizable, so that dispersion forces may be established between the substituents. This attractive force must be in the order of 1 kcal mol$^{-1}$ for dihaloethanes. Such attractions between halogens fit the earlier observations on 2,2′-dihalobiphenyls,[5,38,39] and 1,3-dihalopropanes,[40,41] and were also proposed earlier by Abraham for 1,2-difluoroethane.[7]

Why the discrepancy appears larger in difluoroethane than in dichloroethane, and why the energy difference is too small in dicyanoethane is not easily understood, but may be connected with the estimate of the dipole moments, and thereby with the set of basis functions applied. The discrepancies between the experimental and calculated $C-X$ bond vectors are consistent with an error in the calculated energy differences of about $-0.4$ kcal mol$^{-1}$ for difluoroethane and 0.2 kcal mol$^{-1}$ for dicyanoethane due to dipole/dipole repulsions.[37]

This is also consistent with the somewhat too large calculated $\phi_g$ for difluoroethane. Although the effect is too small to account for the error in $\Delta E$ for dicyanoethane, it seems reasonable that the apparent difference in correlation energy between difluoro- and dichloro-ethane, is due to a somewhat too large estimate of the calculated $C-F$ bond vector.

The difference in correlation energy seems negligible in dicyanoethane. While each halogen has three lone pairs, which may interact in *gauche*, the electrons on C(N) are mainly localized on the "backside", in the triple bond to nitrogen, and therefore not so easily polarized by the other $-C\equiv N$ group in *gauche*. The lone pairs on N are too far apart to get in van der Waals' contact with each other.

If one expands the torsional potential as a Fourier series, terminated after the third term $[V(\phi)=\frac{1}{2}\sum_{n=1}^{3} V_n(1+\cos n\,\phi)]$, one can associate the steric and electrostatic repulsions with the $V_1$ term, the electronegativity with the $V_2$ term and bond/bond repulsion with the $V_3$ term.[2] The relative size of $V_1$ to $V_2$ determines whether *gauche* or *anti* is the most stable form. In the case of difluoroethane, where the steric effect is relatively small,[7] the correlation energy makes $V_1$ sufficiently small, and the most stable conformer is *gauche*. For dichloroethane the steric and electrostatic repulsions dominate. Even though approximately the same correlation effect is found, $V_1$ is dominating and *anti* is the most stable conformer.

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