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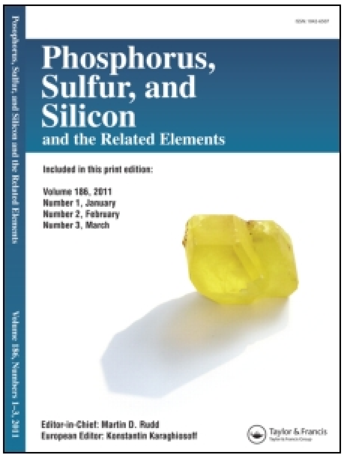

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STRUCTURES OF ARYLSELENENYL IODIDES: THE ROLE OF ARYL STACKING AND „SOFT-SOFT“ SE···I AND I···I INTERACTIONS

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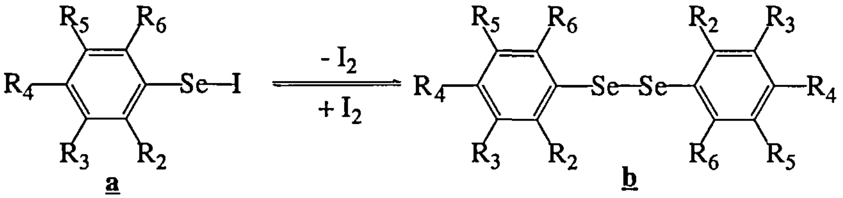
The influence of packing effects and Se...I / I...I interactions on the stability of Iodoselanes are discussed.

Keywords: selenium, iodoselanes, secondary interactions, packing effects



1a, 1b R_2, R_4, R_6 = *t* - Bu // R_3, R_5 = H
2a, 2b R_2, R_4, R_6 = *i* - Prop // R_3, R_5 = H
3a, 3b R_2, R_4, R_6 = Me // R_3, R_5 = H
4a, 4b R_2, R_3, R_5, R_6 = Me // R_4 = H

When 2,4,6-t-$Bu_3C_6H_2SeI$ **1a** was characterised as first stable solid selenenyl iodide, it was assumed, that its existence was due to steric destabilisation of the congested diselenide (2,4,6-t-$Bu_3C_6H_2Se)_2$ **1b** [1].

The less crowded selenenyl iodide 2,4,6-i-$Pr_3C_6H_2SeI$ **2a**, exists in solution in equilibrium with its parent diselenide (2,4,6-i-$Pr_3C_6H_2Se)_2$ **2b**. However, **2a** cannot be isolated. The solid product from **2a/2b** is (Fig.1) an inclusion compound of two equivalents of **2b** with one I_2 molecule [2.].

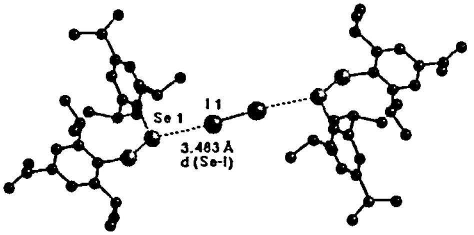


FIGURE 1: Iodine inclusion between two molecules of (2,4,6-i-$Pr_3C_6H_2Se)_2$ (**2b**)

Like **1a** and **2a**, even less crowded 2,4,6-$Me_3C_6H_2SeI$ **3a** exists in solution in equilibrium with its parent diselenide (2,4,6-$Me_3C_6H_2Se)_2$ **3b**. In this case, however, the selenenyl iodide **3a** was isolated as pure solid.

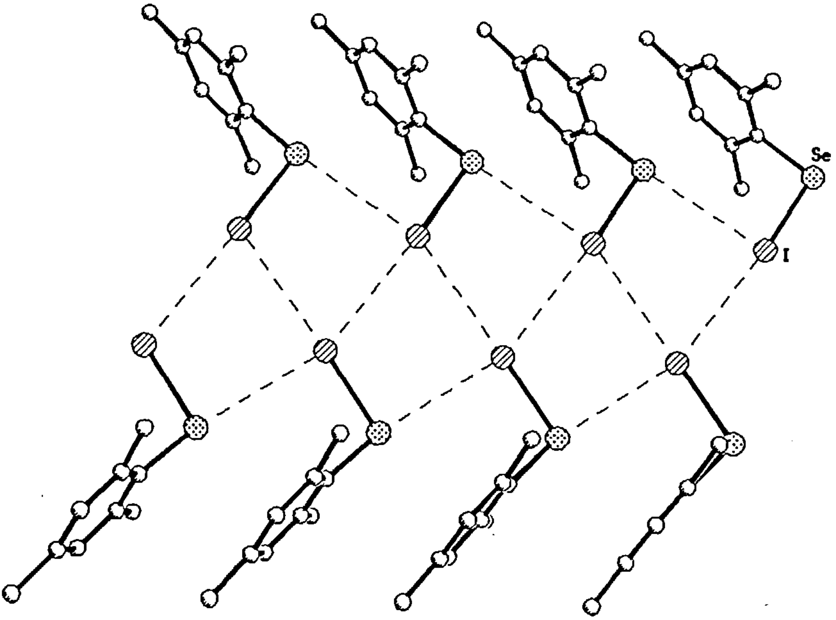
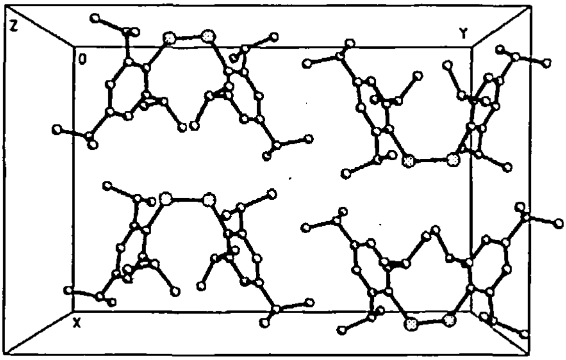


FIGURE 2: Interactions within the layers of 2,4,6-$Me_3C_6H_2SeI$ (3a); [d(Se-I): 383.9 pm ; d(I-I): 384.1 pm]

In the solid state structure of selenenyl iodide **3a** (Fig.2) aryl stacking of the mesityl groups is accompanied by significant intermolcular Se⋯I and I⋯I contacts (L-type patterns related to those of $(I_2)_2$).

The comparison of the structures of diselenide **2b** and **3b** is very interesting (Fig.3): The 2,4,6-i-$Pr_3C_6H_2Se$ substituents of **2b** do not allow fair aryl stacking but allow I_2 intercalation! The structure of diselenide **3b**, however, involves slipped-sandwich-like aryl stacking of the mesityl groups.

2b



3b

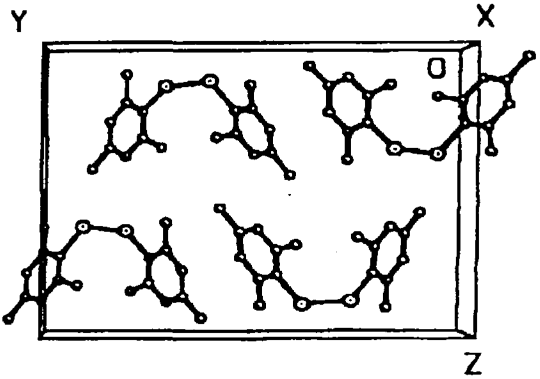
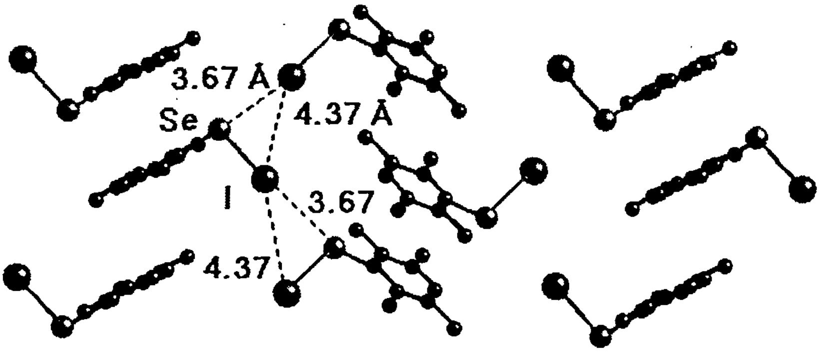


FIGURE 3: Packing of Tip_2Se_2 (**2b**) in comparison with Mes_2Se_2 (**3b**)

The structure of solid 2,3,5,6-Me_4C_6HSeI **4a** is related to that of **3a** (Fig.4): the stability of the Se-I bond in the solid compound **4a** (in equlilibrium with the diselenide (2,3,5,6-$Me_4C_6HSe)_2$ **4b** in toluene solution) will to a significant part be due to favourable intermolecular soft-soft interactions within the columnar structure. Channels of weak soft-soft interactions between Se-I moities of the molecules are bridged by staples of aromatic durene groups.

It appears, that not only steric destabilisation of molecular diselenides may favour the existence of molecular R-Se-I compounds, but also „packing effects" i.e.: cooperative Se¨I and I¨I interactions combined with favourable aryl stacking.



4a

FIGURE 4: Columnar packing of 2,3,5,6-Me_4C_6HSeI (4a) with closest intermolecular Se...I and I...I distances; Bondlength Se-I: 2.53 Å

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[1.] W.-W. du Mont, S. Kubiniok, Angew. Chem. 99, 820 (1987) 8

[2.] W.-W. du Mont, A. Martens-von Salzen, Phosphorus, Sulfur, and Silicon, Vol. 67, 1-4 (1992), 67 - 71