

MS14-P39 | STEREOCHEMISTRY OF Tl(I) IN INORGANIC OXYALS

Markovski, Mishel (Saint Petersburg State University, Sankt-Petersburg, RUS); Siidra, Oleg (Saint Petersburg State University, Sankt-Peterburg, RUS)

183 monovalent thallium oxysalts for which good refinements exist were reviewed. 303 Tl^+-O_n and 11 $Tl^+-O_nX_m$ ($X = F, Cl, Br$) polyhedra consisting of 2449 Tl^+-O ($\leq 3.55 \text{ \AA}$) and 74 $Tl-X$ ($\leq 3.7 \text{ \AA}$) bonds were taken into consideration. Bond-valence calculations and geometrical parameters ($[\Delta]$ displacement parameter, $[Pd]$ distortion, $[V_p]$ polyhedral volume, $[R_{sph}]$ sphere radius, $[V_{sph}]$ sphere volume, $[S]$ sphericity, $[ECC_l]$ linear eccentricity and $[ECC_v]$ volume eccentricity) were calculated in order to evaluate the influence of the 'lone pair' (LP) stereoactivity on the distortion of $Tl-O_n$ polyhedra. In 2/3 of complexes the LP stereoactivity is pronounced. Complexes with active LP are generally built of strong $Tl-O$ bonds ($\leq 3 \text{ \AA}$). $Tl-O_n$ polyhedra were classified into five types: I-hemidirected convex, II-hemidirected concave, III-equatorial, IV-bisdirected and V-holodirected. Different geometrical parameters and trends for each type were evaluated and will be discussed.

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