diffusion, this would mean that the stepwise diffusion of the divalent cation (Pb^{2+}) in KCl may only be considered to be complete after the dissociation of the complex, achieved by a K^+ jump.

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On the Diffusion Parameters of Plumbous Ions in KCl

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WE are in agreement with the comments of Reisfeld, Glasner, and Honigbaum[1] that vacancies already present in a crystal due to aliovalent impurities should be considered in the diffusion of divalent ions in KCl. Treatment of the problem is somewhat complicated by the fact that apparently divalent ions tend to show a higher concentration near the surface compared to that in the bulk.[2] It is not clear, however, that the slow variation of the diffusion coefficient, $D(C)$, with concentration, observed at low temperatures,[3] can readily be explained by the excess surface concentration of the impurity ions and the vacancies introduced by these ions. These authors make this point, but fail to support the argument. Their subsequent treatment assumes instead that the impurity concentration is uniform throughout the crystal.

Although their calculations show that the curve obtained for Pb^{++} diffusion in KCl at 480°C, using their Eq. (1), gave a good fit to the experimental data, the authors do not show results of calculations for lower temperatures, which would demonstrate that the reported large change in the free energy of association, ΔG,[3] can indeed be explained by the presence of impurities in the crystal.

With regard to Eq. (1) of Reisfeld *et al.*, it should be pointed out that in the treatment of Howard and Lidiard,[4] from which Eq. (1) derives, the degree of association p, is obtained from the expression for the equilibrium constant for the reaction of Pb^{++} ions with vacancies to give Pb^{++}–vacancy pairs:

$$C_p/(C_v-C_p)(C_b-C_p)=K(T),$$

where C_p, C_v, and C_b are atomic fractions of pairs, vacancies and impurities, respectively. For C_v one may substitute the sum of the Pb^{++} and other divalent impurity concentrations, $C_{Pb}+C_{b0}$, but one should not substitute this same sum for C in the above equation since this expression holds only for the Pb^{++}–vacancy equilibrium.

It is interesting to note that recent experiments on the diffusion of Cd^{++} in KCl (Harshaw) did not show a large variation in ΔG.[5] If impurities other than Cd^{++} were present, then by the arguments of Reisfeld *et al.* one might expect an apparent large variation in ΔG in this case also.

In the vacancy model of diffusion of divalent-ion–vacancy pairs it is generally assumed that the rate-determining step is the exchange between a divalent ion and its attached vacancy; the movement of the attached vacancy around the divalent ion occurs with a frequency much greater than the divalent-ion–vacancy interchange frequency. This means that the activation energy for diffusion is simply the mobility activation energy of the divalent ion and is not related to the jump activation energy of K^+, as stated by Reisfeld *et al.*

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Errata

Erratum: Exchange Effects on the Electron and Hole Mobility in Crystalline Anthracene and Naphthalene

[J. Chem. Phys. **42**, 733 (1965)]

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WE have found an error in the digital computer program used to calculate the hybrid integrals, and wish to report the values obtained after correction of the program and recomputation. Table I of our paper should be replaced by Table I below.

Because the values of the hybrid integrals originally used were in error, the computed bandwidths and mobility tensor are also in error. We find for the new values, those listed in Tables II, III, and IV. The

TABLE I. Hybrid sums (units 10^{-2} eV).

Molecule coordinates in a, b, c space[a]	$\sum_{i=1}^{a}\langle u_0^k \mid K_n^i \mid u_n^k\rangle$[b]		$\sum_{i=1}^{a}\langle u_0^{k-1} \mid K_n^i \mid u_0^{k-1}\rangle$[b]	
	Naphthalene	Anthracene	Naphthalene	Anthracene
(0, 0, 1)	0.1072	0.0408	−0.0001	0.0268
(0, 1, 0)	−0.5396	−1.529	2.936	3.057
(0, 1, 1)	−0.0078	0.0013	0.0926	0.0091
(1, 0, 0)	0.0003	−0.0134	−0.0142	−0.0110
(1, 0, 1)	−0.0864	0.0435	−0.3850	0.1572
(1, 1, 0)	0.0024	−0.0020	−0.0171	−0.0023
(1, 1, 1)	0.0014	−0.0007	−0.0026	0.0011
$(\frac{1}{2}, \frac{1}{2}, 0)$	1.255	2.789	−1.292	2.187
$(\frac{1}{2}, \frac{1}{2}, 1)$	0.0958	−0.0698	1.135	−0.9685
$(-\frac{1}{2}, \frac{1}{2}, 1)$	0.0016	−0.0012	0.0012	−0.0007
(−1, 0, 1)	0	0	0	0
(−1, 1, 1)	0	0	0	0
$(\frac{1}{2}, \frac{3}{2}, 0)$	−0.0006	0.0001	−0.0021	−0.0007

[a] This gives the vector to the center of the molecule, the unit vectors being the lattice vectors of the crystals in the corresponding directions.
[b] In these, k represents the lowest unfilled orbital of the molecule.

TABLE II. Components of mobility tensor in constant free-time and constant free-path approximations.

	Naphthalene		Anthracene	
	Hole	Electron	Hole	Electron
$\langle V_a^2/\mid \mathbf{V} \mid\rangle$[a]	2.3	13.1	10.0	23.0
$\langle V_b^2/\mid \mathbf{V} \mid\rangle$[a]	26.1	6.8	22.7	9.0
$\langle V_{c'}^2/\mid \mathbf{V} \mid\rangle$[a]	6.5	0.5	4.4	0.8
$\langle V_a V_{c'}/\mid \mathbf{V} \mid\rangle$[a]	0.75	−0.2	2.0	0.06
$\langle V_a^2\rangle$[b]	94	343	454	9.0
$\langle V_b^2\rangle$[b]	1254	164	1171	29.0
$\langle V_{c'}^2\rangle$[b]	234	8.6	178	4.0
$\langle V_a V_{c'}\rangle$[b]	21	−6.2	97	2.1

[a] Constant free-path approximation; units: 10^{-5} cm sec^{-1}.
[b] Constant free-time approximation; units: 10^{-10} cm^2 sec^{-2}.

TABLE III. Widths of excess electron and hole bands (units 10^{-2} eV).

Direction	Naphthalene		Anthracene	
	Hole	Electron	Hole	Electron
a^+	2.6	7.3	7.6	15.1
a^-	1.7	8.1	6.2	14.9
b^+	15.8	4.6	23.6	6.5
b^-	16.8	10.8	10.4	23.7
c^+	10.8	1.2	9.2	0.4
c^-	12.8	0.9	11.2	1.2

TABLE IV. Ratios of components of mobility tensor in constant free-time and constant free-path approximation.

	Hole		Electron		Hole		Electron	
	a	b	a	b	a	b	a	b
μ_{aa}/μ_{bb}	0.07	0.08	2.1	1.9	0.39	0.44	2.6	2.6
$\mu_{c'c'}/\mu_{bb}$	0.19	0.25	0.05	0.07	0.15	0.19	0.03	0.09
$\mu_{c'c'}/\mu_{aa}$	2.5	2.9	0.02	0.04	0.44	0.44	0.01	0.04

[a] Constant free time.
[b] Constant free path.

vibrational overlap squared has the value 1.0 for all the entires in these tables.

Thus, the calculated ratios of the components of the mobility tensor are in fair agreement with experiment for the hole, but not for the electron.

Erratum: Energy-Transfer Processes in Monochromatically Excited Iodine. I. Experimental Results

[J. Chem. Phys. **42**, 3475 (1965)]

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IN Fig. 15, on p. 3487, the cuts for Figs. 15(b) and 15(d) have been transposed in printing. The broad rotational distribution in the left-hand figure is for $\Delta v' = +2$, while that in the right-hand figure is for $\Delta v' = -2$.

Erratum: Analysis of Charge Distributions: Hydrogen Fluoride

[J. Chem. Phys. **40**, 1374 (1964)]

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WITH the sign convention that the direction of positive force corresponds to nuclear repulsion, the Hellman–Feynman force on the fluorine nucleus in LiF obtained from McLean's extended basis set LCAO-MO-SCF function should be −0.102 a.u. (rather than +0.102 a.u. as given on p. 1388 of the paper). This change has no effect on our qualitative conclusions, although quantitatively it strengthens the force criterion evidence that McLean's function is much closer to the molecular Hartree–Fock solution than was the earlier BAMO treatment.

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