

Erratum: Mass-Spectrometric Study of the Reactions of O Atoms with NO and NO2

Fritz S. Klein and John T. Herron

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Errata

Erratum: Polarization Effects in the Ionic Conductivity of Alkali Halide Crystals. II. Current-Time Dependence

[J. Chem. Phys. 43, 2526 (1965)]

A. R. Allnatt, P. W. M. Jacobs, and J. N. Maycock
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N p. 2527 Eq. (6) should read

$$p = p_{\infty} + \sum_{n=1}^{\infty} A_n [\exp(-\lambda_n t)] X_n.$$
 (6)

On p. 2529 Ref. Nos. 13 and 14 should be interchanged. The wrong block was used for Fig. 6. The correct figure is shown below. On p. 2532 the first equation in the

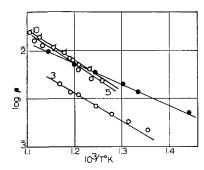


Fig. 6. Plots of $\log \beta$ vs T^{-1} . Open circles, pure KCl; filled circles, KCl+SrCl₂. Lines are identified by run numbers.

first sentence in the right-hand column should read $\log \xi_0 = \log \xi - \frac{1}{2} \text{ eV}/2.303 \text{ kT}$ against T^{-1} .

Erratum: Anomalous ESR Spectrum Spread for Pentacene Anion and Cation Radicals

[J. Chem. Phys. 44, 416 (1966)]

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MPROVED signal to noise in the wing lines of the pentacene cation radical spectrum (via continuous time-averaging technique) has indicated the previously reported values to be incorrect. Due to linewidth variations there are several reasonable combinations but the best seems to be a(1), a(2) = 0.98, 0.76; a(5) = 3.56; a(6) = 2.60. The combination of short lifetime, impurities, and linewidth variations have made these assignments difficult.

Erratum: Thermal Expansion of a Uranium Monocarbide-Zirconium Monocarbide Solid Solution

[J. Chem. Phys. 43, 1736 (1965)]

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(Received 20 January 1966)

THE following two errors should be corrected in Table I on p. 1737:

Column 3, Line 4: for 892 read 982, Column 4, Line 2: for 4.8722₅ read 4.7822₅.

Erratum: Mass-Spectrometric Study of the Reactions of O Atoms with NO and NO₂

[J. Chem. Phys. 41, 1285 (1964)]

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IN an earlier paper¹ the reactions of O atoms with O₂, NO, and NO₂ were discussed in terms of the general mechansim

$$O+XO \xrightarrow{A} [OXO]^* + M \xrightarrow{C} XO_2 + M$$

$$\xrightarrow{D} X+O_2$$

$$\xrightarrow{B} XO + h\nu.$$

The derived rate constants k_B and k_D for the NO₂ reaction were anomalously low (see Footnote 18 of Ref. 1) due to an arithmetic error on our part and the use of a misquoted rate constant from the literature. Table I is a revised form of our original Table II rewritten to more clearly distinguish between measured, derived, and estimated rate constants. k_X is the measured rate constant of the isotopic exchange of O atoms with O_2 , NO, or NO_2 ; k_1 is the rate constant of the reaction $O+XO+M\rightarrow XO_2+M$; and k_2 the rate constant of O+XO₂→XO+O₂. These rate constants in conjunction with the above mechanism permit the ratios k_B/k_C , k_D/k_C , and the rate constant k_A to be calculated. k_B and k_D are derived using estimated values of k_c . The revised values of the rate constants do not affect our qualitative conclusions1 except inasmuch as they predict different lifetimes for the excited inter-

TABLE I. Measured and derived rate constants for the reactions of O atoms with O₂, NO, and NO₂ at 298°K.

	O_2	NO	NO_2
$k_{\mathbf{X}} (\text{cm}^3 \text{mole}^{-1} \cdot \text{sec}^{-1})$	0.6×10 ¹² s	1.1×10 ¹² a	4.2×10 ¹² a
$K_1(\text{cm}^6\text{mole}^{-2}\cdot\text{sec}^{-1})$	2.0×10 ¹⁴ b	3.73×1016 c	10 ¹⁷ d
$k_2(\text{cm}^3\text{mole}^{-1}\cdot\text{sec}^{-1})$		3.8×10 ^{-17 e}	3.28×1012 0
k_B/k_C (mole cm ⁻³)	4.5×10^{-3}	5.9×10^{-5}	6.3×10 ⁻⁵
k_D/k_C (mole cm ⁻³)	4.5×10 ⁻³	1.0×10^{-38}	3.3×10 ⁻⁵
$k_A (\text{cm}^3 \text{mole}^{-1} \cdot \text{sec}^{-1})$	0.9×10^{12}	2.2×10^{12}	9.6×10^{12}
$k_C(\text{cm}^3\text{mole}^{-1}\cdot\text{sec}^{-1})$	4×10 ^{11 f}	1.2×10 ¹² #	8×10 ¹¹
$k_B (\sec^{-1})$	1.8×10^{9}	7.1×10^{7}	5×10 ⁷
$k_D \text{ (sec}^{-1}\text{)}$	1.8×109	1.2×10^{-21}	2.6×10 ⁷

^a J. T. Herron and F. S. Klein, J. Chem. Phys. 40, 2731 (1964).

mediates (OXO)*. Thus NO₂* and NO₃* have comparable lifetime whereas O₃* is about 25 times more labile, as predicted by Benson.²

The lifetime of NO_3^* , $\Gamma_{NO_3}^* \sim 10^{-7}$ sec, although considerably shorter than suggested before, is still sufficiently long to permit internal rearrangement of the asymmetric peroxy configuration to explain isotopic exchange.

Benson and DeMore³ have criticized our choice of a common intermediate for the NO₂ reactions, contending that exchange and formation of NO₃ involve the symmetric form of NO₃* whereas the formation of NO+O₂ involves the peroxy form of NO₃*, ONOO.*

Rate constants calculated on the basis of such a mechanism are the same as those calculated for a mechanism with a common intermediate except that the value of k_A would become 6.3×10^{12} cm³ mole⁻¹·sec⁻¹ and k_D could not longer be derived.

¹ F. S. Klein and J. T. Herron, J. Chem. Phys. **41**, 1285 (1964). ² S. W. Benson, *The Foundations of Chemical Kinetics* (McGraw-Hill Book Co., Inc., New York, 1960), p. 312.

³ S. W. Benson and W. B. DeMore, Ann. Rev. Phys. Chem. **16**, 405 (1965).

Erratum: Some Comparisons of the Classical RRK and the RRKM Theoretical Rate Formulations

[J. Chem. Phys. 43, 4071 (1965)]

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ON p. 4075, right column, 16th line from bottom, change $s = \langle \epsilon_{\rm th}^{\infty} \rangle_f / RT$ to $s = \langle \epsilon_{\rm th}^{+\infty} \rangle_f / RT = (\langle \epsilon_{\rm th}^{\infty} \rangle_f - \epsilon_0) / RT$ (cf. footnotes, Tables VI and VII). On p. 4077, Line 7 from the end of the section, change z to s. On p. 4079, fourth line above table, change RT to sRT, and on p. 4080, second line, change sRT to RT.

In Table XI, last column, last two entries, change 1.21 to 1.48, and 3.74 to 4.33. In Table XIII, last four columns, interchange the frequency descriptions of Models 8 and 9 and in the fourth column from the end change the fifth entry from 0.512 to 0.512–2. In the second column from the end multiply all entries from 1.76–3 to 1.01, inclusive, by 10.

No conclusions or discussion are affected.

b Averaged value from F. Kaufman and J. R. Kelso, J. Chem. Phys. 40, 1162 (1964); and S. W. Benson and A. E. Axworthy, Jr., ibid. 42, 2614 (1965).

c Reference 1.

^d H. W. Ford and N. Endow, J. Chem. Phys. 27, 1156 (1957).

^e F. Kaufman and L. J. Decker, Symp. Combust. 7th London Oxford, 1958, 57 (1959).

f S. W. Benson and A. E. Axworthy, Jr., J. Chem. Phys. 26, 1718 (1957).

Reference 2.