$60^\circ \leqslant \alpha \leqslant 120^\circ$; $0^\circ \leqslant \beta \leqslant 54^\circ$ or $136^\circ \leqslant \beta \leqslant 180^\circ$; $51^\circ \leqslant \gamma \leqslant 129^\circ$;

$120^\circ \geqslant \alpha' \geqslant 60^\circ$; $180^\circ \geqslant \beta' \geqslant 136^\circ$ or $54^\circ \geqslant \beta' \geqslant 0^\circ$; $129^\circ \geqslant \gamma' \geqslant 51^\circ$.

These ranges may be compared with the angles found of 74°, 33°, 62°, and 116°, 136°, 57°, respectively.

The values for the measured structure factors were derived from the intensities in the usual way, applying Waser's (1951) Lorentz and polarization correction in the zero layer measured with the precession camera, and the Tunell (1939) rotation factor for the upper-layer equi-inclination Weissenberg intensities. The calculated structure factors are based on the atomic coordinates given in Table 2. The least-squares and structure-factor calculations were carried out on International Business Machines. A Patterson series was computed on Whirlwind* (the Massachusetts Institute of Technology high-speed digital computer) and the Fourier series were summed, with the aid of Beevers–Lipson strips, at intervals of $a/60$, $b/30$ and $c/30$. The positions of the contour lines were obtained from the summation totals by careful interpolation on a scale of 5 cm. and 6 cm. to 1 Å, in directions parallel with each axis.

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The Crystal Structure of Di-*p*-Tolyl Selenide*

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Di-*p*-tolyl selenide forms orthorhombic crystals, space group $P2_12_12_1$, with a unit cell of constants $a = 25{\cdot}12$, $b = 7{\cdot}99$ and $c = 5{\cdot}88$ Å, containing four molecules. The crystal structure has been determined, and the 45 positional parameters refined by double-Fourier-series and least-squares methods, employing 401 terms. The intensities were measured visually by two observers. The Se–C distance is 1·93 Å and the C–Se–C valence angle is 106°. The normals to the two aromatic rings form an angle of 55° with each other.

Introduction

A series of investigations on the crystal structures of organo-selenium compounds have been reported by McCullough and his co-workers, and their results are summarized in Table 1. The present crystal has been

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Table 1. *Values of the* Se–C *bond distance and the* Se *valency angle*

Molecule	Se–C distance (Å)	C–Se–X angle (°)	Reference
Di-*p*-tolyl selenium dichloride	$1{\cdot}93\pm0{\cdot}03$	$106{\cdot}5\pm1$	McCullough & Marsh (1950)
Di-*p*-tolyl selenium dibromide	$1{\cdot}95\pm0{\cdot}03$	108 ± 1	McCullough & Marsh (1950)
Diphenyl diselenide	$1{\cdot}93\pm0{\cdot}05$	$104{\cdot}6$, $107{\cdot}5\pm2$	Marsh (1952)
p,p'-Dichlorodiphenyl diselenide	$1{\cdot}86\pm0{\cdot}04$	$101{\cdot}7$, $100{\cdot}2\pm1$	Marsh, Kruse & McCullough (1953)
Benzeneseleninic acid	$1{\cdot}903\pm0{\cdot}021$	$99{\cdot}0$, $98{\cdot}5\pm0{\cdot}9$	Bryden & McCullough (1954)

studied to examine further the bond distribution in divalent selenium as well as to determine whether the selenium–carbon distance changes from the above values when the selenium atom is linked directly only to two aromatic rings.

Crystal data

Di-*p*-tolyl selenide, (p-$CH_3.C_6H_4)_2Se$; m.p. 69·5° C.; $D_{\text{meas.}} = 1{\cdot}45$ g.cm.$^{-3}$ (measured by flotation in aqueous $ZnCl_2$ solution); $D_{\text{calc.}} = 1{\cdot}47$ g.cm.$^{-3}$; orthorhombic with

$$a=25{\cdot}12\pm0{\cdot}02,\ b=7{\cdot}99\pm0{\cdot}02 \text{ and } c=5{\cdot}88\pm0{\cdot}02 \text{ Å};$$

absent spectra: ($h00$) only when $h = 2n+1$, ($0k0$) only when $k = 2n+1$ and ($00l$) only when $l = 2n+1$. The space group is uniquely $P2_12_12_1$. There are four molecules per unit cell. No molecular symmetry is required. The absorption coefficient for Mo $K\alpha$ radiation ($\lambda = 0{\cdot}7107$ Å) is 33·5 cm.$^{-1}$, and for Cu $K\alpha$ ($\lambda = 1{\cdot}5418$ Å) is 42·0 cm.$^{-1}$. The volume of the unit cell is 1180·1 Å^3. The total number of electrons per unit cell, $F(0, 0, 0)$, is 528.

Analysis of the structure

The great similarity between the cell dimensions of this crystal and those of di-*p*-tolyl telluride (Blackmore & Abrahams, 1955*a*), together with the space-group identity, suggested the possibility of isomorphism in the two crystals. The general similarity in the corresponding intensities strengthened this chance. Accordingly, structure factors were computed with atomic positions in the present crystal being identical with an almost refined set of coordinates for the telluride structure. The temperature factor B in the expression $\exp\{-B[(\sin\theta)/\lambda]^2\}$ was found by Wilson's (1942) method to be 4·0 Å^2. The agreement factor R_1 between the observed and calculated structure factors thus obtained was about 0·45 in both the ($hk0$) and ($h0l$) layers.

Three Fourier series in the ($h0l$) layer based upon this trial model led to no further changing of structure-factor signs, and the final electron-density map is shown in Fig. 1(*a*). At this stage, $R_1(h0l) = 0{\cdot}20$. Five least-squares cycles then further reduced R_1 to 0·150, and this value remained stationary when a sixth cycle was performed. The process of refinement was then taken as having converged. As was the case with di-*p*-tolyl telluride (Blackmore & Abrahams, 1955*a*), the off-diagonal terms were omitted in applying the method of least squares, and all observations were given a weight of unity, except for $F(020)$ and $F(210)$, which appeared to suffer from extinction. These planes were given zero weight.

In the ($hk0$) layer, four Fourier series led to the projection in Fig. 1(*b*). Preparatory to the application of the method of least squares, it was observed that the scale factor was not constant, but varied with k. The scale factor was taken as $F_o = A.F'_o$, where $A = \sum\limits_{hk}|F_cF'_o| \div \sum\limits_{hk}|F'_o|^2$. When the expression $D = (1/n)\Sigma(|F_c| \div |F_o|)$ (where the sum is over all h associated with a constant k, and n is the number of F_o with this index k) was examined, it was found that D steadily increased for $k > 6$. Thus for $k \leqslant 6$, D was close to unity, but for $k = 10$, $D = 2{\cdot}7$. This variation could be written in the form $D\exp(-uk^m) = 1$, where u and m are empirical constants. Since D and k are known, u and m were determined to be 0·0012 and 3, respectively. McCullough & Marsh (1950) observed a similar dependence on h, k and l in the structure factors of the diaryl-selenium dihalides.

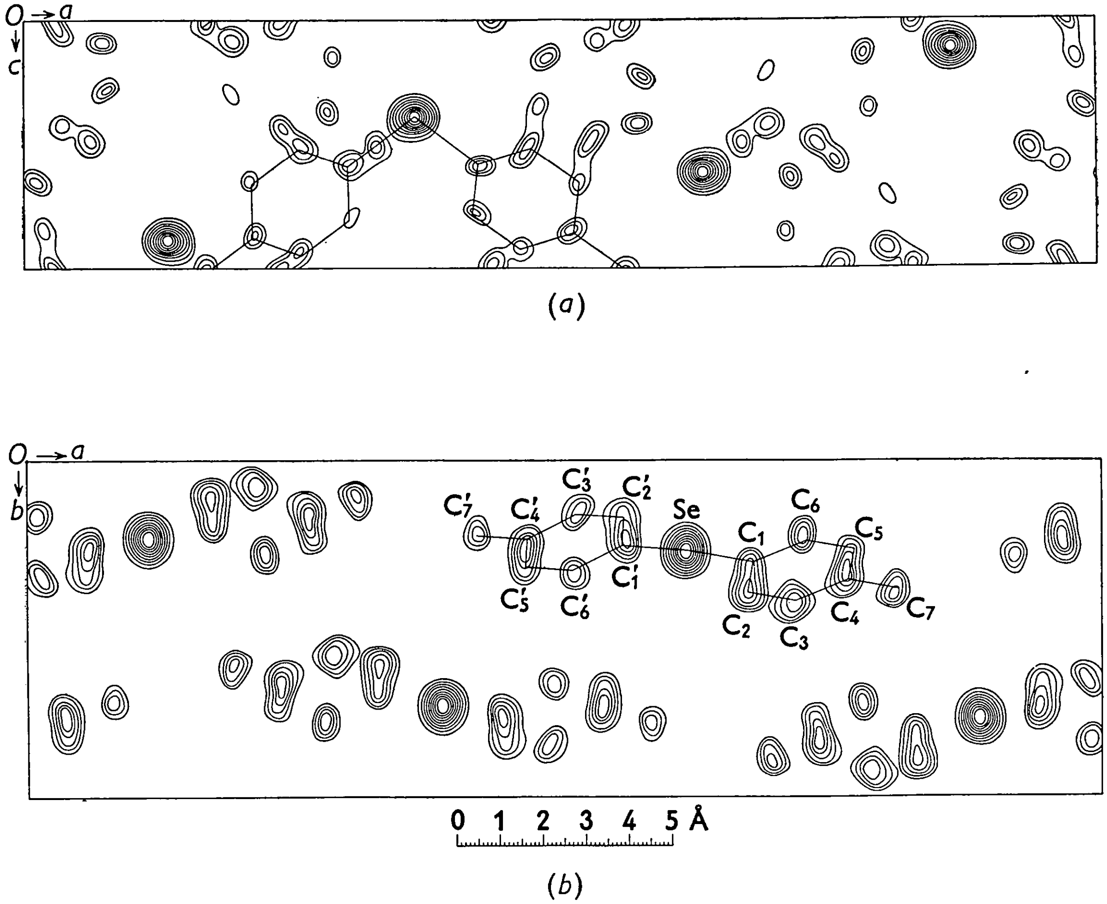
The least-squares method was now applied to the coordinates taken from Fig. 1(*b*), using corrected structure factors of the form $F_c\exp(-0{\cdot}0012\times k^3)$. Six iterations produced a stationary R_1 value, which was accompanied by a considerable oscillation in the signs of the $\Delta\xi_j$'s to be added to the atomic coordinate ξ_j, as was also the case with the ($h0l$) layer. Hence, convergence in this process was reached with R_1 ($hk0$) = 0·169, omitting $F(020)$ and $F(210)$. In the least-squares process, 401 observations were used to determine 45 unknowns.

Atomic coordinates

The method used for selecting the final set of coordinates from the sets of oscillating $\Delta\xi_j$'s resulting from the last few least-squares applications has previously been described (Blackmore & Abrahams, 1955*a*). The final combined coordinates from the ($h0l$) and ($hk0$) layers are given in Table 2. The ($hk1$) intensities were recorded as an independent check of these coordinates, and the final values of R_1 are 0·208 for ($hk0$), 0·168 for ($h0l$) and 0·171 for ($hk1$). In obtaining these R_1 values, all the structure factors given in Table 3 were used. If the two largest $F(hk0)$ terms are omitted, $R_1(hk0) = 0{\cdot}177$.

Dimensions in the di-*p*-tolyl selenide molecule

The Se–C distance is measured twice in the molecule, with no crystallographic relation between the two



(a)

(b)

Fig. 1. (*a*) Projection of the unit cell of di-*p*-tolyl selenide along the *b* axis. Each contour for the carbon atoms represents a density increment of 1 e.$Å^{-2}$, and for the selenium atom of 5 e.$Å^{-2}$. The first contour for both atoms is of 5 e.$Å^{-2}$. The outline of one molecule is marked.

(*b*) Projection of the unit cell along the *c* axis. Contour scale as in (*a*), except that the first contour for carbon is here 4 e.$Å^{-2}$.

Table 2. *Atomic coordinates in* $(p\text{-}CH_3.C_6H_4)_2Se$

The origin is half way between three pairs of non-intersecting screw axes

	Atom	*x*	*y*	*z*
	Se	0·1360	0·2328	0·1381
Ring *A*	C_1	0·0754	0·1977	0·3299
	C_2	0·0809	0·1089	0·5353
	C_3	0·0366	0·0826	0·6748
	C_4	0·9876	0·1452	0·6081
	C_5	0·9821	0·2365	0·4030
	C_6	0·0263	0·2621	0·2643
	C_7	0·9405	0·1061	0·7567
Ring *B*	C_1'	0·1962	0·2475	0·3401
	C_2'	0·1918	0·3311	0·5479
	C_3'	0·2362	0·3409	0·6921
	C_4'	0·2841	0·2678	0·6275
	C_5'	0·2876	0·1852	0·4214
	C_6'	0·2437	0·1735	0·2772
	C_7'	0·3317	0·2778	0·7840

observations. These distances were found to be 1·92 and 1·93 Å. The valency angle C–Se–C is 106·2°. The angle made by the normals of ring *A* (Table 2) with the *a*, *b* and *c* axes are 79°, 31° and 61°. The angles for ring *B* are 106°, 149° and 64°, respectively. These normals make an angle of 55° with each other.

Intermolecular distances

No intermolecular distance was found less than 3·5 Å, and it therefore seems that the only forces binding these molecules together in the crystal are van der Waals forces.

Accuracy of the coordinates

The treatment used in the study of di-*p*-tolyl telluride was employed in the present case. Retaining the same terminology, $\sigma(\Delta x_{\mathrm{Se}}) = 0{\cdot}005$ Å and hence $\sigma(r_{\mathrm{Se}}) = 0{\cdot}005$ Å, assuming that the dependence of the (*hk*0) scale factor upon *k* is not caused by a strong anisotropy in the thermal vibrations of the selenium atom. Here, $\bar{f}_{\mathrm{Se}}/\bar{f}_{\mathrm{C}}$ was found to be 8·9, and hence $\sigma(r_{\mathrm{C}}) = 0{\cdot}045$ Å. The standard deviation in the Se–C bond length is

Table 3. *Observed and calculated structure factors for di-p-tolyl selenide*

$h0l$	F_{obs}	F_{calc}	$h0l$	F_{obs}	F_{calc}	$h0l$	F_{obs}	F_{calc}	$hk0$	F_{obs}	F_{corr}
200	*	-22	23,0,2	22	+20	605	< 4	-4	910	7	+7
400	14	-11	24,0,2	< 4	-1	705	16	-11	10,1,0	57	-52
600	31	+38	25,0,2	14	+9	805	4	-6	11,1,0	< 1	+2
800	48	+57	26,0,2	< 5	-5	905	< 4	-4	12,1,0	49	-53
10,0,0	50	-45	27,0,2	16	-15	10,0,5	17	-15	13,1,0	6	-7
12,0,0	40	-46	28,0,2	5	+1	11,0,5	19	+20	14,1,0	53	+44
14,0,0	60	+59	29,0,2	6	-5	12,0,5	4	+6	15,1,0	6	-7
16,0,0	27	+23	30,0,2	7	+8	13,0,5	4	-4	16,1,0	57	+50
18,0,0	68	-59	31,0,2	7	+8	14,0,5	< 4	-5	17,1,0	< 1	+2
20,0,0	20	-16	32,0,2	< 4	0	15,0,5	37	-33	18,1,0	27	-22
22,0,0	28	+20	103	16	-16	16,0,5	10	-9	19,1,0	12	+12
24,0,0	< 5	-1	203	53	+52	17,0,5	10	+8	20,1,0	88	-74
26,0,0	23	-22	303	17	+21	18,0,5	7	-7	21,1,0	14	-13
28,0,0	< 5	+5	403	17	-18	19,0,5	14	+11	22,1,0	< 2	-4
30,0,0	13	+11	503	27	+27	20,0,5	6	+3	23,1,0	8	+10
32,0,0	< 5	-8	603	65	-62	21,0,5	8	-8	24,1,0 †	3	+1
002	62	+57	703	25	-28	22,0,5	6	+1	25,1,0 †	8	+2
004	60	-48	803	17	+22	23,0,5	8	-8	26,1,0	2	+4
006	12	-7	903	4	-2	24,0,5	6	-3	27,1,0 †	3	+3
101	64	+68	10,0,3	32	+37	25,0,5	7	+7	28,1,0	16	-16
201	38	+46	11,0,3	32	+37	26,0,5	4	-2	29,1,0	3	+4
301	90	-103	12,0,3	29	-27	106	20	-16	30,1,0	4	-6
401	25	-30	13,0,3	< 4	-3	206	< 4	+4	31,1,0	1	-2
501	9	-18	14,0,3	21	-21	306	12	-7	32,1,0	8	+10
601	49	-60	15,0,3	30	-23	406	15	+15	120	67	-73
701	65	+78	16,0,3	34	+36	506	23	+18	220	53	-49
801	35	+39	17,0,3	4	+2	606	< 5	0	320	32	+25
901	6	+12	18,0,3	6	+7	706	8	+5	420	48	+53
10,0,1	70	+78	19,0,3	8	+8	806	< 5	-5	520	38	+29
11,0,1	41	-40	20,0,3	15	-16	906	30	-21	620	61	+53
12,0,1	25	-34	21,0,3	8	-10	10,0,6	6	+6	720	14	+18
13,0,1	< 3	+8	22,0,3	5	-1	11,0,6	5	0	820	63	-69
14,0,1	7	-14	23,0,3	7	-6	12,0,6	6	+5	920	17	+15
15,0,1	36	+39	24,0,3	30	+25	13,0,6	20	+13	10,2,0	26	-31
16,0,1	30	+36	25,0,3	13	+12	14,0,6	5	-5	11,2,0	6	-11
17,0,1	20	-22	26,0,3	5	-5	15,0,6	5	-4	12,2,0	51	+44
18,0,1	< 4	+6	27,0,3	5	+3	16,0,6	5	-3	13,2,0	20	-14
19,0,1	32	-33	28,0,3	6	-5	17,0,6	8	-6	14,2,0	61	+51
20,0,1	< 4	-4	29,0,3	< 5	-4	18,0,6	9	+9	15,2,0	13	+13
21,0,1	7	+6	30,0,3	< 5	+2	19,0,6	4	+3	16,2,0	26	-19
22,0,1	< 4	-1	104	< 4	+4	20,0,6	4	+1	17,2,0 †	6	+3
23,0,1	14	+13	204	6	+7	21,0,6	12	+6	18,2,0	62	-48
24,0,1	34	+28	304	< 4	+2	22,0,6	8	-6	19,2,0	10	-10
25,0,1	14	-14	404	39	+38	107	< 4	+4	20,2,0	18	+14
26,0,1	< 5	-.5	504	11	-9	207	21	-15	21,2,0	< 1	+2
27,0,1	7	-9	604	30	-25	307	4	-2	22,2,0	27	+18
28,0,1	12	-12	704	7	-10	407	7	+5	23,2,0	7	+7
29,0,1	9	+12	804	42	-39	507	< 4	+2	24,2,0	2	+3
30,0,1	5	+6	904	24	+26	607	17	+11	25,2,0	2	+2
31,0,1	< 5	+1	10,0,4	12	+9	707	4	+3	26,2,0	28	-24
32,0,1	< 5	+3	11,0,4	4	+5	807	8	-8	27,2,0	2	-2
102	68	+70	12,0,4	34	+30	907	4	+2	28,2,0	4	-4
202	< 3	-1	13,0,4	14	-18	10,0,7	13	-9	29,2,0	3	-4
302	53	+50	14,0,4	42	-33	11,0,7	4	-4	30,2,0	9	+10
402	3	+5	15,0,4	< 4	+2	12,0,7	9	+9	31,2,0	3	-2
502	64	-67	16,0,4	6	-7	13,0,7	< 4	-1	130	21	-17
602	< 3	-3	17,0,4	< 4	-3	14,0,7	11	+3	230	69	+77
702	24	-25	18,0,4	24	+20	15,0,7	< 4	-2	330	20	+20
802	7	+14	19,0,4	< 4	-3	16,0,7	< 4	-4	430	11	+14
902	78	+86	20,0,4	4	+4	$hk0$	F_{obs}	F_{corr}	530	22	+17
10.0.2	31	-38	21,0,4	5	-6	020	115	-218	630	81	-73
11,0,2	< 3	+6	22,0,4	19	-18	040	58	+63	730	36	-30
12,0,2	< 4	-2	23,0,4	5	+7	060	34	-32	830	38	-38
13,0,2	50	-57	24,0,4	< 5	+1	080	9	+10	930	7	-13
14,0,2	7	-7	25,0,4	< 5	+4	0,10,0	2	-2	10,3,0	37	+41
15,0,2	7	+11	26,0,4	14	+11	110	10	+10	11,3,0	17	-11
16,0,2	4	+6	27,0,4	4	-6	210	105	-140	12,3,0	35	+40
17,0,2	31	+32	28,0,4	4	-4	310	22	-22	13,3,0	27	+25
18,0,2	< 4	-4	105	34	-25	410	6	-9	14,3,0	55	-44
19,0,2	20	-20	205	32	-24	510	< 1	+1	15,3,0	11	+8
20,0,2	4	-2	305	42	+35	610	83	+92	16,3,0	51	-42
21,0,2	30	-29	405	< 4	+3	710	20	+15	17,3,0	7	-11
22,0,2	< 4	-1	505	20	+13	810	33	+35	18,3,0	21	+18

* Not observable; cut off by layer-line screen.

† This structure factor was entered in the Fourier series for Fig. 1(*b*) with the wrong sign.

Table 3 (*cont.*)

hk0	F_{obs}	F_{corr}	hk0	F_{obs}	F_{corr}	hk0	F_{obs}	F_{corr}	hkl	F_{obs}	$\lvert F_{calc}\rvert$
19, 3, 0	14	-13	560	7	+ 8	990	1	+ 3	25, 2, 1	< 9	12
20, 3, 0	44	+32	660	17	+17	10, 9, 0	2	- 3	26, 2, 1	< 9	4
21, 3, 0	14	+12	760	12	+18	11, 9, 0	1	0	131	42	47
22, 3, 0	8	+13	860	9	-12	12, 9, 0	1	- 3	231	28	26
23, 3, 0 †	3	- 6	960	< 2	- 2	13, 9, 0	2	- 4	331	48	51
24, 3, 0	24	-16	10, 6, 0	10	-14	14, 9, 0	3	- 3	431	61	59
25, 3, 0 †	6	- 6	11, 6, 0	18	-15	15, 9, 0	< 1	- 1	531	36	41
26, 3, 0	5	- 6	12, 6, 0	23	+20	16, 9, 0	< 1	+ 2	631	10	17
27, 3, 0	7	- 8	13, 6, 0	5	- 4	1, 10, 0	2	- 2	731	9	15
28, 3, 0	13	+16	14, 6, 0	10	+14	2, 10, 0	< 1	- 1	831	38	37
29, 3, 0	4	- 4	15, 6, 0	8	+ 8	3, 10, 0	5	- 4	931	50	51
30, 3, 0	< 1	+ 2	16, 6, 0	< 2	0	4, 10, 0	2	0	10, 3, 1	41	35
140	13	+17	17, 6, 0	3	+ 2	5, 10, 0	< 1	0	11, 3, 1	24	21
240	13	+17	18, 6, 0	11	-13	6, 10, 0	2	+ 2	12, 3, 1	24	23
340	27	+21	19, 6, 0	8	-10	hkl	F_{obs}	$\lvert F_{calc}\rvert$	13, 3, 1	40	36
440	58	-56	20, 6, 0	4	+ 5	011	37	25	14, 3, 1	17	21
540	30	-19	21, 6, 0	5	- 4	021	28	26	15, 3, 1	10	12
640	50	-42	22, 6, 0	6	+ 8	031	37	44	16, 3, 1	15	14
740	38	-36	23, 6, 0	4	+ 5	041	50	60	17, 3, 1	33	33
840	41	+42	24, 6, 0	< 1	+ 1	051	26	34	18, 3, 1	25	27
940	1	+ 3	25, 6, 0	2	+ 3	061	26	34	19, 3, 1	26	25
10, 4, 0	18	+20	26, 6, 0	2	- 8	111	49	71	20, 3, 1	11	14
11, 4, 0	10	+11	27, 6, 0	< 1	- 2	211	14	14	21, 3, 1	24	23
12, 4, 0	48	-37	170	10	-12	311	91	72	22, 3, 1	21	20
13, 4, 0	25	+15	270	13	+15	411	111	107	23, 3, 1	< 8	6
14, 4, 0	34	-29	370	10	+ 9	511	39	43	141	58	66
15, 4, 0	17	-16	470	2	+ 4	611	25	26	241	46	50
16, 4, 0	6	+ 5	570	7	+ 9	711	24	22	341	36	39
17, 4, 0	3	0	670	10	-14	811	65	60	441	< 6	12
18, 4, 0	33	+28	770	2	- 5	911	48	58	541	14	14
19, 4, 0	10	+11	870	8	- 7	10, 1, 1	63	58	641	28	28
20, 4, 0	8	-10	970	10	-12	11, 1, 1	11	10	741	29	32
21, 4, 0	3	+ 1	10, 7, 0	8	+11	12, 1, 1	34	31	841	13	16
22, 4, 0	20	-14	11, 7, 0	< 2	+ 1	13, 1, 1	52	54	941	18	18
23, 4, 0	4	- 6	12, 7, 0	2	+ 4	14, 1, 1	16	22	10, 4, 1	36	31
24, 4, 0	< 1	- 2	13, 7, 0	10	+11	15, 1, 1	9	11	11, 4, 1	36	35
25, 4, 0	7	- 6	14, 7, 0	6	- 7	16, 1, 1	17	17	12, 4, 1	19	24
26, 4, 0	15	+17	15, 7, 0	3	+ 2	17, 1, 1	50	49	13, 4, 1	< 7	7
27, 4, 0	6	+ 5	16, 7, 0	10	-13	18, 1, 1	22	21	14, 4, 1	< 7	14
28, 4, 0	11	+ 4	17, 7, 0 †	12	-11	19, 1, 1	10	21	15, 4, 1	19	25
29, 4, 0	3	+ 5	18, 7, 0	3	- 3	20, 1, 1	< 8	2	16, 4, 1	21	21
150	23	+17	19, 7, 0	4	- 5	21, 1, 1	19	13	17, 4, 1	15	16
250	46	-39	20, 7, 0	5	+ 8	22, 1, 1	23	24	18, 4, 1	< 8	12
350	7	-12	21, 7, 0	3	+ 5	23, 1, 1	11	13	19, 4, 1	< 8	20
450	4	- 2	22, 7, 0	4	- 4	24, 1, 1	< 8	2	20, 4, 1	8	17
550	26	-16	23, 7, 0	3	+ 5	25, 1, 1	13	8	21, 4, 1	< 8	8
650	39	+34	180	11	+11	26, 1, 1	13	14	151	24	30
750	19	+16	280	2	- 3	27, 1, 1	13	14	251	16	20
850	36	+28	380	13	+11	28, 1, 1	< 9	5	351	21	26
950	15	+17	480	5	- 7	121	88	95	451	21	29
10, 5, 0	30	-28	580	1	- 3	221	95	82	551	24	33
11, 5, 0	9	+ 7	680	7	- 6	321	68	61	651	14	23
12, 5, 0	11	-15	780	2	- 4	421	5	13	751	7	14
13, 5, 0	32	-27	880	4	+ 6	521	31	23	851	17	23
14, 5, 0	26	+22	980	< 1	- 1	621	48	43	951	17	24
15, 5, 0 †	4	- 2	10, 8, 0	< 1	+ 3	721	54	56	10, 5, 1	7	19
16, 5, 0	30	+28	11, 8, 0	7	+ 8	821	44	36	11, 5, 1	7	12
17, 5, 0	11	+15	12, 8, 0	4	- 4	921	24	20	12, 5, 1	< 7	14
18, 5, 0	2	- 1	13, 8, 0	3	+ 2	10, 2, 1	65	55	13, 5, 1	15	24
19, 5, 0	5	+ 3	14, 8, 0	4	- 5	11, 2, 1	49	50	14, 5, 1	11	16
20, 5, 0	13	-15	15, 8, 0	5	- 6	12, 2, 1	37	32	15, 5, 1	8	10
21, 5, 0	< 1	- 1	16, 8, 0	1	+ 2	13, 2, 1	< 6	4	16, 5, 1	8	16
22, 5, 0	< 1	+ 1	17, 8, 0	3	- 2	14, 2, 1	6	14	17, 5, 1	8	21
23, 5, 0	6	+ 7	18, 8, 0	3	+ 4	15, 2, 1	31	33	18, 5, 1	8	14
24, 5, 0	10	+12	19, 8, 0	4	+ 4	16, 2, 1	38	33	19, 5, 1	8	15
25, 5, 0	5	+ 5	190	4	+ 4	17, 2, 1	21	22	20, 5, 1	9	17
26, 5, 0	6	+ 4	290	< 1	- 4	18, 2, 1	< 8	11	21, 5, 1	9	13
27, 5, 0	5	+ 7	390	5	- 3	19, 2, 1	36	29	22, 5, 1	< 9	12
28, 5, 0	4	- 7	490	5	- 3	20, 2, 1	8	12	161	18	22
160	12	-11	590	6	- 6	21, 2, 1	< 8	7	261	18	20
260	12	+10	690	3	+ 3	22, 2, 1	< 8	6	361	23	29
360	35	-23	790	1	+ 3	23, 2, 1	17	15	461	18	20
460	35	+27	890	< 1	+ 1	24, 2, 1	28	21	561	< 7	15

† This structure factor was entered in the Fourier series for Fig. 1(*b*) with the wrong sign.

0·045 Å, in the averaged bond length is 0·03 Å, and in the C–Se–C bond angle is 2°.

Discussion

The Se–C bond distance of 1·92 Å in the present study compares very closely with the other values for this distance given in Table 1. The Se–Se distance in the element has been intensively studied (Grison, 1951; Burbank, 1951; Marsh, Pauling & McCullough, 1953) and is close to 2·34 Å. Taking half this value as the single covalent bond radius, and 0·75 Å for the single covalent radius of carbon, the resulting single bond between selenium and carbon is 1·92 Å, assuming additivity and correcting for the electronegativity difference (Schomaker & Stevenson, 1941). It thus appears that this bond remains very close to a single bond, and is rather insensitive to its surroundings. This behavior appears to be in contrast with that of sulfur (Blackmore & Abrahams, 1955*b*), which has a tendency to conjugate with adjacent double bonds, with the consequence that the S–C bond itself may take on some double-bond character.

The C–Se–C bond angle found in di-*p*-tolyl selenide of 106° lies within the range of comparable angles in Table 1. In the element, the selenium atom exhibits a valence angle of 105·5°, and hence this angle also seems to remain rather constant in a variety of environments.

The dihedral angle of 55° between the normals to the aromatic rings in the present molecule may be compared with ~~the~~ corresponding angle of 80±10° found in di-*p*-tolyl selenium dichloride and dibromide (McCullough & Marsh, 1950). ~~The~~ small dihedral angle found in the present study results in a distance of 3·31 Å between C_2 and C_2'. It is possible that this rather close approach may be due to a tendency for the molecule to assume a planar configuration, which would greatly increase the chance of conjugation in the Se–C bond.

It is of interest to note the great similarity between the molecular orientation of the di-*p*-tolyl selenide molecule in the present crystal, and of the corresponding part of the molecule in the di-*p*-tolyl selenium dichloride and dibromide crystal (McCullough & Marsh, 1950), although the latter crystals belong to a different space group.

Experimental

The colorless needles of di-*p*-tolyl selenide may be prepared as described by McCullough & Campbell (1945) and by Leicester (1938). The crystals used in this study were kindly sent to us by Dr J. D. McCullough, and recrystallized from aqueous alcohol in this laboratory. These crystals are stable in contact with the atmosphere. The largest of the three crystals used was 0·25×0·35×1·10 mm.^{3} and the smallest was 0·08×0·09×0·60 mm.^{3}. The experimental procedures used in this study are the same as those described by Blackmore & Abrahams (1955*a*). The ratio of the strongest intensity to the weakest in each layer was 7230:1 in (*hk*0), 1160:1 in (*h*0*l*) and 1160:1 in (*hk*1). No absorption corrections were made. The largest crystals were used only for the weakest intensities.

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