Crystal structure of bis(triphenylphosphine)hexakis(μ-phenylselenido)-bis(phenylselenido)tetramercury(II), $Hg_4[P(C_6H_5)_3]_2(C_6H_5Se)_8$

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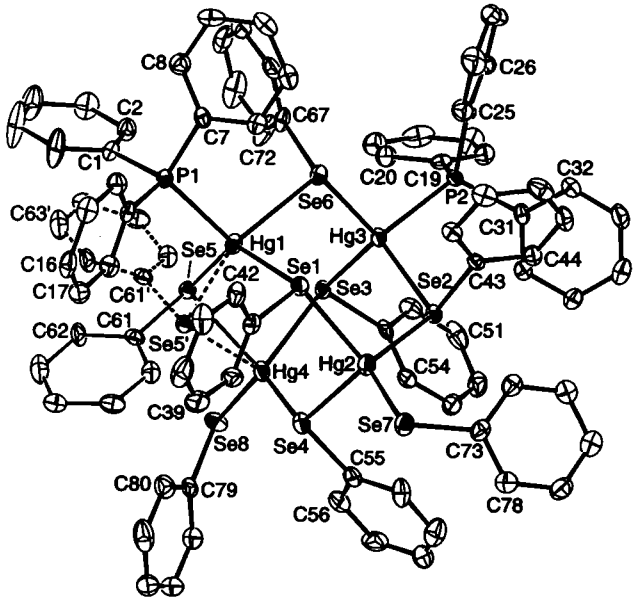

Abstract

$C_{84}H_{70}Hg_4P_2Se_8$, triclinic, $P\bar{1}$ (no. 2), a = 13.732(1) Å, b = 14.788(1) Å, c = 22.641(2) Å, α = 73.095(2)°, β = 73.579(2)°, γ = 65.783(1)°, V = 3940.8 Å^3, Z = 2, $R_{gt}(F)$ = 0.032, $wR_{ref}(F^2)$ = 0.071, T = 100 K.

Source of material

The reactions were carried out under a nitrogen atmosphere using standard Schlenk techniques. All solvents were dried and freshly distilled. Benzeneselenol was prepared by the modified literature procedure [1]. At room temperature, a solution of mercury bromide (0.180 g, 0.5 mmol) and triphenylphosphine (0.131 g, 0.5 mmol) in acetonitrile (15 ml) was added to a mixture of benzeneselenol (0.15 ml, 1.5 mmol) and triethylamine (0.24 ml, 1.5 mmol) in acetonitrile (5.0 ml). Three days later, crystals were obtained from slow evaporation of an acetonitrile and methanol solution of the compound (m.p. 407.5-408.5 K).

Experimental details

One phenylselenido ligand is disordered over two positions on equal terms.

Discussion

Main group metal chalcogenolates with a d^{10} electronic configuration have been found to have wide applications and importance in structural chemistry, photocatalysis, medicinal and bioinorganic chemistry [2]. We are interested in the synthesis and investigation of mercury(II) complexes with chalcogenide ligands because they are extremely rare and have unusual bonding characteristics [3].

Here we reported the structure of tetranuclear mercury(II) complex with Se,P-contained ligands. It features eight benzeneselenol ligands with six bridging selenium atoms bound to four mercury atom leading to the formation of a Hg_4Se_6 adamantane-like mercury-selenium core. Similar mercury complex structures had only been reported for $[(\mu\text{-}ER)^6(HgL)^4]^{2+}$ (E = S, Se or Te; L = tertiary phosphine or arsine) [4-6].

Table 1. Data collection and handling.

Crystal:	yellow, tabular, size 0.15 × 0.30 × 0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	115.46 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	56.66°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	47011, 19531
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 14983
$N(param)_{refined}$:	905
Programs:	SHELXS-97 [6], SHELXL-97 [7]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{iso}
H(2A)	2*i*		0.0829	0.2960	0.4102	0.031
H(3A)	2*i*		0.1353	0.2445	0.5078	0.043
H(4A)	2*i*		0.0717	0.1315	0.5879	0.056
H(5A)	2*i*		−0.0541	0.0763	0.5728	0.076
H(6A)	2*i*		−0.1041	0.1238	0.4743	0.056
H(8A)	2*i*		0.1390	0.0724	0.3756	0.030
H(9A)	2*i*		0.2988	−0.0080	0.3106	0.035
H(10A)	2*i*		0.3243	0.0546	0.2028	0.035
H(11A)	2*i*		0.1907	0.1963	0.1591	0.032
H(12A)	2*i*		0.0275	0.2741	0.2229	0.026
H(14A)	2*i*		−0.0711	0.0750	0.3361	0.029
H(15A)	2*i*		−0.2153	0.0224	0.3500	0.034
H(16A)	2*i*		−0.3918	0.1226	0.3889	0.035
H(17A)	2*i*		−0.4249	0.2794	0.4093	0.034
H(18A)	2*i*		−0.2802	0.3339	0.3934	0.027
H(20A)	2*i*		0.2230	0.6344	0.2877	0.030
H(21A)	2*i*		0.2897	0.6812	0.3535	0.039
H(22A)	2*i*		0.3901	0.7871	0.3113	0.045
H(23A)	2*i*		0.4223	0.8480	0.2049	0.042
H(24A)	2*i*		0.3533	0.8066	0.1377	0.030
H(26A)	2*i*		0.4639	0.5957	0.1385	0.030
H(27A)	2*i*		0.5986	0.4599	0.0960	0.042
H(28A)	2*i*		0.5506	0.3572	0.0583	0.040
H(29A)	2*i*		0.3699	0.3863	0.0628	0.045
H(30A)	2*i*		0.2342	0.5235	0.1049	0.032

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Table 2. Continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(32A)	2i		0.3432	0.7160	0.0267	0.031
H(33A)	2i		0.3120	0.8503	–0.0581	0.036
H(34A)	2i		0.1624	0.9976	–0.0484	0.035
H(35A)	2i		0.0386	1.0104	0.0464	0.027
H(36A)	2i		0.0668	0.8754	0.1319	0.022
H(38A)	2i		–0.4077	0.5590	0.2540	0.031
H(39A)	2i		–0.5499	0.4976	0.2803	0.048
H(40A)	2i		–0.5156	0.3352	0.2666	0.050
H(41A)	2i		–0.3418	0.2382	0.2258	0.042
H(42A)	2i		–0.1997	0.2956	0.2028	0.032
H(44A)	2i		0.0678	0.7832	0.0060	0.026
H(45A)	2i		0.1878	0.6976	–0.0735	0.033
H(46A)	2i		0.2135	0.5309	–0.0682	0.039
H(47A)	2i		0.1235	0.4452	0.0177	0.034
H(48A)	2i		0.0031	0.5283	0.0977	0.024
H(50A)	2i		0.0780	0.8797	0.2780	0.030
H(51A)	2i		0.0679	1.0392	0.2168	0.041
H(52A)	2i		–0.0746	1.1347	0.1604	0.041
H(53A)	2i		–0.2015	1.0670	0.1643	0.037
H(54A)	2i		–0.1909	0.9077	0.2218	0.028
H(56A)	2i		–0.4249	0.9551	0.3020	0.037
H(57A)	2i		–0.4826	1.1291	0.2597	0.041
H(58A)	2i		–0.4984	1.1873	0.1542	0.043
H(59A)	2i		–0.4525	1.0717	0.0913	0.044
H(60A)	2i		–0.3899	0.8995	0.1312	0.039

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(62A)	2i	0.5005	–0.2796	0.4678	0.5206	0.030
H(62B)	2i	0.4995	–0.2356	0.3971	0.5022	0.030
H(63A)	2i	0.5005	–0.4531	0.4518	0.5653	0.045
H(63B)	2i	0.4995	–0.1299	0.3345	0.5825	0.045
H(64A)	2i	0.5005	–0.5687	0.4707	0.4990	0.037
H(64B)	2i	0.4995	0.0018	0.3955	0.5772	0.037
H(65A)	2i	0.5005	–0.5234	0.5318	0.3888	0.032
H(65B)	2i	0.4995	0.0218	0.5323	0.5013	0.032
H(66A)	2i	0.5005	–0.3634	0.5644	0.3468	0.030
H(66B)	2i	0.4995	–0.0861	0.6058	0.4194	0.030
H(68A)	2i		0.2644	0.2626	0.2674	0.030
H(69A)	2i		0.3702	0.1790	0.3451	0.040
H(70A)	2i		0.3602	0.2633	0.4204	0.049
H(71A)	2i		0.2431	0.4289	0.4196	0.055
H(72A)	2i		0.1320	0.5124	0.3435	0.043
H(74A)	2i		–0.1474	0.7288	0.0059	0.029
H(75A)	2i		–0.0926	0.8487	–0.0720	0.031
H(76A)	2i		–0.2228	0.9973	–0.1149	0.035
H(77A)	2i		–0.4057	1.0194	–0.0825	0.038
H(78A)	2i		–0.4615	0.9034	–0.0016	0.038
H(80A)	2i		–0.4711	0.7403	0.4281	0.034
H(81A)	2i		–0.6578	0.7792	0.4403	0.052
H(82A)	2i		–0.7788	0.9386	0.4572	0.058
H(83A)	2i		–0.7146	1.0600	0.4591	0.056
H(84A)	2i		–0.5294	1.0225	0.4453	0.037

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Hg(1)	2i		–0.10001(2)	0.43988(2)	0.308962(9)	0.0258(1)	0.0166(1)	0.0172(1)	–0.00887(8)	–0.00266(8)	–0.00286(8)
Hg(2)	2i		–0.24204(2)	0.67577(2)	0.15562(1)	0.0248(1)	0.0255(1)	0.0180(1)	–0.01126(9)	–0.00389(8)	–0.00112(9)
Hg(3)	2i		0.05193(2)	0.64741(1)	0.210331(9)	0.0202(1)	0.0156(1)	0.0150(1)	–0.00813(8)	0.00130(8)	–0.00427(8)
Hg(4)	2i		–0.24752(2)	0.74796(2)	0.341095(9)	0.0248(1)	0.0204(1)	0.0167(1)	–0.00933(8)	0.00346(8)	–0.00545(8)
Se(1)	2i		–0.16769(4)	0.47650(4)	0.20288(2)	0.0203(3)	0.0210(3)	0.0181(3)	–0.0090(2)	–0.0032(2)	–0.0022(2)
Se(2)	2i		–0.07412(4)	0.73732(4)	0.12424(2)	0.0192(2)	0.0184(3)	0.0145(3)	–0.0079(2)	–0.0003(2)	–0.0044(2)
Se(3)	2i		–0.04004(4)	0.74245(4)	0.30496(2)	0.0208(3)	0.0166(3)	0.0120(2)	–0.0059(2)	0.0004(2)	–0.0036(2)
Se(4)	2i		–0.35496(4)	0.76588(4)	0.25724(2)	0.0262(3)	0.0231(3)	0.0181(3)	–0.0120(2)	0.0010(2)	–0.0047(2)
Se(5)	2i	0.5005(8)	–0.17255(8)	0.54164(7)	0.39767(5)	0.0173(3)	0.0163(4)	0.0169(4)	–0.0074(3)	–0.0031(3)	–0.0026(3)
Se(5')	2i	0.4995	–0.24824(8)	0.55390(7)	0.38552(5)	0.0173(3)	0.0163(4)	0.0169(4)	–0.0074(3)	–0.0031(3)	–0.0026(3)
Se(6)	2i		0.09138(4)	0.45288(4)	0.23889(2)	0.0238(3)	0.0152(3)	0.0178(3)	–0.0097(2)	–0.0048(2)	–0.0023(2)
Se(7)	2i		–0.36108(4)	0.70886(4)	0.07761(3)	0.0273(3)	0.0301(3)	0.0217(3)	–0.0146(2)	–0.0072(2)	0.0000(2)
Se(8)	2i		–0.33002(4)	0.85154(4)	0.42685(3)	0.0182(3)	0.0284(3)	0.0244(3)	–0.0077(2)	–0.0019(2)	–0.0135(2)
P(1)	2i		–0.0525(1)	0.2529(1)	0.35623(6)	0.0193(6)	0.0139(7)	0.0156(7)	–0.0087(5)	–0.0021(5)	–0.0012(5)
P(2)	2i		0.2279(1)	0.6795(1)	0.15607(6)	0.0142(6)	0.0168(7)	0.0139(6)	–0.0051(5)	–0.0009(5)	–0.0041(5)
C(1)	2i		–0.0174(4)	0.2155(4)	0.4330(2)	0.024(3)	0.016(3)	0.015(3)	–0.009(2)	–0.006(2)	0.000(2)
C(2)	2i		0.0550(4)	0.2508(4)	0.4429(3)	0.025(3)	0.032(3)	0.021(3)	–0.015(2)	–0.007(2)	0.001(2)
C(3)	2i		0.0864(5)	0.2197(5)	0.5010(3)	0.035(3)	0.050(4)	0.035(4)	–0.025(3)	–0.019(3)	0.000(3)
C(4)	2i		0.0481(6)	0.1536(5)	0.5488(3)	0.064(5)	0.062(5)	0.025(4)	–0.039(4)	–0.021(3)	0.010(3)
C(5)	2i		–0.0248(7)	0.1198(6)	0.5395(3)	0.113(7)	0.086(6)	0.026(4)	–0.085(5)	–0.031(4)	0.025(4)
C(6)	2i		–0.0559(6)	0.1495(5)	0.4810(3)	0.077(5)	0.062(5)	0.028(4)	–0.060(4)	–0.022(3)	0.016(3)
C(7)	2i		0.0674(4)	0.1816(4)	0.3065(2)	0.022(3)	0.019(3)	0.019(3)	–0.013(2)	0.001(2)	–0.004(2)
C(8)	2i		0.1487(4)	0.0977(4)	0.3316(3)	0.025(3)	0.026(3)	0.025(3)	–0.010(2)	–0.005(2)	–0.004(2)
C(9)	2i		0.2439(4)	0.0500(4)	0.2930(3)	0.020(3)	0.023(3)	0.044(4)	–0.001(2)	–0.008(3)	–0.013(3)
C(10)	2i		0.2589(4)	0.0870(4)	0.2291(3)	0.023(3)	0.038(4)	0.032(3)	–0.015(3)	0.006(2)	–0.019(3)
C(11)	2i		0.1794(4)	0.1707(4)	0.2031(3)	0.035(3)	0.024(3)	0.024(3)	–0.017(3)	0.003(2)	–0.009(2)
C(12)	2i		0.0830(4)	0.2176(4)	0.2411(3)	0.027(3)	0.015(3)	0.026(3)	–0.012(2)	–0.005(2)	–0.004(2)
C(13)	2i		–0.1620(4)	0.2089(4)	0.3638(2)	0.025(3)	0.020(3)	0.012(3)	–0.013(2)	–0.007(2)	0.002(2)
C(14)	2i		–0.1431(4)	0.1167(4)	0.3509(2)	0.026(3)	0.026(3)	0.023(3)	–0.012(2)	–0.004(2)	–0.004(2)
C(15)	2i		–0.2283(5)	0.0853(4)	0.3595(3)	0.040(3)	0.027(3)	0.026(3)	–0.019(3)	–0.009(3)	–0.005(3)
C(16)	2i		–0.3333(5)	0.1453(4)	0.3820(3)	0.035(3)	0.038(4)	0.023(3)	–0.026(3)	–0.011(3)	0.009(3)
C(17)	2i		–0.3529(4)	0.2379(4)	0.3944(3)	0.023(3)	0.036(4)	0.025(3)	–0.012(2)	–0.007(2)	–0.002(3)
C(18)	2i		–0.2670(4)	0.2700(4)	0.3852(2)	0.028(3)	0.024(3)	0.019(3)	–0.010(2)	–0.004(2)	–0.006(2)
C(19)	2i		0.2814(4)	0.7162(4)	0.2058(2)	0.017(3)	0.014(3)	0.023(3)	0.000(2)	–0.006(2)	–0.007(2)
C(20)	2i		0.2629(4)	0.6786(4)	0.2706(3)	0.026(3)	0.027(3)	0.022(3)	–0.008(2)	–0.005(2)	–0.006(2)
C(21)	2i		0.3029(5)	0.7058(5)	0.3094(3)	0.034(3)	0.039(4)	0.019(3)	–0.005(3)	–0.009(3)	–0.008(3)
C(22)	2i		0.3622(5)	0.7689(5)	0.2843(3)	0.037(4)	0.033(4)	0.050(4)	–0.002(3)	–0.026(3)	–0.019(3)

Table 3. Continued.

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(23)	2*i*		0.3810(5)	0.8051(5)	0.2216(3)	0.043(4)	0.035(4)	0.035(4)	−0.018(3)	−0.011(3)	−0.008(3)
C(24)	2*i*		0.3407(4)	0.7802(4)	0.1816(3)	0.024(3)	0.030(3)	0.023(3)	−0.011(2)	−0.008(2)	−0.002(2)
C(25)	2*i*		0.3358(4)	0.5716(4)	0.1262(2)	0.019(3)	0.020(3)	0.013(3)	−0.002(2)	0.000(2)	−0.003(2)
C(26)	2*i*		0.4444(4)	0.5533(4)	0.1232(2)	0.024(3)	0.028(3)	0.021(3)	−0.004(2)	−0.003(2)	−0.007(2)
C(27)	2*i*		0.5241(4)	0.4730(5)	0.0980(3)	0.022(3)	0.041(4)	0.026(3)	0.000(3)	0.002(2)	−0.006(3)
C(28)	2*i*		0.4953(5)	0.4121(4)	0.0757(3)	0.034(3)	0.026(3)	0.019(3)	0.004(3)	0.004(2)	−0.006(3)
C(29)	2*i*		0.3889(5)	0.4291(5)	0.0781(3)	0.049(4)	0.036(4)	0.028(3)	−0.014(3)	0.001(3)	−0.017(3)
C(30)	2*i*		0.3085(4)	0.5104(4)	0.1034(3)	0.029(3)	0.024(3)	0.025(3)	−0.009(2)	−0.001(2)	−0.007(3)
C(31)	2*i*		0.2092(4)	0.7829(4)	0.0879(2)	0.021(3)	0.025(3)	0.011(2)	−0.013(2)	−0.002(2)	−0.004(2)
C(32)	2*i*		0.2812(4)	0.7759(4)	0.0310(3)	0.019(3)	0.030(3)	0.023(3)	−0.008(2)	0.001(2)	−0.004(3)
C(33)	2*i*		0.2627(4)	0.8554(4)	−0.0191(3)	0.029(3)	0.041(4)	0.018(3)	−0.016(3)	0.004(2)	−0.005(3)
C(34)	2*i*		0.1737(5)	0.9425(4)	−0.0135(3)	0.040(3)	0.029(3)	0.021(3)	−0.018(3)	−0.011(3)	0.003(3)
C(35)	2*i*		0.1005(4)	0.9503(4)	0.0427(2)	0.026(3)	0.022(3)	0.021(3)	−0.010(2)	−0.008(2)	−0.001(2)
C(36)	2*i*		0.1174(4)	0.8707(4)	0.0933(2)	0.019(3)	0.023(3)	0.015(3)	−0.009(2)	−0.004(2)	−0.005(2)
C(37)	2*i*		−0.2907(4)	0.4342(4)	0.2253(2)	0.023(3)	0.025(3)	0.014(3)	−0.012(2)	−0.009(2)	−0.001(2)
C(38)	2*i*		−0.3939(4)	0.4932(4)	0.2485(3)	0.020(3)	0.025(3)	0.032(3)	−0.008(2)	−0.006(2)	−0.003(3)
C(39)	2*i*		−0.4784(5)	0.4568(5)	0.2641(3)	0.023(3)	0.044(4)	0.046(4)	−0.012(3)	−0.012(3)	0.007(3)
C(40)	2*i*		−0.4582(5)	0.3606(5)	0.2559(3)	0.047(4)	0.048(4)	0.042(4)	−0.036(3)	−0.021(3)	0.016(3)
C(41)	2*i*		−0.3554(5)	0.3033(5)	0.2323(3)	0.051(4)	0.039(4)	0.027(3)	−0.029(3)	−0.005(3)	−0.006(3)
C(42)	2*i*		−0.2714(5)	0.3376(4)	0.2179(2)	0.040(3)	0.025(3)	0.016(3)	−0.014(3)	−0.003(2)	−0.005(2)
C(43)	2*i*		0.0245(4)	0.6629(4)	0.0598(2)	0.014(2)	0.022(3)	0.014(3)	−0.005(2)	−0.001(2)	−0.006(2)
C(44)	2*i*		0.0789(4)	0.7145(4)	0.0086(2)	0.022(3)	0.024(3)	0.020(3)	−0.010(2)	−0.003(2)	−0.003(2)
C(45)	2*i*		0.1498(4)	0.6634(4)	−0.0386(3)	0.026(3)	0.043(4)	0.017(3)	−0.019(3)	−0.002(2)	−0.003(3)
C(46)	2*i*		0.1655(4)	0.5646(5)	−0.0354(3)	0.023(3)	0.049(4)	0.028(3)	−0.009(3)	−0.003(2)	−0.019(3)
C(47)	2*i*		0.1118(4)	0.5140(4)	0.0153(3)	0.026(3)	0.030(3)	0.035(3)	−0.011(2)	−0.006(3)	−0.013(3)
C(48)	2*i*		0.0407(4)	0.5631(4)	0.0630(2)	0.020(3)	0.020(3)	0.023(3)	−0.008(2)	−0.002(2)	−0.009(2)
C(49)	2*i*		−0.0549(4)	0.8767(4)	0.2561(2)	0.021(3)	0.019(3)	0.015(3)	−0.008(2)	0.008(2)	−0.008(2)
C(50)	2*i*		0.0215(4)	0.9172(4)	0.2545(3)	0.023(3)	0.027(3)	0.028(3)	−0.009(2)	−0.002(2)	−0.012(3)
C(51)	2*i*		0.0149(5)	1.0124(4)	0.2185(3)	0.039(4)	0.032(3)	0.036(4)	−0.025(3)	0.015(3)	−0.019(3)
C(52)	2*i*		−0.0694(5)	1.0692(4)	0.1847(3)	0.046(4)	0.016(3)	0.029(3)	−0.009(3)	0.007(3)	−0.003(3)
C(53)	2*i*		−0.1440(5)	1.0286(4)	0.1871(3)	0.036(3)	0.022(3)	0.020(3)	0.000(2)	0.002(2)	−0.003(2)
C(54)	2*i*		−0.1383(4)	0.9343(4)	0.2214(2)	0.022(3)	0.023(3)	0.018(3)	−0.004(2)	0.003(2)	−0.008(2)
C(55)	2*i*		−0.4009(4)	0.9093(4)	0.2211(3)	0.018(3)	0.026(3)	0.027(3)	−0.011(2)	0.002(2)	−0.002(2)
C(56)	2*i*		−0.4294(4)	0.9784(4)	0.2587(3)	0.026(3)	0.032(3)	0.026(3)	−0.006(2)	0.005(2)	−0.010(3)
C(57)	2*i*		−0.4647(4)	1.0823(4)	0.2337(3)	0.028(3)	0.020(3)	0.046(4)	−0.001(2)	0.000(3)	−0.013(3)
C(58)	2*i*		−0.4736(4)	1.1168(5)	0.1713(3)	0.024(3)	0.036(4)	0.041(4)	−0.015(3)	−0.001(3)	0.006(3)
C(59)	2*i*		−0.4461(5)	1.0480(5)	0.1343(3)	0.045(4)	0.037(4)	0.033(4)	−0.024(3)	−0.013(3)	0.004(3)
C(60)	2*i*		−0.4094(5)	0.9456(5)	0.1580(3)	0.042(4)	0.038(4)	0.024(3)	−0.027(3)	0.000(3)	−0.001(3)
C(61)	2*i*	0.5005	−0.3084(7)	0.5190(7)	0.4293(5)	0.014(3)	0.014(4)	0.026(4)	−0.005(3)	0.001(3)	−0.006(3)
C(61′)	2*i*	0.4995	−0.1677(7)	0.5065(7)	0.4523(5)	0.014(3)	0.014(4)	0.026(4)	−0.005(3)	0.001(3)	−0.006(3)
C(62)	2*i*	0.5005	−0.3328(8)	0.4840(8)	0.4939(5)	0.027(4)	0.034(5)	0.011(4)	−0.014(3)	0.001(3)	−0.003(3)
C(62′)	2*i*	0.4995	−0.1822(8)	0.4251(9)	0.5012(5)	0.027(4)	0.034(5)	0.011(4)	−0.014(3)	0.001(3)	−0.003(3)
C(63)	2*i*	0.5005	−0.433(1)	0.468(1)	0.5197(6)	0.047(6)	0.039(5)	0.023(5)	−0.022(4)	0.004(4)	−0.002(4)
C(63′)	2*i*	0.4995	−0.121(1)	0.389(1)	0.5478(6)	0.047(6)	0.039(5)	0.023(5)	−0.022(4)	0.004(4)	−0.002(4)
C(64)	2*i*	0.5005	−0.502(1)	0.484(1)	0.4822(6)	0.022(4)	0.028(5)	0.035(5)	−0.003(3)	−0.002(4)	−0.005(4)
C(64′)	2*i*	0.4995	−0.0442(9)	0.4260(9)	0.5463(6)	0.022(4)	0.028(5)	0.035(5)	−0.003(3)	−0.002(4)	−0.005(4)
C(65)	2*i*	0.5005	−0.4736(8)	0.5190(8)	0.4161(5)	0.023(4)	0.025(4)	0.033(5)	−0.004(4)	−0.005(4)	−0.014(4)
C(65′)	2*i*	0.4995	−0.0308(7)	0.5068(9)	0.5000(6)	0.023(4)	0.025(4)	0.033(5)	−0.004(4)	−0.005(4)	−0.014(4)
C(66)	2*i*	0.5005	−0.3799(8)	0.5373(8)	0.3918(5)	0.027(4)	0.025(4)	0.021(4)	−0.012(3)	−0.002(3)	−0.002(3)
C(66′)	2*i*	0.4995	−0.0940(8)	0.5477(8)	0.4517(5)	0.027(4)	0.025(4)	0.021(4)	−0.012(3)	−0.002(3)	−0.002(3)
C(67)	2*i*		0.1858(4)	0.3947(4)	0.2991(2)	0.031(3)	0.025(3)	0.018(3)	−0.020(2)	−0.008(2)	0.005(2)
C(68)	2*i*		0.2584(4)	0.2962(4)	0.2989(3)	0.018(3)	0.036(3)	0.021(3)	−0.015(2)	0.001(2)	−0.003(3)
C(69)	2*i*		0.3221(4)	0.2471(5)	0.3445(3)	0.020(3)	0.043(4)	0.027(3)	−0.009(3)	−0.002(2)	0.002(3)
C(70)	2*i*		0.3159(5)	0.2971(5)	0.3893(3)	0.037(4)	0.048(4)	0.038(4)	−0.027(3)	−0.018(3)	0.021(3)
C(71)	2*i*		0.2465(6)	0.3947(5)	0.3890(3)	0.077(5)	0.053(5)	0.031(4)	−0.047(4)	−0.024(4)	0.005(3)
C(72)	2*i*		0.1804(5)	0.4445(5)	0.3437(3)	0.064(4)	0.025(3)	0.031(3)	−0.027(3)	−0.025(3)	0.008(3)
C(73)	2*i*		−0.3110(4)	0.8036(4)	0.0116(2)	0.031(3)	0.023(3)	0.015(3)	−0.006(2)	−0.007(2)	−0.005(2)
C(74)	2*i*		−0.2006(4)	0.7890(4)	−0.0112(2)	0.031(3)	0.023(3)	0.020(3)	−0.009(2)	−0.007(2)	−0.005(2)
C(75)	2*i*		−0.1678(4)	0.8597(4)	−0.0576(3)	0.028(3)	0.031(3)	0.024(3)	−0.014(2)	−0.006(2)	−0.008(3)
C(76)	2*i*		−0.2449(5)	0.9473(4)	−0.0835(3)	0.041(3)	0.026(3)	0.026(3)	−0.016(3)	−0.009(3)	−0.005(3)
C(77)	2*i*		−0.3530(5)	0.9611(4)	−0.0634(3)	0.035(3)	0.027(3)	0.026(3)	−0.004(3)	−0.010(3)	−0.002(3)
C(78)	2*i*		−0.3860(5)	0.8914(4)	−0.0159(3)	0.028(3)	0.031(3)	0.030(3)	−0.007(3)	−0.005(3)	−0.005(3)
C(79)	2*i*		−0.4817(4)	0.8773(4)	0.4343(2)	0.020(3)	0.028(3)	0.011(3)	−0.008(2)	0.000(2)	−0.004(2)
C(80)	2*i*		−0.5205(4)	0.8060(5)	0.4338(3)	0.029(3)	0.036(4)	0.019(3)	−0.013(3)	−0.002(2)	−0.006(3)
C(81)	2*i*		−0.6313(5)	0.8286(6)	0.4416(3)	0.042(4)	0.076(5)	0.023(3)	−0.040(4)	−0.009(3)	0.003(3)
C(82)	2*i*		−0.7028(5)	0.9231(6)	0.4513(3)	0.017(3)	0.070(5)	0.036(4)	−0.009(3)	−0.011(3)	0.017(4)
C(83)	2*i*		−0.6649(5)	0.9949(5)	0.4525(3)	0.025(3)	0.049(4)	0.034(4)	0.005(3)	0.000(3)	0.008(3)
C(84)	2*i*		−0.5554(4)	0.9726(4)	0.4443(3)	0.028(3)	0.035(3)	0.023(3)	−0.008(3)	−0.003(2)	−0.001(3)

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