Tetrel bond between X2TO (T= C, Si, Ge, Sn; X = H, F, Cl, Br, CH3) and CO2. An effective absorbent for CO2

Mingchang Hou[1], Zhenbo Liu[1], and Qingzhong Li[1]

[1]Yantai University

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Abstract

Quantum chemical calculations are applied to study the complexes between X2TO (X=H, F, Cl, Br, CH3; T=C, Si, Ge, Sn) and CO2. The carbon atom of CO2 as a Lewis acid participates in the O***C carbon bond, whereas its oxygen atom as a base engages in the O***T tetrel bond with X2TO. Most of complexes are stabilized by a combination of both O***C and O***T interactions. The interaction energies are dependent on the nature of T and X atoms/groups. Both the electron-withdrawing halogen group and the electron-donating methyl group increase the interaction energy, up to 51 kJ/mol in F2SiO***CO2. One F2SiO molecule can bind with different number of CO2 molecules from one to four; as the number of CO2 increases, the average interaction energy for each CO2 is decreased but it can contribute at least 27 kJ/mol stabilization energy. Therefore, silicon-containing molecules are good absorbents for CO2.

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