## Multipole Moments and Static (hyper)Polarizabilities of the O<sub>2</sub> molecule for Atmospheric Applications

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The elucidation of the energy transfer processes between oxygen molecules can provide a better understanding of the reactions occurring in the Earth's atmosphere.<sup>1</sup> Although the oxygen molecule does not possess a permanent dipole moment, collision-induced dipoles facilitate the light absorption in the roto-translational region. This effect can potentially change the role of the molecular oxygen in the atmospheric processes. It is therefore crucial to understand the underlying physics of the O<sub>2</sub>-O<sub>2</sub> interaction and how each molecule is polarized in the electric field of its neighbor. To this end, we have calculated several multipole moments, polarizabilities and hyperpolarizabilities for O<sub>2</sub> at different bond lengths, at both the MRCl<sup>2</sup> and CASPT2<sup>3,4</sup> levels employing the d-aug-cc-pVXZ and aug-cc-pVXZ basis sets of Dunning<sup>5</sup>, where X = D,T,Q, and 5. Our multipole moments and polarizabilities are compared to earlier values, <sup>6,7,8</sup> and will be plugged in the long range approximation expressions for the O<sub>2</sub>-O<sub>2</sub> interaction energy and collision induced dipole moment. Finally, the potential energy curves for O<sub>2</sub> in its ground electric state have been used for the calculation of the vibrationally averaged electric properties of O<sub>2</sub> for the first six vibrational levels ( $\nu$ =0-5).

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