THE CO_2 MOLECULE IS NEVER LINEAR

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In spectroscopic parlance, a linear triatomic molecule is one whose potential energy minimum occurs at a linear geometry. We have recently discussed[a] how any linear triatomic molecule will be observed as being bent on ro-vibronic average in any ro-vibronic state.

To provide further support for this idea we make here an *ab initio* calculation of the bending distribution functions for low lying vibrational states of the CO_2 molecule (which is well known to be linear in the sense mentioned above) in its ground electronic state. These functions have their maximum values at a non-linear geometry, and the value zero at linearity, despite the fact that the potential surface has its minimum value at linearity. They are in accord with experimental distribution functions inferred by analysis of Coulomb Explosion Imaging experiments.[b] Thus in a femto-second 'snapshot' of a room temperature ensemble of gas phase rotating-vibrating CO_2 molecules, none would be linear. The same can be said for any triatomic molecule or, for that matter, for any chain molecule with a linear equilibrium structure.

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[a] T. Hirano, U. Nagashima, P. Jensen, H. Li, Journal of Molecular Spectroscopy 362 (2019) 29–36. URL https://doi.org/10.1016/j.jms.2019.05.005; P. Jensen, Canadian Journal of Physics (2020). URL https://doi.org/10.1139/cjp-2019-0395, and references therein.

[b] B. Siegmann, U. Werner, H. O. Lutz, R. Mann, Journal of Physics B: Atomic, Molecular and Optical Physics 35(17) (2002) 3755–3765. URL https://doi.org/10.1088%2F0953-4075%2F35%2F17%2F311; J. P. Brichta, S. J. Walker, R. Helsten, J. H. Sanderson, Journal of Physics B: Atomic, Molecular and Optical Physics 40(1) (2006) 117–129. URL https://doi.org/10.1088%2F0953-4075%2F40%2F1%2F011.