QUASI-JAHN-TELLER EFFECT IN CHEMICAL REACTIONS

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It will be demonstrated that the quasi-Jahn-Teller effect in chemical reactions is a nuclear quantum effect, T^q, induced by electronic nonadiabaticity[a]. Further, T^q is equivalent to the Diagonal Born-Oppenheimer Correction. Results including and without T^q for a model system will be presented[b]. The research shows clearly that one has to consider this effect in order to obtain various quantities within a spectroscopic accuracy for systems where this effect is no longer negligible.

[a] L. Wang, Chem. Phys. Lett. (a) 285 (1998) 359; (b) submitted.
[b] L. Wang, Chem. Phys. 237 (1998) 305.