



Electron localization function (ELF) study on intramolecular delocalization of the electron density in the H_2X , $H_2C=X$ and XO_2 ($X = O, S, Se, Te$) molecules: role of the atomic core and lone pair.

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Streszczenie

A nature of the chemical bond and delocalization of the electron density in the H_2X , $H_2C@X$ and XO_2 ($X = O, S, Se$ and Te) molecules is systematically studied by means of the topological analysis of the electron localization function (ELF). The covariance parameter $cov[XI, Xj]$, which reveals a correlation between the electron density distributions in basins XI and Xj is analyzed. Going from the oxygen to tellurium atom one observes gradual decrease of the electron delocalization between the lone pairs of chalcogen: $V1(X)MV2(X)$ and increase of delocalization between the lone pairs and core basin $V1(X)MC(X)MV2(X)$. In H_2O , H_2S and $H_2C@O$, $H_2C@S$ dominates an exchange between lone electron pairs: $cov[V1(X), V2(X)] > cov[V1(X), C(X)]$, meanwhile for Se and Te containing molecules prevails a delocalization with core region: $cov[V1(X), C(X)] > cov[V1(X), V2(X)]$. It is proposed that this effect is associated with not negligible penetration of d electrons from the outermost shell of the atomic core into valence shell. A study on the O_3 molecule reveals dominating delocalization between the lone pair $V(O)$ and electron density of the $O-Oi=1,2$ bonds: $V(O, Oi=1)MV(O)MV(O, Oi=2)$, meanwhile an exchange between the chalcogen core $C(X)$ and lone pair $V(X)$: $C(X)MV(X)$ prevails in SO_2 , SeO_2 and TeO_2 .

Słowa kluczowe

Electron localisation function, Ab initio calculations, Selenium compounds, Sulphur compounds, Tellurium compounds, Chemical bond

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