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Density Functional Study of the Hexamethyl(Dewar Benzene) Radical Cation and Some Related Compounds†

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A theoretical study has been undertaken of the hexamethyl(Dewar benzene) radical cation (both $^2B_2$ and $^2A_1$ states in C_{2v} symmetry) as well as of two related ions, the pentamethylbenzene and the pentamethylbenzyl trifluoroacetate radical cations, which have been suggested as alternative assignments of the EPR spectrum attributed to the hexamethyl(Dewar benzene) cation. The geometries were optimized at the HF and LDA levels of theory using a standard 6-31G basis set. Single point calculations of the hyperfine coupling constants (hfcc) were then performed at the more accurate MP2, B3PW91, B3LYP and PWP86 levels using larger basis sets. The theoretical results of the present study support the assignment of $^2B_2$ as the ground state of the hexamethyl(Dewar benzene) cation, yielding hydrogen atom hfcc's in very good agreement with experiment.

In recent years, the characterization of the hexamethyl(Dewar benzene) (hexamethylbicyclo[2,2,0]-hexa-2,5-diene) radical cation has been the target of several detailed experimental studies. This strained cation, hereafter denoted $\mathbf{1}^{\cdot+}$, is reported to be elusive and particularly difficult to study because of its propensity to undergo a facile rearrangement to its planar isomer, the hexamethylbenzene cation.[1] An indication of the existence of the discrete cation derived from hexamethyl(Dewar benzene) was first shown by Roth *et al.*[2] by means of chemically induced dynamic nuclear polarization (CIDNP) measurements. This study was complemented by *ab initio* calculations on the parent Dewar benzene cation, predicting the presence of two distinct states on the potential energy surface of this cation (in C_{2v} symmetry): a $^2B_2$ ground state and an 8.0 kcal mol^{-1} less stable $^2A_1$ state with an elongated transannular bond. The spin density was furthermore found to be localized on the bond between the two pairs of olefinic carbon atoms in the $^2B_2$ state, whereas in the $^2A_1$ state most of the spin density was confined to the bridgehead carbons, as computed by Roth *et al.*[2] In turn, the CIDNP measurements on $\mathbf{1}^{\cdot+}$ provided indirect evidence for the formation of both $^2A_1$ and $^2B_2$ states, generated via competing pathways, the ground state not being assigned in these experiments.[2]

The isolation of $\mathbf{1}^{\cdot+}$ was also possible in a low temperature matrix isolation experiment, by γ-irradiation of a dilute solution of neutral **1** in a frozen chlorofluorocarbon (CFC) matrix at 77 K.[3] A 13-line EPR spectrum with a 9.5 G hyperfine splitting was detected by Rhodes[3] and assigned to the $^2B_2$ state of $\mathbf{1}^{\cdot+}$. This result was later re-examined and confirmed in a series of three papers by different authors.[4–6] Trifunac and coauthors [4] performed a time-resolved fluorescence detected magnetic resonance study of $\mathbf{1}^{\cdot+}$ in non-polar alkane solvents between 205 and 245 K and observed also a 13-line pattern with a 9.2 G splitting assigned to the $^2B_2$ state of $\mathbf{1}^{\cdot+}$. Rhodes' assignment was furthermore confirmed by Arnold and Gerson[5] who examined the EPR spectrum of $\mathbf{1}^{\cdot+}$ in different CFC matrices. Finally, Williams *et al.*[6] repeated Rhodes' experiment and also reported on a similar EPR spectrum with a hyperfine splitting of 9.1 G.

Recently, Roth reported on an EPR spectrum with a 9.8 G splitting of the product of oxidation of **1** with $SbCl_5$–$SOCl_2$[7] and later observed a value of 10.7 G from the spectrum generated at room temperature by stabilizing **1** on the surface of a solid oxidant, dioxygenyl hexafluoroantimonate.[8] In addition, Roth *et al.* also reported the deposition of pentamethylbenzene (**2**-H) onto ($O_2^{\cdot+}SbF_6^-$), generating a very similar 13-line spectrum with a single spacing of 10.3 G due to the

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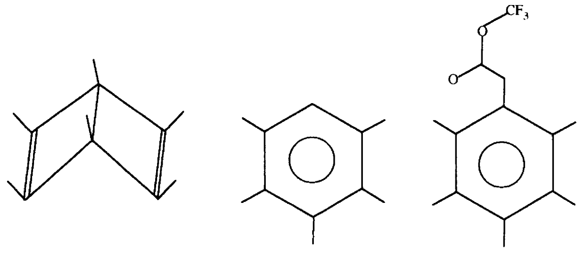

1 2-H 2-OCOCF$_3$

Scheme 1.

pentamethylbenzene cation.[8] Very recently, however, Eberson *et al.* showed that the oxidation of **1** by Tl^{III} in a solution of trifluoroacetic acid (TFA) at -11 °C generates the cation of the parent hexamethylbenzene, which then reacts with TFA to yield the pentamethylbenzyl trifluoroacetate cation.[9] A 13-line EPR spectrum [$a^H = 10.4$ G (12 H), $a^H = 0.80$ G (2 H) and $a^H = 0.40$ G (3 H)] was reported by Eberson *et al.* for the pentamethylbenzyl trifluoroacetate (**2**-OCOCF$_3$) cation,[9] which in part appears to overlap with the data reported in some of the earlier studies of **1**. Finally, in a very detailed study, Eberson *et al.* have reported the 13-line EPR spectra of $\mathbf{1}^{\cdot +}$, **2**-H$^{\cdot +}$, and **2**-OCOCF$_3$$^{\cdot +}$ as well as of some isotopomers and other related compounds, obtained by photolysis in TFA at -11 °C.[10]

In order to try to resolve some ambiguities remaining in the above-mentioned studies, a theoretical investigation was here undertaken for the hexamethyl(Dewar benzene) (**1**) radical cation (both $^2B_2$ and $^2A_1$ states in C_{2v} symmetry) as well as for two related ions, the pentamethylbenzene (**2**-H) and the pentamethylbenzyl trifluoroacetate (**2**-OCOCF$_3$) radical cations.

Methods

Calculations were performed using different levels of density functional theory (DFT) and at the *ab initio* HF and MP2 levels. The geometries were obtained by complete optimizations at the HF and local density approximation (LDA) levels, using the 6-31G basis set. The LDA functional uses Slater's exchange term[11] and the Vosko–Wilks–Nusair parametrization for the correlation term.[12] This functional will be denoted SVWN throughout. Using the LDA optimized geometries, single-point computations of the hyperfine coupling constants (hfcc's) were subsequently performed at the gradient corrected B3PW91/6-31G, B3LYP/6-31G and B3LYP/6-31G(d,p) levels of theory and at the PWP86 level in conjunction with a DZVP basis set on the carbon atoms and the IGLO-III basis set[13] on the hydrogens. The gradient-corrected (non-local) functionals use the three-parameter hybrid exchange by Becke (B3)[14] in conjunction with the correlation corrections by Perdew *et al.* (PW91)[15] or by Lee-Yang-Parr (LYP),[16] or the Perdew–Wang exchange (PW)[17] together with Perdew's 1986 correlation correction (PW86).[18] In addition, single-point MP2/6-31G calculations at the HF/6-31G geometry were carried out for the smallest cations ($\mathbf{1}^{\cdot +}$ and **2**-H$^{\cdot +}$). The GAUSSIAN 94 program package[19] was used for all but the PWP86 calculations, which were performed using the program deMon.[20]

Results

The isotropic proton hyperfine coupling constants (hfcc) obtained in the various calculations and in the experimental measurements are collected in Tables 1–4. Only the average of the hfcc's in the different groups of chemically equivalent hydrogen atoms are reported in the tables. In Figs. 1–4 we show the optimized SVWN/6-31G geometries of the different systems, also indicating the average of the hydrogen atom hfcc's of each methyl group.

Table 1. The EPR parameters of the $^2B_2$ state of the hexamethyl(Dewar benzene) radical cation ($\mathbf{1}^{\cdot +}$), as calculated at different levels of theory. The average over the hyperfine coupling constants (hfcc's) of the hydrogen atoms of the allylic methyl groups (12 H) and of the bridgehead methyl groups (6 H) are given in gauss (G).

Level of calculation	hfc/G	
SVWN/6-31G	9.9 (12 H),	−0.02 (6 H)
B3PW91/6-31G//SVWN/6-31G	9.9 (12 H),	−0.13 (6 H)
B3LYP/6-31G//SVWN/6-31G	10.2 (12 H),	−0.09 (6 H)
B3LYP/6-31G(d,p)//SVWN/6-31G	9.5 (12 H),	−0.05 (6 H)
PWP86/(DZVP, IGLO-III)// SVWN/6-31G[a]	9.9 (12 H),	+0.02 (6 H)
HF/6-31G	8.8 (12 H),	−0.53 (6 H)
MP2/6-31G//HF/6-31G	9.1 (12 H),	−0.21 (6 H)
Experiment[b]	9.5 (12 H)	

[a]The PWP86 calculation is performed in conjunction with the DZVP basis set on the C atoms and the IGLO-III basis set on the H atoms, using the SVWN/6-31G geometry (see also the text). [b]Rhodes, C. J. *J. Am. Chem. Soc. 110* (1988) 4446.

Table 2. The EPR parameters of the $^2A_1$ state of the hexamethyl(Dewar benzene) radical cation ($\mathbf{1}^{\cdot +}$), as calculated at different levels of theory. The average over the hyperfine coupling constants (hfcc's) of the hydrogen atoms of the allylic methyl groups (12 H) and of the bridgehead methyl groups (6 H) are given in gauss (G).

Level of calculation	hfcc/G	
SVWN/6-31G	4.3 (12 H),	8.3 (6 H)
B3PW91/6-31G//SVWN/6-31G	3.7 (12 H),	9.6 (6 H)
B3LYP/6-31G//SVWN/6-31G	3.9 (12 H),	9.7 (6 H)
B3LYP/6-31G(d,p)//SVWN/6-31G	3.6 (12 H),	9.2 (6 H)
PWP86/(DZVP, IGLO-III) //SVWN/6-31G	4.1 (12 H),	8.7 (6 H)
HF/6-31	0.7 (12 H),	12.1 (6 H)
MP2/6-31G//HF/6-31G	1.8 (12 H),	10.8 (6 H)
Experiment[a]	9.5 (12 H)	

[a]Rhodes, C. J. *J. Am. Chem. Soc. 110* (1988) 4446.

Table 3. The EPR parameters of the pentamethylbenzene radical cation (**2**-H$^{\cdot+}$) as calculated at different levels of theory. The average over the hyperfine coupling constants (hfcc's) of the hydrogen atoms of the four *ortho* and *meta* methyl groups (12 H) and of the *para* methyl group (3 H) are given in gauss (G) (the methyl groups are labelled Me′ and Me, respectively, in Fig. 3). The hfcc of the hydrogen atom on the non-substituted carbon atom of the benzene ring is also reported (1 H).

Level of calculation	hfcc/G		
SVWN/6-31G	12.4 (12 H),	−1.0 (3 H),	0.2 (1 H)
B3PW91/6-31G //SVWN/6-31G	13.0 (12 H),	−2.6 (3 H),	2.2 (1 H)
B3LYP/6-31G //SVWN/6-31G	13.3 (12 H),	−2.5 (3 H),	1.9 (1 H)
B3LYP/6-31G(d,p) //SVWN/6-31G	12.4 (12 H),	−2.3 (3 H),	1.5 (1 H)
PWP86/(DZVP, IGLO-III) //SVWN/6-31G	12.9 (12 H),	−1.6 (3 H),	0.7 (1 H)
HF/6-31G	11.7 (12 H),	−7.5 (3 H),	10.5 (1 H)
MP2/6-31G//HF/6-31G	9.9 (12 H),	−2.6 (3 H),	3.6 (1 H)
Experiment[a]	10.2 (12 H),	0.47 (3 H),	0.40 (1 H)

[a] Eberson, L., Hartshorn, M. P., Persson, O. and Svensson, J. O. *J. Chem. Soc., Perkin Trans. 2* (1995) 1253.

Table 4. The EPR parameters of the pentamethylbenzyl trifluoroacetate radical cation (**2**-OCOCF$_3$$^{\cdot+}$), as calculated at different levels of theory. The average over the hyperfine coupling constants (hfcc's) of the hydrogen atoms of the four *ortho* and *meta* methyl groups (12 H) and of the *para* methyl group (3 H) are given in gauss (G) (the methyl groups are labelled Me′ and Me, respectively, in Fig. 4). The intermediate value in each line corresponds to the average of the hfcc's of the two hydrogen atoms of the trifluoroacetate tail (2 H).

Level of calculation	hfcc/G		
SVWN/6-31G	10.9 (12 H),	0.70 (2 H),	1.12 (3 H)
B3PW91/6-31G //SVWN/6-31G	11.5 (12 H),	0.04 (2 H),	0.02 (3 H)
B3LYP/6-31G //SVWN/6-31G	11.8 (12 H),	0.10 (2 H),	0.14 (3 H)
B3LYP/6-31G(d,p) //SVWN/6-31G	11.2 (12 H),	0.03 (2 H),	0.01 (3 H)
PWP86/(DZVP, IGLO-III) //SVWN/6-31G	11.1 (12 H),	0.74 (2 H),	1.02 (3 H)
HF/6-31G	11.5 (12 H),	−3.90 (2 H),	−6.42 (3 H)
Experiment[a]	10.2 (12 H),	0.80 (2 H),	0.40 (3 H)

[a] Eberson, L., Hartshorn, M. P., Persson, O. and Svensson, J. O. *J. Chem. Soc., Perkin Trans. 2* (1995) 1253.

Our preliminary results for the hexamethyl(Dewar benzene) cation indicate that, irrespective of the method employed, the $^2B_2$ state has most of its spin density on the olefinic positions (cf. Table 1 and Fig. 1) whereas, for the $^2A_1$ state, the spin density is instead concentrated on the bridgehead positions, as reported in Table 2 and Fig. 2. These predictions agree with the earlier theoretical results obtained at the MP2/6-31G(d) level for the unsubstituted Dewar benzene cation.[2]

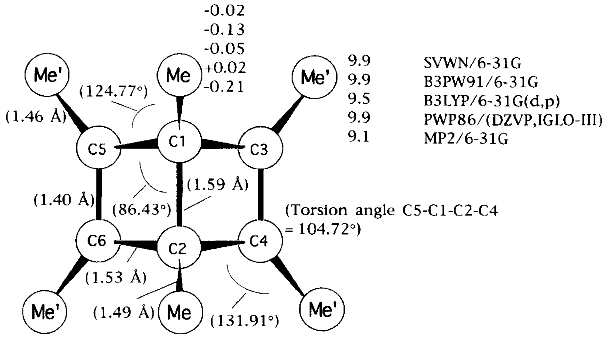

Fig. 1. The optimized SVWN/6-31G geometry of the $^2B_2$ state of the hexamethyl(Dewar benzene) radical cation (**1**$^{\cdot+}$). The average over the hyperfine coupling constants (hfcc's) of the hydrogen atoms of the allylic and bridgehead methyl groups, Me′ and Me, respectively, as calculated at the different levels of theory indicated on the figure, are reported in gauss. Selected geometrical parameters, obtained from full geometry optimization calculations at the SVWN/6-31G level, are given in parentheses.

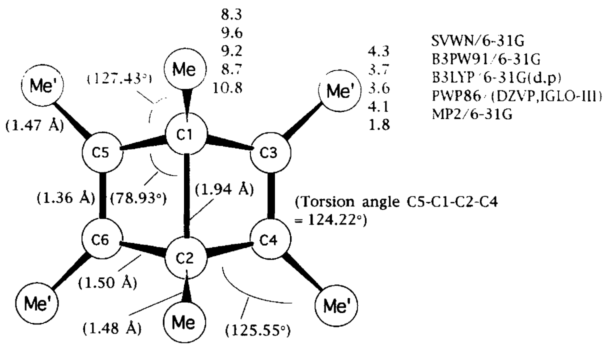

Fig. 2. The optimized SVWN/6-31G geometry of the $^2A_1$ state of **1**$^{\cdot+}$ and averaged hfcc's of the hydrogen atoms of the allylic and bridgehead methyl groups, Me′ and Me, respectively.

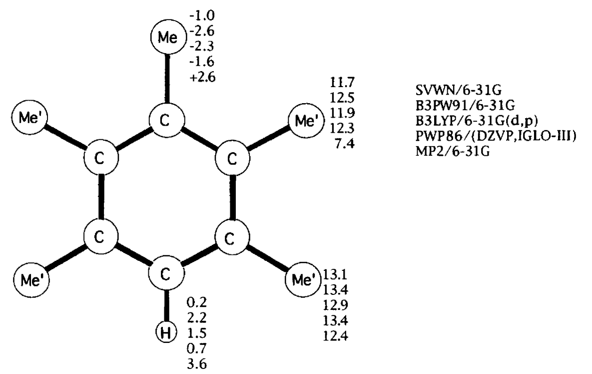

Fig. 3. Pentamethylbenzene (**2**-H$^{\cdot+}$) radical cation: average hfcc's of the hydrogen atoms of the methyl groups as well as the hfcc of the hydrogen atom on the non-substituted carbon atom of the benzene ring, as calculated at different levels of theory, are shown.

For the $^2B_2$ state, the computed values of the hfcc's of the H atoms of the allylic methyl groups (12 hydrogens), especially using the highest levels of calculation, i.e., B3LYP/6-31G(d,p)//SVWN/6-31G, PWP86 and MP2/6-31G//HF/6-31G, are in very good agreement with

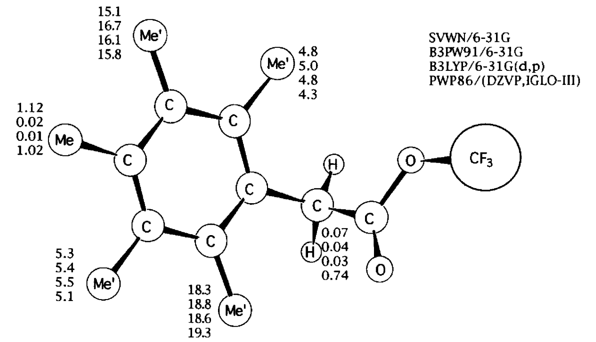

Fig. 4. Average hfcc's of the hydrogen atoms of the methyl groups and the average of the hfcc's of the two hydrogen atoms of the trifluoroacetate tail of the pentamethylbenzyl trifluoroacetate (**2**-OCOCF$_3^{\cdot +}$) radical cation.

the experimental observations of a 13-line spectrum with a single splitting of 9.5 G,[3] 9.2 G,[4] 9.1 G,[6] 9.8 G[7] or 10.7 G,[8] depending on experimental conditions. For the $^2A_1$ state, the computed hyperfine pattern is instead 4 G (12 H) and 9 G (6 H), which does not match that observed experimentally. The theoretical results of the present study hence provide definite confirmation of the assignment of $^2B_2$ as the ground state of the hexamethyl(Dewar benzene) cation. The $^2B_2$ state is, moreover, predicted to be 2.5 kcal mol^{-1} more stable than the $^2A_1$ state in our MP2/6-31G calculations, again in line with the theoretical results of Roth *et al.*[2] obtained for the parent non-substituted Dewar benzene cation [8.0 kcal mol^{-1} at the MP2/6-31G(d) level]. The HF/6-31G geometry obtained in the present study for the Dewar benzene skeleton is essentially the same as that obtained by Roth *et al.* for the Dewar benzene cation,[2] at the same level of calculation.

In the case of the pentamethylbenzene cation, most of the spin density is found to be localized on the four *ortho* and *meta* positions (cf. Table 3 and Fig. 3), as was also observed by Eberson *et al.*[10] However, the calculated average hfcc's are found to be up to ca. 3 G larger than the measured splittings, resulting in the largest deviation between our results and the experimental measurements (cf. the next section).

Finally, as can be seen from an examination of Table 4 (see also Fig. 4), the theoretical hyperfine structure of the fourth molecular species considered, the pentamethylbenzyl trifluoroacetate cation, is reasonably close to the observed EPR spectrum.[10]

Discussion

Previous experience[21–25] has shown that proton hfcc's in most cases are predicted with good reliability ($\leqslant 10\%$ error) by both the PWP86 and B3LYP functionals, provided basis sets of at least DZVP quality are used. This can be seen to be true for the $^2B_2$ state of **1**$^{\cdot +}$ in Table 1 and also for the results of the **2**-OCOCF$_3^{\cdot +}$ radical cation in Table 4. The experimental assignments are hence strongly supported by the calculations in these cases. It is, likewise, clearly shown by the computations (Tables 1 and 2) that a $^2A_1$ assignment of the 13-line spectrum of **1**$^{\cdot +}$ can be ruled out. The agreement between calculation and experiment for the pentamethylbenzene (**2**-H$^{\cdot +}$) radical cation, as shown in Table 3, is not quite as good, with a deviation of about 20% for the largest couplings. At the present stage, it is an open question whether the source of this discrepancy lies in the experiments or in the calculations. More detailed investigations, both theoretical and experimental, would be needed for a definitive answer.

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