The gas-phase structure of octaphenyloctasilsesquioxane $Si_8O_{12}Ph_8$ and the crystal structures of Si_8O_{12}(*p*-tolyl)$_8$ and Si_8O_{12}(*p*-$ClCH_2C_6H_4$)$_8$

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Supplementary Information

The X-ray crystal structure of Si_8O_{12}(*p*-tolyl)$_8$ (2)

The included solvent was found to be highly disordered, and the best approach to handling this electron density was found to be the SQUEEZE routine of PLATON.[45] This suggested a total of 809 electrons per unit cell, equivalent to approximately 51 electrons per asymmetric unit. The crystal was grown from a 3:1 mixture of acetone [Me_2C=O, C_3H_6O, 32 electrons] and dichloromethane [CH_2Cl_2, 42 electrons]. The shape and flat electron density profile of the residual electron density peaks observed in the disordered solvent region before the use of SQUEEZE suggest that the included solvent is slightly more likely to be acetone rather than dichloromethane. 51 electrons equates to *ca.* 1.5 acetone molecules (48 electrons), and so this interpretation of the included solvent was used for the calculations of the contents of the asymmetric unit. The equates to 6 acetone molecules per cage.

As a result of the absence of the solvent atoms from the asymmetric unit, the atom list is low by $C_{4.5}H_9O_{1.5}$ (and the unit cell low by $C_{72}H_{144}O_{24}$) compared to what is actually presumed to be present. The middle of the cage is at a 2/*m* special position. The structure of the asymmetric unit of **2**, showing 30% probability ellipsoids, is shown in Figure S2 below.

The X-ray crystal structure of Si_8O_{12}(*p*-$ClCH_2C_6H_4$)$_8$ (3)

Disorder was found for two of the eight chlorobenzyl moieties in the structure of **3**. For the Si(5)-bound unit, three partial occupancy orientations of *ca.* 49, 31 and 20% occupancy were identified, their geometries optimised, and only the chlorine atoms were refined anisotropically. For the Si(8)-bound unit, two partial occupancy orientations of ca. 60 and 40% occupancy were identified, their geometries optimised, and the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (the others were refined isotropically).

The crystals of **3** were very weak scatterers of X-rays, so the target resolution of the data collection was trimmed to 0.90 Å with 98.5% completeness. Despite these measures, the three-day data collection resulted in a data set that was only 97% complete. The molecular structure of **3**, showing 30% probability ellipsoids, is shown in Figure S3 below.

Table S1 Nozzle-to-camera distances (mm), temperatures (K), accelerating voltages (kV), individual *R* factors (%), scale factors and electron wavelengths ($Å^{-1}$) used in the GED study of $Si_8O_{12}Ph_8$ (**1**).

Nozzle-to-plate distance	338	598
Temperature	615(10)	615(10)
Accelerating Voltage	74.2	72.9
R factor	5.7	4.7
Scale factor	1.18	1.46
Electron wavelength	0.04350	0.04390

Table S2 Cartesian coordinates for the calculated [B3LYP/cc-pVTZ] structure of **1**.

	x	*y*	*z*
Si(1)	-1.5613	1.5996	1.5786
Si(2)	-1.5996	-1.5613	1.5786
Si(3)	1.5613	-1.5996	1.5786
Si(4)	1.5996	-1.5613	-1.5786
Si(5)	1.5613	1.5996	-1.5786
Si(6)	-1.5996	1.5613	-1.5786
Si(7)	-1.5613	-1.5996	-1.5786
Si(8)	1.5996	1.5613	1.5786
O(9)	-1.8922	1.8922	0.0000
O(10)	-1.8922	-1.8922	0.0000
O(11)	1.8922	-1.8922	0.0000
O(12)	1.8922	1.8922	0.0000
O(13)	0.0203	1.8860	1.8883
O(14)	-1.8860	0.0203	1.8883
O(15)	-0.0203	-1.8860	1.8883
O(16)	1.8860	0.0203	-1.8883
O(17)	-0.0203	1.8860	-1.8883
O(18)	-1.8860	-0.0203	-1.8883
O(19)	0.0203	-1.8860	-1.8883
O(20)	1.8860	-0.0203	1.8883
C(21)	-2.6078	2.6984	2.6485
C(22)	-2.6984	-2.6078	2.6485
C(23)	2.6078	-2.6984	2.6485
C(24)	2.6984	-2.6078	-2.6485
C(25)	2.6078	2.6984	-2.6485
C(26)	-2.6984	2.6078	-2.6485
C(27)	-2.6078	-2.6984	-2.6485
C(28)	2.6984	2.6078	2.6485
C(29)	-3.9376	2.9755	2.3062
C(30)	-2.9755	-3.9376	2.3062
C(31)	3.9376	-2.9755	2.3062
C(32)	2.9755	-3.9376	-2.3062

C(33)	3.9376	2.9755	-2.3062
C(34)	-2.9755	3.9376	-2.3062
C(35)	-3.9376	-2.9755	-2.3062
C(36)	2.9755	3.9376	2.3062
C(37)	-2.0993	3.2524	3.8294
C(38)	-3.2524	-2.0993	3.8294
C(39)	2.0993	-3.2524	3.8294
C(40)	3.2524	-2.0993	-3.8294
C(41)	2.0993	3.2524	-3.8294
C(42)	-3.2524	2.0993	-3.8294
C(43)	-2.0993	-3.2524	-3.8294
C(44)	3.2524	2.0993	3.8294
C(45)	-4.7334	3.7749	3.1178
C(46)	-3.7749	-4.7334	3.1178
C(47)	4.7334	-3.7749	3.1178
C(48)	3.7749	-4.7334	-3.1178
C(49)	4.7334	3.7749	-3.1178
C(50)	-3.7749	4.7334	-3.1178
C(51)	-4.7334	-3.7749	-3.1178
C(52)	3.7749	4.7334	3.1178
C(53)	-2.8933	4.0522	4.6437
C(54)	-4.0522	-2.8933	4.6437
C(55)	2.8933	-4.0522	4.6437
C(56)	4.0522	-2.8933	-4.6437
C(57)	2.8933	4.0522	-4.6437
C(58)	-4.0522	2.8933	-4.6437
C(59)	-2.8933	-4.0522	-4.6437
C(60)	4.0522	2.8933	4.6437
C(61)	-4.2119	4.3134	4.2894
C(62)	-4.3134	-4.2119	4.2894
C(63)	4.2119	-4.3134	4.2894
C(64)	4.3134	-4.2119	-4.2894
C(65)	4.2119	4.3134	-4.2894
C(66)	-4.3134	4.2119	-4.2894
C(67)	-4.2119	-4.3134	-4.2894
C(68)	4.3134	4.2119	4.2894
H(69)	-4.3550	2.5704	1.3928
H(70)	-2.5704	-4.3550	1.3928
H(71)	4.3550	-2.5704	1.3928
H(72)	2.5704	-4.3550	-1.3928
H(73)	4.3550	2.5704	-1.3928
H(74)	-2.5704	4.3550	-1.3928
H(75)	-4.3550	-2.5704	-1.3928
H(76)	2.5704	4.3550	1.3928
H(77)	-1.0711	3.0645	4.1106
H(78)	-3.0645	-1.0711	4.1106
H(79)	1.0711	-3.0645	4.1106
H(80)	3.0645	-1.0711	-4.1106
H(81)	1.0711	3.0645	-4.1106
H(82)	-3.0645	1.0711	-4.1106
H(83)	-1.0711	-3.0645	-4.1106
H(84)	3.0645	1.0711	4.1106

H(85)	-5.7581	3.9798	2.8355
H(86)	-3.9798	-5.7581	2.8355
H(87)	5.7581	-3.9798	2.8355
H(88)	3.9798	-5.7581	-2.8355
H(89)	5.7581	3.9798	-2.8355
H(90)	-3.9798	5.7581	-2.8355
H(91)	-5.7581	-3.9798	-2.8355
H(92)	3.9798	5.7581	2.8355
H(93)	-2.4817	4.4740	5.5516
H(94)	-4.4740	-2.4817	5.5516
H(95)	2.4817	-4.4740	5.5516
H(96)	4.4740	-2.4817	-5.5516
H(97)	2.4817	4.4740	-5.5516
H(98)	-4.4740	2.4817	-5.5516
H(99)	-2.4817	-4.4740	-5.5516
H(100)	4.4740	2.4817	5.5516
H(101)	-4.8304	4.9375	4.9217
H(102)	-4.9375	-4.8304	4.9217
H(103)	4.8304	-4.9375	4.9217
H(104)	4.9375	-4.8304	-4.9217
H(105)	4.8304	4.9375	-4.9217
H(106)	-4.9375	4.8304	-4.9217
H(107)	-4.8304	-4.9375	-4.9217
H(108)	4.9375	4.8304	4.9217

Energy = –5072.4567 Hartrees

Table S3 Cartesian coordinates for the GED-refined structure of **1**.

	x	*y*	*z*
Si(1)	-1.5616	1.5999	1.5790
Si(2)	-1.5999	-1.5616	1.5790
Si(3)	1.5616	-1.5999	1.5790
Si(4)	1.5999	-1.5616	-1.5790
Si(5)	1.5616	1.5999	-1.5790
Si(6)	-1.5999	1.5616	-1.5790
Si(7)	-1.5616	-1.5999	-1.5790
Si(8)	1.5999	1.5616	1.5790
O(9)	-1.9059	1.9059	0.0000
O(10)	-1.9059	-1.9059	0.0000
O(11)	1.9059	-1.9059	0.0000
O(12)	1.9059	1.9059	0.0000
O(13)	0.0188	1.8837	1.8801
O(14)	-1.8837	0.0188	1.8801
O(15)	-0.0188	-1.8837	1.8801
O(16)	1.8837	0.0188	-1.8801
O(17)	-0.0188	1.8837	-1.8801
O(18)	-1.8837	-0.0188	-1.8801
O(19)	0.0188	-1.8837	-1.8801
O(20)	1.8837	-0.0188	1.8801
C(21)	-2.6251	2.6920	2.6420
C(22)	-2.6920	-2.6251	2.6420
C(23)	2.6251	-2.6920	2.6420
C(24)	2.6920	-2.6251	-2.6420

C(25)	2.6251	2.6920	-2.6420
C(26)	-2.6920	2.6251	-2.6420
C(27)	-2.6251	-2.6920	-2.6420
C(28)	2.6920	2.6251	2.6420
C(29)	-3.9383	2.9662	2.2579
C(30)	-2.9662	-3.9383	2.2579
C(31)	3.9383	-2.9662	2.2579
C(32)	2.9662	-3.9383	-2.2579
C(33)	3.9383	2.9662	-2.2579
C(34)	-2.9662	3.9383	-2.2579
C(35)	-3.9383	-2.9662	-2.2579
C(36)	2.9662	3.9383	2.2579
C(37)	-2.1746	3.2171	3.8528
C(38)	-3.2171	-2.1746	3.8528
C(39)	2.1746	-3.2171	3.8528
C(40)	3.2171	-2.1746	-3.8528
C(41)	2.1746	3.2171	-3.8528
C(42)	-3.2171	2.1746	-3.8528
C(43)	-2.1746	-3.2171	-3.8528
C(44)	3.2171	2.1746	3.8528
C(45)	-4.7850	3.7301	3.0424
C(46)	-3.7301	-4.7850	3.0424
C(47)	4.7850	-3.7301	3.0424
C(48)	3.7301	-4.7850	-3.0424
C(49)	4.7850	3.7301	-3.0424
C(50)	-3.7301	4.7850	-3.0424
C(51)	-4.7850	-3.7301	-3.0424
C(52)	3.7301	4.7850	3.0424
C(53)	-3.0113	3.9826	4.6479
C(54)	-3.9826	-3.0113	4.6479
C(55)	3.0113	-3.9826	4.6479
C(56)	3.9826	-3.0113	-4.6479
C(57)	3.0113	3.9826	-4.6479
C(58)	-3.9826	3.0113	-4.6479
C(59)	-3.0113	-3.9826	-4.6479
C(60)	3.9826	3.0113	4.6479
C(61)	-4.3286	4.2439	4.2454
C(62)	-4.2439	-4.3286	4.2454
C(63)	4.3286	-4.2439	4.2454
C(64)	4.2439	-4.3286	-4.2454
C(65)	4.3286	4.2439	-4.2454
C(66)	-4.2439	4.3286	-4.2454
C(67)	-4.3286	-4.2439	-4.2454
C(68)	4.2439	4.3286	4.2454
H(69)	-4.3130	2.5869	1.3264
H(70)	-2.5869	-4.3130	1.3264
H(71)	4.3130	-2.5869	1.3264
H(72)	2.5869	-4.3130	-1.3264
H(73)	4.3130	2.5869	-1.3264
H(74)	-2.5869	4.3130	-1.3264
H(75)	-4.3130	-2.5869	-1.3264
H(76)	2.5869	4.3130	1.3264

H(77)	-1.1660	3.0341	4.1690
H(78)	-3.0341	-1.1660	4.1690
H(79)	1.1660	-3.0341	4.1690
H(80)	3.0341	-1.1660	-4.1690
H(81)	1.1660	3.0341	-4.1690
H(82)	-3.0341	1.1660	-4.1690
H(83)	-1.1660	-3.0341	-4.1690
H(84)	3.0341	1.1660	4.1690
H(85)	-5.7883	3.9233	2.7155
H(86)	-3.9233	-5.7883	2.7155
H(87)	5.7883	-3.9233	2.7155
H(88)	3.9233	-5.7883	-2.7155
H(89)	5.7883	3.9233	-2.7155
H(90)	-3.9233	5.7883	-2.7155
H(91)	-5.7883	-3.9233	-2.7155
H(92)	3.9233	5.7883	2.7155
H(93)	-2.6494	4.3818	5.5754
H(94)	-4.3818	-2.6494	5.5754
H(95)	2.6494	-4.3818	5.5754
H(96)	4.3818	-2.6494	-5.5754
H(97)	2.6494	4.3818	-5.5754
H(98)	-4.3818	2.6494	-5.5754
H(99)	-2.6494	-4.3818	-5.5754
H(100)	4.3818	2.6494	5.5754
H(101)	-4.9792	4.8379	4.8576
H(102)	-4.8379	-4.9792	4.8576
H(103)	4.9792	-4.8379	4.8576
H(104)	4.8379	-4.9792	-4.8576
H(105)	4.9792	4.8379	-4.8576
H(106)	-4.8379	4.9792	-4.8576
H(107)	-4.9792	-4.8379	-4.8576
H(108)	4.8379	4.9792	4.8576

Table S4 First least-squares correlation matrix (×100) for $Si_8O_{12}Ph_8$.[a]

	p_1	p_4
p_5		–79.2
p_6	–70.6	

[a] Only elements with absolute values ≥50% are shown.

Table S5 Second least-squares correlation matrix (×100) for $Si_8O_{12}Ph_8$.[a]

	p_9	p_{12}	p_{14}	p_{16}	p_{18}
p_{13}	81.9	–50.8			
p_{14}		–95.0			
p_{18}		–53.8	63.2	–80.0	
p_{20}		–51.6		–98.2	85.1

[a] Only elements with absolute values ≥50% are shown.

Table S6 Interatomic distances (r_a / Å), experimental and theoretical amplitudes of vibration (u_{h1} / Å), and k_{h1} values for the GED structure of $Si_8O_{12}Ph_8$ (**1**).[a,b]

	Atom pair	r_a	Expt. u_{h1}	Calc. u_{h1}	k_{h1}
u_1	C(37)-H(77)	1.0705(16)	0.0540(23)	0.0828	0.0022
u_2	C(61)-H(101)	1.0717(16)	0.0468(tied to u_1)	0.0756	0.0011
u_3	C(29)-H(69)	1.0711(16)	0.0544(tied to u_1)	0.0832	0.0023
u_4	C(29)-C(45)	1.3840(16)	0.0318(7)	0.0475	0.0001
u_5	C(53)-C(61)	1.4003(88)	0.0479(tied to u_4)	0.0637	0.0016
u_6	C(37)-C(53)	1.3849(16)	0.0318(tied to u_4)	0.0476	0.0001
u_7	C(45)-C(61)	1.3840(16)	0.0472(tied to u_4)	0.0629	0.0015
u_8	C(21)-C(37)	1.3930(16)	0.0480(tied to u_4)	0.0638	0.0016
u_9	C(21)-C(29)	1.3937(16)	0.0494(tied to u_4)	0.0652	0.0018
u_{10}	Si(1)-O(13)	1.6334(49)	0.0391(6)	0.0545	0.0003
u_{11}	Si(1)-O(9)	1.6446(62)	0.0389(tied to u_{10})	0.0543	0.0001
u_{12}	Si(1)-O(14)	1.6414(79)	0.0395(tied to u_{10})	0.0549	0.0000
u_{13}	Si(1)-C(21)	1.8597(14)	0.0455(20)	0.0585	-0.0014
u_{14}	C(45)...H(69)	2.1166(141)	0.0824(30)	0.1149	-0.0013
u_{15}	C(53)...H(77)	2.1306(135)	0.0811(tied to u_{14})	0.1137	-0.0012
u_{16}	C(29)...H(85)	2.1340(19)	0.0842(tied to u_{14})	0.1168	-0.0015
u_{17}	C(37)...H(93)	2.1331(19)	0.0823(tied to u_{14})	0.1148	-0.0001
u_{18}	C(61)...H(93)	2.1156(150)	0.0754(tied to u_{14})	0.108	0.0309
u_{19}	C(53)...H(101)	2.1593(85)	0.0879(tied to u_{14})	0.1205	-0.0033
u_{20}	C(45)...H(101)	2.1380(19)	0.0855(tied to u_{14})	0.1181	-0.0026
u_{21}	C(61)...H(85)	2.1077(142)	0.0761(tied to u_{14})	0.1086	0.0311
u_{22}	C(21)...H(77)	2.1109(19)	0.0759(tied to u_{14})	0.1084	0.0287
u_{23}	C(21)...H(69)	2.1123(19)	0.0759(tied to u_{14})	0.1085	0.0303
u_{24}	C(29)...C(37)	2.3624(57)	0.0564(11)	0.0733	0.0287
u_{25}	C(45)...C(53)	2.3755(93)	0.0558(tied to u_{24})	0.0727	0.0302
u_{26}	C(29)...C(61)	2.4018(177)	0.0699(tied to u_{24})	0.0868	-0.0070
u_{27}	C(37)...C(61)	2.4263(137)	0.0731(tied to u_{24})	0.09	-0.0080
u_{28}	C(21)...C(53)	2.4215(150)	0.0700(tied to u_{24})	0.0869	-0.0052
u_{29}	C(21)...C(45)	2.4361(138)	0.0741(tied to u_{24})	0.091	-0.0064
u_{30}	H(69)...H(85)	2.4125(211)	0.1676(fixed)	0.1676	0.0148
u_{31}	H(77)...H(93)	2.4338(206)	0.1678(fixed)	0.1678	0.0147
u_{32}	O(9)...O(14)	2.6530(35)	0.1057(23)	0.1117	0.0109
u_{33}	O(13)...O(14)	2.6534(62)	0.1072(tied to u_{32})	0.1132	0.0107
u_{34}	O(9)...O(13)	2.6789(73)	0.1056(tied to u_{32})	0.1116	0.0118
u_{35}	O(13)...H(77)	3.0445(513)	0.6963(fixed)	0.6963	-0.2221
u_{36}	C(29)...C(53)	2.7526(224)	0.1019(12)	0.1143	0.0050
u_{37}	C(37)...C(45)	2.7729(270)	0.0978(tied to u_{36})	0.1102	0.0082
u_{38}	C(21)...C(61)	2.7953(55)	0.0598(tied to u_{36})	0.0722	0.0121
u_{39}	Si(1)...C(29)	2.8265(108)	0.1073(tied to u_{36})	0.1197	-0.0022
u_{40}	Si(1)...C(37)	2.8571(114)	0.1012(tied to u_{36})	0.1136	-0.0003
u_{41}	O(13)...C(21)	2.8670(279)	0.0993(tied to u_{36})	0.1117	0.0006

u_{42}	O(9)...C(21)	2.8477(146)	0.1053(tied to u_{36})	0.1177	0.0010
u_{43}	O(13)...C(28)	2.8749(140)	0.1051(tied to u_{36})	0.1176	0.0019
u_{44}	O(9)...H(69)	2.8876(539)	0.8249(fixed)	0.8248	-0.0561
u_{45}	Si(1)...H(69)	2.9310(173)	0.2202(fixed)	0.2202	0.0030
u_{46}	Si(1)...H(77)	2.9854(210)	0.2167(fixed)	0.2167	0.0016
u_{47}	Si(1)...Si(6)	3.1184(8)	0.0904(15)	0.109	0.0400
u_{48}	Si(1)...Si(2)	3.1215(8)	0.0918(tied to u_{47})	0.1104	0.0403
u_{49}	O(13)...C(37)	3.3867(386)	0.5061(667)	0.3694	-0.1494
u_{50}	O(9)...C(29)	3.3044(419)	0.5743(tied to u_{49})	0.4377	-0.0867
u_{51}	C(61)...H(69)	3.3590(214)	0.1149(58)	0.1535	-0.0024
u_{52}	C(61)...H(77)	3.3891(184)	0.1135(tied to u_{51})	0.1522	-0.0021
u_{53}	C(29)...H(77)	3.3228(49)	0.0759(tied to u_{51})	0.1146	0.0451
u_{54}	C(53)...H(85)	3.3357(158)	0.0766(tied to u_{51})	0.1153	0.0480
u_{55}	C(45)...H(93)	3.3296(104)	0.0760(tied to u_{51})	0.1147	0.0470
u_{56}	C(29)...H(101)	3.3628(131)	0.0710(tied to u_{51})	0.1096	0.0054
u_{57}	C(37)...H(69)	3.3238(49)	0.0762(tied to u_{51})	0.1148	0.0456
u_{58}	C(37)...H(101)	3.3880(97)	0.0747(tied to u_{51})	0.1133	0.0036
u_{59}	C(21)...H(93)	3.3855(109)	0.1131(tied to u_{51})	0.1517	0.0000
u_{60}	C(21)...H(85)	3.3962(95)	0.1181(tied to u_{51})	0.1568	-0.0010
u_{61}	O(13)...H(76)	3.3314(484)	0.8694(tied to u_{51})	0.908	0.2468
u_{62}	O(13)...C(36)	3.5436(332)	0.3462(225)	0.5006	0.0691
u_{63}	H(69)...H(74)	1.4677(2156)	2.9385(tied to u_{51})	2.9771	2.1372
u_{64}	O(13)...O(15)	3.6728(88)	0.2650(tied to u_{62})	0.4193	0.0948
u_{65}	O(13)...C(44)	3.6638(313)	0.3063(tied to u_{62})	0.4606	0.1052
u_{66}	O(13)...O(17)	3.6658(261)	0.2563(tied to u_{62})	0.4106	0.0946
u_{67}	O(9)...O(10)	3.7207(313)	0.2542(tied to u_{62})	0.4086	0.0911
u_{68}	Si(1)...O(17)	3.7395(134)	0.3082(84)	0.2268	0.0587
u_{69}	Si(1)...O(12)	3.7658(154)	0.3049(tied to u_{68})	0.2235	0.0566
u_{70}	Si(1)...O(20)	3.7606(36)	0.3084(tied to u_{68})	0.227	0.0579
u_{71}	Si(1)...O(15)	3.7629(70)	0.3123(tied to u_{68})	0.2309	0.0590
u_{72}	Si(1)...O(18)	3.7741(111)	0.3036(tied to u_{68})	0.2222	0.0585
u_{73}	Si(1)...O(10)	3.8025(155)	0.3061(tied to u_{68})	0.2248	0.0578
u_{74}	O(13)...H(84)	3.5934(557)	0.7661(tied to u_{51})	0.8048	0.2597
u_{75}	C(29)...H(93)	3.8117(225)	0.1190(tied to u_{51})	0.1576	0.0186
u_{76}	C(53)...H(69)	3.8124(226)	0.1200(tied to u_{51})	0.1587	0.0184
u_{77}	C(45)...H(77)	3.8322(270)	0.1142(tied to u_{51})	0.1528	0.0215
u_{78}	C(37)...H(85)	3.8318(268)	0.1161(tied to u_{51})	0.1548	0.0219
u_{79}	C(21)...H(101)	3.8555(57)	0.0630(tied to u_{51})	0.1016	0.0248
u_{80}	Si(1)...H(78)	4.3248(700)	0.8119(fixed)	0.8119	-0.2595
u_{81}	C(21)...H(78)	4.4916(834)	0.8428(578)	1.2012	-0.3223
u_{82}	O(9)...C(37)	3.9320(193)	0.2429(79)	0.2788	0.1467
u_{83}	O(13)...C(29)	3.9683(169)	0.1786(tied to u_{82})	0.2146	0.1515
u_{84}	Si(1)...C(45)	4.1223(142)	0.1096(25)	0.1082	0.0092
u_{85}	Si(1)...C(53)	4.1350(141)	0.1037(tied to u_{84})	0.1023	0.0119

u_{86}	Si(1)...H(74)	4.1860(723)	0.9379(tied to u_{84})	0.9365	-0.0807
u_{87}	C(29)...H(74)	3.3891(1882)	1.8457(tied to u_{81})	2.2041	0.6714
u_{88}	H(69)...H(101)	4.2341(170)	-0.1818(tied to u_{81})	0.1766	0.0062
u_{89}	H(77)...H(101)	4.2684(147)	-0.1786(tied to u_{81})	0.1798	0.0058
u_{90}	H(69)...H(77)	4.1942(42)	-0.2079(tied to u_{81})	0.1505	0.0701
u_{91}	O(9)...H(77)	4.1265(230)	0.1304(tied to u_{81})	0.4888	0.2554
u_{92}	C(21)...H(74)	4.2793(1078)	1.0352(tied to u_{81})	1.3936	0.0076
u_{93}	C(37)...H(78)	4.7439(645)	1.1305(tied to u_{81})	1.4889	-0.2662
u_{94}	Si(1)...Si(5)	4.3851(11)	0.1244(tied to u_{84})	0.123	0.0564
u_{95}	O(13)...H(69)	4.1616(174)	0.0110(tied to u_{81})	0.3694	0.2617
u_{96}	Si(1)...Si(3)	4.4142(11)	0.1264(tied to u_{84})	0.125	0.0572
u_{97}	Si(1)...C(22)	4.4483(299)	0.1503(tied to u_{84})	0.1489	0.0526
u_{98}	Si(1)...C(26)	4.4371(154)	0.1531(tied to u_{84})	0.1517	0.0511
u_{99}	Si(1)...Si(7)	4.4381(11)	0.1238(tied to u_{84})	0.1224	0.0575
u_{100}	Si(1)...C(28)	4.4482(150)	0.1552(tied to u_{84})	0.1537	0.0545
u_{101}	C(29)...H(78)	4.4085(1799)	1.3674(tied to u_{81})	1.7258	0.2331
u_{102}	O(13)...C(53)	4.7123(350)	0.2899(tied to u_{82})	0.3258	-0.1029
u_{103}	H(77)...H(78)	4.3741(898)	1.5549(tied to u_{81})	1.9133	0.2227
u_{104}	O(13)...O(16)	4.5136(268)	0.2316(tied to u_{82})	0.2676	0.0794
u_{105}	O(9)...C(45)	4.6306(491)	0.3364(tied to u_{82})	0.3724	-0.0619
u_{106}	O(9)...O(15)	4.5547(100)	0.2323(tied to u_{82})	0.2682	0.0775
u_{107}	O(9)...O(19)	4.5697(126)	0.2348(tied to u_{82})	0.2708	0.0779
u_{108}	O(13)...O(18)	4.5442(218)	0.2325(tied to u_{82})	0.2684	0.0795
u_{109}	Si(1)...C(38)	4.8337(496)	0.4450(tied to u_{84})	0.4435	-0.1265
u_{110}	Si(1)...C(61)	4.6362(45)	0.0890(tied to u_{84})	0.0876	0.0282
u_{111}	H(69)...H(78)	3.8147(2094)	1.9380(tied to u_{81})	2.2964	1.0638
u_{112}	Si(1)...C(34)	4.7620(535)	0.5114(tied to u_{84})	0.5099	-0.0543
u_{113}	C(29)...C(34)	4.6732(1668)	1.4779(31)	1.5133	0.0473
u_{114}	O(13)...H(78)	5.1732(485)	0.6584(tied to u_{113})	0.6937	-0.2885
u_{115}	O(13)...H(74)	5.0569(596)	0.6684(tied to u_{113})	0.7037	-0.2640
u_{116}	O(13)...C(52)	4.8088(500)	0.3758(tied to u_{113})	0.4111	0.0433
u_{117}	H(69)...H(93)	4.8691(228)	0.1627(tied to u_{113})	0.198	0.0343
u_{118}	H(77)...H(85)	4.8887(269)	0.1608(tied to u_{113})	0.1962	0.0377
u_{119}	Si(1)...H(76)	4.6737(541)	1.0174(tied to u_{113})	1.0527	0.2897
u_{120}	C(21)...C(38)	5.2298(514)	0.6676(tied to u_{113})	0.7029	-0.1801
u_{121}	Si(1)...H(85)	4.9445(115)	0.1523(tied to u_{113})	0.1877	0.0107
u_{122}	O(13)...C(60)	4.8863(329)	0.3485(tied to u_{113})	0.3838	0.0780
u_{123}	Si(1)...H(93)	4.9753(112)	0.1433(tied to u_{113})	0.1786	0.0141
u_{124}	C(45)...H(74)	4.5321(2261)	2.1763(tied to u_{113})	2.2117	0.3931
u_{125}	C(21)...C(34)	5.1294(923)	0.7768(tied to u_{113})	0.8122	-0.0620
u_{126}	O(13)...H(93)	5.3590(411)	0.4494(tied to u_{113})	0.4848	-0.1613
u_{127}	Si(1)...O(16)	5.0553(122)	0.1767(tied to u_{113})	0.2121	0.0765
u_{128}	C(53)...H(78)	5.5468(1190)	1.4897(tied to u_{113})	1.5251	-0.3760
u_{129}	Si(1)...C(36)	5.0181(361)	0.5518(tied to u_{113})	0.5871	0.1230

u_{130}	Si(1)...O(11)	5.1026(210)	0.1761(tied to u_{113})	0.2115	0.0750
u_{131}	Si(1)...O(19)	5.0807(102)	0.1776(tied to u_{113})	0.2129	0.0767
u_{132}	O(9)...H(78)	5.3191(768)	0.8551(tied to u_{113})	0.8905	-0.0191
u_{133}	O(9)...C(53)	5.0838(396)	0.2086(tied to u_{113})	0.244	0.1256
u_{134}	C(45)...H(78)	5.2857(2212)	1.7023(tied to u_{113})	1.7376	0.0347
u_{135}	O(9)...H(85)	5.2465(617)	0.5150(tied to u_{113})	0.5504	-0.0971
u_{136}	O(13)...C(45)	5.1497(226)	0.1598(tied to u_{113})	0.1952	0.1263
u_{137}	O(9)...C(22)	5.2328(229)	0.2039(tied to u_{113})	0.2392	0.0707
u_{138}	O(9)...H(75)	5.2463(483)	0.8712(tied to u_{113})	0.9065	0.0205
u_{139}	O(13)...C(25)	5.2092(123)	0.2104(tied to u_{113})	0.2457	0.0724
u_{140}	C(21)...C(26)	5.2122(440)	0.2854(tied to u_{113})	0.3207	0.0725
u_{141}	Si(1)...H(84)	4.9779(605)	0.9072(tied to u_{113})	0.9426	0.3153
u_{142}	O(13)...C(22)	5.2432(226)	0.2006(tied to u_{113})	0.236	0.0726
u_{143}	C(21)...C(22)	5.2384(211)	0.2842(tied to u_{113})	0.3196	0.0790
u_{144}	H(69)...H(90)	4.3993(2643)	2.6666(tied to u_{113})	2.702	0.7715
u_{145}	O(13)...C(23)	5.2453(57)	0.2111(tied to u_{113})	0.2465	0.0754
u_{146}	Si(1)...C(44)	5.1629(340)	0.5042(tied to u_{113})	0.5396	0.1603
u_{147}	O(13)...O(19)	5.2341(232)	0.2434(tied to u_{113})	0.2787	0.0887
u_{148}	O(13)...C(26)	5.2519(227)	0.1953(tied to u_{113})	0.2307	0.0722
u_{149}	C(29)...C(38)	5.3021(1275)	1.2670(tied to u_{113})	1.3023	0.1285
u_{150}	O(9)...C(27)	5.2777(227)	0.2013(tied to u_{113})	0.2367	0.0737
u_{151}	O(9)...O(11)	5.3053(442)	0.2421(tied to u_{113})	0.2774	0.0854
u_{152}	C(37)...H(74)	5.2959(1017)	1.1599(tied to u_{113})	1.1953	0.0141
u_{153}	C(37)...H(76)	4.7731(1567)	1.9174(tied to u_{113})	1.9527	0.7274
u_{154}	O(13)...C(61)	5.4558(265)	0.1625(tied to u_{113})	0.1978	0.0273
u_{155}	O(13)...C(68)	5.3789(413)	0.1915(tied to u_{113})	0.2268	0.0454
u_{156}	O(9)...C(61)	5.3773(474)	0.1759(tied to u_{113})	0.2112	0.0411
u_{157}	Si(1)...Si(4)	5.4037(14)	0.0793(tied to u_{113})	0.1147	0.0701
u_{158}	C(37)...C(38)	5.5067(560)	1.0865(tied to u_{113})	1.1219	-0.0152
u_{159}	O(13)...H(73)	5.2584(691)	0.9399(tied to u_{113})	0.9753	0.1468
u_{160}	C(61)...H(78)	5.9530(1872)	1.4225(tied to u_{113})	1.4579	-0.3900
u_{161}	O(13)...C(38)	5.6625(401)	0.3791(tied to u_{113})	0.4145	-0.1099
u_{162}	O(13)...H(79)	5.4275(497)	0.9041(tied to u_{113})	0.9395	0.1169
u_{163}	O(13)...C(34)	5.5877(460)	0.3838(tied to u_{113})	0.4192	-0.0872
u_{164}	C(21)...H(76)	5.0496(1018)	1.5137(tied to u_{113})	1.5491	0.5649
u_{165}	C(37)...H(84)	5.2052(833)	1.6354(tied to u_{113})	1.6707	0.4017
u_{166}	O(13)...H(92)	5.5121(574)	0.5718(tied to u_{113})	0.6072	0.0726
u_{167}	Si(1)...C(42)	5.4843(196)	0.3059(tied to u_{113})	0.3413	0.2232
u_{168}	O(9)...C(38)	5.7703(473)	0.4736(tied to u_{113})	0.5089	-0.0071
u_{169}	C(29)...C(50)	5.6161(2149)	1.5142(tied to u_{113})	1.5495	-0.0085
u_{170}	C(21)...C(36)	5.5214(835)	0.8771(tied to u_{113})	0.9124	0.2200
u_{171}	Si(1)...H(101)	5.6919(46)	0.0790(tied to u_{113})	0.1143	0.0452
u_{172}	H(77)...H(100)	5.9661(1222)	1.7474(tied to u_{113})	1.7827	-0.2299
u_{173}	Si(1)...C(30)	5.5104(158)	0.2380(tied to u_{113})	0.2734	0.2433

u_{174}	O(9)...C(35)	5.7200(314)	0.4873(tied to u_{113})	0.5226	0.0216
u_{175}	O(13)...H(100)	5.6442(412)	0.5301(tied to u_{113})	0.5655	0.1245
u_{176}	Si(1)...H(75)	5.9561(489)	0.6867(247)	0.6485	-0.1646
u_{177}	O(13)...C(33)	5.7269(466)	0.2274(263)	0.5577	0.0747
u_{178}	C(29)...H(90)	5.5638(2583)	2.0676(tied to u_{176})	2.0295	0.1545
u_{179}	H(69)...H(75)	6.4010(1165)	1.2652(tied to u_{176})	1.2271	-0.5867
u_{180}	H(69)...H(82)	5.5735(699)	1.2807(tied to u_{176})	1.2425	0.2449
u_{181}	H(77)...H(92)	5.5771(2614)	2.1494(tied to u_{176})	2.1112	0.3894
u_{182}	O(13)...C(39)	5.8146(284)	0.2214(tied to u_{177})	0.5517	0.0640
u_{183}	Si(1)...H(82)	5.5981(287)	0.6314(tied to u_{176})	0.5933	0.3513
u_{184}	C(61)...H(74)	5.8635(2063)	1.7382(tied to u_{176})	1.7001	-0.0254
u_{185}	Si(1)...H(79)	6.0804(403)	0.7462(tied to u_{176})	0.7081	-0.1120
u_{186}	Si(1)...C(54)	6.1196(482)	0.4757(tied to u_{176})	0.4376	-0.0746
u_{187}	C(21)...C(44)	5.7178(468)	0.8679(tied to u_{176})	0.8298	0.2709
u_{188}	Si(1)...C(25)	5.9693(111)	0.2155(tied to u_{176})	0.1774	0.0752
u_{189}	Si(1)...H(70)	5.6235(190)	0.5007(tied to u_{176})	0.4626	0.3830
u_{190}	C(53)...H(74)	6.0253(1577)	1.3825(tied to u_{176})	1.3444	-0.0269
u_{191}	Si(1)...C(50)	6.0345(681)	0.5208(tied to u_{176})	0.4826	-0.0175
u_{192}	C(21)...H(84)	5.4946(689)	1.4044(tied to u_{176})	1.3663	0.5624
u_{193}	Si(1)...C(23)	6.0110(110)	0.2150(tied to u_{176})	0.1769	0.0782
u_{194}	C(37)...C(52)	6.1150(1691)	1.3581(tied to u_{176})	1.32	0.0478
u_{195}	C(21)...C(54)	6.3170(550)	0.7830(tied to u_{176})	0.7448	-0.1207
u_{196}	Si(1)...C(27)	6.0357(219)	0.2078(tied to u_{176})	0.1697	0.0771
u_{197}	O(9)...H(93)	5.9577(351)	0.3868(tied to u_{176})	0.3487	0.1879
u_{198}	O(13)...H(81)	5.9591(524)	0.8966(tied to u_{176})	0.8585	0.3044
u_{199}	C(37)...C(60)	6.2805(1030)	1.1929(tied to u_{176})	1.1548	-0.0688
u_{200}	O(13)...H(85)	6.0209(164)	0.3033(tied to u_{176})	0.2652	0.1903
u_{201}	C(21)...H(94)	6.5884(766)	1.0941(tied to u_{176})	1.0559	-0.2464
u_{202}	C(21)...C(50)	6.1822(1260)	0.8627(tied to u_{176})	0.8245	-0.0248
u_{203}	O(13)...C(41)	6.0855(275)	0.5518(tied to u_{176})	0.5137	0.1828
u_{204}	C(29)...C(42)	6.0408(954)	0.8412(tied to u_{176})	0.8031	0.1631
u_{205}	O(13)...H(71)	5.8822(444)	0.8915(tied to u_{176})	0.8534	0.3415
u_{206}	O(13)...C(31)	6.0443(334)	0.5513(tied to u_{176})	0.5132	0.2029
u_{207}	H(77)...H(108)	6.7616(2103)	1.4476(4119)	1.491	-0.4131
u_{208}	C(29)...C(54)	6.2810(1227)	1.3934(1785)	1.3974	0.1567
u_{209}	C(45)...H(90)	5.9591(3547)	2.1997(tied to u_{207})	2.2431	0.2160
u_{210}	O(9)...C(30)	6.1284(202)	0.6441(2271)	0.4753	0.2260
u_{211}	C(53)...H(76)	5.8090(1549)	2.0270(tied to u_{207})	2.0703	0.7088
u_{212}	C(29)...H(94)	6.4016(1568)	1.6713(tied to u_{207})	1.7146	0.1358
u_{213}	Si(1)...C(52)	6.2285(586)	0.4899(71)	0.5336	0.1188
u_{214}	C(45)...C(50)	6.2520(2926)	1.6737(tied to u_{208})	1.6776	0.0130
u_{215}	Si(1)...H(94)	6.6381(618)	0.6053(tied to u_{207})	0.6486	-0.1588
u_{216}	O(9)...C(43)	6.1993(296)	0.6057(tied to u_{210})	0.4369	0.2164
u_{217}	C(21)...H(90)	6.3839(1578)	1.1401(tied to u_{207})	1.1834	-0.0614

u_{218}	O(9)...H(70)	6.0235(392)	0.7338(tied to u_{207})	0.7772	0.3716
u_{219}	Si(1)...H(81)	6.3834(662)	0.7992(tied to u_{207})	0.8425	0.1386
u_{220}	C(37)...H(94)	6.6126(805)	1.4489(tied to u_{207})	1.4922	-0.1122
u_{221}	Si(1)...C(35)	6.4557(353)	0.3368(tied to u_{213})	0.3805	-0.0355
u_{222}	Si(1)...C(39)	6.5311(303)	0.3665(tied to u_{213})	0.4102	-0.0247
u_{223}	O(13)...H(101)	6.4795(274)	0.1884(tied to u_{207})	0.2317	0.0453
u_{224}	O(13)...H(108)	6.3898(495)	0.2200(tied to u_{207})	0.2633	0.0655
u_{225}	O(9)...H(101)	6.3931(511)	0.2022(tied to u_{207})	0.2456	0.0596
u_{226}	O(9)...H(83)	6.1776(468)	0.6530(tied to u_{207})	0.6964	0.3287
u_{227}	H(77)...H(79)	6.4433(1271)	1.8141(tied to u_{207})	1.8574	0.0575
u_{228}	C(37)...C(54)	6.4669(651)	1.2263(tied to u_{208})	1.2303	0.0672
u_{229}	C(37)...C(68)	6.6867(1516)	1.0003(tied to u_{208})	1.0042	-0.1609
u_{230}	Si(1)...C(60)	6.3382(425)	0.4500(tied to u_{213})	0.4936	0.1540
u_{231}	Si(1)...H(90)	6.5085(908)	0.6743(tied to u_{207})	0.7176	-0.0616
u_{232}	C(21)...C(42)	6.2102(507)	0.5373(tied to u_{208})	0.5413	0.3320
u_{233}	H(69)...H(94)	5.9629(1895)	2.2929(tied to u_{207})	2.3362	0.7809
u_{234}	O(13)...C(30)	6.2933(209)	0.4811(tied to u_{210})	0.3123	0.2603
u_{235}	O(13)...C(42)	6.3420(182)	0.4507(tied to u_{210})	0.2819	0.2475
u_{236}	C(37)...H(92)	6.3923(2064)	1.7265(tied to u_{207})	1.7698	0.3225
u_{237}	C(21)...C(30)	6.2946(138)	0.4644(tied to u_{208})	0.4683	0.3555
u_{238}	H(77)...H(94)	6.3532(961)	1.9634(tied to u_{207})	2.0067	0.3268
u_{239}	C(29)...H(75)	7.0794(1001)	0.9421(tied to u_{207})	0.9855	-0.4594
u_{240}	C(53)...H(84)	6.2080(876)	1.7598(tied to u_{207})	1.8031	0.4785
u_{241}	Si(1)...H(73)	6.3780(558)	0.7962(tied to u_{207})	0.8395	0.2497
u_{242}	C(29)...H(76)	6.0298(567)	1.5952(tied to u_{207})	1.6385	0.6978
u_{243}	C(21)...C(52)	6.4971(1247)	0.8889(tied to u_{208})	0.8929	0.2058
u_{244}	C(45)...H(94)	6.7693(2088)	1.8434(tied to u_{207})	1.8867	0.1065
u_{245}	C(29)...C(66)	6.6832(2004)	1.1173(tied to u_{208})	1.1212	-0.0317
u_{246}	H(69)...H(106)	6.7184(2240)	1.7120(tied to u_{207})	1.7553	-0.0671
u_{247}	Si(1)...C(41)	6.6963(369)	0.4343(tied to u_{213})	0.478	0.0918
u_{248}	C(29)...H(82)	6.3108(664)	0.9868(tied to u_{207})	1.0301	0.4245
u_{249}	O(13)...H(70)	6.3569(192)	0.3969(tied to u_{207})	0.4403	0.3882
u_{250}	C(53)...H(94)	6.9828(1419)	1.6267(tied to u_{207})	1.67	-0.1475
u_{251}	O(13)...H(82)	6.4637(195)	0.3575(tied to u_{207})	0.4008	0.3500
u_{252}	Si(1)...C(58)	6.6138(444)	0.2807(tied to u_{213})	0.3244	0.2145
u_{253}	C(37)...H(100)	6.6757(1179)	1.4966(tied to u_{207})	1.5399	0.1269
u_{254}	O(13)...C(54)	6.9537(487)	0.5979(tied to u_{210})	0.4291	-0.0521
u_{255}	C(21)...H(75)	7.0623(883)	0.7696(tied to u_{207})	0.8129	-0.2459
u_{256}	Si(1)...C(33)	6.6903(332)	0.4349(tied to u_{213})	0.4785	0.1535
u_{257}	C(45)...C(54)	6.8514(1683)	1.4875(tied to u_{208})	1.4914	0.1248
u_{258}	Si(1)...C(46)	6.6733(234)	0.2240(tied to u_{213})	0.2677	0.2268
u_{259}	O(13)...C(50)	6.8604(528)	0.5984(tied to u_{210})	0.4296	-0.0265
u_{260}	C(61)...H(94)	7.2551(1969)	1.5525(tied to u_{207})	1.5958	-0.2344
u_{261}	O(13)...C(24)	6.8276(139)	0.1864(187)	0.2247	0.0952

u_{262}	H(69)...H(98)	6.8309(1518)	1.2969(tied to u_{207})	1.3403	0.0715
u_{263}	C(29)...C(58)	6.7754(1534)	0.9053(tied to u_{208})	0.9092	0.1306
u_{264}	O(9)...C(23)	6.8801(187)	0.1854(tied to u_{261})	0.2237	0.0948
u_{265}	C(21)...C(60)	6.6548(837)	0.8175(tied to u_{208})	0.8214	0.2579
u_{266}	O(13)...C(27)	6.8597(113)	0.1852(tied to u_{261})	0.2235	0.0956
u_{267}	C(21)...H(82)	6.4632(398)	0.7831(tied to u_{207})	0.8264	0.5286
u_{268}	Si(1)...C(68)	6.8300(541)	0.2737(tied to u_{213})	0.3174	0.1169
u_{269}	Si(1)...C(62)	6.9399(344)	0.2389(tied to u_{213})	0.2826	0.0923
u_{270}	C(29)...C(30)	6.5122(420)	1.0185(tied to u_{208})	1.0225	0.4605
u_{271}	Si(1)...C(66)	6.8615(609)	0.2503(tied to u_{213})	0.294	0.1073
u_{272}	C(21)...H(79)	7.1826(503)	0.8702(tied to u_{207})	0.9135	-0.1476
u_{273}	O(9)...C(54)	7.0561(453)	0.4539(tied to u_{261})	0.4922	0.0216
u_{274}	Si(1)...H(92)	6.8252(704)	0.7551(tied to u_{207})	0.7984	0.1689
u_{275}	C(53)...C(54)	7.0208(1177)	1.3263(tied to u_{208})	1.3303	0.0402
u_{276}	O(13)...H(75)	7.0323(447)	0.4702(tied to u_{207})	0.5135	-0.0299
u_{277}	O(9)...C(51)	6.9672(411)	0.4622(tied to u_{261})	0.5005	0.0549
u_{278}	C(37)...H(79)	7.2466(904)	1.3427(tied to u_{207})	1.3861	-0.1518
u_{279}	O(9)...H(79)	7.1909(374)	0.4837(tied to u_{207})	0.5271	-0.0340
u_{280}	O(13)...C(49)	7.0074(634)	0.4888(tied to u_{261})	0.5271	0.0889
u_{281}	O(13)...C(55)	7.0596(460)	0.4837(tied to u_{261})	0.522	0.0838
u_{282}	H(69)...H(70)	6.3089(343)	1.6299(tied to u_{207})	1.6733	0.8037
u_{283}	C(21)...H(70)	6.5715(263)	0.6120(tied to u_{207})	0.6554	0.5561
u_{284}	Si(1)...C(31)	6.9509(245)	0.3063(tied to u_{213})	0.3499	0.2296
u_{285}	C(53)...C(68)	7.3555(1615)	1.1704(tied to u_{208})	1.1744	-0.0809
u_{286}	Si(1)...H(71)	6.8764(299)	0.5240(tied to u_{207})	0.5674	0.3420
u_{287}	O(13)...H(94)	7.4645(637)	0.5626(tied to u_{207})	0.6059	-0.1453
u_{288}	C(21)...H(92)	6.9020(1507)	1.2601(tied to u_{207})	1.3035	0.3419
u_{289}	C(21)...C(68)	7.0784(1180)	0.5959(tied to u_{208})	0.5999	0.1626
u_{290}	C(61)...H(90)	7.1012(3421)	1.7135(tied to u_{207})	1.7568	0.0405
u_{291}	Si(1)...H(100)	7.0156(556)	0.6960(tied to u_{207})	0.7393	0.2230
u_{292}	Si(1)...C(43)	7.0603(198)	0.2152(tied to u_{213})	0.2589	0.2255
u_{293}	C(37)...H(108)	7.4454(1793)	1.0435(tied to u_{207})	1.0868	-0.1455
u_{294}	C(37)...C(50)	6.9847(1374)	0.8922(tied to u_{208})	0.8961	0.2556
u_{295}	O(13)...H(90)	7.3151(697)	0.5594(tied to u_{207})	0.6027	-0.1106
u_{296}	C(21)...C(66)	7.1192(1201)	0.5692(tied to u_{208})	0.5732	0.1427
u_{297}	C(21)...C(62)	7.2581(389)	0.5555(tied to u_{208})	0.5594	0.1230
u_{298}	C(53)...H(92)	6.9596(2094)	1.9907(tied to u_{207})	2.034	0.4622
u_{299}	Si(1)...C(24)	7.2410(22)	0.0836(tied to u_{213})	0.1273	0.0911
u_{300}	O(13)...H(80)	7.3306(507)	0.5441(tied to u_{207})	0.5875	0.0846
u_{301}	C(37)...H(90)	7.0965(1729)	1.1974(259)	1.1702	0.1707
u_{302}	Si(1)...H(83)	7.0827(282)	0.4351(tied to u_{301})	0.4078	0.3112
u_{303}	C(61)...H(76)	6.8414(1149)	1.9479(tied to u_{301})	1.9206	0.6653
u_{304}	C(29)...C(44)	6.7945(471)	1.3508(2262)	0.9026	0.5791
u_{305}	C(45)...C(66)	7.2927(2794)	1.7074(tied to u_{304})	1.2592	0.0396

u_{306}	C(21)...C(25)	7.3554(302)	0.7120(tied to u_{304})	0.2638	0.0933
u_{307}	C(21)...C(58)	7.0993(920)	1.0248(tied to u_{304})	0.5766	0.3227
u_{308}	O(13)...C(57)	7.3006(431)	0.4411(87)	0.4799	0.1810
u_{309}	C(29)...C(62)	7.2785(829)	1.6722(tied to u_{304})	1.224	0.2884
u_{310}	O(13)...C(47)	7.2534(585)	0.4474(tied to u_{308})	0.4861	0.2019
u_{311}	C(29)...H(84)	6.6264(666)	1.4291(tied to u_{301})	1.4018	0.8240
u_{312}	O(13)...H(72)	7.2677(468)	0.6118(tied to u_{301})	0.5846	0.1671
u_{313}	C(21)...C(23)	7.4204(298)	0.7090(tied to u_{304})	0.2607	0.0996
u_{314}	C(29)...H(70)	6.8125(322)	1.1665(tied to u_{301})	1.1393	0.6495
u_{315}	O(9)...H(94)	7.6170(597)	0.7520(tied to u_{301})	0.7247	-0.0034
u_{316}	C(45)...H(76)	6.8697(729)	1.8265(tied to u_{301})	1.7993	0.7218
u_{317}	C(29)...H(106)	7.4740(2216)	1.2298(tied to u_{301})	1.2026	-0.0247
u_{318}	C(29)...C(35)	7.7363(904)	1.1453(tied to u_{304})	0.697	-0.2807
u_{319}	C(21)...C(46)	7.2317(241)	0.9664(tied to u_{304})	0.5181	0.3371
u_{320}	O(13)...C(35)	7.4559(287)	0.2974(tied to u_{308})	0.3361	0.0477
u_{321}	O(9)...C(39)	7.5595(252)	0.3009(tied to u_{308})	0.3397	0.0391
u_{322}	O(9)...C(46)	7.3580(281)	0.4063(tied to u_{308})	0.4451	0.2151
u_{323}	C(21)...C(27)	7.4477(595)	0.6938(tied to u_{304})	0.2455	0.0959
u_{324}	O(9)...H(91)	7.4732(503)	0.7533(tied to u_{301})	0.726	0.0385
u_{325}	C(53)...H(100)	7.2719(1426)	1.8256(tied to u_{301})	1.7983	0.2975
u_{326}	O(9)...C(59)	7.3617(330)	0.3817(tied to u_{308})	0.4205	0.2211
u_{327}	C(21)...C(35)	7.6687(758)	0.9464(tied to u_{304})	0.4982	-0.0695
u_{328}	C(21)...H(100)	7.1838(983)	1.2194(tied to u_{301})	1.1922	0.4124
u_{329}	C(21)...C(39)	7.7525(481)	0.9967(tied to u_{304})	0.5485	-0.0441
u_{330}	O(13)...C(40)	7.6201(280)	0.3237(tied to u_{308})	0.3625	0.0977
u_{331}	C(21)...H(81)	7.5828(871)	1.1586(tied to u_{301})	1.1314	0.2196
u_{332}	O(13)...H(89)	7.5452(900)	0.8006(tied to u_{301})	0.7734	0.1077
u_{333}	O(13)...C(46)	7.4848(370)	0.2755(tied to u_{308})	0.3143	0.2532
u_{334}	O(13)...H(95)	7.6405(615)	0.7875(tied to u_{301})	0.7603	0.0947
u_{335}	C(37)...C(39)	7.9292(792)	1.3956(tied to u_{304})	0.9474	-0.1631
u_{336}	H(69)...H(81)	7.4115(216)	1.9392(tied to u_{301})	1.912	0.3614
u_{337}	C(53)...H(90)	7.4778(2642)	1.4250(tied to u_{301})	1.3977	0.1584
u_{338}	Si(1)...H(98)	7.4571(399)	0.4914(tied to u_{301})	0.4642	0.3044
u_{339}	C(29)...C(46)	7.3355(499)	1.5852(tied to u_{304})	1.1369	0.4581
u_{340}	O(13)...C(32)	7.5851(261)	0.3226(tied to u_{308})	0.3614	0.1419
u_{341}	O(13)...C(58)	7.4884(339)	0.2507(tied to u_{308})	0.2894	0.2508
u_{342}	C(45)...H(75)	8.1398(1059)	1.0823(tied to u_{301})	1.0551	-0.4447
u_{343}	C(37)...C(62)	7.4769(611)	1.5706(tied to u_{304})	1.1224	0.3572
u_{344}	O(9)...H(71)	7.5445(294)	0.4857(tied to u_{301})	0.4584	0.2414
u_{345}	Si(1)...H(80)	7.7910(358)	0.4117(tied to u_{301})	0.3845	0.0709
u_{346}	Si(1)...C(51)	7.7390(372)	0.4184(tied to u_{301})	0.3912	0.0170
u_{347}	Si(1)...C(55)	7.8229(453)	0.4411(tied to u_{301})	0.4138	0.0188
u_{348}	C(37)...C(42)	7.2422(605)	1.1997(tied to u_{304})	0.7514	0.6032
u_{349}	Si(1)...H(72)	7.6718(386)	0.4102(tied to u_{301})	0.383	0.1137

u_{350}	C(45)...C(58)	7.5269(2149)	1.4949(tied to u_{304})	1.0467	0.2385
u_{351}	O(9)...C(62)	7.7775(350)	0.3028(tied to u_{308})	0.3416	0.1192
u_{352}	Si(1)...H(86)	7.5168(172)	0.3851(tied to u_{301})	0.3579	0.3225
u_{353}	O(13)...C(65)	7.7232(576)	0.3136(tied to u_{308})	0.3524	0.1296
u_{354}	O(13)...H(83)	7.6694(262)	0.4226(tied to u_{301})	0.3954	0.2161
u_{355}	O(13)...C(62)	7.7752(439)	0.2900(tied to u_{308})	0.3288	0.1215
u_{356}	O(13)...C(63)	7.7191(580)	0.3186(tied to u_{308})	0.3574	0.1369
u_{357}	C(53)...H(108)	7.9719(1977)	1.3308(tied to u_{301})	1.3035	-0.0569
u_{358}	C(29)...H(98)	7.5530(1502)	1.0641(tied to u_{301})	1.0368	0.2992
u_{359}	O(9)...C(67)	7.7130(372)	0.3040(tied to u_{308})	0.3427	0.1427
u_{360}	C(45)...H(82)	7.3158(979)	1.1681(tied to u_{301})	1.1408	0.5356
u_{361}	O(13)...C(66)	7.7158(449)	0.2840(tied to u_{308})	0.3228	0.1372
u_{362}	H(69)...H(91)	8.3558(1186)	1.2603(tied to u_{301})	1.2331	-0.5522
u_{363}	O(9)...C(31)	7.7486(243)	0.2662(tied to u_{308})	0.305	0.1881
u_{364}	C(29)...C(52)	7.4141(874)	1.5003(tied to u_{304})	1.0521	0.5060
u_{365}	C(61)...H(84)	7.2825(834)	1.7418(tied to u_{301})	1.7146	0.6980
u_{366}	O(13)...C(43)	7.8008(125)	0.2317(tied to u_{308})	0.2704	0.1801
u_{367}	Si(1)...H(108)	7.8016(675)	0.3996(tied to u_{301})	0.3723	0.1434
u_{368}	Si(1)...H(102)	7.9334(368)	0.3590(tied to u_{301})	0.3318	0.1145
u_{369}	H(77)...H(90)	7.4471(1264)	1.3535(tied to u_{301})	1.3263	0.4640
u_{370}	C(37)...H(70)	7.1852(464)	0.9445(tied to u_{301})	0.9173	0.7681
u_{371}	Si(1)...H(106)	7.8429(684)	0.3715(tied to u_{301})	0.3443	0.1310
u_{372}	C(21)...C(41)	7.9677(543)	1.1139(tied to u_{304})	0.6656	0.1251
u_{373}	Si(1)...C(57)	7.9758(401)	0.4821(tied to u_{301})	0.4549	0.1088
u_{374}	H(69)...H(84)	7.0542(593)	1.3393(tied to u_{301})	1.3121	0.9508
u_{375}	C(29)...H(79)	8.0855(717)	0.9705(tied to u_{301})	0.9433	0.0206
u_{376}	C(21)...H(73)	7.6396(532)	1.1442(tied to u_{301})	1.117	0.3539
u_{377}	C(45)...C(62)	7.8502(1242)	1.7686(tied to u_{304})	1.3204	0.3157
u_{378}	C(45)...H(106)	7.9390(3139)	1.4130(tied to u_{301})	1.3858	0.0593
u_{379}	Si(1)...C(40)	8.0621(195)	0.2491(tied to u_{301})	0.2219	0.0980
u_{380}	C(37)...H(75)	8.1027(922)	0.9505(tied to u_{301})	0.9233	-0.0352
u_{381}	C(29)...H(81)	7.9464(475)	1.5698(tied to u_{301})	1.5426	0.2611
u_{382}	Si(1)...C(32)	7.9965(204)	0.2492(tied to u_{301})	0.2219	0.1211
u_{383}	Si(1)...C(49)	7.9745(453)	0.4786(tied to u_{301})	0.4514	0.1603
u_{384}	C(21)...H(108)	7.9197(1423)	0.7147(tied to u_{301})	0.6875	0.1943
u_{385}	C(53)...H(79)	8.3552(1126)	1.4584(tied to u_{301})	1.4312	-0.1752
u_{386}	C(37)...C(46)	7.6046(574)	1.4715(tied to u_{304})	1.0233	0.5875
u_{387}	C(21)...H(102)	8.1404(465)	0.6631(tied to u_{301})	0.6359	0.1453
u_{388}	C(21)...H(106)	7.9785(1349)	0.6799(tied to u_{301})	0.6527	0.1684
u_{389}	C(21)...C(33)	7.9940(303)	1.1027(tied to u_{304})	0.6545	0.2013
u_{390}	H(69)...H(102)	7.7138(1228)	2.0223(tied to u_{301})	1.995	0.6523
u_{391}	O(13)...H(97)	8.0399(460)	0.7144(tied to u_{301})	0.6872	0.2514
u_{392}	Si(1)...H(91)	8.2168(483)	0.5932(tied to u_{301})	0.5659	-0.0429
u_{393}	O(13)...H(87)	7.9477(660)	0.7193(tied to u_{301})	0.6921	0.2807

u_{394}	H(69)...H(79)	8.0883(765)	1.1881(tied to u_{301})	1.1609	0.2601
u_{395}	C(37)...H(82)	7.5717(481)	0.9561(tied to u_{301})	0.9288	0.7527
u_{396}	C(29)...H(102)	8.1066(858)	1.3310(tied to u_{301})	1.3037	0.3015
u_{397}	Si(1)...H(95)	8.3650(616)	0.6386(tied to u_{301})	0.6113	-0.0292
u_{398}	C(45)...H(84)	7.4405(743)	1.5963(tied to u_{301})	1.5691	0.8651
u_{399}	C(29)...C(60)	7.6570(787)	1.3917(tied to u_{304})	0.9434	0.6167
u_{400}	C(37)...H(73)	7.9867(380)	1.5818(tied to u_{301})	1.5546	0.3386
u_{401}	C(53)...C(62)	8.0324(1068)	1.6704(tied to u_{304})	1.2221	0.3793
u_{402}	C(29)...H(92)	7.7347(1068)	1.5116(tied to u_{301})	1.4843	0.6307
u_{403}	C(21)...H(98)	7.9307(907)	0.7882(tied to u_{301})	0.761	0.4724
u_{404}	Si(1)...C(47)	8.1829(451)	0.3715(tied to u_{301})	0.3443	0.2332
u_{405}	O(9)...H(86)	8.1012(442)	0.6466(tied to u_{301})	0.6193	0.3038
u_{406}	C(61)...H(92)	7.9645(1568)	1.9159(tied to u_{301})	1.8887	0.5690
u_{407}	H(77)...H(95)	8.5779(1390)	1.8175(tied to u_{301})	1.7902	-0.1203
u_{408}	H(69)...H(86)	7.7023(583)	1.9011(tied to u_{301})	1.8739	0.7962
u_{409}	O(9)...H(99)	8.1324(408)	0.6116(tied to u_{301})	0.5843	0.3041
u_{410}	C(37)...C(66)	7.9566(1333)	1.2666(tied to u_{304})	0.8184	0.4754
u_{411}	H(77)...H(81)	8.1462(1471)	1.3516(tied to u_{301})	1.3244	0.5118
u_{412}	Si(1)...C(59)	8.2502(250)	0.2936(tied to u_{301})	0.2663	0.2374
u_{413}	C(61)...C(62)	8.3307(1332)	1.4639(tied to u_{304})	1.0156	0.2422
u_{414}	H(69)...H(83)	8.3211(994)	1.0333(tied to u_{301})	1.0061	0.1465
u_{415}	C(37)...H(81)	8.3355(1186)	1.1948(tied to u_{301})	1.1676	0.3560
u_{416}	C(45)...C(46)	8.0581(946)	1.6600(tied to u_{304})	1.2118	0.5221
u_{417}	C(21)...H(86)	8.0935(271)	0.6549(tied to u_{301})	0.6276	0.4858
u_{418}	C(29)...C(68)	8.0116(986)	1.2338(tied to u_{304})	0.7856	0.5181
u_{419}	C(61)...C(66)	8.2390(2703)	1.4504(tied to u_{304})	1.0022	0.2527
u_{420}	C(45)...H(70)	7.7876(734)	1.2083(tied to u_{301})	1.181	0.7252
u_{421}	C(29)...C(41)	8.4468(385)	1.5559(tied to u_{304})	1.1077	0.2003
u_{422}	C(37)...H(102)	8.2972(634)	1.2290(tied to u_{301})	1.2018	0.3793
u_{423}	Si(1)...C(65)	8.5619(427)	0.3274(tied to u_{301})	0.3001	0.1334
u_{424}	C(21)...C(31)	8.3686(501)	0.9358(tied to u_{304})	0.4876	0.3056
u_{425}	O(13)...H(86)	8.3153(304)	0.4011(tied to u_{301})	0.3738	0.3506
u_{426}	Si(1)...H(97)	8.6220(505)	0.7136(tied to u_{301})	0.6864	0.1334
u_{427}	H(77)...H(82)	7.9061(474)	1.0116(tied to u_{301})	0.9844	0.8405
u_{428}	C(29)...C(51)	8.8228(999)	1.2084(tied to u_{304})	0.7602	-0.2408
u_{429}	Si(1)...C(63)	8.5765(488)	0.3215(tied to u_{301})	0.2943	0.1386
u_{430}	C(37)...C(58)	8.0536(1032)	1.2805(tied to u_{304})	0.8323	0.6397
u_{431}	O(13)...H(98)	8.3490(255)	0.3691(tied to u_{301})	0.3419	0.3422
u_{432}	C(37)...C(41)	8.6339(901)	1.2585(tied to u_{304})	0.8103	0.2143
u_{433}	Si(1)...C(67)	8.5537(295)	0.3062(tied to u_{301})	0.2789	0.1486
u_{434}	C(29)...H(86)	8.1686(290)	1.2644(tied to u_{301})	1.2371	0.5979
u_{435}	C(45)...H(98)	8.2473(2144)	1.2515(tied to u_{301})	1.2243	0.4473
u_{436}	C(45)...H(102)	8.5510(1220)	1.4694(tied to u_{301})	1.4422	0.3456
u_{437}	C(29)...C(39)	8.6684(744)	1.1416(tied to u_{304})	0.6934	0.1715

u_{438}	C(21)...C(43)	8.4922(547)	0.8067(tied to u_{304})	0.3585	0.2999
u_{439}	C(21)...H(71)	8.3492(480)	0.7755(tied to u_{301})	0.7482	0.4675
u_{440}	H(77)...H(102)	8.1290(869)	1.8198(tied to u_{301})	1.7926	0.7124
u_{441}	C(29)...H(91)	9.0538(1121)	0.9997(tied to u_{301})	0.9725	-0.3577
u_{442}	O(9)...H(102)	8.7777(435)	0.4792(420)	0.3868	0.1441
u_{443}	Si(1)...H(89)	8.6075(696)	0.7661(tied to u_{442})	0.6737	0.2165
u_{444}	O(13)...H(105)	8.7175(690)	0.4909(tied to u_{442})	0.3985	0.1555
u_{445}	O(13)...H(102)	8.7723(479)	0.4635(tied to u_{442})	0.371	0.1470
u_{446}	O(13)...H(103)	8.7034(707)	0.4975(tied to u_{442})	0.4051	0.1652
u_{447}	C(37)...C(55)	9.0558(1149)	1.0027(308)	0.9863	-0.1474
u_{448}	O(9)...H(107)	8.6896(467)	0.4809(tied to u_{442})	0.3885	0.1715
u_{449}	O(13)...H(106)	8.6996(478)	0.4567(tied to u_{442})	0.3643	0.1641
u_{450}	C(21)...C(51)	8.8529(818)	0.5509(tied to u_{447})	0.5346	-0.0088
u_{451}	C(61)...H(75)	9.0757(1016)	1.1021(tied to u_{442})	1.0097	-0.2607
u_{452}	O(13)...C(51)	8.7895(285)	0.3559(370)	0.338	0.0886
u_{453}	O(9)...C(55)	8.8913(311)	0.3589(tied to u_{452})	0.3409	0.0784
u_{454}	C(21)...C(55)	8.8851(768)	0.6153(tied to u_{447})	0.599	0.0782
u_{455}	C(45)...H(92)	8.2559(1150)	1.8164(tied to u_{442})	1.724	0.6983
u_{456}	C(45)...C(60)	8.3010(957)	1.1211(tied to u_{447})	1.1047	0.6413
u_{457}	C(61)...H(100)	8.3136(1381)	1.8186(tied to u_{442})	1.7262	0.6409
u_{458}	C(21)...H(83)	8.5911(531)	0.6076(tied to u_{442})	0.5152	0.4259
u_{459}	C(53)...H(70)	8.1096(709)	1.0722(tied to u_{442})	0.9798	0.8363
u_{460}	C(45)...H(79)	9.0916(1126)	1.1157(tied to u_{442})	1.0233	-0.0121
u_{461}	C(37)...H(71)	8.6717(704)	1.0668(tied to u_{442})	0.9744	0.3924
u_{462}	C(29)...H(100)	8.1668(999)	1.4068(tied to u_{442})	1.3143	0.7960
u_{463}	H(69)...H(92)	8.1241(854)	1.6530(tied to u_{442})	1.5606	0.8210
u_{464}	O(13)...C(56)	8.9457(266)	0.3677(tied to u_{452})	0.3497	0.1255
u_{465}	C(53)...C(66)	8.4926(2090)	0.9665(tied to u_{447})	0.9501	0.4923
u_{466}	C(61)...H(79)	9.2663(1213)	1.2426(tied to u_{442})	1.1502	-0.1468
u_{467}	C(61)...H(82)	8.3326(963)	1.1859(tied to u_{442})	1.0935	0.7201
u_{468}	C(53)...H(75)	9.0468(994)	1.0903(tied to u_{442})	0.9979	-0.0722
u_{469}	C(29)...H(73)	8.4776(888)	1.1622(tied to u_{442})	1.0698	0.5266
u_{470}	O(13)...C(48)	8.9191(298)	0.3632(tied to u_{452})	0.3453	0.1626
u_{471}	C(53)...H(102)	8.7330(1092)	1.4330(tied to u_{442})	1.3406	0.4155
u_{472}	C(29)...C(33)	8.7260(732)	0.7610(tied to u_{447})	0.7446	0.3534
u_{473}	C(45)...C(68)	8.6036(1131)	0.9462(tied to u_{447})	0.9298	0.5247
u_{474}	H(69)...H(73)	8.3379(1040)	1.2421(tied to u_{442})	1.1497	0.6869
u_{475}	C(37)...H(95)	9.3424(1392)	1.4116(tied to u_{442})	1.3192	-0.1783
u_{476}	C(21)...C(24)	9.0751(36)	0.1558(tied to u_{447})	0.1394	0.1152
u_{477}	C(61)...H(108)	8.9249(1706)	1.2613(tied to u_{442})	1.1689	0.2914
u_{478}	C(61)...H(102)	8.9816(1329)	1.2440(tied to u_{442})	1.1516	0.2758
u_{479}	C(21)...H(91)	9.1837(963)	0.8497(tied to u_{442})	0.7573	-0.1024
u_{480}	C(21)...C(57)	9.1654(575)	0.6765(tied to u_{447})	0.6601	0.1391
u_{481}	C(53)...H(82)	8.4353(768)	1.1272(tied to u_{442})	1.0348	0.8206

u_{482}	C(61)...H(106)	8.8543(3063)	1.2363(tied to u_{442})	1.1439	0.2925
u_{483}	C(37)...H(86)	8.4933(556)	1.1619(tied to u_{442})	1.0695	0.7505
u_{484}	O(9)...C(47)	9.0577(243)	0.3126(tied to u_{452})	0.2946	0.2046
u_{485}	C(21)...H(95)	9.3635(959)	0.9308(tied to u_{442})	0.8384	-0.0649
u_{486}	C(29)...H(83)	8.9019(801)	0.8365(tied to u_{442})	0.7441	0.3174
u_{487}	C(61)...H(70)	8.4407(868)	1.0293(tied to u_{442})	0.9369	0.7666
u_{488}	Si(1)...H(87)	8.9446(450)	0.5676(tied to u_{442})	0.4752	0.3192
u_{489}	O(13)...C(59)	9.0831(137)	0.2809(tied to u_{452})	0.2629	0.2018
u_{490}	C(45)...H(81)	9.0916(684)	1.7153(tied to u_{442})	1.6229	0.2840
u_{491}	C(37)...H(106)	8.7601(1509)	0.9976(tied to u_{442})	0.9052	0.5173
u_{492}	H(77)...H(86)	8.3603(718)	1.6755(tied to u_{442})	1.5831	0.9965
u_{493}	C(21)...C(49)	9.1913(500)	0.6612(tied to u_{447})	0.6449	0.2054
u_{494}	Si(1)...H(99)	9.0689(226)	0.4432(tied to u_{442})	0.3508	0.3198
u_{495}	C(53)...C(58)	8.7075(1638)	0.9687(tied to u_{447})	0.9524	0.6892
u_{496}	C(29)...H(108)	8.8023(1260)	0.9814(tied to u_{442})	0.889	0.5696
u_{497}	O(13)...H(91)	9.3473(409)	0.5541(tied to u_{442})	0.4617	0.0635
u_{498}	Si(1)...C(56)	9.3975(174)	0.3044(tied to u_{442})	0.212	0.1300
u_{499}	O(9)...H(95)	9.5073(466)	0.5662(tied to u_{442})	0.4738	0.0515
u_{500}	Si(1)...C(48)	9.3441(183)	0.3033(tied to u_{442})	0.2109	0.1494
u_{501}	C(53)...H(73)	9.1753(662)	1.7262(tied to u_{442})	1.6338	0.3790
u_{502}	C(45)...H(86)	8.8594(732)	1.4367(tied to u_{442})	1.3443	0.7035
u_{503}	C(21)...H(80)	9.5686(397)	0.5020(tied to u_{442})	0.4096	0.0905
u_{504}	C(45)...H(100)	8.7022(1248)	1.6407(tied to u_{442})	1.5482	0.8693
u_{505}	C(21)...H(72)	9.4446(421)	0.4990(tied to u_{442})	0.4066	0.1461
u_{506}	C(53)...H(81)	9.4286(1191)	1.3757(tied to u_{442})	1.2833	0.3737
u_{507}	O(13)...C(64)	9.5357(230)	0.2851(tied to u_{452})	0.2671	0.1579
u_{508}	O(9)...C(63)	9.5730(265)	0.2839(tied to u_{452})	0.2659	0.1590
u_{509}	C(37)...H(98)	8.9068(1023)	1.0728(tied to u_{442})	0.9804	0.7930
u_{510}	Si(1)...H(105)	9.5704(537)	0.4419(tied to u_{442})	0.3495	0.1608
u_{511}	O(13)...H(96)	9.6217(367)	0.5876(tied to u_{442})	0.4952	0.1338
u_{512}	O(13)...C(67)	9.5280(168)	0.2789(tied to u_{452})	0.2609	0.1658
u_{513}	Si(1)...H(103)	9.5781(574)	0.4342(tied to u_{442})	0.3418	0.1676
u_{514}	C(37)...C(49)	9.5983(737)	1.1629(tied to u_{447})	1.1466	0.2121
u_{515}	H(69)...H(100)	8.6818(886)	1.3575(tied to u_{442})	1.2651	0.9959
u_{516}	Si(1)...H(107)	9.5455(323)	0.4160(tied to u_{442})	0.3236	0.1784
u_{517}	H(77)...H(89)	9.4933(779)	2.0158(tied to u_{442})	1.9234	0.3326
u_{518}	C(45)...C(51)	9.8255(1177)	0.8635(tied to u_{447})	0.8471	-0.1985
u_{519}	C(21)...C(47)	9.5051(812)	0.5220(tied to u_{447})	0.5056	0.3087
u_{520}	C(29)...C(57)	9.6227(725)	1.1633(tied to u_{447})	1.147	0.2272
u_{521}	C(53)...H(106)	9.1857(2357)	1.1632(tied to u_{442})	1.0708	0.5448
u_{522}	C(21)...H(97)	9.7186(738)	1.0773(tied to u_{442})	0.9849	0.1910
u_{523}	O(13)...H(88)	9.5635(502)	0.5761(tied to u_{442})	0.4837	0.1948
u_{524}	H(69)...H(107)	9.9386(1073)	1.1649(tied to u_{442})	1.0724	-0.2529
u_{525}	C(37)...C(47)	9.7147(1163)	0.7594(tied to u_{447})	0.743	0.1522

u_{526}	C(45)...H(91)	9.9650(1341)	1.1803(tied to u_{442})	1.0879	-0.3352
u_{527}	C(29)...C(67)	9.7546(966)	0.7052(tied to u_{447})	0.6888	-0.0370
u_{528}	C(21)...C(65)	9.7546(566)	0.4704(tied to u_{447})	0.454	0.1549
u_{529}	C(37)...C(63)	9.9232(1283)	0.7792(tied to u_{447})	0.7628	-0.0181
u_{530}	C(37)...C(57)	9.7602(1016)	0.8853(tied to u_{447})	0.869	0.2268
u_{531}	C(29)...C(31)	9.3487(593)	0.6190(tied to u_{447})	0.6027	0.5121
u_{532}	H(77)...H(87)	9.8170(1300)	1.2478(tied to u_{442})	1.1554	0.1268
u_{533}	C(45)...H(108)	9.2838(1465)	1.1596(tied to u_{442})	1.0672	0.5882
u_{534}	C(21)...C(63)	9.7870(883)	0.4564(tied to u_{447})	0.44	0.1644
u_{535}	H(69)...H(97)	9.5807(609)	2.0341(tied to u_{442})	1.9417	0.3858
u_{536}	H(69)...H(80)	9.8182(502)	0.7911(tied to u_{442})	0.6987	0.0946
u_{537}	C(29)...C(59)	9.6988(895)	0.6988(tied to u_{447})	0.6824	0.1417
u_{538}	C(21)...C(59)	9.5781(651)	0.4094(tied to u_{447})	0.393	0.3133
u_{539}	C(53)...C(55)	10.1113(1664)	1.0703(tied to u_{447})	1.0539	-0.1256
u_{540}	C(21)...C(40)	9.8785(218)	0.2577(tied to u_{447})	0.2414	0.1213
u_{541}	H(77)...H(103)	10.1443(1420)	1.3169(tied to u_{442})	1.2245	-0.1340
u_{542}	H(77)...H(106)	9.1665(1091)	1.2596(tied to u_{442})	1.1671	0.7706
u_{543}	C(21)...C(32)	9.8101(223)	0.2567(tied to u_{447})	0.2403	0.1514
u_{544}	C(21)...C(67)	9.7463(745)	0.4280(tied to u_{447})	0.4117	0.1756
u_{545}	C(61)...H(81)	9.8127(1001)	1.5075(tied to u_{442})	1.415	0.3094
u_{546}	C(61)...H(98)	9.2342(2100)	1.2771(tied to u_{442})	1.1847	0.7154
u_{547}	C(29)...H(71)	9.3496(496)	0.8400(tied to u_{442})	0.7476	0.6400
u_{548}	C(53)...H(86)	9.1606(915)	1.2760(tied to u_{442})	1.1836	0.8411
u_{549}	C(37)...C(43)	9.5174(486)	0.4402(tied to u_{447})	0.4238	0.5213
u_{550}	O(9)...H(87)	9.7680(259)	0.4764(tied to u_{442})	0.384	0.2596
u_{551}	H(69)...H(99)	9.8887(1031)	1.1847(tied to u_{442})	1.0923	0.0595
u_{552}	C(29)...C(55)	9.8700(1046)	0.7750(tied to u_{447})	0.7587	0.2441
u_{553}	C(21)...H(89)	9.7516(772)	1.0485(tied to u_{442})	0.9561	0.2984
u_{554}	H(77)...H(80)	10.0875(1009)	0.7894(tied to u_{442})	0.697	0.1499
u_{555}	O(13)...H(99)	9.8456(164)	0.4250(tied to u_{442})	0.3326	0.2520
u_{556}	H(69)...H(71)	9.3401(485)	0.8530(tied to u_{442})	0.7606	0.7186
u_{557}	C(53)...H(95)	10.3161(1986)	1.5115(tied to u_{442})	1.419	-0.1737
u_{558}	Si(1)...C(64)	9.9784(46)	0.2470(tied to u_{442})	0.1546	0.1593
u_{559}	C(61)...H(86)	9.4168(1021)	1.1652(tied to u_{442})	1.0728	0.7394
u_{560}	H(69)...H(72)	9.8482(728)	0.7586(tied to u_{442})	0.6662	0.2640
u_{561}	H(69)...H(108)	9.2665(1110)	1.1207(tied to u_{442})	1.0283	0.8297
u_{562}	Si(1)...H(96)	10.0885(292)	0.4150(tied to u_{442})	0.3226	0.1373
u_{563}	C(37)...H(83)	9.5831(452)	0.6508(tied to u_{442})	0.5584	0.6367
u_{564}	Si(1)...H(88)	9.9856(308)	0.4101(tied to u_{442})	0.3177	0.1688
u_{565}	C(45)...H(73)	9.6058(1027)	1.2847(tied to u_{442})	1.1923	0.5513
u_{566}	C(37)...C(51)	9.8927(888)	0.6845(tied to u_{447})	0.6681	0.2376
u_{567}	H(77)...H(83)	9.5815(474)	0.7677(tied to u_{442})	0.6753	0.7309
u_{568}	C(29)...H(97)	10.0731(772)	1.5814(tied to u_{442})	1.489	0.2596
u_{569}	C(29)...C(49)	9.8712(962)	0.8180(tied to u_{447})	0.8017	0.3647

u_{570}	H(77)...H(98)	9.3268(757)	1.1921(tied to u_{442})	1.0997	0.9418
u_{571}	C(29)...H(80)	10.2393(281)	0.6049(tied to u_{442})	0.5125	0.1046
u_{572}	C(37)...H(89)	10.0536(972)	1.5758(tied to u_{442})	1.4834	0.2928
u_{573}	C(37)...C(65)	10.2411(965)	0.9136(tied to u_{447})	0.8973	0.1958
u_{574}	C(37)...H(72)	10.1733(370)	0.6115(tied to u_{442})	0.5191	0.1319
u_{575}	C(53)...H(71)	9.9045(906)	1.1447(tied to u_{442})	1.0523	0.4799
u_{576}	C(29)...H(95)	10.2432(1298)	1.0584(tied to u_{442})	0.966	0.1682
u_{577}	H(77)...H(97)	10.0648(1383)	1.4927(tied to u_{442})	1.4003	0.4864
u_{578}	C(37)...H(80)	10.3868(701)	0.6042(tied to u_{442})	0.5118	0.1341
u_{579}	C(61)...H(73)	9.9562(949)	1.4856(tied to u_{442})	1.3932	0.4586
u_{580}	C(53)...H(98)	9.5195(1637)	1.2338(tied to u_{442})	1.1414	0.8810
u_{581}	C(29)...H(72)	10.1890(553)	0.4972(440)	0.494	0.2232
u_{582}	C(37)...H(91)	10.2035(1087)	0.9029(tied to u_{581})	0.8997	0.1496
u_{583}	C(37)...H(97)	10.3342(1199)	1.1090(tied to u_{581})	1.1058	0.3204
u_{584}	C(29)...C(65)	10.3156(963)	0.8798(tied to u_{581})	0.8766	0.2801
u_{585}	C(45)...H(83)	10.1136(891)	0.7948(tied to u_{581})	0.7916	0.4152
u_{586}	H(69)...H(95)	10.2953(1161)	1.2386(tied to u_{581})	1.2354	0.4329
u_{587}	C(21)...H(87)	10.2663(862)	0.6867(tied to u_{581})	0.6835	0.4365
u_{588}	C(37)...H(87)	10.4524(1276)	0.9340(tied to u_{581})	0.9308	0.3033
u_{589}	C(29)...C(40)	10.5773(149)	0.3480(tied to u_{581})	0.3448	0.1451
u_{590}	C(29)...H(107)	10.6282(1035)	0.7620(tied to u_{581})	0.7588	-0.0160
u_{591}	O(13)...H(104)	10.5700(286)	0.2971(tied to u_{581})	0.2939	0.1873
u_{592}	C(37)...C(40)	10.6947(468)	0.3404(tied to u_{581})	0.3371	0.1458
u_{593}	O(9)...H(103)	10.6032(316)	0.2955(tied to u_{581})	0.2923	0.1894
u_{594}	C(37)...H(103)	10.8155(1489)	0.8444(tied to u_{581})	0.8412	0.0043
u_{595}	O(13)...H(107)	10.5530(185)	0.2885(tied to u_{581})	0.2853	0.1967
u_{596}	C(29)...C(32)	10.5492(391)	0.3326(tied to u_{581})	0.3293	0.2090
u_{597}	C(21)...H(105)	10.7089(729)	0.5308(tied to u_{581})	0.5275	0.1849
u_{598}	C(45)...C(57)	10.7096(1196)	1.2097(tied to u_{581})	1.2065	0.2442
u_{599}	C(21)...H(99)	10.4080(604)	0.5017(tied to u_{581})	0.4985	0.4347
u_{600}	C(21)...H(103)	10.7322(1026)	0.5130(tied to u_{581})	0.5097	0.1964
u_{601}	C(29)...H(99)	10.5382(907)	0.7941(tied to u_{581})	0.7909	0.2792
u_{602}	C(53)...C(57)	10.8331(1355)	0.9451(tied to u_{581})	0.9419	0.2431
u_{603}	H(77)...H(91)	10.4759(1141)	0.9977(tied to u_{581})	0.9944	0.3485
u_{604}	H(77)...H(105)	10.7303(1119)	1.5014(tied to u_{581})	1.4982	0.3375
u_{605}	C(21)...H(107)	10.6762(784)	0.4797(tied to u_{581})	0.4765	0.2089
u_{606}	C(45)...C(67)	10.7805(1165)	0.7744(tied to u_{581})	0.7712	0.0317
u_{607}	C(53)...C(63)	10.9998(1802)	0.8423(tied to u_{581})	0.8391	0.0324
u_{608}	C(29)...C(47)	10.4802(905)	0.6634(tied to u_{581})	0.6602	0.5449
u_{609}	C(29)...H(89)	10.4786(1231)	1.0009(tied to u_{581})	0.9977	0.4876
u_{610}	C(45)...C(55)	10.8546(1577)	0.8321(tied to u_{581})	0.8288	0.2290
u_{611}	C(61)...H(91)	10.9286(1353)	1.0418(tied to u_{581})	1.0386	-0.0987
u_{612}	H(69)...H(89)	10.2837(1252)	1.2470(tied to u_{581})	1.2438	0.6780
u_{613}	C(29)...C(63)	10.7284(1070)	0.6787(tied to u_{581})	0.6755	0.4196

u_{614}	C(61)...H(95)	11.2324(2158)	1.1643(tied to u_{581})	1.1611	-0.0582
u_{615}	C(45)...C(59)	10.8025(1058)	0.7542(tied to u_{581})	0.751	0.2325
u_{616}	C(37)...C(59)	10.6078(622)	0.4763(tied to u_{581})	0.4731	0.5635
u_{617}	Si(1)...H(104)	11.0196(49)	0.1822(tied to u_{581})	0.179	0.1905
u_{618}	C(45)...H(71)	10.5102(699)	0.8384(tied to u_{581})	0.8352	0.6980
u_{619}	C(45)...H(95)	11.1501(1912)	1.0770(tied to u_{581})	1.0738	0.1411
u_{620}	C(37)...H(105)	11.1614(1151)	0.9796(tied to u_{581})	0.9764	0.2261
u_{621}	C(37)...C(67)	10.7857(779)	0.5325(tied to u_{581})	0.5293	0.4342
u_{622}	C(45)...H(97)	11.1039(1288)	1.6060(tied to u_{581})	1.6027	0.2962
u_{623}	C(45)...C(49)	10.9610(1337)	0.8727(tied to u_{581})	0.8694	0.3797
u_{624}	C(53)...H(91)	11.0272(1272)	1.0135(tied to u_{581})	1.0102	0.1277
u_{625}	C(21)...C(56)	11.2150(194)	0.2370(tied to u_{581})	0.2338	0.1573
u_{626}	C(61)...H(71)	10.7722(850)	0.9522(tied to u_{581})	0.9489	0.6233
u_{627}	C(21)...C(48)	11.1569(203)	0.2345(tied to u_{581})	0.2312	0.1835
u_{628}	H(69)...H(105)	10.8943(1102)	1.4764(tied to u_{581})	1.4731	0.4923
u_{629}	C(53)...C(65)	11.3189(1440)	0.9452(tied to u_{581})	0.942	0.2151
u_{630}	C(53)...H(83)	10.7198(566)	0.6143(tied to u_{581})	0.6111	0.6984
u_{631}	C(53)...H(89)	11.1260(1463)	1.5975(tied to u_{581})	1.5943	0.3481
u_{632}	C(29)...H(105)	11.2480(1164)	0.9897(375)	0.9518	0.3130
u_{633}	C(53)...H(97)	11.3453(1541)	1.2788(tied to u_{632})	1.241	0.3473
u_{634}	C(61)...H(83)	10.9698(738)	0.7093(tied to u_{632})	0.6714	0.5963
u_{635}	C(45)...C(65)	11.3895(1445)	0.9543(tied to u_{632})	0.9164	0.2910
u_{636}	C(45)...H(80)	11.5726(331)	0.5527(tied to u_{632})	0.5148	0.1370
u_{637}	C(53)...H(72)	11.4823(344)	0.5619(tied to u_{632})	0.524	0.1731
u_{638}	C(53)...H(80)	11.7025(644)	0.5484(tied to u_{632})	0.5106	0.1631
u_{639}	C(45)...H(72)	11.4991(551)	0.5348(tied to u_{632})	0.497	0.2535
u_{640}	C(45)...H(107)	11.5997(1270)	0.9357(tied to u_{632})	0.8978	0.0561
u_{641}	C(61)...H(97)	11.7522(1596)	1.3880(tied to u_{632})	1.3501	0.2960
u_{642}	C(53)...H(87)	11.5834(1679)	1.0830(tied to u_{632})	1.0451	0.4028
u_{643}	C(29)...H(87)	11.2561(882)	0.8074(tied to u_{632})	0.7696	0.6721
u_{644}	C(21)...C(64)	11.8050(47)	0.2060(tied to u_{632})	0.1681	0.1911
u_{645}	C(21)...H(96)	11.8825(341)	0.3928(tied to u_{632})	0.3549	0.1654
u_{646}	C(61)...C(65)	11.9022(1645)	0.7674(tied to u_{632})	0.7296	0.2239
u_{647}	C(21)...H(88)	11.7703(354)	0.3854(tied to u_{632})	0.3475	0.2087
u_{648}	C(61)...C(63)	11.8870(1883)	0.7388(tied to u_{632})	0.701	0.2369
u_{649}	C(45)...H(89)	11.5225(1617)	1.1669(tied to u_{632})	1.1291	0.5185
u_{650}	C(29)...H(103)	11.6677(1213)	0.7810(tied to u_{632})	0.7431	0.4643
u_{651}	C(37)...C(48)	11.9220(157)	0.3803(tied to u_{632})	0.3424	0.1793
u_{652}	C(29)...C(56)	11.9038(139)	0.3835(tied to u_{632})	0.3456	0.1860
u_{653}	C(45)...C(47)	11.5535(1336)	0.7726(tied to u_{632})	0.7348	0.5807
u_{654}	C(45)...C(63)	11.7394(1595)	0.7800(tied to u_{632})	0.7421	0.4297
u_{655}	H(69)...H(87)	11.2948(637)	0.8977(tied to u_{632})	0.8599	0.8027
u_{656}	C(37)...C(56)	12.0250(429)	0.3706(tied to u_{632})	0.3327	0.1801
u_{657}	C(37)...H(99)	11.4206(548)	0.6012(tied to u_{632})	0.5634	0.6980

u_{658}	C(61)...C(67)	11.7337(1134)	0.6910(tied to u_{632})	0.6531	0.2720
u_{659}	C(45)...H(99)	11.6355(1085)	0.9112(tied to u_{632})	0.8734	0.3908
u_{660}	C(29)...C(48)	11.8813(392)	0.3649(tied to u_{632})	0.3271	0.2422
u_{661}	C(61)...H(89)	11.8646(1743)	1.3431(tied to u_{632})	1.3053	0.4199
u_{662}	C(37)...H(107)	11.7081(838)	0.6336(tied to u_{632})	0.5957	0.4829
u_{663}	C(53)...C(67)	11.7284(979)	0.6468(tied to u_{632})	0.609	0.4577
u_{664}	H(77)...H(88)	12.1392(592)	0.6832(tied to u_{632})	0.6454	0.1544
u_{665}	H(69)...H(96)	12.1010(415)	0.6941(tied to u_{632})	0.6562	0.1732
u_{666}	C(53)...H(105)	12.1980(1710)	1.0798(tied to u_{632})	1.0419	0.2492
u_{667}	C(53)...C(59)	11.6311(808)	0.5806(tied to u_{632})	0.5427	0.6103
u_{668}	H(77)...H(99)	11.5086(464)	0.7244(tied to u_{632})	0.6865	0.8264
u_{669}	C(61)...H(80)	12.2561(414)	0.4928(tied to u_{632})	0.455	0.1648
u_{670}	H(69)...H(103)	11.7298(948)	1.0511(tied to u_{632})	1.0132	0.6776
u_{671}	C(61)...H(72)	12.1028(402)	0.4937(tied to u_{632})	0.4559	0.2297
u_{672}	H(77)...H(96)	12.3722(827)	0.6752(tied to u_{632})	0.6373	0.1990
u_{673}	H(69)...H(88)	12.1141(637)	0.6514(tied to u_{632})	0.6135	0.3084
u_{674}	C(45)...H(105)	12.2806(1719)	1.0498(tied to u_{632})	1.012	0.3280
u_{675}	H(77)...H(107)	11.9152(782)	0.7638(tied to u_{632})	0.7259	0.6542
u_{676}	C(29)...H(96)	12.5449(218)	0.5084(tied to u_{632})	0.4706	0.1878
u_{677}	C(37)...H(88)	12.5061(385)	0.5043(tied to u_{632})	0.4664	0.1991
u_{678}	C(37)...C(64)	12.5961(219)	0.3156(tied to u_{632})	0.2777	0.1991
u_{679}	C(29)...C(64)	12.5114(231)	0.3174(tied to u_{632})	0.2796	0.2344
u_{680}	C(37)...H(96)	12.6942(577)	0.4928(tied to u_{632})	0.4549	0.2013
u_{681}	C(29)...H(88)	12.4918(476)	0.4789(tied to u_{632})	0.441	0.2824
u_{682}	C(61)...H(105)	12.7745(1957)	0.8733(tied to u_{632})	0.8354	0.2583
u_{683}	C(61)...H(103)	12.7450(2145)	0.8394(tied to u_{632})	0.8015	0.2738
u_{684}	C(45)...H(87)	12.3241(1307)	0.9154(tied to u_{632})	0.8776	0.7325
u_{685}	C(61)...H(87)	12.4877(1629)	0.9958(tied to u_{632})	0.9579	0.6041
u_{686}	C(45)...H(103)	12.6381(1794)	0.8662(tied to u_{632})	0.8284	0.4785
u_{687}	C(61)...H(107)	12.5631(1245)	0.7841(tied to u_{632})	0.7463	0.3119
u_{688}	C(21)...H(104)	12.8427(50)	0.2313(tied to u_{632})	0.1935	0.2258
u_{689}	C(53)...H(107)	12.6052(1063)	0.7174(1082)	0.6919	0.5108
u_{690}	C(53)...H(99)	12.4467(748)	0.6725(tied to u_{689})	0.647	0.7673
u_{691}	C(61)...H(99)	12.5546(973)	0.7578(tied to u_{689})	0.7323	0.6238
u_{692}	H(77)...H(104)	13.2821(439)	0.5048(tied to u_{689})	0.4793	0.1990
u_{693}	H(69)...H(104)	13.1204(432)	0.5069(tied to u_{689})	0.4814	0.2672
u_{694}	C(45)...C(56)	13.2471(127)	0.3703(tied to u_{689})	0.3448	0.2234
u_{695}	C(53)...C(56)	13.3551(410)	0.3557(tied to u_{689})	0.3302	0.2183
u_{696}	C(45)...C(48)	13.2125(417)	0.3518(tied to u_{689})	0.3263	0.2797
u_{697}	C(37)...H(104)	13.6299(227)	0.3269(tied to u_{689})	0.3013	0.2346
u_{698}	C(29)...H(104)	13.5406(254)	0.3296(tied to u_{689})	0.3041	0.2718
u_{699}	C(45)...H(96)	13.8798(185)	0.5031(tied to u_{689})	0.4776	0.2268
u_{700}	C(53)...H(88)	13.8164(328)	0.5022(tied to u_{689})	0.4767	0.2469
u_{701}	C(53)...C(64)	13.9287(201)	0.2986(tied to u_{689})	0.2731	0.2418

u_{702}	C(45)...C(64)	13.8536(234)	0.2993(tied to u_{689})	0.2737	0.2735
u_{703}	C(53)...H(96)	14.0143(535)	0.4849(tied to u_{689})	0.4594	0.2390
u_{704}	C(45)...H(88)	13.8057(502)	0.4742(tied to u_{689})	0.4487	0.3218
u_{705}	C(61)...H(96)	14.5747(280)	0.4336(tied to u_{689})	0.4081	0.2522
u_{706}	C(61)...C(64)	14.5203(98)	0.2256(tied to u_{689})	0.2001	0.2807
u_{707}	C(61)...H(88)	14.4319(351)	0.4306(tied to u_{689})	0.405	0.3055
u_{708}	C(53)...H(104)	14.9605(205)	0.3239(tied to u_{689})	0.2983	0.2802
u_{709}	C(45)...H(104)	14.8804(263)	0.3256(tied to u_{689})	0.3001	0.3137
u_{710}	C(61)...H(104)	15.5521(103)	0.2517(tied to u_{689})	0.2262	0.3210

[a] Estimated standard deviations, obtained in the least squares refinement, are given in parentheses. [b] Amplitudes not refined were fixed at the values obtained using the B3LYP/cc-pVTZ force field.

Figure S1 Experimental and difference (experimental minus theoretical) molecular-scattering intensities for **1**.

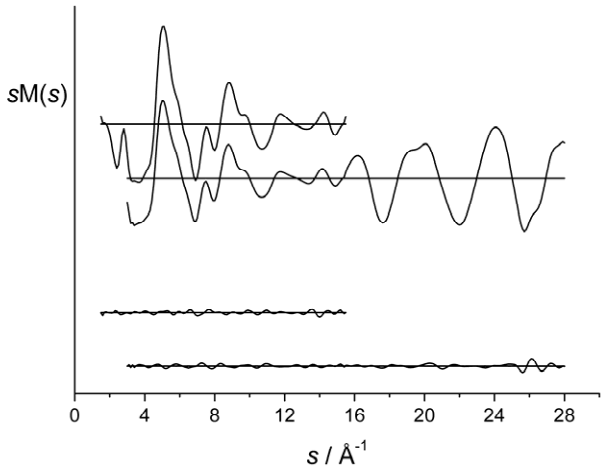

Figure S2 The molecular structure of the asymmetric unit in the structure of **2** (30% probability ellipsoids).

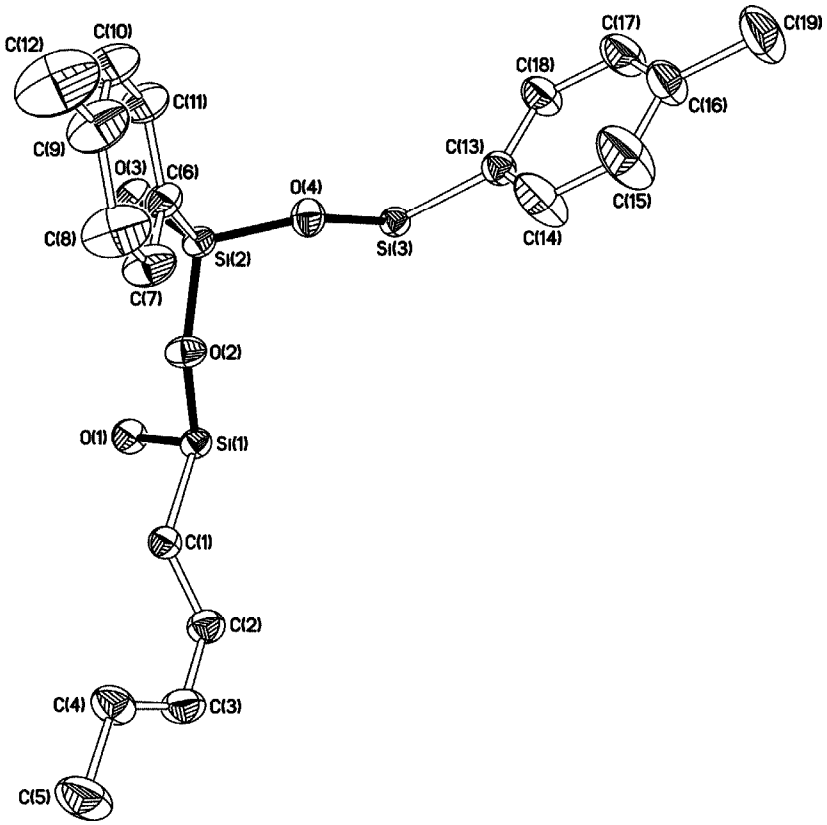

Figure S3 The molecular structure of **3** (30% probability ellipsoids).