S-O Valence force constants of sulfoxides by quantum chemical methods

Victor Vargas,

Morales, Raul G.E.

S-O stretching force constants in a series of synmetrical sulfoxide compounds were calculated from quantum chemical methods. Molecular geometries were obtained from experimental data and from MNDO and PM3 calculations. S-O bond potential energy curves were constructed around the zero-point energy and the MNDO force constants calculated in the armonic approximation were compared to force constants calculated in a point-charge bond model in the CNDO approximation. The present force constants range between 5 and 12 mdyn/A.