

Quantum Chemical Predictions of Dipole Moments and Dipole Polarizabilities for Known and Postulated Astromolecules

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Quantum chemical calculations of dipole moments and dipole polarizabilities were performed for about 200 neutral molecules with up to 12 atoms that are known or postulated to be present in interstellar or circumstellar sources in order to make new predictions for chemical rate coefficients of ion-molecule reactions. Optimized structures and the response properties were computed at the RCCSD(T) level with basis sets as large as aug-cc-pVTZ, depending on the size of the molecule. Comparisons are made to existing experimental data, which are particularly limited in the case of dipole polarizabilities.

The predictions are available online at <http://www.astrochymist.org/properties/>.

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