

Reply to “Accuracy of a b i n i t i o C–H bond length differences and their correlation with isolated C–H stretching frequencies”

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Citation: *The Journal of Chemical Physics* **88**, 7257 (1988); doi: 10.1063/1.454336

View online: <http://dx.doi.org/10.1063/1.454336>

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Reply to "Accuracy of *ab initio* C–H bond length differences and their correlation with isolated C–H stretching frequencies"

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(Received 8 February 1988; accepted 23 February 1988)

A major point of our papers^{1,2} is that the experimental C–H vibrational frequencies of *n*-alkanes and cyclohexane correlate with calculated (*ab initio*) bond lengths with a precision of about 10^{-4} Å in bond length or 1 cm^{-1} in frequency. We demonstrated this correlation for *ab initio* calculations in which 4-31G and 6-31G basis sets were used. Schäfer and Siam show that the correlation also holds with 4-21G and 5-31G** basis sets.³ Contrary to the statements in Schäfer and Siam,³ we noted^{1,2} that different basis sets need not give the same slope to provide useful correlations. *Relative differences* between bond lengths can be estimated, with the stated high precision, from these correlations independent of their slope. *Accuracy* is another matter, of course, since *experimental* bond lengths correlate with experimental

frequencies with still a different slope. The difference between the various correlations is discussed in detail in the original publications.^{1,2}

We gratefully acknowledge support from the National Science Foundation (CHE-83-16674) and the National Institutes of Health (GM 27690).

¹R. G. Snyder, A. L. Aljibury, H. L. Strauss, H. L. Casal, K. M. Gough, and W. J. Murphy, *J. Chem. Phys.* **81**, 5352 (1984).

²A. L. Aljibury, R. G. Snyder, H. L. Strauss, and K. Raghavachari, *J. Chem. Phys.* **84**, 6872 (1986).

³L. Schäfer and K. Siam, *J. Chem. Phys.* **88**, 7255 (1988).

ERRATA

Erratum: Electronic states and spectra of 1, 4-naphthoquinone: Evidence for the dual phosphorescence from T_1 $^3(n,\pi^*)$ and T_2 $^3(n,\pi^*)$ states [*J. Chem. Phys.* **87**, 4361 (1987)]

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There is at least one confusing error which the author would like to correct: In the line between Eqs. (5) and (6a), in column 2 on p. 4365, the two matrix elements should be $\langle ^1A_1|H_{so}(b_1)|^3B_1\rangle$ and $\langle ^1B_2|H_{so}(b_1)|^3A_2\rangle$, instead of $\langle ^1A_1|H_{so}(b_1)|^3A_2\rangle$ and $\langle ^1A_2|H_{so}(b_1)|^3B_2\rangle$. Equations (6a) and (6b) are correct as printed.

Another less important error is that the first term on the right-hand side of Eq. (3) should be $k(T_1)$, not $1k(T_1)$.