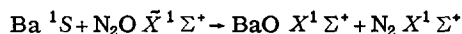is that our original diagram[2] focusses on the transition state region. Our $Ba + N_2O$ correlation diagram, *augmented* by local $Ba + O + N_2$ correlation and energetic arguments, predicts that the adiabatic (spin conserving)

$$Ba\ ^1S + N_2O\ \tilde{X}^1\Sigma^+ \to BaO\ X^1\Sigma^+ + N_2\ X^1\Sigma^+$$

surface *may not be the lowest energy surface in the transition region.* The augmented correlation diagram was drawn in an attempt to clarify an apparently paradoxical situation by suggesting that a smaller activation energy permits a spin nonconserving reaction to occur with larger yield than a spin conserving reaction.[2] Augmented correlation diagrams of the type

$$M + AB \to M + A + B \to MA + B$$
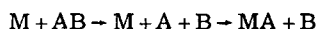
may prove to be useful for understanding reactions which, as in the $Ba + N_2O$ reaction, involve transfer of an initially weakly bound atom.

Several mechanisms have been postulated in an attempt to explain the high BaO $a^3\Pi$ yield from the $Ba + N_2O$ reaction. These include direct but nonadiabatic formation of BaO $a^3\Pi$ from ground state reactants[2]; direct adiabatic formation of BaO $a^3\Pi$ from metastable $Ba\ ^3D$ which is formed by a precursor reaction[5]; direct adiabatic formation of BaO $X^1\Sigma^+(v \gg 0)$ from ground state reactants followed by collision induced transitions into $a^3\Pi^{3b}$; collision induced surface crossing in a long lived $Ba - N_2O$ complex.[5] If only because of its simplicity we continue to prefer the direct nonadiabatic mechanism

$$Ba\ ^1S + N_2O\ \tilde{X}^1\Sigma^+ \to BaO\ a^3\Pi + N_2\ X^1\Sigma^+$$
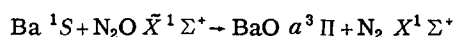
and do not believe that this mechanism is ruled out by the correlation arguments of Husain and Wiesenfeld.[5] It remains to be determined whether the total $Ba + N_2O$ reactive cross section for ground state reactants,[9] measured under single collision conditions, is too large to be consistent with a 20–100% yield of products formed *via* a spin nonconserving reaction which should be well described by the weak spin–orbit coupling limit.

[1]C. R. Jones and H. P. Broida, J. Chem. Phys. 60, 4369 (1974).

[2]R. W. Field, C. R. Jones, and H. P. Broida, J. Chem. Phys. 60, 4377 (1974).

[3](a) D. J. Eckstrom, S. A. Edelstein, and S. W. Benson, J. Chem. Phys. 60, 2930 (1974); (b) S. A. Edelstein, D. J. Eckstrom, and D. L. Huestis, Status Report 2 (March 1974) for SRI Project PYU-3190.

[4]C. J. Hsu, W. D. Krugh, and H. B. Palmer, J. Chem. Phys. 60, 5118 (1974).

[5]D. Husain and J. R. Wiesenfeld, J. Chem. Phys. 62, 2010 (1975), accompanying Comment.

[6]R. W. Field, J. Chem. Phys. 60, 2400 (1974).

[7]Semiempirical estimates of diagonal and off-diagonal spin–orbit matrix elements are made by replacing molecular orbitals of the dominant electronic configuration by a dominant atomic orbital and using the observed spin–orbit splitting of an appropriate atomic state to estimate the radial part of the spin–orbit matrix element.

[8]A. G. Gaydon, *Dissociation Energies and Spectra of Diatomic Molecules* (Chapman and Hall, London, 1968), Appendix 1.

[9]An upper limit of 3×10^{-15} cm^2 is obtained by C. D. Jonah, R. N. Zare, and Ch. Ottinger [J. Chem. Phys. 56, 263 (1972)], who measure reactive plus nonreactive attenuation of a Ba atomic beam by N_2O.

ERRATA

Erratum: Crystal-field model study of the xenon hexafluoride molecule. I. Energy levels and molecular geometry [J. Chem. Phys. 60, 3901 (1974)]

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The calculated t_{1u} bending frequency reported as 109 cm^{-1} on pp. 3908 and 3913 is in error. The zero point energy is also in error. The correct frequency is 240 cm^{-1} using a harmonic oscillator approximation matching the curvature of the potential energy at the C_{4v} radial minimum. Alternatively a fit of the potential $V(x) = -ax^2 + bx^4$ to the position and depth of the C_{4v} radial minimum yields[1] a spacing of 319 cm^{-1} between the first two levels (ignoring inversion splittings) and a zero point energy of 163 cm^{-1}. The reduced mass of 8.7×10^{-23} g molecule^{-1} = 52.4 amu molecule^{-1} used for this mode is $4m_F m_{XeF_2} / m_{XeF_6}$ (m_F and m_{Xe} are fluorine and xenon masses), an expression which is eight times larger than that obtained using Wilson's high frequency approximation[2] for the separation of the t_{1u} bending and stretching modes. However, our treatment is equivalent to the latter, as it is used with a molecular force constant eight times larger than that associated with the t_{1u} symmetry coordinate in Eq. (27) on p. 3906. The t_{1u} displacement is taken as the bond length times the change in a F–Xe–F angle. For the t_{2g} mode our mass is $4m_F$ rather than $\frac{1}{4} m_F$ and is used with a force constant 16 times larger than that associated with the t_{2g} symmetry coordinate in Eq. (27). The displacement for this mode is the bond length times one-half of the change in a F–Xe–F angle. For the t_{2u} mode our mass is $4m_F$ rather than $\frac{1}{2} m_F$ and is used with a force constant eight times larger than that associated with the t_{2u} symmetry coordinate in Eq. (27).

The pseudorotational frequency $2B_e$ estimated as 0.61 cm^{-1} on p. 3908 is in error by a factor of eight and should be 4.9 cm^{-1}. In addition, the value of ΔE_{5s-5p}

for Te(+ 4)in Table III should be 11.10 eV instead of 16.10 eV, the $I(s,0;p,0)$ matrix element in Eq. (20) should contain the factor R_k^{-3} instead of R_k^{-1}, the two references to Eq. (35) in the second column of p. 3911 should be instead to Eq. (40), and the subscript on Q_5

in Eq. (59) for V_{445} (C_{2V}) should be 110 instead of 100.

[1]S. Y. Wang and L. L. Lohr, Jr., J. Chem. Phys. 61, 4110 (1974).
[2]E. B. Wilson, Jr., J. Chem. Phys. 9, 76 (1941).

Erratum: Rates of collision-induced emission from metastable O(^1S) atoms [J. Chem. Phys. 61, 1118 (1974)]

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Table II and associated discussion should be corrected to show that the apparent rate constant for collisionally induced emission from O(^1S) in xenon $(k_g + k_G)$ is 25% of the total deactivation rate constant (k_q), rather than 40% as asserted in the paper.

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Erratum: Some theoretical aspects of chemically-induced dynamic nuclear polarization [J. Chem. Phys. 61, 1517 (1974)]

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Printer's errors were made in Eq. (3.8) and (3.6). They should read

$$P^\infty(\text{R.I.})/\mathcal{F}(\text{R.I.}) = -P_{k=0}^\infty(S) = +P_{k=0}^\infty(T) \ . \tag{3.6}$$

$$\Lambda = k\tau_1/(1 + k\tau_1) \ . \tag{3.8}$$