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New Crystal Structures of *p-tert*-butylthiacalix[6]arene Complexes with Toluene and Benzyl Alcohol

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It is well known that *p-tert*-butylthiacalixarenes can make host-guest complexation with organic guest molecules and metal cations. In order to study crystal structural properties of the titled host molecule with organic compounds, we tried to make a new crystal of the *p-tert*-butylthiacalix[6]arene. Fortunately, two new crystal structures of *p-tert*-butylthiacalix[6]arenes complexed with toluene and with benzyl alcohol were obtained. The conformation of the complex with toluene is the cone conformation; on the other hand, the conformation of the complex with benzyl alcohol is 1,2,3-alternate.

Key Words : calixarene, thiacalixarene, crystal structure, hydrogen bonding.

1. Introduction

Considerable attention has been recently focused on thiacalixarenes because of their capability of making of a host-guest complexation with organic compounds or metal cations [1]. Thiacalixarene is much more versatile host compound than calixarene because thiacalixarene itself can make a hot-guest complexation with metal cations because sulfide functional group has affinity for metal cations [2]. The crystal structures of thiacalixarene analogues have been reported by couple groups such as Miyano and Hosseini groups [3-4]. Recently, Miyano et al. has reported that crystal structures derived from *p-tert*-butyl thiacalix[6]arene, of which the crystal is a complex with dichloromethane [5]. Quite recently, Miyano et al. also reported the beautiful crystal structure of decacopper (II) cluster complex of *p-tert*-butylthiacalix[6]arene [6]. Hamada and Endo et al. have investigated the synthesis and crystal structure of K_4[*p-tert*-butylthiacalix[6]arene^{4-}]•14MeOH•$2H_2O$ [7]. We report herein that the crystal structure and properties of *p-tert*-butylthiacalix[6]arene with two kinds of organic compounds, which is the first example of complexes with aromatic residues.

2. Experimental

X-Ray crystallography

Single crystal of *p-tert*-butylthiacalix[6]arene was obtained by slow evaporation of the solvent from the toluene or benzyl alcohol solution. Crystal data for *p-tert*-butylthiacalix[6]arene with toluene: $C_{60}H_{72}O_6S_6(C_7H_8)$, FW=1173.73, Crystal color: colorless, Size (mm)=0.15 x 0.15 x 0.30, Crystal System: monoclinic, space group; $P2_1/n$ a(Å)=17.3876(3), b(Å)=18.9409(5), c(Å)=19.1486(5), β(deg)=96.7710(6), V(Å^3)=6262.4(2), Dc=1.245 g cm^{-3}, Z=4, m=μ(Mo-Kα) 2.69 cm^{-1}, Rigaku RAXIS-RAPID imaging Plate diffractometer, T=103K, Number of Reflections:54073, Independent Reflections:14533 (R_{int} =0.076), Observed Reflections:14118($I_0 > -10.00\ \sigma\ (I_0)$), Rw=0.169, R=0.066, GOF=1.57.

Crystal data for *p-tert*-butylthiacalix[6]arene with benzyl alcohol: $C_{60}H_{72}O_6S_6(C_7H_8O)$, FW=1189.72, Crystal color: colorless, Size (mm)=0.30 x 0.20 x 0.20, Crystal System: triclinic, space group;P-1 a(Å)=14.3002(1), b(Å)=14.9248(4), c(Å)=17.1777(4), α(deg)=84.248(1), β(deg)=66.241(1), γ(deg)=73.2676(5), V(Å^3)=3212.9(1), Dc=1.230gcm^{-3}, Z=2, m=μ(Mo-Kα) 2.64cm^{-1} Rigaku RAXIS-RAPID imaging Plate diffractometer, T=103K, Number of Reflections: 24705, Independent Reflections: 13264 (R_{int} =0.068),Observed Reflections:13253 ($I_0 > -10.00\ \sigma\ (I_0)$), Rw=0.145, R=0.075, GOF=1.43.

3. Results and discussion

It is reported that calix[6]arenes are more flexible than those of calix[4]arenes and crystal structure determination show that the cone conformation is lost. Two classes have been described; one has a conformation with symmetry planes, the other a centro symmetric conformation [8]. In principle thiacalix[4]arenes is cone conformation, although there are few examples of conformation data of *p-tert*-butylthiacalix[6]arene. Only a data of solid-state conformation with dichloromethane as a guest shows that *p-tert*-butylthiacalix[6]arene adopts a distorted cone conformation, which has two cavities comprising BAB' and CDC' rings [5]. In the structure of *p-tert*-butylthiacalix[6]arene•toluene, Figure 1, such as two cavities is also evident, and adopts winged cone conformation, which is stabilized by strong hydrogen bondings between six hydroxyl groups of lower rim of thiacalixarene because the phenolic O-O distances of O(1)-O(2), O(2)-O(3), O(3)-O(4), O(4)-O(5), O(5)-O(6) and O(6)-O(1) are 2.838Å, 2.8 39Å, 2.718Å, 2.688Å, 2.765Å and 2.755Å, respectively. The dihedral angels of benzene units such as A/D, B/F, C/E are 132. 23°, 90.58°, and 85.22°, respectively. These data supports that the

conformation of *p-tert*-butylthiacalix[6]arene•toluene is similar those of *p-tert*-butylthiacalix[6]arene•dichloromethane and *p-tert*-butylcalix[6]arene itself reported by Ungaro et al. [8]. The only one difference of the structure between *p-tert*-butylthiacalix[6]arene • toluene and of *p-tert*-butylthiacalix[6]arene • dichloromethane was observed. The structure of *p-tert*-butylthiacalix[6]arene•toluene has not a crystallographic mirror plane. Miyano et al. reported that *p-tert*-butylthiacalix[4]arene formed 2:1=host : guest complex with toluene [9]. It is recognized that *p-tert*-butylthiacalix[6]arene should be more capable of inclusion ability than that of *p-tert*-butylthiacalix[4]arene, because of a larger guest-binding domain. Bond lengths, bond angles, and dihedral angles (Table Ⅰ, Ⅱ and, Ⅲ, respectively) were within the expected ranges.

Figure 2 shows the crystal structure of *p-tert*-butylthiacalix[6]arene•benzyl alcohol, which indicates 1,2,3-alternate structure because ring inversion between ring IJK and ring HGL are recognized. It is indicated that intra-hydrogen bonding between six hydroxyl groups of lower rim of thiacalixarene observed in the case of *p-tert*-butylthiacalix[6]arene•toluene was prohibited because there are two hydrogen-bonding systems,which are intra molecular hydrogen bonding between ring IJK and ring HGL and inter hydrogen bonding between -OH of benzyl alcohol and phenolic -OH of H, I, and K benzene ring of the thiacalix[6]arene. The intra- hydrogen bonding among ring K, J, and I of which the phenolic O-O distances of O(1)-O(2), O(1)-O(6) are 2.879 Å and 2.838 Å, respectively and among ring L, G, and H of which the phenolic O-O distances of O(4)-O(3), O(4)-O(5) are 2.948 Å and 2.934 Å, respectively. The distances of benzyl alcoholic- O and phenolic O of H, I, and K are 2.978 Å, 2.802 Å and 2.760 Å, respectively. Bond lengths, bond angles, and dihedral angles (Table Ⅳ, Ⅴ and, Ⅵ, respectively) were within the expected ranges. It seems that the guest binding behavior of this system is mixed up hydrogen bonding and hydrophobic interaction to elevate the guest binding ability.

4. Conclusion

Two new crystal structures of *p-tert*-butylthiacalix[6]arene including toluene and benzyl alcohol, of which the conformations are winged cone and 1,2,3-alternate, respectively. It is recognized that the conformation of *p-tert*-butylthiacalix[6]arene in the solid state is depended on a kind of guest species. We are now investigating to make new crystals of *p-tert*-butylthiacalix[6]arene and aromatic guest molecules.

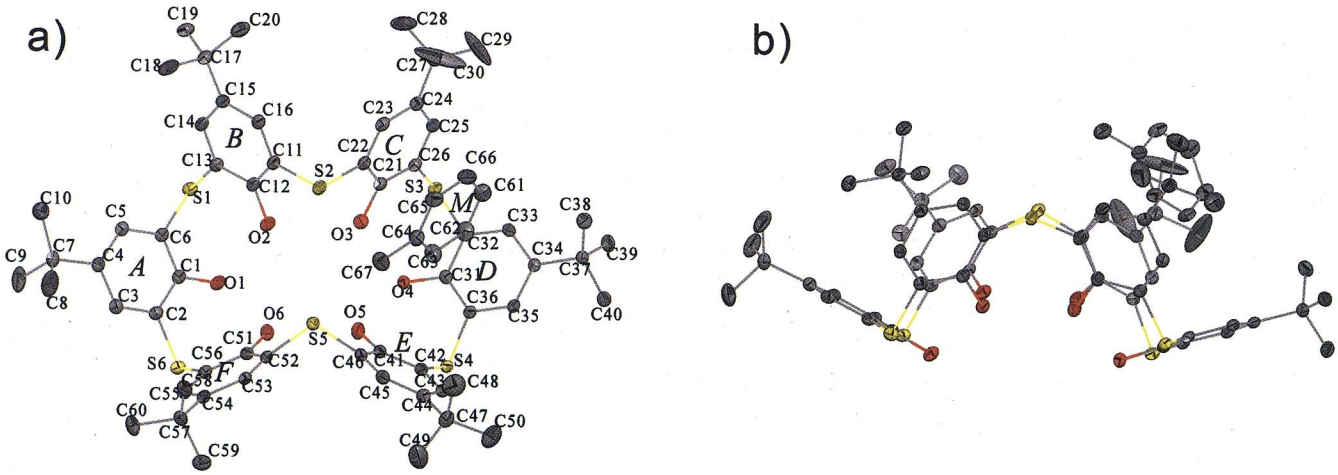

Figure 1. Crystal structure of thiacalix[6]arene with toluene. a) top view b) side view

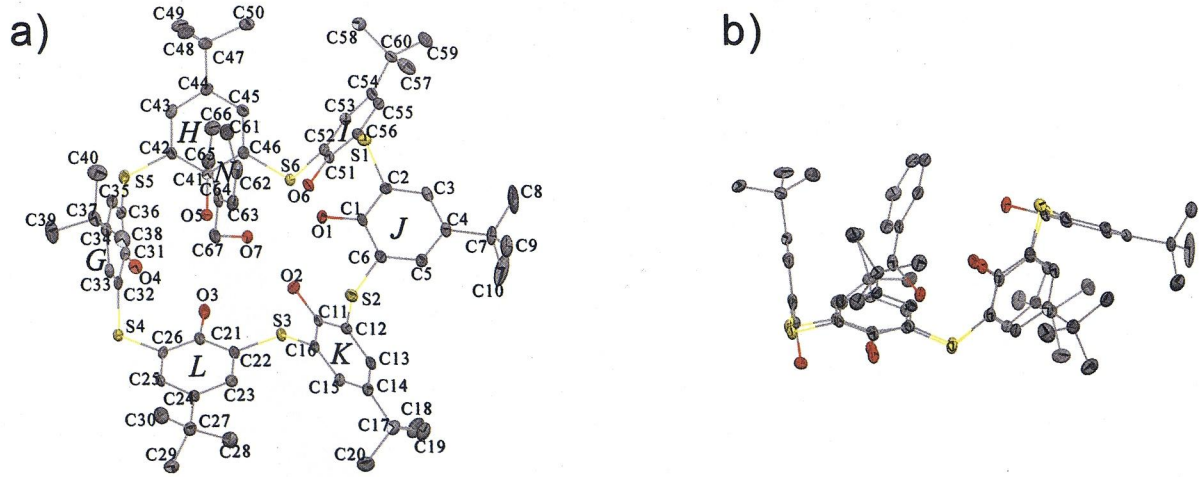

Figure 2. Crystal structure of thiacalix[6]arene with benzyl alcohol. a) top view b) side view

Table I Intermolecular bond lengths for TC6A with toluene (Å)

atom	atom	distance	atom	atom	distance
S(1)	C(6)	1.792(3)	S(1)	C(13)	1.780(3)
S(2)	C(11)	1.790(3)	S(2)	C(22)	1.785(3)
S(3)	C(26)	1.787(3)	S(3)	C(32)	1.791(3)
S(4)	C(36)	1.788(3)	S(4)	C(42)	1.789(3)
S(5)	C(46)	1.786(3)	S(5)	C(52)	1.781(3)
S(6)	C(2)	1.791(3)	S(6)	C(56)	1.789(3)
O(1)	C(1)	1.369(4)	O(2)	C(12)	1.358(4)
O(3)	C(21)	1.368(4)	O(4)	C(31)	1.369(3)
O(5)	C(41)	1.364(3)	O(6)	C(51)	1.352(4)
C(1)	C(2)	1.399(4)	C(1)	C(6)	1.386(4)
C(2)	C(3)	1.394(4)	C(3)	C(4)	1.397(4)
C(4)	C(5)	1.396(4)	C(4)	C(7)	1.535(4)
C(5)	C(6)	1.397(4)	C(7)	C(8)	1.522(5)
C(7)	C(9)	1.524(5)	C(7)	C(10)	1.515(5)
C(11)	C(12)	1.397(4)	C(11)	C(16)	1.392(4)
C(12)	C(13)	1.406(4)	C(13)	C(14)	1.394(4)
C(14)	C(15)	1.400(4)	C(15)	C(16)	1.396(4)
C(15)	C(17)	1.528(4)	C(17)	C(18)	1.543(5)
C(17)	C(19)	1.539(4)	C(17)	C(20)	1.522(5)
C(21)	C(22)	1.404(4)	C(21)	C(26)	1.393(4)
C(22)	C(23)	1.377(4)	C(23)	C(24)	1.396(4)
C(24)	C(25)	1.397(4)	C(24)	C(27)	1.534(4)
C(25)	C(26)	1.392(4)	C(27)	C(28)	1.477(6)
C(27)	C(29)	1.500(6)	C(27)	C(30)	1.474(6)
C(31)	C(32)	1.409(4)	C(31)	C(36)	1.390(4)
C(32)	C(33)	1.385(4)	C(33)	C(34)	1.404(4)
C(34)	C(35)	1.396(4)	C(34)	C(37)	1.525(4)
C(35)	C(36)	1.402(4)	C(37)	C(38)	1.543(4)
C(37)	C(39)	1.524(4)	C(37)	C(40)	1.529(4)
C(41)	C(42)	1.403(4)	C(41)	C(46)	1.398(4)
C(42)	C(43)	1.397(4)	C(43)	C(44)	1.385(4)
C(44)	C(45)	1.391(4)	C(44)	C(47)	1.537(4)
C(45)	C(46)	1.387(4)	C(47)	C(48)	1.538(6)
C(47)	C(49)	1.511(5)	C(47)	C(50)	1.527(5)
C(51)	C(52)	1.412(4)	C(51)	C(56)	1.398(4)
C(52)	C(53)	1.381(4)	C(53)	C(54)	1.395(4)
C(54)	C(55)	1.399(4)	C(54)	C(57)	1.531(4)
C(55)	C(56)	1.397(4)	C(57)	C(58)	1.535(4)
C(57)	C(59)	1.521(4)	C(57)	C(60)	1.529(4)
C(61)	C(62)	1.380(5)	C(61)	C(66)	1.387(5)
C(62)	C(63)	1.375(5)	C(63)	C(64)	1.381(5)
C(64)	C(65)	1.379(5)	C(64)	C(67)	1.506(5)
C(65)	C(66)	1.384(5)			

Table II Intermolecular bond angles of TC6A with toluene (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(6)	S(1)	C(13)	102.6(1)	C(11)	S(2)	C(22)	100.7(1)
C(26)	S(3)	C(32)	102.4(1)	C(36)	S(4)	C(42)	103.9(1)
C(46)	S(5)	C(52)	107.2(1)	C(2)	S(6)	C(56)	99.8(1)
O(1)	C(1)	C(2)	120.5(3)	O(1)	C(1)	C(6)	120.1(3)
C(2)	C(1)	C(6)	119.3(3)	S(6)	C(2)	C(1)	120.1(2)
S(6)	C(2)	C(3)	120.3(2)	C(1)	C(2)	C(3)	119.6(3)
C(2)	C(3)	C(4)	122.0(3)	C(3)	C(4)	C(5)	117.2(3)
C(3)	C(4)	C(7)	120.2(3)	C(5)	C(4)	C(7)	122.5(3)
C(4)	C(5)	C(6)	121.5(3)	S(1)	C(6)	C(1)	119.0(2)
S(1)	C(6)	C(5)	120.6(2)	C(1)	C(6)	C(5)	120.2(3)
C(4)	C(7)	C(8)	110.5(3)	C(4)	C(7)	C(9)	109.2(3)
C(8)	C(7)	C(9)	107.0(4)	C(4)	C(7)	C(10)	112.7(3)
C(8)	C(7)	C(10)	108.9(4)	C(9)	C(7)	C(10)	108.4(3)
S(2)	C(11)	C(12)	120.4(2)	S(2)	C(11)	C(16)	119.6(2)
C(12)	C(11)	C(16)	120.0(3)	O(2)	C(12)	C(11)	121.2(3)
O(2)	C(12)	C(13)	119.9(3)	C(11)	C(12)	C(13)	119.0(3)
S(1)	C(13)	C(12)	121.6(2)	S(1)	C(13)	C(14)	118.6(2)
C(12)	C(13)	C(14)	119.7(3)	C(13)	C(14)	C(15)	122.1(3)
C(14)	C(15)	C(16)	117.0(3)	C(14)	C(15)	C(17)	121.1(3)
C(16)	C(15)	C(17)	121.8(3)	C(11)	C(16)	C(15)	122.2(3)
C(15)	C(17)	C(18)	108.2(3)	C(15)	C(17)	C(19)	110.9(3)
C(18)	C(17)	C(19)	108.2(3)	C(15)	C(17)	C(20)	112.1(3)
C(18)	C(17)	C(20)	110.0(3)	C(19)	C(17)	C(20)	107.4(3)
O(3)	C(21)	C(22)	119.0(3)	O(3)	C(21)	C(26)	121.7(3)
C(22)	C(21)	C(26)	119.3(3)	S(2)	C(22)	C(21)	119.6(2)
S(2)	C(22)	C(23)	120.9(3)	C(21)	C(22)	C(23)	119.5(3)
C(22)	C(23)	C(24)	122.8(3)	C(23)	C(24)	C(25)	116.6(3)
C(23)	C(24)	C(27)	120.7(3)	C(25)	C(24)	C(27)	122.6(3)
C(24)	C(25)	C(26)	122.1(3)	S(3)	C(26)	C(21)	120.7(2)
S(3)	C(26)	C(25)	119.4(2)	C(21)	C(26)	C(25)	119.7(3)
C(24)	C(27)	C(28)	109.9(3)	C(24)	C(27)	C(29)	112.0(3)
C(28)	C(27)	C(29)	108.1(6)	C(24)	C(27)	C(30)	111.6(3)
C(28)	C(27)	C(30)	107.9(5)	C(29)	C(27)	C(30)	107.2(6)
O(4)	C(31)	C(32)	119.5(3)	O(4)	C(31)	C(36)	121.3(3)
C(32)	C(31)	C(36)	119.2(3)	S(3)	C(32)	C(31)	120.4(2)
S(3)	C(32)	C(33)	120.1(2)	C(31)	C(32)	C(33)	119.5(3)
C(32)	C(33)	C(34)	122.5(3)	C(33)	C(34)	C(35)	116.8(3)
C(33)	C(34)	C(37)	120.0(3)	C(35)	C(34)	C(37)	123.2(3)
C(34)	C(35)	C(36)	121.8(3)	S(4)	C(36)	C(31)	120.3(2)
S(4)	C(36)	C(35)	119.5(2)	C(31)	C(36)	C(35)	120.1(3)
C(34)	C(37)	C(38)	108.2(3)	C(34)	C(37)	C(39)	109.5(3)
C(38)	C(37)	C(39)	110.0(3)	C(34)	C(37)	C(40)	112.2(3)
C(38)	C(37)	C(40)	108.8(3)	C(39)	C(37)	C(40)	108.2(3)
O(5)	C(41)	C(42)	121.0(3)	O(5)	C(41)	C(46)	119.8(3)
C(42)	C(41)	C(46)	119.2(3)	S(4)	C(42)	C(41)	121.2(2)
S(4)	C(42)	C(43)	119.6(2)	C(41)	C(42)	C(43)	119.3(3)

Table II Intermolecular bond angles of TC6A with toluene (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(42)	C(43)	C(44)	122.5(3)	C(43)	C(44)	C(45)	116.9(3)
C(43)	C(44)	C(47)	122.8(3)	C(45)	C(44)	C(47)	120.4(3)
C(44)	C(45)	C(46)	122.8(3)	S(5)	C(46)	C(41)	120.4(2)
S(5)	C(46)	C(45)	119.4(2)	C(41)	C(46)	C(45)	119.4(3)
C(44)	C(47)	C(48)	108.3(3)	C(44)	C(47)	C(49)	110.0(3)
C(48)	C(47)	C(49)	109.3(4)	C(44)	C(47)	C(50)	113.1(3)
C(48)	C(47)	C(50)	106.0(3)	C(49)	C(47)	C(50)	110.1(3)
O(6)	C(51)	C(52)	120.6(3)	O(6)	C(51)	C(56)	121.0(3)
C(52)	C(51)	C(56)	118.4(3)	S(5)	C(52)	C(51)	119.5(2)
S(5)	C(52)	C(53)	119.2(2)	C(51)	C(52)	C(53)	119.8(3)
C(52)	C(53)	C(54)	123.1(3)	C(53)	C(54)	C(55)	116.5(3)
C(53)	C(54)	C(57)	120.6(3)	C(55)	C(54)	C(57)	122.9(3)
C(54)	C(55)	C(56)	122.1(3)	S(6)	C(56)	C(51)	120.5(2)
S(6)	C(56)	C(55)	119.3(2)	C(51)	C(56)	C(55)	120.2(3)
C(54)	C(57)	C(58)	110.2(3)	C(54)	C(57)	C(59)	108.9(3)
C(58)	C(57)	C(59)	109.8(3)	C(54)	C(57)	C(60)	111.5(3)
C(58)	C(57)	C(60)	107.8(3)	C(59)	C(57)	C(60)	108.7(3)
C(62)	C(61)	C(66)	118.9(4)	C(61)	C(62)	C(63)	120.1(4)
C(62)	C(63)	C(64)	122.1(4)	C(63)	C(64)	C(65)	117.3(3)
C(63)	C(64)	C(67)	121.9(3)	C(65)	C(64)	C(67)	120.8(3)
C(64)	C(65)	C(66)	121.7(3)	C(61)	C(66)	C(65)	119.9(4)

Table Ⅲ Intermolecular dihedral angles of TC6A with toluene (°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(13)	S(1)	C(6)	C(1)	-102.6(5)	C(13)	S(1)	C(6)	C(5)	82.3(5)
C(6)	S(1)	C(13)	C(12)	73.9(5)	C(6)	S(1)	C(13)	C(14)	-110.0(5)
C(22)	S(2)	C(11)	C(12)	94.5(5)	C(22)	S(2)	C(11)	C(16)	-86.4(5)
C(11)	S(2)	C(22)	C(21)	-89.8(5)	C(11)	S(2)	C(22)	C(23)	90.7(5)
C(32)	S(3)	C(26)	C(21)	-77.1(5)	C(32)	S(3)	C(26)	C(25)	107.6(5)
C(26)	S(3)	C(32)	C(31)	94.1(5)	C(26)	S(3)	C(32)	C(33)	-88.1(5)
C(42)	S(4)	C(36)	C(31)	-90.1(5)	C(42)	S(4)	C(36)	C(35)	95.2(5)
C(36)	S(4)	C(42)	C(41)	81.9(5)	C(36)	S(4)	C(42)	C(43)	-100.2(5)
C(52)	S(5)	C(46)	C(41)	92.2(5)	C(52)	S(5)	C(46)	C(45)	-98.1(5)
C(46)	S(5)	C(52)	C(51)	-92.9(5)	C(46)	S(5)	C(52)	C(53)	101.2(5)
C(56)	S(6)	C(2)	C(1)	94.2(5)	C(56)	S(6)	C(2)	C(3)	-87.3(5)
C(2)	S(6)	C(56)	C(51)	-82.1(5)	C(2)	S(6)	C(56)	C(55)	96.4(5)
O(1)	C(1)	C(2)	S(6)	0.8(5)	O(1)	C(1)	C(2)	C(3)	-177.7(3)
C(6)	C(1)	C(2)	S(6)	-178.8(3)	C(6)	C(1)	C(2)	C(3)	2.7(6)
O(1)	C(1)	C(6)	S(1)	3.4(5)	O(1)	C(1)	C(6)	C(5)	178.5(3)
C(2)	C(1)	C(6)	S(1)	-177.1(3)	C(2)	C(1)	C(6)	C(5)	-2.0(6)
S(6)	C(2)	C(3)	C(4)	179.0(3)	C(1)	C(2)	C(3)	C(4)	-2.5(6)
C(2)	C(3)	C(4)	C(5)	1.4(6)	C(2)	C(3)	C(4)	C(7)	177.5(4)
C(3)	C(4)	C(5)	C(6)	-0.6(6)	C(7)	C(4)	C(5)	C(6)	-176.6(4)
C(3)	C(4)	C(7)	C(8)	51.6(6)	C(3)	C(4)	C(7)	C(9)	-65.8(6)
C(3)	C(4)	C(7)	C(10)	173.7(4)	C(5)	C(4)	C(7)	C(8)	-132.5(5)
C(5)	C(4)	C(7)	C(9)	110.0(5)	C(5)	C(4)	C(7)	C(10)	-10.5(7)
C(4)	C(5)	C(6)	S(1)	175.9(3)	C(4)	C(5)	C(6)	C(1)	0.9(6)
S(2)	C(11)	C(12)	O(2)	-1.9(4)	S(2)	C(11)	C(12)	C(13)	177.7(3)
C(16)	C(11)	C(12)	O(2)	179.0(4)	C(16)	C(11)	C(12)	C(13)	-1.4(6)
S(2)	C(11)	C(16)	C(15)	-178.7(3)	C(12)	C(11)	C(16)	C(15)	0.5(6)
O(2)	C(12)	C(13)	S(1)	-3.3(5)	O(2)	C(12)	C(13)	C(14)	-179.4(3)
C(11)	C(12)	C(13)	S(1)	177.1(3)	C(11)	C(12)	C(13)	C(14)	1.0(6)
S(1)	C(13)	C(14)	C(15)	-175.8(3)	C(12)	C(13)	C(14)	C(15)	0.4(6)
C(13)	C(14)	C(15)	C(16)	-1.4(6)	C(13)	C(14)	C(15)	C(17)	-177.6(4)
C(14)	C(15)	C(16)	C(11)	0.9(6)	C(17)	C(15)	C(16)	C(11)	177.1(4)
C(14)	C(15)	C(17)	C(18)	82.8(5)	C(14)	C(15)	C(17)	C(19)	-35.7(6)
C(14)	C(15)	C(17)	C(20)	-155.7(4)	C(16)	C(15)	C(17)	C(18)	-93.2(5)
C(16)	C(15)	C(17)	C(19)	148.3(4)	C(16)	C(15)	C(17)	C(20)	28.3(6)
O(3)	C(21)	C(22)	S(2)	2.8(5)	O(3)	C(21)	C(22)	C(23)	-177.7(3)
C(26)	C(21)	C(22)	S(2)	-178.7(3)	C(26)	C(21)	C(22)	C(23)	0.8(6)
O(3)	C(21)	C(26)	S(3)	2.0(5)	O(3)	C(21)	C(26)	C(25)	177.3(3)
C(22)	C(21)	C(26)	S(3)	-176.5(3)	C(22)	C(21)	C(26)	C(25)	-1.2(6)
S(2)	C(22)	C(23)	C(24)	-179.5(3)	C(21)	C(22)	C(23)	C(24)	1.0(6)
C(22)	C(23)	C(24)	C(25)	-2.3(6)	C(22)	C(23)	C(24)	C(27)	176.3(4)
C(23)	C(24)	C(25)	C(26)	1.9(6)	C(27)	C(24)	C(25)	C(26)	-176.6(4)
C(23)	C(24)	C(27)	C(28)	-74.7(6)	C(23)	C(24)	C(27)	C(29)	165.1(6)
C(23)	C(24)	C(27)	C(30)	45.0(7)	C(25)	C(24)	C(27)	C(28)	103.7(6)
C(25)	C(24)	C(27)	C(29)	-16.4(8)	C(25)	C(24)	C(27)	C(30)	-136.6(6)
C(24)	C(25)	C(26)	S(3)	175.2(3)	C(24)	C(25)	C(26)	C(21)	-0.2(6)
O(4)	C(31)	C(32)	S(3)	1.8(4)	O(4)	C(31)	C(32)	C(33)	-176.1(3)

Table Ⅲ Intermolecular dihedral angles of TC6A with toluene (°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(36)	C(31)	C(32)	S(3)	-178.3(3)	C(36)	C(31)	C(32)	C(33)	3.9(6)
O(4)	C(31)	C(36)	S(4)	2.8(5)	O(4)	C(31)	C(36)	C(35)	177.5(3)
C(32)	C(31)	C(36)	S(4)	-177.1(3)	C(32)	C(31)	C(36)	C(35)	-2.4(6)
S(3)	C(32)	C(33)	C(34)	179.0(3)	C(31)	C(32)	C(33)	C(34)	-3.1(6)
C(32)	C(33)	C(34)	C(35)	0.8(6)	C(32)	C(33)	C(34)	C(37)	-179.2(4)
C(33)	C(34)	C(35)	C(36)	0.7(6)	C(37)	C(34)	C(35)	C(36)	-179.2(4)
C(33)	C(34)	C(37)	C(38)	57.5(5)	C(33)	C(34)	C(37)	C(39)	-62.4(5)
C(33)	C(34)	C(37)	C(40)	177.4(4)	C(35)	C(34)	C(37)	C(38)	-122.6(4)
C(35)	C(34)	C(37)	C(39)	117.6(4)	C(35)	C(34)	C(37)	C(40)	-2.6(6)
C(34)	C(35)	C(36)	S(4)	174.9(3)	C(34)	C(35)	C(36)	C(31)	0.1(6)
O(5)	C(41)	C(42)	S(4)	-0.6(5)	O(5)	C(41)	C(42)	C(43)	-178.6(3)
C(46)	C(41)	C(42)	S(4)	179.3(3)	C(46)	C(41)	C(42)	C(43)	1.4(6)
O(5)	C(41)	C(46)	S(5)	-12.4(5)	O(5)	C(41)	C(46)	C(45)	177.8(3)
C(42)	C(41)	C(46)	S(5)	167.6(3)	C(42)	C(41)	C(46)	C(45)	-2.1(6)
S(4)	C(42)	C(43)	C(44)	-177.5(3)	C(41)	C(42)	C(43)	C(44)	0.5(6)
C(42)	C(43)	C(44)	C(45)	-1.5(6)	C(42)	C(43)	C(44)	C(47)	-179.6(4)
C(43)	C(44)	C(45)	C(46)	0.7(6)	C(47)	C(44)	C(45)	C(46)	178.8(4)
C(43)	C(44)	C(47)	C(48)	116.6(5)	C(43)	C(44)	C(47)	C(49)	-124.0(5)
C(43)	C(44)	C(47)	C(50)	-0.5(7)	C(45)	C(44)	C(47)	C(48)	-61.4(6)
C(45)	C(44)	C(47)	C(49)	58.0(6)	C(45)	C(44)	C(47)	C(50)	-178.5(4)
C(44)	C(45)	C(46)	S(5)	-168.7(3)	C(44)	C(45)	C(46)	C(41)	1.2(6)
O(6)	C(51)	C(52)	S(5)	13.6(5)	O(6)	C(51)	C(52)	C(53)	179.5(3)
C(56)	C(51)	C(52)	S(5)	-165.1(3)	C(56)	C(51)	C(52)	C(53)	0.8(6)
O(6)	C(51)	C(56)	S(6)	-0.1(5)	O(6)	C(51)	C(56)	C(55)	-178.7(3)
C(52)	C(51)	C(56)	S(6)	178.6(3)	C(52)	C(51)	C(56)	C(55)	0.1(6)
S(5)	C(52)	C(53)	C(54)	164.8(3)	C(51)	C(52)	C(53)	C(54)	-1.1(6)
C(52)	C(53)	C(54)	C(55)	0.6(6)	C(52)	C(53)	C(54)	C(57)	-177.2(4)
C(53)	C(54)	C(55)	C(56)	0.3(6)	C(57)	C(54)	C(55)	C(56)	178.1(4)
C(53)	C(54)	C(57)	C(58)	46.2(6)	C(53)	C(54)	C(57)	C(59)	-74.2(5)
C(53)	C(54)	C(57)	C(60)	165.8(4)	C(55)	C(54)	C(57)	C(58)	-131.5(4)
C(55)	C(54)	C(57)	C(59)	108.1(5)	C(55)	C(54)	C(57)	C(60)	-11.8(6)
C(54)	C(55)	C(56)	S(6)	-179.2(3)	C(54)	C(55)	C(56)	C(51)	-0.6(6)
C(66)	C(61)	C(62)	C(63)	0.7(8)	C(62)	C(61)	C(66)	C(65)	-1.2(8)
C(61)	C(62)	C(63)	C(64)	0.0(8)	C(62)	C(63)	C(64)	C(65)	-0.2(7)
C(62)	C(63)	C(64)	C(67)	178.6(5)	C(63)	C(64)	C(65)	C(66)	-0.4(7)
C(67)	C(64)	C(65)	C(66)	-179.1(5)	C(64)	C(65)	C(66)	C(61)	1.1(8)

Table IV Intermolecular bond lengths for TC6A with benzyl alcohol (Å)

atom	atom	distance	atom	atom	distance
S(1)	C(2)	1.771(4)	S(1)	C(56)	1.773(3)
S(2)	C(6)	1.776(4)	S(2)	C(12)	1.775(3)
S(3)	C(16)	1.776(4)	S(3)	C(22)	1.784(3)
S(4)	C(26)	1.781(3)	S(4)	C(32)	1.782(4)
S(5)	C(36)	1.771(3)	S(5)	C(42)	1.777(4)
S(6)	C(46)	1.791(4)	S(6)	C(52)	1.782(4)
O(1)	C(1)	1.355(4)	O(2)	C(11)	1.362(4)
O(3)	C(21)	1.365(4)	O(4)	C(31)	1.361(4)
O(5)	C(41)	1.370(4)	O(6)	C(51)	1.355(4)
O(7)	C(67)	1.444(4)	C(1)	C(2)	1.393(5)
C(1)	C(6)	1.413(5)	C(2)	C(3)	1.403(5)
C(3)	C(4)	1.384(5)	C(4)	C(5)	1.386(5)
C(4)	C(7)	1.531(5)	C(5)	C(6)	1.382(5)
C(7)	C(8)	1.516(6)	C(7)	C(9)	1.495(7)
C(7)	C(10)	1.523(5)	C(11)	C(12)	1.398(5)
C(11)	C(16)	1.390(5)	C(12)	C(13)	1.398(5)
C(13)	C(14)	1.384(5)	C(14)	C(15)	1.404(5)
C(14)	C(17)	1.528(5)	C(15)	C(16)	1.383(5)
C(17)	C(18)	1.546(6)	C(17)	C(19)	1.512(5)
C(17)	C(20)	1.521(6)	C(21)	C(22)	1.389(5)
C(21)	C(26)	1.382(5)	C(22)	C(23)	1.387(5)
C(23)	C(24)	1.399(5)	C(24)	C(25)	1.388(5)
C(24)	C(27)	1.521(5)	C(25)	C(26)	1.380(5)
C(27)	C(28)	1.525(5)	C(27)	C(29)	1.522(6)
C(27)	C(30)	1.550(5)	C(31)	C(32)	1.384(5)
C(31)	C(36)	1.395(5)	C(32)	C(33)	1.384(5)
C(33)	C(34)	1.392(5)	C(34)	C(35)	1.385(5)
C(34)	C(37)	1.536(5)	C(35)	C(36)	1.401(5)
C(37)	C(38)	1.527(6)	C(37)	C(39)	1.533(5)
C(37)	C(40)	1.519(5)	C(41)	C(42)	1.391(5)
C(41)	C(46)	1.390(5)	C(42)	C(43)	1.390(5)
C(43)	C(44)	1.395(5)	C(44)	C(45)	1.382(5)
C(44)	C(47)	1.532(5)	C(45)	C(46)	1.398(5)
C(47)	C(48)	1.528(5)	C(47)	C(49)	1.508(5)
C(47)	C(50)	1.533(5)	C(51)	C(52)	1.410(5)
C(51)	C(56)	1.407(5)	C(52)	C(53)	1.385(5)
C(53)	C(54)	1.396(5)	C(54)	C(55)	1.399(5)
C(54)	C(60)	1.531(5)	C(55)	C(56)	1.382(5)
C(57)	C(60)	1.525(5)	C(58)	C(60)	1.527(5)
C(59)	C(60)	1.520(5)	C(61)	C(62)	1.372(6)
C(61)	C(66)	1.376(6)	C(62)	C(63)	1.377(5)
C(63)	C(64)	1.382(5)	C(64)	C(65)	1.395(5)
C(64)	C(67)	1.512(5)	C(65)	C(66)	1.378(5)

Table V Intermolecular bond angles of TC6A with benzyl alcohol (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	S(1)	C(56)	105.4(2)	C(6)	S(2)	C(12)	100.0(2)
C(16)	S(3)	C(22)	102.1(2)	C(26)	S(4)	C(32)	101.9(2)
C(36)	S(5)	C(42)	104.6(2)	C(46)	S(6)	C(52)	102.3(2)
O(1)	C(1)	C(2)	122.9(3)	O(1)	C(1)	C(6)	117.9(3)
C(2)	C(1)	C(6)	119.2(3)	S(1)	C(2)	C(1)	119.2(3)
S(1)	C(2)	C(3)	121.0(3)	C(1)	C(2)	C(3)	119.2(3)
C(2)	C(3)	C(4)	122.5(3)	C(3)	C(4)	C(5)	117.0(3)
C(3)	C(4)	C(7)	122.9(3)	C(5)	C(4)	C(7)	120.0(3)
C(4)	C(5)	C(6)	122.9(4)	S(2)	C(6)	C(1)	119.8(3)
S(2)	C(6)	C(5)	120.8(3)	C(1)	C(6)	C(5)	119.3(3)
C(4)	C(7)	C(8)	109.3(4)	C(4)	C(7)	C(9)	112.6(4)
C(8)	C(7)	C(9)	106.4(5)	C(4)	C(7)	C(10)	108.5(3)
C(8)	C(7)	C(10)	109.3(4)	C(9)	C(7)	C(10)	110.6(4)
O(2)	C(11)	C(12)	121.8(3)	O(2)	C(11)	C(16)	118.7(3)
C(12)	C(11)	C(16)	119.5(3)	S(2)	C(12)	C(11)	120.3(3)
S(2)	C(12)	C(13)	120.3(3)	C(11)	C(12)	C(13)	119.5(3)
C(12)	C(13)	C(14)	122.2(4)	C(13)	C(14)	C(15)	116.6(3)
C(13)	C(14)	C(17)	122.7(3)	C(15)	C(14)	C(17)	120.7(3)
C(14)	C(15)	C(16)	122.5(3)	S(3)	C(16)	C(11)	119.7(3)
S(3)	C(16)	C(15)	120.6(3)	C(11)	C(16)	C(15)	119.6(3)
C(14)	C(17)	C(18)	108.8(3)	C(14)	C(17)	C(19)	109.8(3)
C(18)	C(17)	C(19)	109.4(4)	C(14)	C(17)	C(20)	112.8(3)
C(18)	C(17)	C(20)	106.7(3)	C(19)	C(17)	C(20)	109.3(3)
O(3)	C(21)	C(22)	117.5(3)	O(3)	C(21)	C(26)	123.8(3)
C(22)	C(21)	C(26)	118.6(3)	S(3)	C(22)	C(21)	116.4(3)
S(3)	C(22)	C(23)	123.3(3)	C(21)	C(22)	C(23)	120.2(3)
C(22)	C(23)	C(24)	121.6(3)	C(23)	C(24)	C(25)	116.8(3)
C(23)	C(24)	C(27)	123.3(3)	C(25)	C(24)	C(27)	119.9(3)
C(24)	C(25)	C(26)	121.9(3)	S(4)	C(26)	C(21)	120.0(3)
S(4)	C(26)	C(25)	119.2(3)	C(21)	C(26)	C(25)	120.8(3)
C(24)	C(27)	C(28)	110.2(3)	C(24)	C(27)	C(29)	112.9(3)
C(28)	C(27)	C(29)	108.7(3)	C(24)	C(27)	C(30)	107.1(3)
C(28)	C(27)	C(30)	107.9(3)	C(29)	C(27)	C(30)	110.0(3)
O(4)	C(31)	C(32)	118.3(3)	O(4)	C(31)	C(36)	122.2(3)
C(32)	C(31)	C(36)	119.5(3)	S(4)	C(32)	C(31)	119.0(3)
S(4)	C(32)	C(33)	121.3(3)	C(31)	C(32)	C(33)	119.7(3)
C(32)	C(33)	C(34)	122.5(3)	C(33)	C(34)	C(35)	117.0(3)
C(33)	C(34)	C(37)	119.8(3)	C(35)	C(34)	C(37)	123.1(3)
C(34)	C(35)	C(36)	121.8(3)	S(5)	C(36)	C(31)	118.4(3)
S(5)	C(36)	C(35)	121.9(3)	C(31)	C(36)	C(35)	119.5(3)
C(34)	C(37)	C(38)	110.6(3)	C(34)	C(37)	C(39)	111.7(3)
C(38)	C(37)	C(39)	107.7(3)	C(34)	C(37)	C(40)	107.7(3)
C(38)	C(37)	C(40)	110.6(4)	C(39)	C(37)	C(40)	108.5(4)
O(5)	C(41)	C(42)	119.0(3)	O(5)	C(41)	C(46)	122.2(3)
C(42)	C(41)	C(46)	118.8(3)	S(5)	C(42)	C(41)	123.0(3)
S(5)	C(42)	C(43)	116.7(3)	C(41)	C(42)	C(43)	120.1(3)

Table V Intermolecular bond angles of TC6A with benzyl alcohol (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(42)	C(43)	C(44)	121.8(3)	C(43)	C(44)	C(45)	117.4(3)
C(43)	C(44)	C(47)	119.9(3)	C(45)	C(44)	C(47)	122.7(3)
C(44)	C(45)	C(46)	121.7(3)	S(6)	C(46)	C(41)	118.2(3)
S(6)	C(46)	C(45)	121.5(3)	C(41)	C(46)	C(45)	120.2(3)
C(44)	C(47)	C(48)	109.1(3)	C(44)	C(47)	C(49)	112.5(3)
C(48)	C(47)	C(49)	108.4(3)	C(44)	C(47)	C(50)	109.6(3)
C(48)	C(47)	C(50)	108.5(3)	C(49)	C(47)	C(50)	108.6(3)
O(6)	C(51)	C(52)	124.1(3)	O(6)	C(51)	C(56)	117.7(3)
C(52)	C(51)	C(56)	118.1(3)	S(6)	C(52)	C(51)	119.2(3)
S(6)	C(52)	C(53)	120.5(3)	C(51)	C(52)	C(53)	120.3(3)
C(52)	C(53)	C(54)	122.1(3)	C(53)	C(54)	C(55)	116.6(3)
C(53)	C(54)	C(60)	121.3(3)	C(55)	C(54)	C(60)	122.0(3)
C(54)	C(55)	C(56)	122.7(3)	S(1)	C(56)	C(51)	120.8(3)
S(1)	C(56)	C(55)	119.0(3)	C(51)	C(56)	C(55)	119.9(3)
C(54)	C(60)	C(57)	108.6(3)	C(54)	C(60)	C(58)	111.2(3)
C(57)	C(60)	C(58)	108.9(3)	C(54)	C(60)	C(59)	111.6(3)
C(57)	C(60)	C(59)	108.0(3)	C(58)	C(60)	C(59)	108.5(3)
C(62)	C(61)	C(66)	119.9(4)	C(61)	C(62)	C(63)	119.7(4)
C(62)	C(63)	C(64)	121.6(4)	C(63)	C(64)	C(65)	117.9(4)
C(63)	C(64)	C(67)	121.3(4)	C(65)	C(64)	C(67)	120.8(3)
C(64)	C(65)	C(66)	120.5(4)	C(61)	C(66)	C(65)	120.4(4)
O(7)	C(67)	C(64)	111.1(3)				

Table VI Intermolecular dihedral angles of TC6A with benzyl alcohol (°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(56)	S(1)	C(2)	C(1)	-105.9(6)	C(56)	S(1)	C(2)	C(3)	83.3(6)
C(2)	S(1)	C(56)	C(51)	69.7(7)	C(2)	S(1)	C(56)	C(55)	-117.2(6)
C(12)	S(2)	C(6)	C(1)	103.1(6)	C(12)	S(2)	C(6)	C(5)	-81.1(6)
C(6)	S(2)	C(12)	C(11)	-80.2(6)	C(6)	S(2)	C(12)	C(13)	100.2(6)
C(22)	S(3)	C(16)	C(11)	-81.9(6)	C(22)	S(3)	C(16)	C(15)	102.3(6)
C(16)	S(3)	C(22)	C(21)	163.1(5)	C(16)	S(3)	C(22)	C(23)	-21.0(7)
C(32)	S(4)	C(26)	C(21)	-67.4(6)	C(32)	S(4)	C(26)	C(25)	114.8(6)
C(26)	S(4)	C(32)	C(31)	109.8(6)	C(26)	S(4)	C(32)	C(33)	-73.9(7)
C(42)	S(5)	C(36)	C(31)	-107.3(6)	C(42)	S(5)	C(36)	C(35)	78.4(6)
C(36)	S(5)	C(42)	C(41)	61.3(7)	C(36)	S(5)	C(42)	C(43)	-123.5(5)
C(52)	S(6)	C(46)	C(41)	-152.5(5)	C(52)	S(6)	C(46)	C(45)	30.9(7)
C(46)	S(6)	C(52)	C(51)	88.5(6)	C(46)	S(6)	C(52)	C(53)	-91.5(6)
O(1)	C(1)	C(2)	S(1)	9.6(6)	O(1)	C(1)	C(2)	C(3)	-179.4(4)
C(6)	C(1)	C(2)	S(1)	-169.5(4)	C(6)	C(1)	C(2)	C(3)	1.4(8)
O(1)	C(1)	C(6)	S(2)	-3.9(6)	O(1)	C(1)	C(6)	C(5)	-179.7(4)
C(2)	C(1)	C(6)	S(2)	175.3(4)	C(2)	C(1)	C(6)	C(5)	-0.5(8)
S(1)	C(2)	C(3)	C(4)	169.7(4)	C(1)	C(2)	C(3)	C(4)	-1.1(8)
C(2)	C(3)	C(4)	C(5)	-0.2(8)	C(2)	C(3)	C(4)	C(7)	-175.8(5)
C(3)	C(4)	C(5)	C(6)	1.1(8)	C(7)	C(4)	C(5)	C(6)	176.9(5)
C(3)	C(4)	C(7)	C(8)	-120.2(7)	C(3)	C(4)	C(7)	C(9)	-2.1(9)
C(3)	C(4)	C(7)	C(10)	120.7(6)	C(5)	C(4)	C(7)	C(8)	64.3(8)
C(5)	C(4)	C(7)	C(9)	-177.6(6)	C(5)	C(4)	C(7)	C(10)	-54.8(7)
C(4)	C(5)	C(6)	S(2)	-176.6(4)	C(4)	C(5)	C(6)	C(1)	-0.8(8)
O(2)	C(11)	C(12)	S(2)	0.0(6)	O(2)	C(11)	C(12)	C(13)	179.6(4)
C(16)	C(11)	C(12)	S(2)	179.3(4)	C(16)	C(11)	C(12)	C(13)	-1.1(8)
O(2)	C(11)	C(16)	S(3)	3.6(6)	O(2)	C(11)	C(16)	C(15)	179.5(4)
C(12)	C(11)	C(16)	S(3)	-175.7(4)	C(12)	C(11)	C(16)	C(15)	0.2(8)
S(2)	C(12)	C(13)	C(14)	179.8(4)	C(11)	C(12)	C(13)	C(14)	0.2(8)
C(12)	C(13)	C(14)	C(15)	1.5(8)	C(12)	C(13)	C(14)	C(17)	-178.2(5)
C(13)	C(14)	C(15)	C(16)	-2.5(8)	C(17)	C(14)	C(15)	C(16)	177.3(5)
C(13)	C(14)	C(17)	C(18)	115.3(6)	C(13)	C(14)	C(17)	C(19)	-125.0(6)
C(13)	C(14)	C(17)	C(20)	-2.9(8)	C(15)	C(14)	C(17)	C(18)	-64.3(7)
C(15)	C(14)	C(17)	C(19)	55.4(7)	C(15)	C(14)	C(17)	C(20)	177.5(5)
C(14)	C(15)	C(16)	S(3)	177.5(4)	C(14)	C(15)	C(16)	C(11)	1.7(8)
O(3)	C(21)	C(22)	S(3)	-2.1(6)	O(3)	C(21)	C(22)	C(23)	-178.1(4)
C(26)	C(21)	C(22)	S(3)	179.1(4)	C(26)	C(21)	C(22)	C(23)	3.1(7)
O(3)	C(21)	C(26)	S(4)	0.9(6)	O(3)	C(21)	C(26)	C(25)	178.7(4)
C(22)	C(21)	C(26)	S(4)	179.6(4)	C(22)	C(21)	C(26)	C(25)	-2.6(7)
S(3)	C(22)	C(23)	C(24)	-177.0(3)	C(21)	C(22)	C(23)	C(24)	-1.3(8)
C(22)	C(23)	C(24)	C(25)	-1.1(7)	C(22)	C(23)	C(24)	C(27)	176.5(5)
C(23)	C(24)	C(25)	C(26)	1.6(8)	C(27)	C(24)	C(25)	C(26)	-176.1(5)
C(23)	C(24)	C(27)	C(28)	129.1(6)	C(23)	C(24)	C(27)	C(29)	7.4(8)
C(23)	C(24)	C(27)	C(30)	-113.8(6)	C(25)	C(24)	C(27)	C(28)	-53.3(7)
C(25)	C(24)	C(27)	C(29)	-175.0(5)	C(25)	C(24)	C(27)	C(30)	63.8(7)
C(24)	C(25)	C(26)	S(4)	178.0(4)	C(24)	C(25)	C(26)	C(21)	0.2(8)
O(4)	C(31)	C(32)	S(4)	-6.0(6)	O(4)	C(31)	C(32)	C(33)	177.6(4)

Table VI Intermolecular dihedral angles of TC6A with benzyl alcohol (°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(36)	C(31)	C(32)	S(4)	173.6(4)	C(36)	C(31)	C(32)	C(33)	-2.7(8)
O(4)	C(31)	C(36)	S(5)	7.6(6)	O(4)	C(31)	C(36)	C(35)	-178.0(4)
C(32)	C(31)	C(36)	S(5)	-172.1(4)	C(32)	C(31)	C(36)	C(35)	2.4(8)
S(4)	C(32)	C(33)	C(34)	-175.1(4)	C(31)	C(32)	C(33)	C(34)	1.2(8)
C(32)	C(33)	C(34)	C(35)	0.7(8)	C(32)	C(33)	C(34)	C(37)	177.5(5)
C(33)	C(34)	C(35)	C(36)	-1.1(8)	C(37)	C(34)	C(35)	C(36)	-177.8(5)
C(33)	C(34)	C(37)	C(38)	53.8(7)	C(33)	C(34)	C(37)	C(39)	173.7(5)
C(33)	C(34)	C(37)	C(40)	-67.2(7)	C(35)	C(34)	C(37)	C(38)	-129.6(6)
C(35)	C(34)	C(37)	C(39)	-9.6(8)	C(35)	C(34)	C(37)	C(40)	109.4(7)
C(34)	C(35)	C(36)	S(5)	173.8(4)	C(34)	C(35)	C(36)	C(31)	-0.5(8)
O(5)	C(41)	C(42)	S(5)	-4.0(6)	O(5)	C(41)	C(42)	C(43)	-179.0(4)
C(46)	C(41)	C(42)	S(5)	174.6(4)	C(46)	C(41)	C(42)	C(43)	-0.5(8)
O(5)	C(41)	C(46)	S(6)	2.7(6)	O(5)	C(41)	C(46)	C(45)	179.4(4)
C(42)	C(41)	C(46)	S(6)	-175.8(4)	C(42)	C(41)	C(46)	C(45)	0.8(8)
S(5)	C(42)	C(43)	C(44)	-175.3(4)	C(41)	C(42)	C(43)	C(44)	0.1(8)
C(42)	C(43)	C(44)	C(45)	-0.1(8)	C(42)	C(43)	C(44)	C(47)	179.0(5)
C(43)	C(44)	C(45)	C(46)	0.5(8)	C(47)	C(44)	C(45)	C(46)	-178.6(5)
C(43)	C(44)	C(47)	C(48)	64.7(7)	C(43)	C(44)	C(47)	C(49)	-174.9(5)
C(43)	C(44)	C(47)	C(50)	-54.0(7)	C(45)	C(44)	C(47)	C(48)	-116.2(6)
C(45)	C(44)	C(47)	C(49)	4.2(8)	C(45)	C(44)	C(47)	C(50)	125.1(6)
C(44)	C(45)	C(46)	S(6)	175.6(4)	C(44)	C(45)	C(46)	C(41)	-0.9(8)
O(6)	C(51)	C(52)	S(6)	-3.1(6)	O(6)	C(51)	C(52)	C(53)	176.8(4)
C(56)	C(51)	C(52)	S(6)	176.8(4)	C(56)	C(51)	C(52)	C(53)	-3.2(7)
O(6)	C(51)	C(56)	S(1)	-3.3(6)	O(6)	C(51)	C(56)	C(55)	-176.4(4)
C(52)	C(51)	C(56)	S(1)	176.7(4)	C(52)	C(51)	C(56)	C(55)	3.7(7)
S(6)	C(52)	C(53)	C(54)	178.8(3)	C(51)	C(52)	C(53)	C(54)	-1.1(8)
C(52)	C(53)	C(54)	C(55)	4.9(8)	C(52)	C(53)	C(54)	C(60)	-171.2(5)
C(53)	C(54)	C(55)	C(56)	-4.5(8)	C(60)	C(54)	C(55)	C(56)	171.6(5)
C(53)	C(54)	C(60)	C(57)	73.7(7)	C(53)	C(54)	C(60)	C(58)	-46.1(7)
C(53)	C(54)	C(60)	C(59)	-167.4(5)	C(55)	C(54)	C(60)	C(57)	-102.2(6)
C(55)	C(54)	C(60)	C(58)	138.0(6)	C(55)	C(54)	C(60)	C(59)	16.7(8)
C(54)	C(55)	C(56)	S(1)	-173.0(4)	C(54)	C(55)	C(56)	C(51)	0.2(8)
C(66)	C(61)	C(62)	C(63)	0.7(9)	C(62)	C(61)	C(66)	C(65)	-1.1(9)
C(61)	C(62)	C(63)	C(64)	-0.3(9)	C(62)	C(63)	C(64)	C(65)	0.1(9)
C(62)	C(63)	C(64)	C(67)	178.3(5)	C(63)	C(64)	C(65)	C(66)	-0.5(8)
C(67)	C(64)	C(65)	C(66)	-178.7(5)	C(63)	C(64)	C(67)	O(7)	-103.8(6)
C(65)	C(64)	C(67)	O(7)	74.4(7)	C(64)	C(65)	C(66)	C(61)	0.9(9)

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