

# Near-Hartree–Fock Calculations on the Ground State of the Fluoronium Ion, $\text{FH}_2^+$

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SCF wavefunctions have been calculated for the ground state of the fluoronium ion using a variety of contracted gaussian basis sets, ranging from a DZ,  $\{4s2p/2s\}$ , to a near-Hartree–Fock quality basis of  $\{6s5p2d1f/3s2p\}$ . The total energy obtained from the latter is  $-100.265\ 268$  hartree, estimated to be  $0.002 \pm 0.001$  hartree within its Hartree–Fock limit. Equilibrium geometry parameters, energy inversion barriers, harmonic force constants, proton affinities and a few one-electron properties have also been computed.

The fluoronium ion,  $\text{FH}_2^+$ , is isoprotic and isoelectronic with  $\text{H}_2\text{O}$  and it is only natural that it has been proposed as early as 1927 by Hantzsch<sup>1</sup> in the non-aqueous hydrofluoric acid solvent system in an attempt to explain the formation of complexes such as  $\text{FH}_2^+ \cdot \text{ClO}_4^-$ . Since then, it was postulated most frequently<sup>2–5</sup> but its direct existence was not proved until 1972 when Couzi *et al.*<sup>6</sup> reported its infrared spectrum. The analysis of the latter revealed a bent configuration, but its exact geometrical parameters were not determined.

The fluoronium ion has also been studied theoretically by *ab initio* techniques, mostly at the SCF level<sup>7–21</sup> and with a variety of basis sets, ranging from STO-3G<sup>19</sup> to rather extended basis.<sup>11,12</sup> Most of the pertinent results for  $\text{FH}_2^+$  obtained from non-empirical SCF calculations are condensed in table 1. The best calculation reported so far at the Hartree–Fock level, is that of Lischka<sup>11</sup> with an energy of  $0.007–0.009$  hartree above the estimated Hartree–Fock limit (*vide infra*) and with rather limited information for the  $\text{FH}_2^+$  ion.

We feel that the ten-electron “water-like” molecule of fluoronium ion deserves a more thorough examination, and the present report is an effort toward this purpose. We report the results of a systematic series of Hartree–Fock calculations of the ground  $^1A_1$  state of  $\text{FH}_2^+$  using contracted gaussian basis sets, ranging from  $\{4s2p/2s\}$  to  $\{6s5p2d1f/3s2p\}$ . Wavefunctions, energies, Koopmans’ ionization potentials, equilibrium geometry parameters, harmonic force constants and a limited number of one-electron properties have been computed.

## METHOD AND COMPUTATIONAL DETAILS

Most of the Restricted Hartree–Fock (RHF) wavefunctions used in this study were constructed using the POLYATOM SCF routines<sup>22</sup> and the BIGGMOLI integral program of Raffanetti<sup>23</sup> as implemented at Michigan State University. Those

TABLE 1.—ENERGY VALUES, BOND DISTANCES, ANGLES, PROTON AFFINITIES AND ENERGY INVERSION BARRIERS OF  $\text{FH}_2^+$ 

ref.	$E^a$ /hartree	$R(\text{F—H})^b$ /bohr	$\theta/^\circ$	$A_p^c$ /kJ mol <sup>-1</sup>	$E_{\text{IB}}^d$ /kJ mol <sup>-1</sup>
19	-98.864 11	1.840	112.0	-771.4	112.1
9, 21	-100.077 87	1.831	125.5	-500.4	—
13	-100.197 82	1.818	113.9	-511.7	—
16	-100.201 97	—	—	-444.4	—
15	-100.218 16	1.812	127.2	-491.7	32
18	-100.229 54	1.803	120.4	-503.2	42.9
14	-100.242 40	1.818 <sup>e</sup>	113.9 <sup>e</sup>	-516.0	—
10	-100.247 78	1.795	114.75	-502.8	—
12	-100.258 38	1.781	116.0	-509.3	—
11	-100.261 2	1.81 <sup>f</sup>	113.0 <sup>f</sup>	-512.9 <sup>g</sup>	—

<sup>a</sup> 1 hartree = 27.211 608 eV = 627.09 kcal mol<sup>-1</sup> = 2625.5 kJ mol<sup>-1</sup>;

<sup>b</sup> 1 bohr = 0.529 177 × 10<sup>-10</sup> m; <sup>c</sup> proton affinity; <sup>d</sup> (energy) inversion barrier; <sup>e</sup> assumed from ref. (13); <sup>f</sup> obtained from basis (A) of ref. (11); <sup>g</sup> obtained from basis (B) of ref. (11).

calculations involving  $f$  functions were carried out at the Argonne National Laboratory using the Argonne version of BIGGMOLI and the SCF capabilities of GVB TWO. Table 2 shows the basis sets used and their contractions. All contractions were according to Raffanetti's generalized contraction scheme.<sup>24</sup> Basis sets (A) and (B) were taken from Huzinaga's tables,<sup>25</sup> the ( $s, p$ ) parts of bases (C)–(G) from van Duijneveldt's compilation,<sup>26</sup> the three  $d$  and the two  $p$  component functions for the F and H atoms of basis (F) and (G) are those of Dunning,<sup>27</sup> the hydrogen  $s$  functions are those of Huzinaga.<sup>28</sup> They were scaled by semioptimized scale factors of 1.30, 1.30 and 1.10 for the basis sets (A), (B) and (C), respectively. The scale factors were optimized at geometries within 0.01 bohr of the F—H bond and 2° of the internuclear angle, from the corresponding equilibrium geometries for these basis sets. For the basis sets (D), (D') and (E) the scale factor for the hydrogen  $s$  functions was fixed to 1.10 and the exponents for the  $p$  functions on H and  $d$  functions on F were set equal to 1.0. For the set (F) the hydrogen  $s$  and  $p$  functions were scaled with 1.10 and 1.70, respectively, and the fluorine  $d$  functions with 2.30. The 1.70 and 2.30 values are the result of a semioptimization at a geometry of 1.78 bohr for the bond length and 116° for the internuclear angle. For the basis set (G) the exponent of the  $f$  functions was arbitrarily set equal to 1.0 and all other

TABLE 2.—BASIS SETS USED IN THE PRESENT STUDY

primitive set	contracted set	number of contracted gaussian functions	
(9s5p/4s)	{4s2p/2s}	14	(A)
(10s6p/5s)	{5s3p/3s}	20	(B)
(12s6p/6s)	{6s4p/3s}	24	(C)
(12s7p/6s)	{6s4p/3s}	24	(D)
(12s7p/6s)	{6s5p/3s}	27	(D')
(12s7p1d/6s1p)	{6s5p1d/3s1p}	39	(E)
(12s7p3d/6s2p)	{6s5p2d/3s2p}	51	(F)
(12s7p3d1f/6s2p)	{6s5p2d1f/3s2p}	61	(G)

scale factors were as in (F). Notice that, owing to the nature of gaussian functions, the six  $d$  gaussians will form linear combinations which correspond to the traditionally accepted  $3d$  atomic orbitals and one  $3s$  atomic orbital. Similarly, the ten  $f$ -type gaussians will produce seven  $4f$  atomic orbitals and three  $4p$  atomic orbitals. No attempt was made to separate the gaussians into the more traditional forms.

## ENERGIES AND GEOMETRIES

Total energies, geometrical parameters [bond length  $R(\text{F}-\text{H})$  and the apex angle  $\theta$ ], and virial ratios ( $-V/T$ ) obtained from RHF calculations on the ground  $^1A_1$  state of  $\text{FH}_2^+$ , and for all basis sets (A)–(G), are given in table 3. The total energies of calculations (F) and (G) are 0.0028 and 0.0041 hartree lower than that of ref. (11), the best (up to now) SCF calculation on  $\text{FH}_2^+$ .

For a system of the type  $\text{XH}_2$ , where X can be any element from the collection B, C, N, O or F, we can divide its Hartree–Fock space into two parts: a fundamental ( $sp/s$ ) part and a remaining part which we can call “polarization space” with its components being functions of symmetry ( $dfgh\cdots/pdf\cdots$ ). Of course, the sum of the two parts is complete, *i.e.* gives the complete Hartree–Fock space for the corresponding molecular system and its properties. In practice, for systems composed of hydrogen and second-row atoms the polarization space is often truncated to one set of  $d$  functions on the heavy atom or  $d$  functions on the heavy atom and  $p$  functions on the H atom. The total energy decreases monotonically as functions of higher symmetry are added, with the  $d$  contributing more than the  $f$  functions and the  $g$  being less effective than the  $f$  functions, and so on.<sup>29,30</sup> However, it is important to saturate the fundamental space, the ( $sp/s$ ) space in the present case, before polarization  $d$  functions are added. Otherwise, the polarization functions will try to make up for the missing ( $sp/s$ ) part, and they can produce spurious results for molecular properties. It is also advisable to saturate the ( $d/p$ ) part of the polarization space before moving to its higher parts ( $f$ ) or ( $f/d$ ). From table 3, and using the total energy  $E$  as our basic criterion for the completeness of the different expansions, it can be seen that certainly the ( $sp/s$ ) space was saturated before adding the ( $d/p$ ) polarization space, and we can be reasonably confident that the latter has for all practical purposes been saturated before adding the  $f$  functions on the F atom. From the same table we also observe the well-known

TABLE 3.—ENERGIES, BOND DISTANCES, ANGLES, VIRIAL RATIOS, INVERSION BARRIERS AND PROTON AFFINITIES OF  $\text{FH}_2^+$

basis set	$E/\text{hartree}$	$R(\text{F}-\text{H})/\text{bohr}$	$\theta/^\circ$	$-V/T$	$R(\text{F}-\text{H})^a/\text{bohr}$	$E_{\text{IB}}/\text{kJ mol}^{-1}$	$A_{\text{P}}/\text{kJ mol}^{-1}$
(A)	-100.210 070	1.806	127.1	1.998 62	1.814	28.8	-487.8
(B)	-100.222 910	1.811	126.2	2.000 40	1.806	31.4	-489.4
(C)	-100.226 907	1.807	126.6	2.000 11	1.809	31.5	-491.5
(D)	-100.227 766	1.807 <sup>b</sup>	126.6 <sup>b</sup>	2.000 16	—	—	-489.4
(D')	-100.227 929	1.807	126.7	2.000 08	1.808	31.1	-489.4
(E)	-100.260 196	1.783	116.1	2.000 02	1.789	65.8	-512.0
(F)	-100.263 983	1.781	114.68	2.000 08	1.786	73.0	-513.7
(G)	-100.265 268	1.781 <sup>c</sup>	114.68 <sup>c</sup>	—	1.786 <sup>c</sup>	68.5	-515.0

<sup>a</sup> Optimum bond length of  $\text{FH}_2^+$  in the  $|^1\Sigma_g^+$  state, symmetry  $D_{\infty h}$ . <sup>b</sup> No geometry optimization was done; assumed from basis (C). <sup>c</sup> Assumed from basis (F).

effect, at least in neutral and positively charged species, of bond length shortening as the basis set size increases approaching its Hartree-Fock limit.<sup>31,32</sup>

#### ENERGY INVERSION BARRIERS, PROTON AFFINITIES AND HARTREE-FOCK LIMIT

The energy inversion barrier  $E_{\text{IB}}$  can be defined as the relative energy of the linear optimized structure with respect to the optimized bent structure:

$$E_{\text{IB}} \equiv E(|^1A_1\rangle) - E(|^1\Sigma_g^+\rangle).$$

*Ab initio* calculations of near Hartree-Fock quality for closed-shell systems are capable of producing accurate predictions of  $E_{\text{IB}}$ .<sup>33</sup> The requirement for high-quality SCF calculations is also obvious in the  $\text{FH}_2^+$  system, either from results obtained from the literature and shown in table 1 or from results of the present study and listed in table 3. The  $E_{\text{IB}}$  values shown reveal clearly their basis-set sensitivity, and how critical are the polarization functions, a well-established fact.<sup>33</sup> The 70 kJ mol<sup>-1</sup> value obtained differs significantly from all other values given before and listed in table 1, a fact traced to the inadequacy of previously used basis sets. Going from the bent  $|^1A_1\rangle$  state to the linear  $|^1\Sigma_g^+\rangle$  we observe a slight increase in the F—H bond length of  $\text{FH}_2^+$ , table 3. Note, however, that the scale factors and exponents used in obtaining equilibrium geometries in the linear state were the same as those of the  $|^1A_1\rangle$  state.

Fig. 1 presents the Mulliken-Walsh correlation diagram<sup>34,35</sup> for all five doubly occupied molecular orbitals of the ground  $|^1A_1\rangle$  state of  $\text{FH}_2^+$ , in the basis set (F). The diagram shows the variations of one-electron eigenvalues of the Fock operator with the internuclear angle  $\theta$ ; the F—H bond length was fixed at its equilibrium value of the  $|^1A_1\rangle$  state (1.781 bohr). The general features of this diagram are in general agreement with those estimated by Walsh and a bent configuration is clearly predicted. The  $1b_1$  molecular orbital is perpendicular to the plane of the molecule and it is of pure  $p_x$  symmetry for all internuclear angles. Because of this it would be reasonable to assume that this orbital has nothing to do with the geometry of the  $\text{FH}_2^+$  system, and its energy should remain constant.<sup>35</sup> However, an inspection of fig. 1 shows a significant variation in energy of this orbital, the energy increasing in the direction  $1b_1 \rightarrow 1\pi_u$ . The  $1b_1$  energy variation with the angle  $\theta$  (as well as that of the  $1a_1$  molecular orbital) can be rationalized, according to Buenker and Peyerimhoff,<sup>36,37</sup> as being caused by the electron-repulsion interaction of  $1b_1$  with the other orbitals, the electron repulsion being a function of the angle  $\theta$ . For the role of the  $1b_1$  orbital on the geometry of  $\text{XH}_2$  systems and particularly on  $\text{FH}_2^+$  see also ref. (38).

The proton affinity  $A_p$ , or energy of protonation ("gas basicity") may be defined as the energy difference between the protonated system ( $\text{BH}^+$ ) and the parent molecular system

$$A_p \equiv E(\text{BH}^+) - E(\text{B}).$$

The proton affinities listed in table 3 were calculated according to the definition given above and they are not corrected for nuclear motion. The bond length of the parent species FH was optimized in every basis set but (G) and its energy was computed at the corresponding equilibrium points. The SCF energies of hydrogen fluoride, FH, in the basis sets (F) and (G) are -100.068 447 and -100.069 296 hartree, respectively, while its equilibrium bond length obtained from basis (F) is 1.697 bohr. The above energy values should be contrasted with the best SCF value

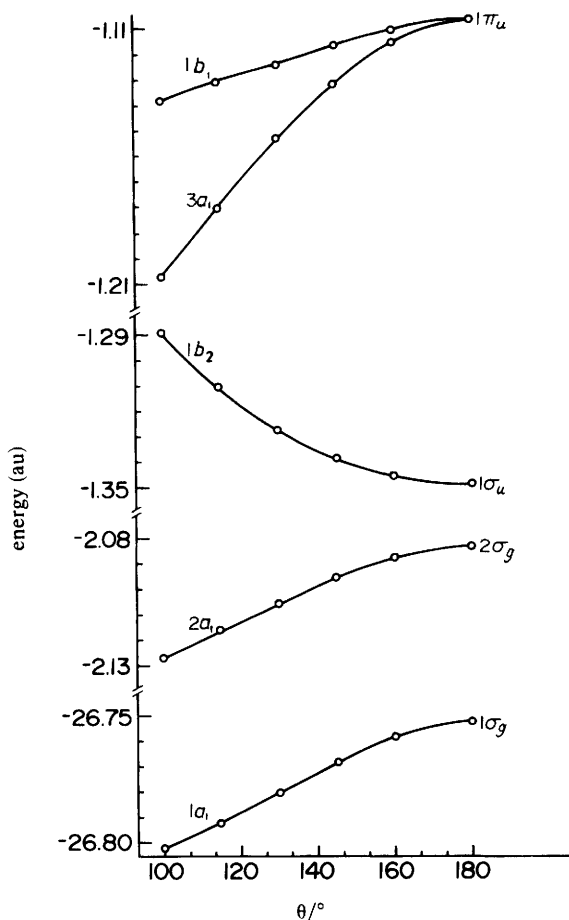


FIG. 1.—Canonical orbital energies of the fluoronium ion as a function of the apex angle; basis set (F).

obtained by McLean and Yoshimine<sup>39</sup> of  $-100.0705$  hartree, an energy which is  $<0.001$  hartree away from its Hartree-Fock limit. From table 4 it can be seen that the proton affinity is a property not very sensitive to basis set size, although values obtained with minimal STO-3G basis overestimate the  $A_p$  of FH by as much as *ca.*  $250 \text{ kJ mol}^{-1}$ .<sup>9,19</sup>

The proton affinity of FH has been determined experimentally by Beauchamp,<sup>40</sup> and his ICR (ion cyclotron resonance) result of  $-469 \pm 8 \text{ kJ mol}^{-1}$  is in relatively good agreement with the best theoretical value of the present study,  $-515 \text{ kJ mol}^{-1}$ . Nevertheless, assuming that correlation effects should not be very significant, owing to the fact that both the parent and the protonated species are isoelectronic, one should expect better agreement between theoretical and experimental results. However, the present theoretical result has not been corrected for nuclear motion. According to the definition of proton affinity given previously we can write

$$A_p \equiv E(\text{FH}_2^+, \text{frozen nuclei}) + E_{\text{vib}}(\text{FH}_2^+, 0 \text{ K}) \\ - \{E(\text{FH}, \text{frozen nuclei}) + E_{\text{vib}}(\text{FH}, 0 \text{ K})\}$$

TABLE 4.—ONE-ELECTRON PROPERTIES OF THE FLUORONIUM ION IN THE HARTREE-FOCK APPROXIMATION. ALL RESULTS ARE IN ATOMIC UNITS (au). ORIGIN AT THE F ATOM.

property	basis sets					
	(A)	(B)	(C)	(D')	(E)	(F)
dipole moment ( $D$ ) <sup>a</sup>	1.128	1.125	1.116	1.115	1.109	1.066
quadrupole moment ( $Q$ ) <sup>b</sup>						
$Q_{xx}$	-2.412	-2.426	-2.415	-2.413	-2.301	-2.288
$Q_{yy}$	3.417	3.404	3.410	3.413	2.722	2.627
$Q_{zz}$	-1.005	-0.978	-0.995	-1.000	-0.421	-0.339
diamagnetic susceptibility ( $\chi^d$ ) <sup>c</sup>						
$\chi^d_{xx}$	-10.439	-10.350	-10.341	-10.336	-10.022	-9.986
$\chi^d_{yy}$	-7.752	-7.694	-7.684	-7.671	-7.559	-7.550
$\chi^d_{zz}$	-7.752	-7.694	-7.684	-7.671	-7.559	-7.550
electric field ( $E$ ) <sup>d</sup> at F						
$E_z$	-0.234	-0.202	-0.148	-0.133	-0.029	-0.027
$E_y$	0.028	0.024	0.022	0.023	0.008	0.008
$E_z$	0.092	0.078	0.075	0.078	0.015	0.005
electric field gradient ( $q$ ) <sup>e</sup>						
$q_{xx}$	2.390	2.534	2.570	2.561	2.554	2.564
$q_{yy}$	-3.037	-3.240	-3.283	-3.276	-2.792	-2.729
$q_{zz}$	0.647	0.686	0.713	0.715	0.238	0.165
$q_{xx}$	0.235	0.227	0.228	0.227	0.230	0.230
$q_{yy}$	-0.325	-0.305	-0.310	-0.309	-0.241	-0.234
$q_{zz}$	0.088	0.078	0.082	0.081	0.010	0.004

<sup>a</sup> 1 au =  $ea_0 = 0.84784 \times 10^{-29}$  C m; note that the dipole moment of a charged species is origin-dependent. <sup>b</sup> 1 au =  $ea_0^2 = 0.44866 \times 10^{-39}$  C m<sup>2</sup>. <sup>c</sup> 1 au =  $e^2 Na_0^3 / 4mc^2 = 1.188012 \times 10^{-5}$  J T<sup>-2</sup> mol<sup>-1</sup>. <sup>d</sup> 1 au =  $ea_0^{-2} = 5.721526 \times 10^4$  C m<sup>-2</sup>. <sup>e</sup> 1 au =  $ea_0^{-3} = 10.812121 \times 10^{11}$  C m<sup>-3</sup>.  $a_0$  is the Bohr radius (= 1 bohr).

where  $E_{\text{vib}}$  is the zero-point nuclear motion. Considering only harmonic vibrational effects as the main source of  $E_{\text{vib}}$ , Pople and Binkley<sup>14</sup> estimated the difference

$$E_{\text{vib}}(\text{FH}_2^+, 0 \text{ K}) - E_{\text{vib}}(\text{FH}, 0 \text{ K}) \approx 25 \text{ kJ mol}^{-1}.$$

This brings the calculated proton affinity down to  $-490 \text{ kJ mol}^{-1}$ , now in respectable agreement with Beauchamp's experimental value.<sup>40</sup>

A proton affinity of  $-395.0 \text{ kJ mol}^{-1}$  has recently been reported by Lee *et al.*<sup>41</sup> using photoionization techniques. Although the discrepancy from Beauchamp's value is very large they did not comment upon their results.

The near Hartree-Fock proton affinity computed here may be used to obtain the energy Hartree-Fock limit of  $\text{FH}_2^+$ . We can write

$$E_{\text{Hartree-Fock}}(\text{FH}_2^+) = E_{\text{Hartree-Fock}}(\text{FH}) + A_{\text{p, Hartree-Fock}}(\text{FH}).$$

It is reasonable to assume that the proton affinity computed in the present study will not change significantly by further extending the basis set. For the term  $E_{\text{Hartree-Fock}}(\text{FH})$  the McLean-Yoshimine<sup>39</sup> result can be used, which is 0.001 hartree within the Hartree-Fock limit. Therefore

$$\begin{aligned} E_{\text{SCF}}(\text{FH}_2^+) &= -100.0705 \text{ hartree} - 515 \text{ kJ mol}^{-1} \\ &= -100.267 \text{ hartree} \end{aligned}$$

or

$$E_{\text{Hartree-Fock}}(\text{FH}_2^+) \approx -100.267 \pm 0.001 \text{ hartree}$$

Pople and Binkley<sup>14</sup> estimated the Hartree-Fock limit to be  $-100.270$  hartree.

A Mulliken population analysis<sup>42,43</sup> on  $\text{FH}_2^+$  and FH employing the basis set (F) gives gross total charges for the fluorine atom of  $-0.051$  and  $-0.390$ , respectively. Notwithstanding the well-known drawbacks of the method and its basis-set sensitivity<sup>43</sup> the following qualitative conclusion may be inferred: as a proton,  $\text{H}^+$ , approaches the molecule FH, its positive charge simply cancels the negative charge on the F atom, or  $0.40e$  are transferred from F to  $\text{H}^+$  leaving the F atom almost neutral and the overlap distribution undisturbed. A previous population analysis<sup>15</sup> assigns gross total charges on F and H atoms of  $-0.30$  and  $+0.65e$ , respectively.

#### FORCE CONSTANTS AND ONE-ELECTRON PROPERTIES

In order to determine the force constants of the totally symmetric vibrations, nine points on the two-dimensional energy surface were calculated with the basis set (F). The previously determined equilibrium geometry of  $1.781$  bohr and  $114.68^\circ$  was surrounded by a fine nine-point grid with bond ( $\Delta R$ ) and angle ( $\Delta\theta$ ) displacements of  $\pm 0.03$  bohr and  $\pm 3^\circ$ , respectively. We can hope that these values correspond to the mean displacement in the ground vibrational state.

The potential-energy surface for a non-linear triatomic molecule of the type  $\text{XH}_2$  in the harmonic approximation is given by the general expression<sup>44</sup>

$$\begin{aligned} E(\Delta R_1, \Delta R_2, \Delta\theta) &= E(000) + 1/2 K_{R^2}(\Delta R_1^2 + \Delta R_2^2) \\ &\quad + \frac{1}{2} K_{\theta^2}(\mathcal{R}_e \Delta\theta)^2 + K_{R\theta}(\Delta R_1 + \Delta R_2)(\mathcal{R}_e \Delta\theta) + K_{R_1 R_2} \Delta R_1 \Delta R_2 \end{aligned}$$

where  $K_{R^2}$  is the force constant of the F-H bonds,  $K_{\theta^2}$  is the angular force constant,  $K_{R\theta}$  is the bond-angle interaction constant and  $K_{R_1 R_2}$  is the interaction constant of the two F-H bonds. The nine energy points calculated are sufficient to determine the three force constants  $K_{R^2}$ ,  $K_{\theta^2}$  and  $K_{R\theta}$ . The following results were obtained:

$K_{R^2} = 8.298 \times 10^2 \text{ N m}^{-1}$ ,  $K_{\theta^2} = 0.638 \times 10^2 \text{ N m}^{-1}$  and  $K_{R\theta} = 0.070 \times 10^2 \text{ N m}^{-1}$ . Previously published results by Lischka<sup>11</sup> and Wild *et al.*<sup>15</sup> are as follows

$$K_{R^2} = 8.227 \times 10^2, \quad K_{\theta^2} = 0.549 \times 10^2, \quad K_{R\theta} = 0.061 \times 10^2 \text{ N m}^{-1} \quad (\text{Lischka})$$

$$K_{R^2} = 6.97 \times 10^2, \quad K_{\theta^2} = 0.463 \times 10^2, \quad K_{R\theta} = 0.050 \times 10^2 \text{ N m}^{-1} \quad (\text{Wild}).$$

Finally, table 4 lists some one-electron properties of the  $\text{FH}_2^+$  molecule computed in all basis sets but (G). The origin was taken as the F atom. Note that even the simplest of moments, the dipole moment, is origin-dependent in a charged species. As far as we know one-electron properties for the  $\text{FH}_2^+$  have not been published before, therefore a comparison is not possible. However, we admit that such results are of limited value owing to the known shortcomings of the Hartree-Fock method. In addition, the complete lack of experimental results caused by the obvious difficulties of measuring properties of charged species makes contact with "reality" impossible. However, we can attempt a comparison with the isoelectronic water molecule. Dunning *et al.*,<sup>45</sup> using an  $(11s7p2d/5s1p)$  gaussian set contracted to  $\{6s5p2d/3s1p\}$  that is quite similar to our (F) basis, predicted the water dipole moment to be 0.799 au as compared with an experimental value of 0.728 au.<sup>46</sup> Our result of 1.066 au (with respect to the F atom as origin) is fairly close to the corresponding water result, implying an analogous charge distribution. Taking the analogy a little further we can propose an "experimental" dipole moment for  $\text{FH}_2^+$  of 1.0 au.

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