QUANTUM CHEMICAL PREDICTIONS OF THE DIPOLE MOMENTS AND DIPOLE POLARIZABILITIES FOR 200+ KNOWN AND POSTULATED NEUTRAL ASTROMOLECULES

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Quantum chemical calculations of dipole moments and dipole polarizabilities were carried out 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 of chemical rate coefficients for ion-molecule reactions. Optimized structures and the response properties were computed at the RCCSD(T) level of coupled cluster theory with basis sets as large as aug-cc-pVTZ, depending on the size of the molecule. The accuracy of the predictions was assessed against existing experimental data, which is particularly limited in the case of dipole polarizabilities. In addition to appearing in publication form, the predictions are available online at http://www.astrochymist.org/properties.