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Crystal Structure of Benzylidene-1,3-indandiones

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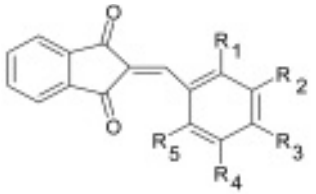
Benzylidene-1,3-indandiones exhibit solid state and solution non-linear optical properties. In the course of structural investigation of indandione derivatives monocrystals of the compound **I-V** were obtained.



I $R_1=R_2=R_4=R_5=H$, $R_3=OH$;
II $R_1=R_2=R_4=R_5=H$, $R_3=NPh_2$;
III $R_1=Me$, $R_2=R_4=R_5=H$, $R_3=NMe_2$;
IV $R_1=OMe$, $R_2=R_4=R_5=H$, $R_3=NMe_2$;
V $R_1=OMe$, $R_2=R_5=H$, $R_3=N(CH_2CH_2Ac)_2$; $R_4=OMe$.

Crystal data are:
I $a=5.1881(2)$, $b=14.5301(7)$, $c=15.7627(9)$ Å; $P\,2_1nb$, $Z=4$
II $a=6.9497(3)$, $b=8.1944(3)$, $c=18.196(1)$ Å, $\alpha=81.226(2)$, $\beta=86.050(2)$, $\gamma=86.093(2)°$; $P(1$, $Z=2$
III $a=9.4410(3)$, $b=9.1493(3)$, $c=17.3840(8)$ Å, $\beta=95.638(1)°$; $P\,2_1/c$, $Z=4$
IV $a=7.6954(1)$, $b=8.3213(2)$, $c=24.0894(6)$ Å; $P\,2_12_12_1$, $Z=4$
V $a=9.8768(4)$, $b=11.1550(4)$, $c=11.6796(6)$ Å, $\alpha=107.120(2)$, $\beta=92.429(2)$, $\gamma=100.776(1)°$; $P(1$, $Z=2$
The X-ray crystallographic study indicates, that indandione system and phenyl ring in **I-V** are near to coplanar. The crystal packing of these compounds is characterized by stacking interactions.

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Specific Features of the Lanthanides Stereochemistry in the Structures of Halide Containing Compounds

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Keywords: lanthanide halides, structure and properties, Voronoi-Dirichlet polyhedron

Voronoi-Dirichlet (VD) polyhedra and the intersecting spheres method were used to perform crystal-chemical analyses of 337 compounds containing in their structures 485 types of monoligand complexes $LnHal_n$ (Ln = La - Lu, Hal = F, Cl, Br or J). Primary crystal-structure information was selected from databases on the structures of inorganic [1] and coordination [2] compounds. All the necessary calculations such as determination of atoms coordination numbers (C.N.), the lanthanides VD polyhedra characteristics calculation and their analysis have been done by means of the TOPOS program package [3]. It was found out that, in the structures of compounds under discussion containing different halides the C.N.s of the Ln very from 6 to 12, 10 different types of $LnHal_n$ (n = 6 - 12) coordination polyhedra exist in the structures. Our findings show that, though the average interatomic distances Ln-Hal increase with an increase in C.N. and various types of coordination polyhedra shapes exist in the structures of compounds under discussion, but the VD polyhedra volume of the Ln atoms depends for all C.N. only on nature and oxidation state of the Ln and nature of the Hal atoms. This fact allows us to use the radius of the sphere with volume equal to the volume of the corresponding VD polyhedron (R_{SD}) as one-dimensional characteristic of the lanthanides atoms in crystal structures. Our results are evidence in favour of the idea that comlexing atoms in crystals should be treated as soft, easily deformable spheres of constant volume. The R_{SD} (Ln(III)) in a series Ln = La - Lu obey lanthanides contraction rule Our findings made it possible to determine Ln oxidation state for some intriguing cases, to establish substances with anisotropic conductivity and find out some misprints made while put structure information in databases [1] and [2].

[1] Inorganic crystal structure database. FIZ Karlsruhe & NIST Gaithersburg. 2004.
[2] Cambridge structural database system. November 2004 Release.
[3] Blatov, V.A., Shevchenko, A.P. & Serezhkin, V.N. (1999) Russ. J. Coord. Chem. 25, 453-456.