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Charge-transfer reactions of $C_{60}^{3+\cdot}$: "bracketing" the third ionization energy of C_{60}

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The occurrence or absence of charge transfer from $C_{60}^{3+\cdot}$ to several neutral molecules is reported. The results, which were obtained using the selected-ion flow tube technique operating at 294±2 K and a helium buffer gas pressure of 0.35±0.01 Torr, are in good agreement with earlier Fourier-transform ion cyclotron resonance experiments. Rapid charge transfer, often in competition with other product channels, was noted for the reactions of $C_{60}^{3+\cdot}$ with several neutrals having $IE \leqslant 11.02$ eV. Charge transfer to OCS (IE=11.1736 eV) was observed to be inefficient, and no charge transfer was seen to C_2H_2 (IE=11.40 eV) or to neutrals having higher ionization energy. Consideration of the effects of Coulombic repulsion upon the occurrence of charge transfer from a triply-charged ion indicates $IE(C_{60}^{2+}) = 15.6 \pm 0.5$ eV, in disagreement with a value $IE(C_{60}^{2+}) = 17.0 \pm 0.75$ eV determined by charge stripping. A value for the fourth ionization energy of C_{60}, 19.5 eV, is estimated by extrapolation of the first three ionization energies.

1. Introduction

Following its discovery in 1985 [1] and synthesis in 1990 [2], buckminsterfullerene, C_{60}, has become one of the most intensively studied chemical species [3]. Among the factors promoting interest in C_{60} are its exceptionally high symmetry and rigidity. It appears unique among polyatomic species in having at least twelve experimentally accessible charge states ranging from C_{60}^{6-} to $C_{60}^{5+\cdot}$ [4,5]. Determination of the thermochemistry of successive ionizations in C_{60} is therefore important as a model for the influence of the charge state upon the ionization energy for molecular species.

Several experimental techniques have been used to study the first few ionization energies of C_{60}. There is good agreement on $IE(C_{60}) = 7.61 \pm 0.02$ eV [10], and on $EA(C_{60}) = 2.7 \pm 0.1$ eV [11,12]. A spread of values for $IE(C_{60}^{+\cdot})$, ranging from 9.7±0.2 eV (determined by FT-ICR bracketing [8,9]) to 12.25±0.5 eV (by charge stripping [13]) has been reported [10,14–17]. We have recently [18] studied the occurrence of charge-transfer reactions of $C_{60}^{2+} + X$ using the selected-ion flow tube (SIFT) technique, and have stated that the threshold for occurrence of charge-transfer reactions, $IE(X) = 9.59 \pm 0.11$ eV [8,9,18], is consistent with a recently reported value [17] of $IE(C_{60}^{+\cdot}) = 11.39 \pm 0.05$ eV when consideration is made of the role of Coulombic repulsion in charge-transfer reactions of doubly-charged ions. The effect of Coulombic repulsion cannot be ignored, since the products of a charge-transfer reaction of the type

$$C_{60}^{n+} + X \rightarrow C_{60}^{(n-1)+} + X^{+} \qquad (1)$$

are initially in close proximity to each other. The threshold for production of such an ion pair will be substantially above the threshold for production of the ions $C_{60}^{(n-1)+}$ and X^{+} at infinite separation from each other.

Previously reported values of $IE(C_{60}^{2+})$ are 11.2±0.2 eV by FT-ICR bracketing [8,9] and 17.0±0.75 eV by charge stripping [13]. The discrepancy between these values is severe: however, the major portion of the discrepancy can be resolved by

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consideration of the Coulombic effect discussed above.

As a component of our studies of the ion–molecule chemistry of fullerenes, we have discussed the role of Coulombic repulsion in promoting and directing adduct formation [19–21] and in impeding charge transfer from fullerene dications [18] and proton transfer from derivatized fullerene dications [22–25]. In a companion Letter [26] to the present work, we have discussed the expected charge distributions and Coulombic constraints to charge transfer from C_{60}^{n+} ($n=3$–6). Here we present the results of an experimental investigation into charge transfer reactions of fullerene trications, and accordingly "bracket" the third ionization energy of C_{60}.

2. Experimental

The measurements presented here were obtained using a SIFT which has been described previously [27,28], operating at 294±2 K and at a helium buffer gas pressure of 0.35±0.01 Torr. $C_{60}^{3+\cdot}$ was generated in the ion source by electron bombardment (100 V) of a vaporised fullerene mixture (C_{60}/C_{70}, 2%–12% C_{70}, obtained from Strem Chemicals Inc.) entrained in argon. Reactant neutrals were of high purity (>99.5%) and were used either undiluted (e.g. OCS, C_2H_2) or as dilute mixtures (1%–10%) of vapour in helium. Rate coefficients and product distributions for the reactions observed have an estimated uncertainty of ±30%.

3. Results and discussion

The results obtained are summarised in table 1. Several of the neutrals used here were also employed in the earlier study of McElvany and Bach [8], who noted, in a qualitative fashion only, the occurrence or absence of charge transfer. In general, our results are in agreement with those of McElvany and Bach, although we have detected a previously unreported minor channel (10%) leading to charge transfer in the reaction with C_3H_8; also we did not detect the O^- transfer reaction which they reported for $C_{60}^{3+\cdot}+CH_3NO_2$. This difference may arise due to the differences in techniques: the SIFT method used here allows much greater probability of collisional stabilisation than does the lower pressure FT-ICR technique. Indeed, for the reaction with CH_3NO_2, we did detect, as a primary product, an adduct ($C_{60}\cdot CH_3NO_2^{3+\cdot}$, $m/z=280.3$) which was not reported in the study of McElvany and Bach. Fig. 1 shows the reaction profile initiated by $C_{60}^{3+\cdot}+CH_3NO_2$ in our experiments.

It is apparent from the products shown in table 1 that several possible product channels may compete with charge transfer from $C_{60}^{3+\cdot}$: hydride abstraction, for example, and addition. We shall deal more fully elsewhere with an exploration of the chemistry of $C_{60}^{3+\cdot}$; we note here that the abundance of competing product channels, often of high efficiency, limits the number of neutrals whose reactivity can be expected to provide useful thermochemical information on the occurrence or absence of charge transfer. For this reason, although several neutrals (other than those employed in this study) also have ionization energies in the range from 10.9 to 11.5 eV, we have not studied the reactions of $C_{60}^{3+\cdot}$ with these neutrals since we anticipate the high probability of rapid hydride abstraction, addition, or other competing channels in these reactions.

We are able to confirm the bracketing value, for the threshold for charge transfer, from the study of McElvany and Bach [8]. Charge transfer to CH_3NO_2 (IE=11.02±0.04 eV), C_3H_8 (IE=10.95±0.05 eV) and to CH_3OH (IE=10.85±0.01 eV) is seen to be efficient in competition with addition or hydride abstraction. Charge transfer to O_2 (IE=12.071±0.001 eV), to C_2H_6 (IE=11.52±0.01 eV), or to HCCH (IE=11.400±0.002 eV) was not observed: in the latter case, adduct formation occurred, but this accounted for only ≈6% of collisions and so the absence of charge transfer in the remaining 94% of collisions is taken as being significant. The observation of slow charge transfer, $k=0.018\ k_c$, from $C_{60}^{3+\cdot}$ to OCS (IE=11.1736±0.0015 eV) – as depicted in fig. 2 – also appears to be significant: a value of $E_a=0.10$ eV can be obtained from the Arrhenius expression

$$k=k_c \exp(-E_a/k_B T) . \qquad (2)$$

This value represents the height of the barrier to charge transfer in this reaction, and would indicate a value of IE(X)=11.07 eV as the threshold for efficient charge transfer from $C_{60}^{3+\cdot}$ to X. We choose to

Table 1
Rate coefficients and product distributions for reactions of the type $C_{60}^{3+\cdot}+X$, used to bracket the occurrence of charge transfer to various neutrals X as a function of IE(X)

X	Products [a]	k_{obs} [b]	k_c [c]	IE(X) [d]
O_2	none	<0.001	1.59	12.071
C_2H_6 [e]	none	<0.005	2.76	11.52
Cl_2	$C_{60}Cl^{2+\cdot}+Cl^+$	obs. [f]	1.89	11.480
C_2H_2 [e]	$C_{60}\cdot C_2H_2^{3+\cdot}$ [g]	0.15	2.67	11.400
HCOOH	$C_{60}H^{2+\cdot}+CO_2H^+$ [0.5] $C_{60}\cdot HCOOH^{3+\cdot}$ [0.5]	2.5	3.41	11.33
CH_3Cl	$C_{60}H^{2+\cdot}+CH_2Cl^+$	obs. [f]	3.95	11.22
COS	$C_{60}^{2+}+COS^{+\cdot}$	0.048	2.61	11.1736
CH_3NO_2 [e]	$C_{60}\cdot CH_3NO_2^{3+\cdot}$ [0.9] $C_{60}^{2+}+CH_3NO_2^{+\cdot}$ [g] [0.1]	5.0	5.60	11.02
C_3H_8 [e]	$C_{60}H^{2+\cdot}+C_3H_7^+$ [g] [0.9] $C_{60}^{2+}+C_3H_8^{+\cdot}$ [0.1]	4.2	2.84	10.95
CH_3OH [e]	$C_{60}^{2+}+CH_3OH^{+\cdot}$ [g] [0.8] $C_{60}\cdot CH_3OH^{3+\cdot}$ [0.2]	2.5	4.38	10.85
H_2S	$C_{60}H^{2+\cdot}+HS^+$ [>0.5] $C_{60}^{2+}+H_2S^{+\cdot}$ [<0.5]	3.5	3.39	10.453
$NO^\cdot$	$C_{60}^{2+}+NO^+$	1.1	1.67	9.264

[a] Where more than one product channel was detected, product ratios are reported in square brackets.

[b] k_{obs} is the observed reaction rate coefficient, in units of 10^{-9} cm^3 $molecule^{-1}$ s^{-1}, at 294 ± 2 K and a helium pressure of 0.35 ± 0.01 Torr.

[c] k_c is the calculated ADO collision rate coefficient, in units of 10^{-9} cm^3 $molecule^{-1}$ s^{-1}, calculated according to the method of Su and Bowers [29].

[d] IE(X) is the ionization energy, in electronvolts, of the neutral in question, as listed in the tabulation of Lias et al. [30] unless specified otherwise.

[e] This neutral was also employed in the study of McElvany and Bach [8].

[f] Reaction was observed as shown, but a rate coefficient was not determined. The reaction appeared to be efficient ($k > 10^{-9}$ cm^3 $molecule^{-1}$ s^{-1}).

[g] Product channel also reported by McElvany and Bach [8].

adopt, instead, a threshold value of 11.09 ± 0.09 eV, encompassing the apparent endothermicity of charge transfer to OCS and the apparent exothermicity of charge transfer to CH_3NO_2.

Having obtained a value for the threshold IE(X) for the occurrence of efficient charge transfer, we must allow for the Coulombic repulsion barrier to charge transfer in order to estimate IE(C_{60}^{2+}). In the companion paper to the present work [26], we have estimated that the Coulombic repulsion barrier, $V_3' + V_2''$, to the reaction

$$C_{60}^{3+\cdot}+X \rightarrow C_{60}^{2+}+X^{+\cdot} \qquad (3)$$

is 4.51 ± 0.4 eV above ΔH^0 for this reaction. This yields a value of IE(C_{60}^{2+}) = 15.6 ± 0.5 eV, in disagreement with the value of 17.0 ± 0.75 eV determined by Lifshitz et al. [13]. While the charge-stripping technique used to measure the ionization energy in the study of Lifshitz et al. [13] is arguably a more direct route than is our estimation, two points should be raised in defence of the value obtained here. Firstly, it seems significant that the charge-stripping study [13] yielded the highest value for IE($C_{60}^{+\cdot}$), 12.25 ± 0.5 eV, while no other method has yet yielded a value in excess of 11.90 eV and the least uncertain determination to date is 11.39 ± 0.05 eV [17], in disagreement with the charge-stripping value. It is conceivable that the charge-stripping technique systematically overestimates the appearance energy for C_{60}^{n+} polycations from the reaction

$$(C_{60}^{(n-1)+})^* + X \rightarrow C_{60}^{n+} + X + e\,, \qquad (4)$$

since the collision, although at high centre-of-mass energy, is still affected by ion–induced dipole interactions which are likely to favour localisation of one of the charges on $C_{60}^{(n-1)+}$ at the point of closest ap-

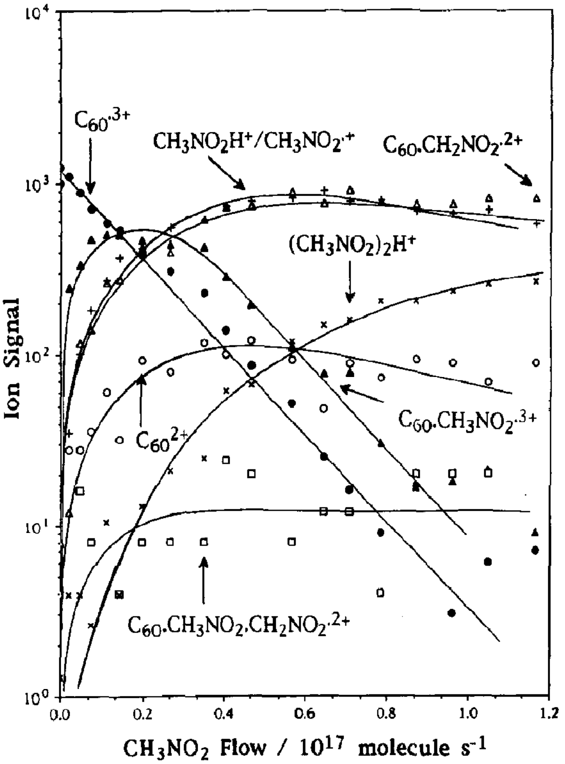

Fig. 1. Experimentally observed data for reaction of $C_{60}^{3+\cdot}$ with CH_3NO_2 in helium buffer gas: $P=0.354$ Torr, He flow velocity$=6.2\times10^3$ cm s^{-1}, reaction length$=46$ cm and $T=294$ K. Primary product channels seen are charge transfer (10%) and adduct formation (90%), with several secondary processes also in evidence. The adduct $C_{60}\cdot CH_3NO_2^{3+\cdot}$ is seen to proton transfer rapidly to CH_3NO_2: some secondary adduct formation evidently occurs also (although this adduct $C_{60}\cdot(CH_3NO_2)_2^{3+\cdot}$ was not directly observable), since the deprotonated secondary adduct $C_{60}\cdot CH_3NO_2\cdot CH_2NO_2^{2+\cdot}$ was detected. Protonated nitromethane, $CH_3NO_2H^+$, was observed to form the proton-bound dimer $(CH_3NO_2)_2H^+$. In the graph shown, data was collected in the high-mass mode of the downstream quadrupole mass spectrometer which did not permit resolution of the signals at *m/z* 61 ($CH_3NO_2^{+\cdot}$, from charge transfer) and *m/z* 62 ($CH_3NO_2H^+$) and so the signal ascribed to $CH_3NO_2H^+$ also contains some component from *m/z* 61; in further experiments performed in the low-mass mode, *m/z* 61 and 62 were well-resolved.

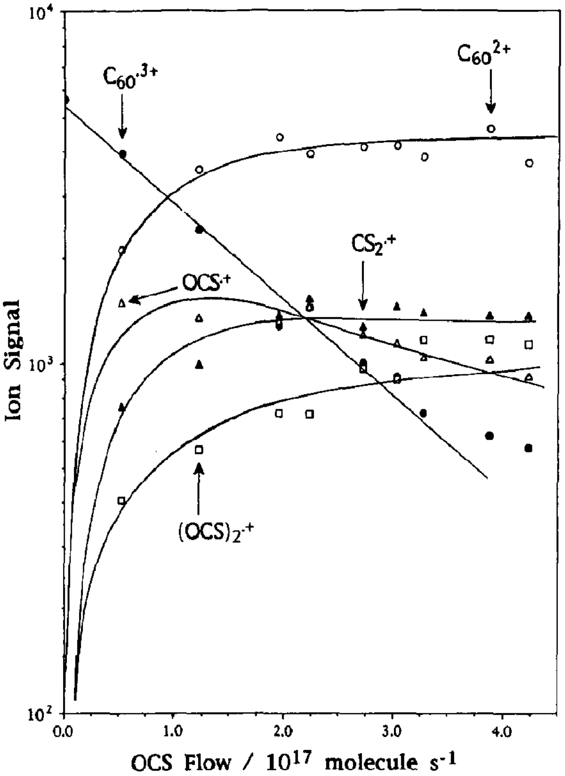

Fig. 2. Experimentally observed data for the reaction of $C_{60}^{3+\cdot}$ with OCS: $P=0.359$ Torr, He flow velocity$=6.1\times10^3$ cm s^{-1}, reaction length$=46$ cm and $T=294$ K. Charge transfer was the sole primary product channel detected. Formation of the OCS dimer ion occurred as a secondary process; the formation of $CS_2^{+\cdot}$, which was also noted, may be due to a slight CS_2 impurity in the OCS sample used or also due to secondary reaction. (●) *m/z* 240; (○) *m/z* 360; (△) *m/z* 60; (▲) *m/z* 74; (□) *m/z* 120.

proach upon the fullerene surface to the neutral X. This is likely to result in the initial formation of a polycation C_{60}^{n+} possessing an unfavourable charge distribution, and hence the appearance potential for this process will be somewhat elevated. This effect is likely to be much more significant for $C_{60}^{(n-1)+}$ than for other ions having little or no charge delocalisation. Secondly, the most questionable assumption in our calculation of the Coulombic repulsion barrier is likely to be that the separation between $C_{60}^{3+\cdot}$ and X at the moment of charge transfer, which we have taken as 1.0 ± 0.7 Å, is indeed equal to the separation between C_{60}^{2+} and X at the moment of charge transfer [18]. If the separation differs with the charge state of the fullerene polycation, then it appears probable that charge transfer occurs at a greater separation for $C_{60}^{3+\cdot}$...X than for C_{60}^{2+}...X, in which case the Coulombic repulsion barrier – and, in consequence, the IE(C_{60}^{2+}) value determined from this – will be lower than that estimated for a separation of 1.0 ± 0.7 Å. We thus anticipate that our bracketed value of IE(C_{60}^{2+}) is likely to be too high rather than too low. A lower value of IE(C_{60}^{2+}) would be in more serious disagreement with that reported previously by Lifshitz et al. [13].

It seems reasonable to assume that the bulk of the energy released in the Coulombic repulsion between the two product ions will be manifested in the translational excitation of these ions. The comparatively large uncertainty in our determination of $\mathrm{IE}(C_{60}^{2+}) = 15.6 \pm 0.5$ eV could therefore be reduced by an accurate measurement of the kinetic energy release upon charge transfer from $C_{60}^{3+\cdot}$ to X. While we recognise the desirability of such a measurement, it is not possible to perform an experiment of this type using the SIFT technique employed in the present study.

A linear relationship between the successive ionization energies of large polycyclic aromatic hydrocarbons has been proposed by Smith [31]. While it is not clear that buckminsterfullerene is sufficiently large to exhibit such behaviour, it is interesting to note that our value of $\mathrm{IE}(C_{60}^{2+}) = 15.6 \pm 0.5$ eV does encompass the value of 15.17 ± 0.12 eV obtained by extrapolation of $\mathrm{IE}(C_{60})$ and $\mathrm{IE}(C_{60}^{+\cdot})$. A value somewhat higher than 15.17 eV for the third IE might be anticipated for two reasons. Firstly, there is considerable charge crowding in $C_{60}^{3+\cdot}$ (intercharge separation is only 6.06 Å for a trigonal planar charge configuration [26]): the approximations inherent in Smith's model [31] will not hold perfectly for a species of such small diameter and high charge state. Secondly, ionization of C_{60} and C_{60}^{2+} produce radical ions while ionization of $C_{60}^{+\cdot}$ produces a non-radical ion: the differences in the contribution of the electron pairing energy to $\mathrm{IE}(C_{60})$ and $\mathrm{IE}(C_{60}^{+\cdot})$ also lead to an underestimate of $\mathrm{IE}(C_{60}^{2+})$ by extrapolation.

Further extrapolation, using the current values of $\mathrm{IE}(C_{60}) = 7.61 \pm 0.02$ eV, $\mathrm{IE}(C_{60}^{+\cdot}) = 11.39 \pm 0.05$ eV, and $\mathrm{IE}(C_{60}^{2+}) = 15.6 \pm 0.5$ eV, yields an estimate for $\mathrm{IE}(C_{60}^{3+\cdot})$ of ≈ 19.5 eV. This is considerably below the value of 21.7 eV estimated by Walter et al. [32], using the same technique but different values (those of Lifshitz et al. [13]) for the second and third ionization energies. Based on our extrapolated value of $\mathrm{IE}(C_{60}^{3+\cdot}) = 19.5$ eV, and the value of $(V'_4 + V''_3) = 7.1 \pm 0.6$ eV which we have obtained for the Coulombic repulsion energy involved in charge transfer from C_{60}^{4+} to X at the assumed C_{60}...X separation of 1.0 ± 0.7 Å, we estimate that C_{60}^{4+} should be capable of undergoing charge transfer with species X having $\mathrm{IE}(X) \leqslant 12.4$ eV. However, the cumulative uncertainties involved in this estimate are high. We are at present attempting to determine $\mathrm{IE}(C_{60}^{3+\cdot})$ using the bracketing technique described here, but confirmation via photoionization or other techniques is also very desirable.

4. Conclusion

Ion/molecule studies bracketing the occurrence of charge transfer from $C_{60}^{3+\cdot}$ favour a lower value, $\mathrm{IE}(C_{60}^{2+}) = 15.6 \pm 0.5$ eV, than the only other experimental determination of this quantity yet reported, even when consideration is made of the maximum Coulombic repulsion barrier expected to impede charge transfer from $C_{60}^{3+\cdot}$. The value reported here is consistent with the progression observed between $\mathrm{IE}(C_{60}) = 7.61 \pm 0.02$ eV and $\mathrm{IE}(C_{60}^{+\cdot}) = 11.39 \pm 0.05$ eV. However, the uncertainty associated with any "bimolecular" method of ionization energy determination, arguably including the charge-stripping technique, is large and it is difficult to pinpoint the third ionization energy, by such methods, as accurately as seems feasible by spectroscopic means. We therefore recommend that a spectroscopic determination of $\mathrm{IE}(C_{60}^{2+})$ be attempted in order to clarify this issue. Alternatively, a measurement of the kinetic energy release upon charge transfer from $C_{60}^{3+\cdot}$ could also assist in refining the third ionization energy.

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