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Molecular Properties of Excited Electronic States: The $\tilde{a}\ ^3A''$ and $\tilde{A}\ ^1A''$ States of Formaldehyde

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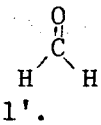
ABSTRACT

Ab initio self-consistent-field wave functions and molecular properties have been calculated for the three lowest electronic states of H_2CO. For the ground state, a variety of basis sets were used, the largest being an uncontracted gaussian basis: C(11s 7p 2d), O(11s 7p 2d), H(6s 1p). For the excited states the above basis was contracted to C(7s 5p 2d), O(7s 5p 2d), H(4s 1p). Ground state molecular properties agree well with the earlier theoretical study of Neumann and Moskowitz, and with available experimental data. The z components (along the CO bond axis) of the excited state dipole moments have been measured, and the present *a priori* predictions reproduce experiment rather closely. Other properties reported include quadrupole moments, octupole moments, and electric field gradients.

INTRODUCTION

One of the most important recent trends in chemical physics has been the development of new experimental and theoretical methods for studying the excited electronic states of molecules.[1] Since excited state properties are often strikingly different from their ground state counterparts, the results of experiments on excited states sometimes force us to reevaluate our thoughts concerning the nature of molecular structure and properties.

As one of the earliest studied examples, consider the lowest two excited states of formaldehyde. For reference, we note the planar C_{2v} structure[2] of the ground state,  , with r(CO) = 1.208 Å, r(CH) = 1.116 Å, θ(HCH) = 116° 31'. The electron configuration for the $^1A_1$ ground state may be written[3]

$$1a_1^2\ 2a_1^2\ 3a_1^2\ 4a_1^2\ 1b_2^2\ 5a_1^2\ 1b_1^2\ 2b_2^2 \qquad (1)$$

In both excited states, the geometries are quite different;[3-5] in fact both are nonplanar, with the methylene group tilted out of the plane defined by the ground state molecular structure. For the lowest triplet state, this out of plane angle is ∿ 35°, while it is ∿ 31° for the first excited singlet state.[3] Although these two states would be labeled $^3A_2$ and $^1A_2$ if they retained the ground state's C_{2v} equilibrium geometry, these labels are not appropriate since only a plane of symmetry is retained. Hence the states are properly designated $\tilde{a}\ ^3A''$ and $\tilde{A}\ ^1A''$ and both arise from the electron configuration

$$1a'^2\ 2a'^2\ 3a'^2\ 4a'^2\ 1a''^2\ 5a'^2\ 6a'^2\ 2a''\ 7a' \qquad (2)$$

Note that the half-filled $2a''$ and $7a'$ orbitals correlate with the C_{2v} orbitals $2b_2$ and $2b_1$, the latter being unoccupied in the ground state. Finally, it should be mentioned that the CO distance in the two excited states is more than 0.1 Å longer than for the ground state: $\tilde{a}$ 1.312 Å, $\tilde{A}$ 1.323 Å.

The above example illustrates some of the interesting relationships that have been established between ground and excited state molecular geometries. For other properties, however, less is known about excited states. For example, there are only a small number of polyatomic molecules for which excited state electric dipole moments have been measured. Again, one of the systems for which experiments have been possible is the $\tilde{A}\ ^1A''$ state of H_2CO. There Freeman and Klemperer[6a] have obtained $\mu_z = 1.56 \pm 0.07$ debyes from the Stark effect of the near-ultraviolet absorption spectrum. For comparison, the $^1A_1$ ground state dipole moment[7] is 2.323 ± 0.015 debye, or 0.76 ± 0.09 debye larger than the excited state value. In addition Buckingham, Ramsay, and Tyrrell[6b] have measured μ_z for the $\tilde{a}$ state and obtained 1.29 ± 0.03 debye.

The purpose of the present paper is to report near Hartree-Fock values of several molecular properties of the $\tilde{a}$ and $\tilde{A}$ states of formaldehyde. In addition to the dipole moment, known experimentally for both states, we report a number of properties (e.g. molecular quadrupole moments and electric field gradients) which are of interest but very difficult to measure for excited

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electronic states. To evaluate the reliability of the predicted properties, the ground state H_2CO properties have also been calculated using a variety of basis sets.

Basis Sets and Geometries

Four basis sets were used in the present work. They have been labeled A, B, C, and D. In each case analogous basis sets were used for C and O.

A. C,O(9s 5p 1d/5s 3p 1d), H(5s 1p/3s 1p).

Here the primitive gaussian basis sets of Huzinaga[8] have been contracted following Dunning's recommendations.[9] Each of the hydrogen gaussian exponents α was multiplied by a scale factor of $(1.2)^2 = 1.44$. The carbon and oxygen d functions were assigned[10] $\alpha = 0.8$, and the hydrogen p functions $\alpha = 1.0$.

B. C,O(10s 6p 1d/6s 4p 1d), H(6s 1p/4s 1p).

This basis was assembled in an analogous fashion, except that the hydrogen primitive s set was taken from van Duijneveldt[11] and contracted (3111), with the three highest exponents grouped together.

C. C,O(11s 7p 2d/7s 5p 2d), H(6s 1p/4s 1p).

The C and O primitive basis sets of van Duijneveldt[11] were contracted to provide maximum flexibility in the valence region. The d exponents chosen were $\alpha = 2.0$ and 0.5. The hydrogen basis was identical to B.

D. Same as C., but completely uncontracted.

In the next section we will be referring to the earlier theoretical studies of Dunning, Winter, and McKoy[12] (hereafter designated DWM) and Neumann and Moskowitz[13] (NM). Therefore, it should be noted that DWM used an uncontracted C,O(9s 5p),

H(3s) basis, while NM employed a C,O(10s 5p 2d/5s 3p 2d), H(4s 1p/2s 1p) set.

For the ground state, the experimental geometry of Oka[2] was adopted. For the excited states, we used the geometries recommended by Herzberg.[3] In addition to the parameter given in our introduction, we assumed r(CH) = 1.09 Å and θ(HCH) = 119° for both $\tilde{a}$ and $\tilde{A}$ states. The molecular plane (for the ground state) was taken to be the xz plane, with the CO bond coincident with the z axis.

Energy Results

The energy quantities obtained in the present research are summarized in Table I.

The best previously reported ground state SCF energy for H_2CO is that of Neumann and Moskowitz (NM),[13] -113.8917 hartrees. The geometry chosen for the present work was identical to that of NM, and Table I shows that our calculations A, B, and C represent successive improvements on the NM total energy.

Calculations were also carried out for a second (nearby) geometry, that used by Dunning, Winter, and McKoy (DWM):[12] r(CO) = 1.21 Å, r(CH) = 1.12 Å, θ(HCH) = 118°. The energy obtained by DWM was -113.8334 hartrees, whereas the present basis sets yielded -113.89883 (A), -113.90741(B), -113.91439 (C), and -113.91455(D). Note that the final result (basis set D) employed the large uncontracted basis set. Comparison of results C and D at this second geometry indicates the

magnitude of the small contraction error in basis C, namely 0.00016 hartree.

The basis D atomic SCF energies obtained by van Duijneveldt[11] were C(-37.68820 hartrees), O(-74.80849 hartrees), and H(-0.49995 hartrees). These may be compared with the estimated[10] Hartree-Fock energies (-37.6886, -74.8094, and -0.5 hartrees, respectively) to yield an SCF error of $\sim$ 0.0013 hartrees for the separated atoms, basis set D. The other principle deficiency in our H_2CO basis is the lack of additional polarization functions. Based on the H_2O study of Clementi and Popkie[14] using even larger basis sets, it is possible that this additional error could be as large as 0.008 hartrees. In any case, it seems very unlikely that the present basis set C results yield total energies more than 0.01 hartrees above the exact Hartree-Fock energies. Thus we estimate the Hartree-Fock energy of ground state H_2CO at its equilibrium geometry[2] to be not lower than -113.925 hartrees. This result is significantly higher than the semi-empirically predicted Hartree-Fock energy, -114.0309 hartrees, of Hollister and Sinanoglu.[15]

Since all three basis sets yield SCF energies lower than any previously reported, it is not too surprising that the orbital energies obtained are very similar. Since basis A is small enough to be used for considerably larger molecules, we note the differences $\varepsilon(A) - \varepsilon(C)$: -0.0007, +0.0009, +0.0001, +0.0013, +0.0007, +0.0028, +0.0016, and +0.0015 hartrees. It is seen that except for the oxygen core orbital, the larger

basis set lowers the orbital energies. The largest difference, for the $5a_1$ orbital, is still rather modest, 0.0028 hartrees = 0.076 eV. Thus it would appear that basis A yields ε values rather close to the true Hartree-Fock values.

For the ground state, the predicted Koopmans' theorem ionization potentials may be compared with photoelectron spectroscopy results.[16] The four highest adiabatic i.p.'s are 10.9, 14.1, 15.9, and 16.3 eV, as compared with the present (vertical) theoretical results 12.0, 14.6, 17.8, and 18.8 eV. The predicted order is correct[16] except for interchange of the $1b_2$ and $5a_1$ orbital energies. The fact that the Koopmans' theorem i.p.'s all lie higher than experiment could in large part be remedied by direct hole state calculations[17] on the appropriate states of H_2CO^+.

Both excited states are predicted to lie about 1 eV below the experimental[3] excitation energies T_o. This would appear to imply that the pair correlation energies[10] associated with the $7a'$ orbital are relatively small. In any case, the calculations verify the low-lying nature of these $n \rightarrow \pi^*$ electronic states.

Another interesting point concerning the excited states is the shifting (relative to the ground state) of the ordering of orbital energies. While $\varepsilon(1a'') < \varepsilon(5a')$ for the ground state, the opposite is true for both excited states. An even more dramatic change occurs for the $2a''$ orbital, where ε is lowered by $\sim$ 5 eV relative to the ground state. This causes

the ordering of the $6a'$ and $2a''$ orbital energies to switch relative to the ground state. It would certainly be significant if these kinds of qualitative changes could be verified experimentally. What would be required, of course, is the photoelectron spectrum of either of the two excited electronic states.

Molecular Properties

Table II gives the predicted one-electron properties of formaldehyde. There it is seen that the Hartree-Fock limit of the dipole moment is $\sim$ 2.86 debye, a full 0.5 debye greater than experiment. Limited variation of the polarization function exponents did not significantly affect the predicted dipole. The earlier *ab initio* calculations of DWM and NM gave qualitatively similar results, 3.03 and 2.82 debye, respectively. This error in the Hartree-Fock dipole moment of H_2CO is analogous to CO, where McLean and Yoshimine[18] found a discrepancy of 0.39 debye with experiment. Green[19] has given an excellent discussion of the effects of electron correlation on *ab initio* dipole moments.

Much better agreement with experiment was obtained for both excited states. Our value of 1.470 debye for u_z ($\tilde{A}$) is in good agreement with Freeman and Klemperer's 1.56 ± 0.07 debye. The polarity of both ground and excited state dipoles is $^{+}CO^{-}$. Our $|\mu|$ value of 1.557 debye is obtained as the vectorial sum of i) a 1.470 debye contribution along the CO axis, and ii) an 0.513

debye out-of-plane contribution. The $\tilde{a}\ ^3A''$ dipole is predicted to be quite similar, with a slightly greater out-of-plane contribution (μ_y = 0.604 debye), consistent with the 35° (vs. 31° for the $\tilde{A}$ state) methylene tilt angle.[3] The calculated u_z (1.321 debye) agrees with the experimental value,[6b] 1.29 ± 0.03 debye.

The elements of the ground state quadrupole moment tensor are all rather small. This is due to the near cancellation of the nuclear and electronic contributions. Our basis C θ values are within 0.05 x 10^{-26} esu of those reported earlier by NM.[13] However, it appears that the DWM[12] values of θ_{xx} (0.57 x 10^{-26} esu) and θ_{zz} (-0.61 x 10^{-26} esu) are noticeably greater in magnitude than the true Hartree-Fock values. All the theoretical results are in qualitative agreement with the experimental values of Huttner, Lo, and Flygare:[20] θ_{xx} = -0.60 ± 0.70, θ_{yy} = 1.35 ± 0.70, θ_{zz} = -0.75 ± 0.80 x 10^{-26} esu. Note that our coordinate system is somewhat different from those of previous workers.

The excited state quadrupole moments are predicted to be much larger, and hence subject to much smaller percentage errors. Note the nonvanishing θ_{yz} element, due to the lower symmetry of the excited states. The remarkable similarity of the $\tilde{a}$ and $\tilde{A}$ θ values provides additional evidence for the conclusion that the electronic structures of these two states are essentially identical.

The ground state octupole moments are rather insensitive to basis set, and again quite similar to those predicted by NM. There are many more nonzero elements of the excited state octupole moment tensors, and the magnitudes are substantial and similar for the $\tilde{a}$ and $\tilde{A}$ states.

A final set of properties of particular interest are the electric field gradients q, related to experiment via the quadrupole coupling constants eqQ where Q is the nuclear electric quadrupole moment. The predicted field gradients are seen to be relatively independent of basis set. This is particularly encouraging because when smaller basis sets are used field gradients can vary significantly from one calculation to the next.[10] In addition our field gradients are in good agreement with those of NM. From Flygare's work,[21] the experimental values of $q_{xx}(O) = 2.19$ a.u. and $q_{zz}(O) = -0.34$ are known. These experimental values assume the nuclear quadrupole moment of O^{17} to be 0.024 barns.[22] For both elements of q, the discrepancy with experiment is ~ 0.1 a.u. Like the results of NM,[13] our hydrogen field gradients are very close to Flygare's experimental values,[21] reported in the bond axis system.

In light of the basis set stability and good agreement with experiment for the ground state, we expect the excited state field gradients to be meaningful, perhaps within 0.1 a.u. of the (unknown) exact values. Thus it is interesting to note that the excited state q(H) values are rather similar to those for the ground state. This implies that this $n \rightarrow \pi^*$ excitation has little effect on the electron distribution in the vicinity of the hydrogen atoms. This conclusion is of course consistent with a picture of the $2b_2$ (n) orbital as a bonding combination of C and O $2p_x$ functions and the $2b_1$ (π^*) as an antibonding

combination of C and O $2p_y$ functions. This same picture can be used to justify the very significant differences between the ground and excited state q(C) and q(O) elements.

We have also computed a number of other properties, including the potential, electric field vector, and charge density at each nucleus. Although not reproduced here, these properties are available in our complete report of this work.[23]

Concluding Remarks

The present results for the $\tilde{X}\ ^1A_1$ ground state of H_2CO confirm the conclusion of Neumann and Moskowitz that their earlier reported properties are rather close to the limiting Hartree-Fock results. The ground state results are of additional value to us, as we intend to calculate the interaction potential between He and H_2CO using basis set C. The dynamics of rotational excitation of H_2CO by He is a problem of considerable astrophysical interest.[24]

Our results for the $\tilde{a}$ and $\tilde{A}$ states represent perhaps the first near-Hartree-Fock theoretical study of polyatomic excited state molecular properties. The agreement with the experimental dipole moments is impressive, and we hope that this work will encourage experimental studies of other properties of these two fascinating excited electronic states.

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Table I. Energy results for the ground and first two excited states of formaldehyde. Unless indicated all energies are in hartrees (1 hartree = 27.21 eV.) Experimental excitation energies[3] are in parentheses.

	State	$^1A_1$	$^1A_1$	$^1A_1$	$^3A''$	$^1A''$
	Basis	A	B	C	C	C
Total energy		-113.89937	-113.90794	-113.91494	-113.83469	-113.82476
Excitation energy (eV)		0.00	0.00	0.00	2.18 (3.12)	2.45 (3.50)
Orbital energies						
$1a_1$ ($1a'$)		-20.5780	-20.5786	-20.5773	-20.6323	-20.6257
$2a_1$ ($2a'$)		-11.3457	-11.3479	-11.3466	-11.2815	-11.2853
$3a_1$ ($3a'$)		- 1.4067	- 1.4080	- 1.4068	- 1.3804	- 1.3717
$4a_1$ ($4a'$)		- 0.8657	- 0.8669	- 0.8670	- 0.8678	- 0.8686
$1b_2$ ($1a''$)		- 0.6908	- 0.6921	- 0.6915	- 0.6320	- 0.6300
$5a_1$ ($5a'$)		- 0.6503	- 0.6514	- 0.6531	- 0.6443	- 0.6401
$1b_1$ ($6a'$)		- 0.5351	- 0.5367	- 0.5367	- 0.5865	- 0.5815
$2b_2$ ($2a''$)		- 0.4408	- 0.4423	- 0.4423	- 0.6272	- 0.6185
$2b_1$ ($7a'$)		-	-	-	- 0.3576	- 0.3601

Table II. Molecular properties of formaldehyde. Multipole moments were calculated with respect to the center of mass in each case. The actual expressions for the quantum mechanical expectation values are given in D. Neumann and J. W. Moskowitz, J. Chem. Phys. 49, 2056 (1968). Unless indicated, properties are in atomic units. For conversion factors between atomic units and conventional units, see S. Rothenberg and H. F. Schaefer, J. Chem. Phys. 53, 3014 (1970).

Property \ State	$^1A_1$	$^1A_1$	$^1A_1$	$^3A''$	$^1A''$
Basis	A	B	C	C	C
Dipole moment (debyes)					
u_y	-	-	-	0.604	0.513
u_z	-2.840	-2.881	-2.859	-1.321	-1.470
$\|u\|$	2.840	2.881	2.859	1.453	1.557
Quadrupole moment (10^{-26} esu)					
θ_{xx}	0.246	0.247	0.238	2.455	2.448
θ_{yy}	-0.122	-0.092	-0.199	-1.917	-1.901
θ_{zz}	-0.124	-0.155	-0.039	-0.538	-0.548
θ_{yz}	-	-	-	-0.372	-0.329

Table II (Continued)

Octupole moment					
Ω_{yyy}	-	-	-	-2.63	-2.37
Ω_{zzz}	0.65	0.71	0.97	-0.93	-1.04
Ω_{xxy}	-	-	-	0.57	0.46
Ω_{xxz}	-2.49	-2.47	-2.71	-2.26	-2.17
Ω_{yyz}	1.84	1.75	1.75	3.19	3.21
Ω_{yzz}	-	-	-	2.06	1.91
Electric field gradients					
$q_{xx}(H)$	-0.146	-0.144	-0.150	-0.195	-0.195
$q_{yy}(H)$	0.126	0.123	0.130	0.137	0.143
$q_{zz}(H)$	0.020	0.021	0.021	0.058	0.052
$q_{xy}(H)$	-	-	-	-0.118	-0.106
$q_{xz}(H)$	0.173	0.170	0.178	0.163	0.169
$q_{yz}(H)$	-	-	-	0.059	0.055

Table II (Continued)

$q_{xx}(C)$	0.305	0.312	0.317	0.163	0.176
$q_{yy}(C)$	-0.635	-0.638	-0.651	0.078	0.058
$q_{zz}(C)$	0.330	0.326	0.334	-0.241	-0.235
$q_{yz}(C)$	-	-	-	0.016	0.021
$q_{xx}(O)$	2.280	2.316	2.302	- 2.138	- 2.233
$q_{yy}(O)$	- 1.860	- 1.851	- 1.867	2.290	2.524
$q_{zz}(O)$	- 0.420	- 0.465	- 0.435	- 0.152	- 0.291
$q_{yz}(O)$	-	-	-	- 0.046	- 0.017

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