

Layered triaqua(phenylselenonato)lithium(I)

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Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
 R factor = 0.042
 wR factor = 0.088
Data-to-parameter ratio = 14.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $[\text{Li}(\text{C}_6\text{H}_5\text{O}_3\text{Se})(\text{H}_2\text{O})_3]$, shows an extensive hydrogen-bonding network in the solid state, forming complex layers parallel to the crystallographic bc plane. The interlayer distance is 11.336 (12) Å. The molecules pack in an alternating up–down fashion in the plane of the layers so that the SeO_3 and $\text{Li}(\text{H}_2\text{O})_3$ groups are adjacent, creating a double net of hydrogen bonding between the two groups. Each of the six H atoms of the water molecules forms hydrogen bonds, with five to O atoms of the phenylselenonate and one to the O atom of a neighboring water molecule. The Li cation has a tetrahedral geometry formed by one O atom of the phenylselenonate anion and three water molecules. The Li–O distances are in the range 1.896 (8)–1.921 (9) Å to the water molecules and 1.988 (8) Å to the phenylselenonate.

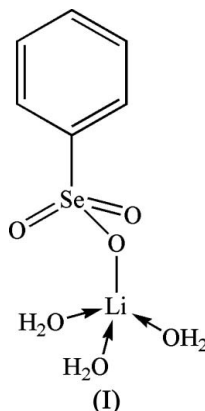
Received 5 January 2006

Accepted 26 January 2006

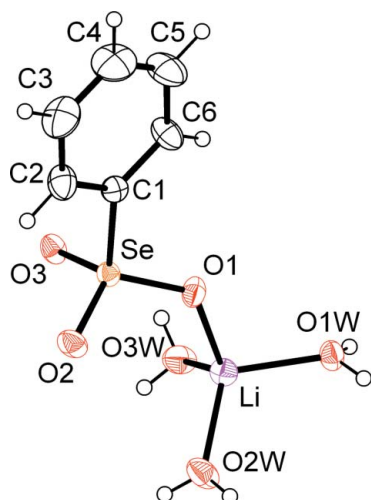
Online 3 February 2006

Comment

Organoselenonates are little studied but offer a coordination chemistry similar to those of the better known organosulfonates (Côté & Shimizu, 2003; Kennedy *et al.*, 2004) and organophosphonates (Clearfield, 2002; Vioux *et al.*, 2004). These coordinating anions usually form laminar structures in the solid state. Continuing our interest in the coordination chemistry of alkali metals (Siquiera *et al.*, 2005), we synthesized phenylselenonic acid and prepared its lithium salt. Crystallization from an aqueous acetone solution produced the title compound, (I) (Fig. 1). Table 1 lists selected distances and angles for (I).



Each Li^+ cation is tetrahedrally coordinated by O atoms from three different water molecules and one O atom from the PhSeO_3^- anion (Table 1). The Se–O distances of the PhSeO_3^- anion are equal within experimental error (Table 1), showing a delocalization of the negative charge across all three O atoms. The molecules of (I) pack in an alternating up–


Figure 1

An ORTEP-3 (Farrugia, 1997) representation (30% probability displacement ellipsoids) of (I), showing the atom numbering scheme.

down fashion across centers of inversion so that the SeO_3 and $\text{Li}(\text{H}_2\text{O})_3$ groups are adjacent in two parallel planes. Each of the six H atoms of the water molecules forms hydrogen bonds, with five to O atoms of the phenylselenonate anion and one to the O atom of a neighboring water molecule (Table 2). This results in a double net of hydrogen bonding that forms a complex two-dimensional layer structure parallel to the crystallographic bc plane (Figs. 2, 3 and 4).

Experimental

Single crystals of the title compound were formed from the slow evaporation of an acetone–water solution (2:1 v/v) of lithium phenylselenonate in a desiccator.

Crystal data

$[\text{Li}(\text{C}_6\text{H}_5\text{O}_3\text{Se})(\text{H}_2\text{O})_3]$
 $M_r = 265.05$
 Monoclinic, $P2_1/c$
 $a = 11.3410$ (11) Å
 $b = 7.6180$ (8) Å
 $c = 12.3021$ (13) Å
 $\beta = 91.720$ (6)°
 $V = 1062.37$ (19) Å³
 $Z = 4$

$D_x = 1.657$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 872 reflections
 $\theta = 3.2$ – 19.0°
 $\mu = 3.53$ mm⁻¹
 $T = 296$ (2) K
 Plate, colorless
 $0.10 \times 0.10 \times 0.02$ mm

Data collection

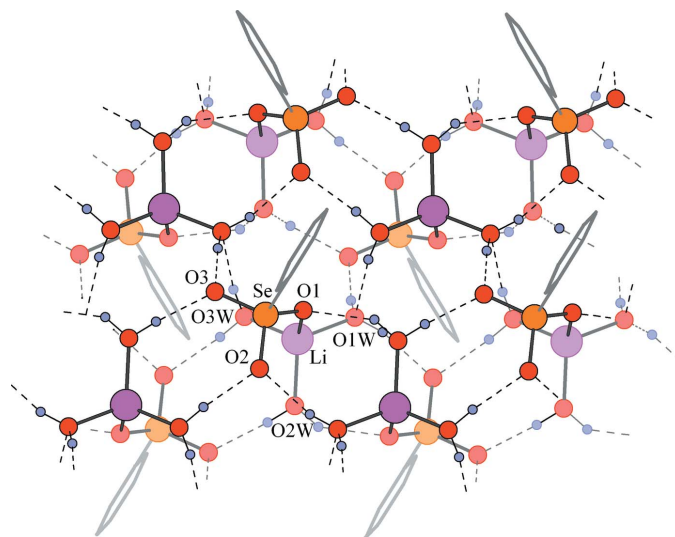
Bruker APEXII CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2004)
 $T_{\min} = 0.63$, $T_{\max} = 0.93$
 8507 measured reflections

2147 independent reflections
 1364 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.082$
 $\theta_{\text{max}} = 26.4^\circ$
 $h = -14 \rightarrow 14$
 $k = -9 \rightarrow 9$
 $l = -15 \rightarrow 14$

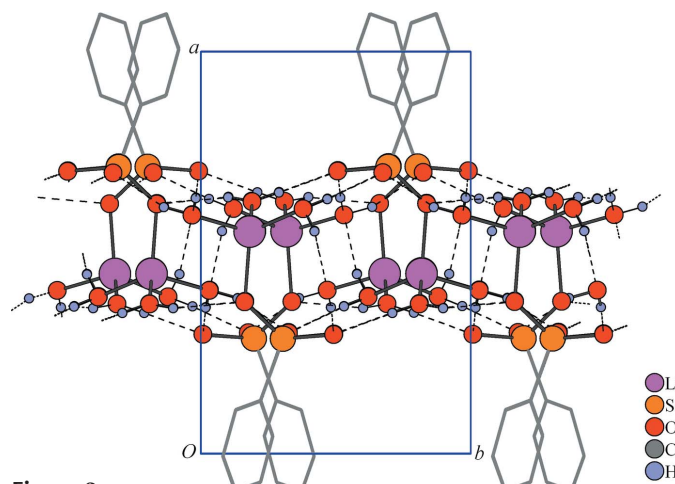
Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.088$
 $S = 0.99$
 2147 reflections
 151 parameters

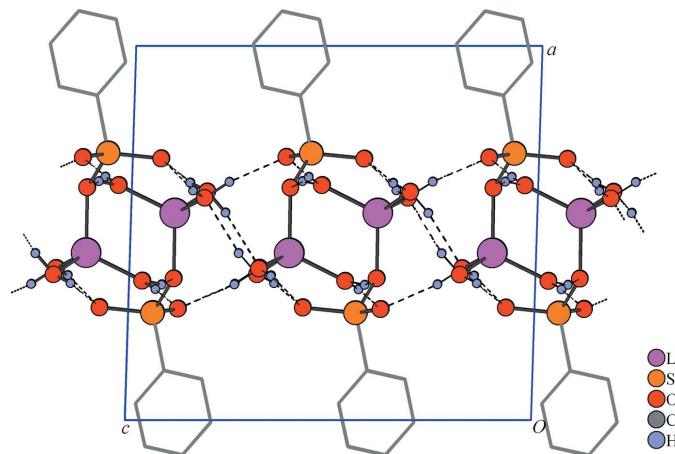
H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0351P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.66$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.58$ e Å⁻³


Figure 2

A view of the hydrogen-bonding (dashed lines) network in (I). The vertical direction is parallel to the c axis and the horizontal direction is parallel to the b axis. The phenyl groups are represented by line figures. H atoms attached to C have been omitted.


Figure 3

View of (I) perpendicular to the ab plane. The phenyl groups are represented as solid grey lines and hydrogen bonds as dashed lines. H atoms attached to C have been omitted.


Figure 4

View of (I) perpendicular to the ac plane. The phenyl groups are represented as solid grey lines and hydrogen bonds as dashed lines. H atoms attached to C have been omitted.

Table 1

Selected geometric parameters (Å, °).

Li1—O1W	1.921 (9)	Se1—O1	1.626 (3)
Li1—O2W	1.896 (8)	Se1—O2	1.622 (3)
Li1—O3W	1.911 (9)	Se1—O3	1.627 (3)
Li1—O1	1.988 (8)		
O2W—Li1—O1W	110.4 (4)	O1W—Li1—O1	100.8 (4)
O3W—Li1—O1W	109.8 (4)	O2—Se1—O1	112.75 (16)
O2W—Li1—O3W	106.3 (4)	O2—Se1—O3	111.74 (16)
O2W—Li1—O1	115.6 (4)	O1—Se1—O3	110.58 (16)
O3W—Li1—O1	113.8 (4)	Se1—O1—Li1	126.7 (3)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H11...O2 ⁱ	0.83 (3)	2.04 (3)	2.852 (5)	166 (5)
O1W—H12...O3 ⁱⁱ	0.86 (3)	1.91 (3)	2.767 (5)	171 (6)
O2W—H21...O1 ⁱ	0.80 (2)	2.12 (3)	2.856 (6)	154 (5)
O2W—H22...O3 ⁱⁱⁱ	0.83 (2)	1.96 (3)	2.781 (6)	176 (5)
O3W—H31...O1W ^{iv}	0.85 (3)	2.05 (3)	2.883 (5)	168 (6)
O3W—H32...O2 ⁱⁱⁱ	0.83 (3)	2.02 (3)	2.836 (5)	170 (6)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, -y, -z+1$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

All H atoms were located in a difference Fourier map. Phenyl H atoms were placed at idealized positions, with C—H distances of 0.93 Å, and refined using a riding model, with $U_{\text{iso}}(\text{H})$ values of $1.2U_{\text{eq}}(\text{C})$. Water H atoms were restrained to a model geometry with O—H and H...H distances of 0.865 (10) and 1.369 (3) Å, based on the average for 81 Li-bound water molecules measured at room temperature found in the Cambridge Structural Database (Version

5.26, update of August 2005; Allen, 2002); $U_{\text{iso}}(\text{H})$ values of $1.5U_{\text{eq}}(\text{O})$ were used.

Data collection: *COSMO/APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Financial support from the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), grants 478831/2003-0 and 475294/2004-1, is gratefully acknowledged, as are fellowships (RAB) from CNPq. The diffractometer was funded by a CT-INFRA grant from the Financiadora de Estudos e Projetos (FINEP).

References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
- Bruker (2004). *APEX2* (Version 1.0.22), *COSMO* (Version 1.48), *SAINT* (Version 7.06A) and *SADABS* (Version 2.10). Bruker AXS Inc., Madison, Wisconsin, USA.
- Clearfield, A. (2002). *Curr. Opin. Solid State Mater. Sci.* **6**, 495–506.
- Côté, A. P. & Shimizu, G. K. H. (2003). *Chem. Eur. J.* **9**, 5361–5370.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Kennedy, A. R., Kirkhouse, J. B. A., McCarney, K. M., Puisegur, O., Smith, W. E., Staunton, E., Teat, S. J., Cherryman, J. C. & James, R. (2004). *Chem. Eur. J.* **10**, 4606–4625.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Siquiera, M. R., Facco, J. T., Lang, E. S., Lorenzini, F., Rizzatti, M. R., Ellena, J. & Burrow, R. A. (2005). *Acta Cryst.* **C61**, m161–m164.
- Vioux, A., Le Bideau, J., Mutin, P. H. & Leclercq, D. (2004). *Top. Curr. Chem.* **232**, 145–174.