QUANTUM CHEMISTRY PREDICTIONS OF MOLECULAR PROPERTIES OF THE ALKOXY RADICALS

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Elements of the electronic spin-rotational tensor have been predicted for the ground electronic state of a series of alkoxy radicals including their possible conformers using the isotope substitution technique. [a] Different types of transformations have been tried and compared. All of these employed the experimentally observed [b] spin-rotational values of ethoxy radical as a reference, while the required rotational constants were obtained by quantum chemical calculations. The predicted values are in good agreement with the experimental ones, and found to be useful parameters to assign the observed rotationally resolved bands to the appropriate conformers.

[a] J. M. Brown, T. J. Sears and J. K. Watson *Mol. Phys.* **41**, 173, 1980.
[b] X. Q. Tan, J. M. Williamson, S. C. Foster and T. A. Miller *J. Phys. Chem.* **97**, 9311, 1993.