use large metal atom clusters which give a realistic treatment of molecular chemisorption.[3(b),7,8]

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ERRATA

Erratum: Observation of thelowest triplet transitions $^3\Sigma_g^+ - ^3\Sigma_u^+$ in Na_2 and K_2 [J. Chem. Phys. 80, 4794 (1984)]

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The factor $3hc$ was inadvertently deleted from the denominator of the right-hand side of Eq. (1). The correct expression is

$$k_v(T) = \frac{4\pi^4 \nu D^2 g^* n^2 [R(v)]^2}{3hc|dv/dR|} e^{-V/kT}. \quad (1)$$

The calculations described in the paper were carried out using this correct expression so that the results shown in the figures are valid.

Erratum: The NMR isotope shift in polyatomic molecules. Estimation of the dynamic factors [J. Chem. Phys. 81, 4300 (1984)]

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In Table I the first line should read ^{2}H HD $^{2/1}$H 0.0469 0.2814 − 0.2814. In Table II the first line should read ^{2}H HD $^{2/1}$H 0.0469 0.7413 21.37 − 11.5 and for ^{19}F in HF the theoretical derivative should read − 441 (Ditchfield's value)[1] instead of − 411 (Stevens and Lipscomb's value).[2] The error arose in attributing the − 0.0469 ppm isotope shift to ^{1}H in the H_2–HD system rather than to ^{2}H in the HD–D_2 system. With the above correction, our estimate of $(2\sigma^D/\partial\Delta r_{HD})_e = -11.5$ ppm Å^{-1} comes closer to the more accurate value calculated by Raynes and Panteli (− 12.5 ppm Å^{-1})[3] which included the term in the second derivative $(\partial^2\sigma/\partial\Delta r^2)_e$ in the interpretation of the isotope shift measured by Beckett and Carr.[4] It is worth noting that if we use $(\partial\sigma^D/\partial\Delta r_{HD})_e = -11.5$ ppm $= (\partial\sigma^H/\partial\Delta r_{HH})_e$ to calculate the ^{1}H isotope shift in the H_2–HD system using $(\partial\sigma^H/\partial\Delta r_{HH})_e[\langle r_{HH}\rangle - \langle r_{HD}\rangle]$, we get − 0.038 ppm which is completely consistent with the value − 0.036 ± 0.002 ppm reported by Evans[5] for H_2 and HD dissolved in organic solvents. The difference between Beckett and Carr's − 0.0469 ± 0.0005 ppm and the earlier value of − 0.036 ± 0.002 ppm is not due to the lower accuracy of the latter experiment, or the intermolecular effects of the organic solvent. It is a real difference which is to be expected from the different dynamic factors involved in the two sets of isotopomers.

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