Ab Initio and DFT Calculations of Eight Membered Chalcogen Rings Using Effective Core Potentials

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We have carried out *ab initio* and density functional calculations using Stuttgarts relativistic large core effective core potentials with two polarization functions implemented on 87 different $E_nE'_{8-n}$-rings (E, E' = S, Se, Te; n = 0-8).

The geometrical opimizations and frequency calculations were done using HF-level of theory. The nuclear magnetic shielding tensor calculations were done using GIAO method at DFT level using B3PW91.

There is a good agreement with the experimental structural and vibrational data where available.[1] The results from the energy calculations show, that $E_nE'_{8-n}$-rings tend to favour structures that have more homoatomic chalcogenbonds.

The calculated isotropic magnetic shielding parameters were compared with the experimental ^{77}Se and ^{125}Te NMR chemical shifts where available.[1, 2] There is a clear correlation between the experimental and the computed values. However, because the ECPs involve only the outer core electrons in to the calculations, the results are comparable only within a group of molecules with very similar structure.

1. Laitinen R.S., Pekonen P., Suontamo R.S., *Coord. Chem. Rev.*, **130**, 1-62 (1994)
2. Laitinen R.S., Pakkanen T.A., *Inorg. Chem.*, **26**, 2598-2603 (1987)