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Polystyrene-Bound Tetrafluorophenylbis(triflyl)methane as an Organic Solvent-Swellable and Strong Brønsted Acid Catalyst

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General. Unless otherwise noted, ^{1}H, ^{13}C, and ^{19}F NMR spectra are referenced against internal tetramethylsilane ($\delta = 0$), $CDCl_3$ ($\delta = 77.0$), and $CF_3C_6H_5$ ($\delta = -64.0$), respectively. High-resolution mass (HRMS) analyses were carried out at Daikin Industries, Ltd.

Pentafluorophenylmethyl Triflone (5) (Scheme 1). A solution of 2,3,4,5,6-pentafluorobenzyl bromide (**4**) (2.6 g, 10 mmol) and sodium triflinate (2.0 g, 13 mmol) in propionitrile (30 mL) was heated at reflux in the presence of tetrabutylammonium iodide (0.37 g, 1 mmol) as catalyst. Monitoring the disappearance of the starting halide by TLC (ca. 1 day), the mixture was cooled, the salts were filtered and the solvent was evaporated under reduced pressure. The residue was purified by column chromatography using a linear EtOAc gradient in hexane to give **5** as a solid (2.9 g, 91% yield): IR (KBr) 1509, 1374, 1210, 1121, 995 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 4.64; ^{13}C NMR ($CDCl_3$, 125 MHz) δ 44.3, 100.0 (dt, J_{CF}=4, 17 Hz, 1C, *ipso*-C), 119.5 (q, J_{CF}=326 Hz, 1C, CF_3), 137.9 (d, J_{CF}=251 Hz, 2C, 2*m*-C), 142.8 (d, J_{CF}=258 Hz, 1C, *p*-C), 145.9 (d, J_{CF}=252 Hz, 2C, 2*o*-C); ^{19}F NMR ($CDCl_3$, 282 MHz) δ –160.0 (d, J=15.2 Hz, 2F, 2*m*-F), 149.0 (s, 1F, *p*-F), 139.4 (d, J=15.2 Hz, 2F, 2*o*-F), –78.3 (s, 3F, CF_3). Anal. Calcd for $C_8H_2O_2F_8S$: C, 30.59; H, 0.64; F, 48.38; S, 10.21. Found C, 30.49; H, 0.73; F, 48.37; S, 10.18.

Pentafluorophenylbis(triflyl)methane (2) (Scheme 1). To a solution of **5** (157 mg, 0.5 mmol) in dry Et_2O (3 mL) was added *t*-BuLi (0.34 mL, 0.5 mmol, 1.6 M solution in pentane) dropwise at –78 °C, and the resulting mixture was stirred for 10 min. Triflic anhydride (42 μL, 0.25 mmol) was then added, and the resulting mixture was allowed to warm to room temperature over a period of 1 h, before the reaction was quenched with water. The resultant mixture was neutralized and washed with hexane. The aqueous phase was acidified with 4 M aqueous HCl and extracted with ether twice. The organic layers were dried over magnesium sulfate, filtrated and concentrated under reduced pressure to give **2** as a solid. Further purification was not required: Mp. 86~87 °C; IR (KBr) 1522, 1501, 1347, 1321, 1198, 1127, 1024, 988, 613 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 6.21 (brs, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 70.4, 98.0 (s, 1C, *ipso*-C), 119.2 (q, J_{CF}=330 Hz, 2C, $2CF_3$), 137.8 (d, J_{CF}=258 Hz, 1C, *m*-C), 138.6 (d, J_{CF}=257 Hz, 1C, *m*-C), 144.7 (d, J_{CF}=264 Hz, 1C, *p*-C), 145.4 (d, J_{CF}=262 Hz, 1C *o*-C), 147.2 (d, J_{CF}=262 Hz, 1C, *o*-C); ^{13}C NMR (CD_3OD (δ 49.0), 125 MHz) δ 56.2, 109.1 (dt, *J*=6, 19 Hz, 1C, *ipso*-C), 122.4 (q, J_{CF}=324 Hz, 2C, $2CF_3$), 138.5 (d, J_{CF}=250 Hz, 2C, 2*m*-C), 143.0 (d, J_{CF}=251 Hz, 1C, *p*-C), 150.0 (d, J_{CF}=245 Hz, 1C, *o*-C), ^{19}F NMR ($CDCl_3$, 282 MHz) δ –157.9 (dt, *J*=6.2, 21.5 Hz, 1F, *m*-F), –156.8 (dt, *J*=6.2, 21.5 Hz, 1F, *m*-F), –142.6 (tt, *J*=5.9, 21.5 Hz, 1F, *p*-F), –140.3 (br, 1F, *o*-F), –127.7 (ddd, *J*=5.9, 15.2, 21.5 Hz, 1F, *o*-F), –75.2 (s, 6F, $2CF_3$); HRMS (EI) calcd for $C_9HO_4F_{11}S_2$ $[M]^+$ 445.9141, found 445.9137.

Preparation of Lithium Pentafluorophenylbis(triflyl)methide. To a solution of **2** (1.36 g, 3.05 mmol) in diethyl ether (20 mL) was neutralized by addition of lithium hydroxide monohydrate (0.13 g, 3.05 mmol). Diethyl ether was evaporated under reduced pressure and the residual salt was dried at 80 °C under vacuum (ca. 1 torr) for 12 h (quantitative yield). ^{13}C NMR (CD_3OD, 125 MHz) δ 56.1, 109.0 (dt, *J*=4, 19 Hz, 1C, *ipso*-C), 122.3 (q, J_{CF}=324 Hz, 2C, $2CF_3$), 138.5 (d, J_{CF}=247 Hz, 2C, 2*m*-C), 143.0

(d, J_{CF}=251 Hz, 1C, *p*-C), 149.5 (d, J_{CF}=245 Hz, 2C, 2*o*-C).

General Procedure for the Preparation of 4-Alkyl-2,3,5,6-tetrafluorophenylbis(triflyl)methanes (6) (Table 1). To a solution of **2** (0.22 g, 0.5 mmol) in Et_2O (3 mL) was added a solution of alkyllithium [*t*-BuLi (1.5 mmol), BuLi (1.5 mmol), and PhLi (1.5 mmol)] at –78 °C, and the mixture was stirred under the following conditions: *t*-BuLi (–78 °C, 1 h), BuLi (–78 °C, 1 h), and PhLi (–78 °C to rt, 1 day) before the reaction was quenched with water. The resultant mixture was neutralized with 1 M aqueous HCl and washed with hexane. The aqueous phase was acidified with 4 M aqueous HCl and extracted with ether twice. The organic layers were dried over magnesium sulfate, filtrated and concentrated under reduced pressure to give **6** as a light brown solid.

4-*tert*-Butyl-2,3,5,6-tetrafluorophenylbis(triflyl)methane (6a): IR ($CHCl_3$) 3021, 1480, 1456, 1408, 1117, 967, 669 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 1.54 (s, 9H), 6.24 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 30.4 (3C), 37.9, 70.8, 99.3 (t, J_{CF}=16 Hz, 1C), 119.2 (q, J_{CF}=328 Hz, 2C, $2CF_3$), 134.2 (t, *J*=13 Hz, 1C), 145.2 (d, J_{CF}=251 Hz, 1C, *m*-C), 145.6 (d, J_{CF}=250 Hz, 1C, *o*-C), 146.4 (d, J_{CF}=251 Hz, 1C, *o*-C), 147.0 (d, J_{CF}=258 Hz, 1C, *m*-C); ^{19}F NMR ($CDCl_3$, 282 MHz) δ –142.8 (m, 1F), –135.1 (dd, *J*=10.6, 18.3 Hz, 1F, *m*-F), –133.9 (dd, *J*=10.6, 18.3 Hz, 1F, *m*-F), –130.3 (m, *J*=9.0, 21.4 Hz, 1F, *o*-F), –75.4 (s, 6F, $2CF_3$); HRMS (EI) calcd for $C_{13}H_{10}O_4F_{10}S_2$ $[M]^+$ 483.9861, found 483.9852.

4-Butyl-2,3,5,6-tetrafluorophenylbis(triflyl)methane (6b): IR ($CHCl_3$) 3021, 1497, 1483, 1410, 1117, 669 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 0.97 (t, *J*=7.6 Hz, 3H), 1.40 (sestet, *J*=7.6 Hz, 2H), 1.64 (quintet, *J*=7.6 Hz, 2H), 2.83 (t, *J*=7.6 Hz, 2H), 6.25 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 13.6, 22.4, 23.3, 30.9, 70.9, 99.2 (t, *J*=16

Hz, 1C), 128.2 (t, J=18 Hz, 1C), 144.4 (d, J_{CF}=251 Hz, 1C), 144.8 (d, J_{CF}=250 Hz, 1C), 145.6 (d, J_{CF}=250 Hz, 1C), 146.3 (d, J_{CF}=258 Hz, 1C); ^{19}F NMR ($CDCl_3$, 282 MHz) δ –142.8 (br, 1F, *o*-F), –141.6 (dd, J=12.3, 21.4 Hz, 1F, *m*-F), –140.4 (dd, J=12.3, 21.4 Hz, 1F, *m*-F), –130.6~–130.4 (m, 1F, *o*-F), –75.4 (s, 6F, $2CF_3$); HRMS (EI) calcd for $C_{13}H_{10}O_4F_{10}S_2$ $[M]^+$ 483.9861, found 483.9873.

4-Phenyl-2,3,5,6-tetrafluorophenylbis(triflyl)methane (6c): IR (KBr) 1487, 1441, 1410, 1395, 1225, 1186, 1117, 1107, 974 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 6.31 (s, 1H), 7.46–7.60 (m, 5H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 70.9, 100.6 (t, J_{CF}=16 Hz, 1C), 119.3 (q, J_{CF}=328 Hz, 2C, $2CF_3$), 125.7, 126.8 (t, J=16 Hz, 1C), 128.9 (2C), 130.0 (2C), 130.3, 139.3 (d, J_{CF}=255 Hz, 1C), 144.5 (d, J_{CF}=245 Hz, 1C), 145.0 (d, J_{CF}=252 Hz, 1C), 146.7 (d, J_{CF}=256 Hz, 1C); ^{19}F NMR ($CDCl_3$, 282 MHz) δ –145.0 (m, 1F, *o*-F), –140.7 (dd, J=12.1, 21.4 Hz, 1F, *m*-F), –139.5 (dd, J=12.1, 21.4 Hz, 1F, *m*-F), –129.6~–129.4 (m, 1F, *o*-F), –75.3 (s, 6F, $2CF_3$); HRMS (EI) calcd for $C_{15}H_6O_4F_{10}S_2$ $[M]^+$ 503.9548, found 503.9560.

Polystyrene-bound tetrafluorophenylbis(triflyl)methane (3): IR (KBr) 1491, 1410, 1350, 1318, 1194, 1111, 1021, 974, 758, 696 cm^{-1}. [*cf.* Polystyrene bead: IR (KBr) 1493, 1451, 750, 692 cm^{-1}.]

Synthesis of Polystyrene-bound 2,3,5,6-tetrafluorophenylbis(triflyl)methane (3) (Eq. 1). To a mixture of poly(4-bromostyrene) [0.37 g, 1 mmol, 2.71 mmol Br/g resin, 2% divinylbenzne (DVB) cross-linked, 200-400 mesh] and benzene (5 mL) was added 1.6 M solution of BuLi in hexanes (1.9 mL, 3.0 mmol) at room temperature. The reaction mixture was stirred at 60 °C for 3 h. After cooling to ambient temperature, the solvents including excess BuLi were removed by decantation. To the residual lithiated resin was added benzene (1 mL), THF (1 mL), and lithium

pentafluorophenylbis(triflyl)methide (1.36 g, 3 mmol) at 0 °C. The reaction mixture was stirred at room temperature for 0.5 h and further at 70 °C for 6 h. After cooling to ambient temperature, water (0.5 mL) and 4 M HCl (0.5 mL) were added to the reaction mixture at 0 °C in this order. Resin **3** was filtered, washed with water (5 mL), a 50% aqueous solution of THF (5 mL), THF (5 mL), and Et_2O (5 mL) in this order, and dried at 80 °C under vacuum (ca. 1 torr) for 12 h. Thus, 0.46 g of **3** was obtained. Loading of **2** onto resin **3** was estimated to be 1.01 mmol $Tf_2CHC_6F_4$-unit/g resin, based on fluorine content as determined by elemental analysis.

General Procedure for the Acylation of *l*-Menthol with Carboxylic Anhydride (Table 3). The mixture of *l*-menthol (0.47 g, 3 mmol) and acetic anhydride (0.42 mL, 4.5 mmol) or benzoic anhydride (1.02 g, 4.5 mmol) in acetonitrile (7 mL) was stirred at 27 °C in the presence of Brønsted acid catalyst. After being stirred at 27 °C for the times indicated in Table 3, resin **3** was filtered, washed with 4 M HCl (5 mL), water (5 mL), a 50% aqueous solution of THF (5 mL), THF (5 mL), and Et_2O (5 mL) in this order, and dried at 80 °C under vacuum (ca. 1 torr) for 12 h to reuse. The filtrate was extracted with hexane twice, and the organic layers were dried over magnesium sulfate, filtered, and concentatrated under reduced pressure. The crude oil was purified by column chromatography on silica gel (hexane-EtOAc) to afford the corresponding ester.

The Esterification of 4-Phenylbutyric Acid with Methanol (Eq. 2): Solid catalyst **3** (20 mg, 1.01 mmol $Tf_2CHC_6F_4$-unit/g resin) or Nafion® SAC-13 (20 mg) was swollen by methanol (2 mL) at 27 °C for 0.5 h. Hydrocinnamic acid (0.28 g, 2 mmol) was added to the mixture at 27 °C. After being stirred at 27 °C for 29 h, resin **3** was filtered, washed with 4 M HCl (5 mL), water (5 mL), a 50% aqueous solution of THF (5 mL), THF (5 mL), and Et_2O (5 mL) in this order, and dried at 80 °C under vacuum (ca. 1 torr) for 12 h to reuse. The filtrate was concentatrated *in vacuo*. The crude oil was

purified by colum chromatography on silica gel (hexane-EtOAc=8:1) to afford the corresponding ester.

The Friedel–Crafts Acylation Reaction of Anisole with Acetic Anhydride (Eq. 3): Solid catalyst **3** (30 mg, 1.01 mmol $Tf_2CHC_6F_4$-unit/g resin) was swollen by nitromethane (1 mL) at room temperature for 0.5 h. After heating to 50 °C, anisole (0.11 mL, 1 mmol) and acetic anhydride (0.11 mL, 1.2 mmol) were added to the mixture. After being stirred at the same temperature for 2 h, resin **3** was filtered, washed with 4 M HCl (5 mL), water (5 mL), a 50% aqueous solution of THF (5 mL), THF (5 mL), and Et_2O (5 mL) in this order, and dried at 80 °C under vacuum (ca. 1 torr) for 12 h to reuse. The filtrate was concentatrated *in vacuo*. The crude oil was purified by colum chromatography on silica gel (hexane-EtOAc=10:1) to afford 4-acetylanisole in quantitative yield.

The Acetalization Reaction of Benzylacetone with Trimethyl Orthoformate (Eq. 4 and Table 5): Solid catalyst **3** (10 mg, 1.01 mmol $Tf_2CHC_6F_4$-unit/g resin) was swollen by toluene (2 mL) at room temperature for 0.5 h. After cooling to 0 °C, benzylacetone (1.5 mL, 10 mmol) and trimethylorthoformate (1.3 mL, 12 mmol) were added to the mixture. After being stirred at the same temperature for 1~2 h, the solution was decanted and the residual catalyst **3** was reused without drying. The conversion of benzylacetone to the corresponding acetal was determined by ^{1}H NMR analysis of the crude products.

The Mukaiyama Aldol Reaction of Benzaldehyde with Trimethylsilyl Enol Ether Derived from Acetophenone (Eq. 5). Solid catalyst **3** (15 mg, 1.01 mmol $Tf_2CHC_6F_4$-unit/g resin) or Nafion® SAC-13 (15 mg) was swollen by toluene (1 mL) at room temperature for 0.5 h. To the mixture were added benzaldehyde (50 μL, 0.5

mmol) and 1-phenyl-1-(trimethylsiloxy)ethylene (0.12 mL, 0.6 mmol) at –78 °C. After being stirred at –78 °C for 7 h, the reaction was quenched with a few drops of triethylamine and then the mixture was allowed to warm to ambient temperature. Resin **3** was filtered, washed with 4 M HCl (5 mL), water (5 mL), a 50% aqueous solution of THF (5 mL), THF (5 mL), and Et_2O (5 mL) in this order, and dried at 80 °C under vacuum (ca. 1 torr) for 12 h to reuse. To hydrolyze the trimethylsilyl ether produced, 1 M HCl (1 mL) and THF (1 mL) were added to the filtrate. After being stirred at room temperature for 15 min, the mixture was neutralized with saturated $NaHCO_3$ aqueous solution. The mixture was extracted with ethyl acetate twice, and the organic layers were dried over sodium sulfate, filtered, and concentrated *in vacuo*. The crude oil was purified by colum chromatography on silica gel (hexane-EtOAc=8:1 to 4:1) to afford the corresponding aldol.

The Sakurai-Hosomi Allylation Reaction of Benzaldehyde with Allyltrimethylsilane (Eq. 6): The mixture of solid catalyst **3** (60 mg, 1.01 mmol $Tf_2CHC_6F_4$-unit/g resin) or Nafion® SAC-13 (60 mg) and allyltrimethylsilane (0.48 mL, 3 mmol) were stirred in dichloromethane (0.42 mL) at room temperature for 0.5 h. After cooling to –40 °C, 1 M solution of benzaldehyde (2 mL, 2 mmol) in dichloromethane was added dropwise over 0.5 h, and the reaction mixture was further stirrred at the same temperature for 1 h. The reaction was quenched with a few drops of triethylamine and then the mixture was allowed to warm to ambient temperature. Resin **3** was filtered, washed with 4 M HCl (5 mL), water (5 mL), a 50% aqueous solution of THF (5 mL), THF (5 mL), and Et_2O (5 mL) in this order, and dried at 80 °C under vacuum (ca. 1 torr) for 12 h to reuse. To hydrolyze the trimethylsilyl ether produced, 1 M HCl (1 mL) and THF (1 mL) were added to the filtrate. After being stirred at room temperature for 30 min, the mixture was neutralized with saturated $NaHCO_3$ aqueous solution. The mixture was extracted with diethyl ether twice, and the organic layers

were dried over sodium sulfate, filtered, and concentatrated *in vacuo*. The crude oil was purified by colum chromatography on silica gel (hexane-EtOAc=20:1 to 5:1) to afford the corresponding homoallylic alcohol.

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4/7=1/1;
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 F                 -0.42004   3.12954  -0.88737
 F                  1.3601    3.19632  -2.26619
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 O                 -0.45536   1.77409   1.88864
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 F                 -2.58542  -4.0917    0.01872
 C                 -0.1891   -4.29819   0.0086
 F                 -0.28887  -5.65636   0.00901
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 F                  2.20299  -4.44327   0.02064
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 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
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  2   2 O     0   2.087305          0.516513          -1.742452
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4	4	C	0	0.193081	2.520344	-1.964854
5	5	F	0	-0.655060	2.565630	-3.055229
6	6	F	0	-0.420041	3.129543	-0.887369
7	7	F	0	1.360102	3.196315	-2.266185
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10	10	O	0	0.448912	-0.223136	2.672220
11	11	O	0	-0.455361	1.774093	1.888643
12	12	C	0	2.238253	1.651085	1.754461
13	13	F	0	3.288846	0.776385	1.556468
14	14	F	0	2.333138	2.692905	0.852097
15	15	F	0	2.293945	2.151652	3.041320
16	16	C	0	0.000000	-1.500670	0.000000
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18	18	F	0	-2.329308	-1.279092	0.028623
19	19	C	0	-1.353416	-3.514025	0.010919
20	20	F	0	-2.585424	-4.091700	0.018721
21	21	C	0	-0.189102	-4.298187	0.008598
22	22	F	0	-0.288871	-5.656357	0.009011
23	23	C	0	1.074192	-3.682968	0.012340
24	24	F	0	2.202990	-4.443275	0.020635
25	25	C	0	1.164086	-2.277062	0.011519
26	26	F	0	2.361338	-1.652330	0.041132
27	27	Li	0	-1.909950	0.611976	0.130056

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.577039	0.781298	-1.542300
2	8	0	2.087305	0.516513	-1.742452
3	8	0	0.010048	-0.085025	-2.692938
4	6	0	0.193081	2.520344	-1.964854
5	9	0	-0.655060	2.565630	-3.055229
6	9	0	-0.420041	3.129543	-0.887369
7	9	0	1.360102	3.196315	-2.266185
8	6	0	0.000000	0.000000	0.000000
9	16	0	0.658332	0.770161	1.504470
10	8	0	0.448912	-0.223136	2.672220
11	8	0	-0.455361	1.774093	1.888643
12	6	0	2.238253	1.651085	1.754461
13	9	0	3.288846	0.776385	1.556468
14	9	0	2.333138	2.692905	0.852097
15	9	0	2.293945	2.151652	3.041320
16	6	0	0.000000	-1.500670	0.000000
17	6	0	-1.243474	-2.112853	0.009083
18	9	0	-2.329308	-1.279092	0.028623
19	6	0	-1.353416	-3.514025	0.010919
20	9	0	-2.585424	-4.091700	0.018721
21	6	0	-0.189102	-4.298187	0.008598
22	9	0	-0.288871	-5.656357	0.009011
23	6	0	1.074192	-3.682968	0.012340
24	9	0	2.202990	-4.443275	0.020635
25	6	0	1.164086	-2.277062	0.011519
26	9	0	2.361338	-1.652330	0.041132
27	3	0	-1.909950	0.611976	0.130056

Distance matrix (angstroms):

		1	2	3	4	5
1	S	0.000000				
2	O	1.546310	0.000000			
3	O	1.547890	2.362259	0.000000		
4	C	1.830371	2.766385	2.711375	0.000000	
5	F	2.644024	3.666446	2.756736	1.382140	0.000000
6	F	2.633886	3.721005	3.711941	1.381309	2.252299
7	F	2.639982	2.825679	3.573787	1.381910	2.254159

8	C	1.822660	2.767628	2.694299	3.201572	4.043017
9	S	3.047875	3.556516	4.332418	3.913542	5.073417
10	O	4.334453	4.766628	5.384849	5.393940	6.465264
11	O	3.717911	4.607766	4.966267	3.978292	5.010816
12	C	3.792729	3.679462	5.268618	4.332626	5.686895
13	F	4.117801	3.520527	5.435991	5.002486	6.326416
14	F	3.531467	3.395409	5.067634	3.541869	4.920643
15	F	5.082835	5.059729	6.565107	5.441630	6.784977
16	C	2.814079	3.385559	3.042378	4.479563	5.128189
17	C	3.754619	4.590809	3.603376	5.237044	5.623561
18	F	3.893566	5.085998	3.782232	4.977159	5.205299
19	C	4.958724	5.581945	4.574704	6.535208	6.844791
20	F	6.015319	6.794980	5.490265	7.441356	7.582580
21	C	5.365950	5.606206	5.008861	7.108653	7.531012
22	F	6.678306	6.842380	6.199163	8.425370	8.782069
23	C	4.753287	4.662760	4.625595	6.570139	7.172536
24	F	5.690575	5.265107	5.582725	7.514911	8.170321
25	C	3.480308	3.425319	3.667549	5.278637	6.013809
26	F	3.407862	2.821373	3.931940	5.112390	6.039644
27	Li	3.001759	4.415138	3.484465	3.528917	3.941770

		6	7	8	9	10
6	F	0.000000				
7	F	2.252665	0.000000			
8	C	3.279923	4.147518	0.000000		
9	S	3.528522	4.538341	1.813830	0.000000	
10	O	4.966509	6.075422	2.718836	1.547299	0.000000
11	O	3.089455	4.751970	2.630918	1.547831	2.328224
12	C	4.028850	4.395962	3.288463	1.826109	2.748950
13	F	5.026483	4.918210	3.720467	2.631035	3.210790
14	F	3.285786	3.305133	3.663515	2.632016	3.920006
15	F	4.874073	5.489353	4.375091	2.635461	3.029851
16	C	4.733152	5.389540	1.500670	2.802410	2.995726
17	C	5.381857	6.335828	2.451624	3.763618	3.677975
18	F	4.890849	6.237560	2.657550	3.911976	3.977707
19	C	6.768686	7.587954	3.765664	4.963071	4.600093
20	F	7.593170	8.596693	4.840122	6.030514	5.586953
21	C	7.485136	7.983873	4.302353	5.352002	4.909988
22	F	8.832482	9.287919	5.663736	6.665863	6.095646
23	C	7.032248	7.252445	3.836443	4.714844	4.408670
24	F	8.065503	8.018936	4.959464	5.636280	5.283679
25	C	5.705159	5.931628	2.557389	3.430781	3.436483
26	F	5.609322	5.462192	2.882326	3.303037	3.552829
27	Li	3.097277	4.807704	2.009810	2.917209	3.567105

		11	12	13	14	15
11	O	0.000000				
12	C	2.699758	0.000000			
13	F	3.889068	1.381321	0.000000		
14	F	3.113578	1.381540	2.254455	0.000000	
15	F	3.004979	1.381910	2.255210	2.255480	0.000000
16	C	3.807676	4.245170	4.292328	4.873979	5.277430
17	C	4.388874	5.416271	5.593212	6.049639	6.316154
18	F	4.036495	5.694477	6.174379	6.180071	6.497755
19	C	5.683005	6.528276	6.507452	7.268029	7.388266
20	F	6.514699	7.698067	7.782671	8.421261	8.480790
21	C	6.362236	6.658373	6.343761	7.479877	7.547407
22	F	7.666311	7.926642	7.521626	8.791809	8.765320
23	C	5.969888	5.730807	5.212950	6.553006	6.686203
24	F	7.015123	6.336294	5.548217	7.185634	7.254369
25	C	4.749533	4.429675	4.028028	5.174343	5.483592
26	F	4.804942	3.723331	3.009181	4.420354	4.845199
27	Li	2.561049	4.574497	5.393437	4.780733	5.340299

		16	17	18	19	20
16	C	0.000000				
17	C	1.386030	0.000000			
18	F	2.339998	1.369151	0.000000		
19	C	2.425995	1.405480	2.438771	0.000000	
20	F	3.660356	2.390974	2.824262	1.360740	0.000000

21	C	2.803914	2.426393	3.700786	1.403760	2.405223
22	F	4.165725	3.669835	4.829515	2.392247	2.778921
23	C	2.432379	2.799437	4.166857	2.433480	3.682376
24	F	3.675937	4.160422	5.527553	3.675816	4.801304
25	C	1.399290	2.413155	3.633186	2.804977	4.165548
26	F	2.366561	3.634251	4.705489	4.155264	5.515567
27	Li	2.850982	2.807760	1.939662	4.165070	4.753233

		21	22	23	24	25
21	C	0.000000				
22	F	1.361830	0.000000			
23	C	1.405141	2.398378	0.000000		
24	F	2.396518	2.771475	1.361000	0.000000	
25	C	2.432298	3.678413	1.408777	2.402474	0.000000
26	F	3.675100	4.801757	2.404384	2.795509	1.350770
27	Li	5.204399	6.475689	5.231205	6.517961	4.220224

		26	27
26	F	0.000000	
27	Li	4.835172	0.000000

Interatomic angles:

O2-S1-O3 = 99.5381 O2-S1-C4 = 109.7363 O3-S1-C4 = 106.4577
O2-O3-C4 = 65.6634 O2-S1-F5 = 119.777 O3-S1-F5 = 77.3881
O2-O3-F5 = 91.1569 S1-C4-F5 = 109.9975 O2-C4-F5 = 120.4866
O3-C4-F5 = 77.1862 O2-S1-F6 = 123.6822 O3-S1-F6 = 123.0355
S1-C4-F6 = 109.3937 O2-C4-F6 = 124.1028 O3-C4-F6 = 127.1058
S1-F6-F5 = 64.9726 O3-F5-F6 = 95.1101 F5-C4-F6 = 109.1809
O2-S1-F7 = 80.2965 O3-S1-F7 = 114.6332 O3-O2-F7 = 86.5956
S1-C4-F7 = 109.7514 O2-C4-F7 = 78.0885 O3-C4-F7 = 117.9361
S1-F7-F5 = 64.841 O2-F7-F5 = 91.6965 O3-F5-F7 = 90.4201
F5-C4-F7 = 109.2791 S1-F6-F7 = 64.8542 O2-F7-F6 = 93.5439
F6-C4-F7 = 109.2206 F5-F6-F7 = 60.0493 O2-S1-C8 = 110.2024
O3-S1-C8 = 105.8511 O2-O3-C8 = 65.9887 C4-S1-C8 = 122.4257
C4-O2-C8 = 70.6939 C4-O3-C8 = 72.6345 F5-S1-C8 = 128.7514
F5-O3-C8 = 95.7456 F6-S1-C8 = 92.9758 F7-S1-C8 = 135.8945
F7-O2-C8 = 95.7156 S1-C8-S9 = 113.8875 O2-C8-S9 = 99.743
O3-C8-S9 = 147.2534 S1-C8-O10 = 144.5458 O2-C8-O10 = 120.6359
O3-C8-O10 = 168.2801 C8-S9-O10 = 107.715 S1-C8-O11 = 111.9121
O2-C8-O11 = 117.1707 O3-C8-O11 = 137.6827 C8-S9-O11 = 102.7161
C8-O11-O10 = 66.1665 O10-S9-O11 = 97.5664 C8-S9-C12 = 129.2275
C8-O10-C12 = 73.9417 O10-S9-C12 = 108.8725 C8-O11-C12 = 76.1672
O11-S9-C12 = 106.0006 O10-O11-C12 = 65.8033 C8-S9-F13 = 112.3508
O10-S9-F13 = 97.003 O11-S9-F13 = 135.4743 S9-C12-F13 = 109.4471
O10-C12-F13 = 96.3838 O11-C12-F13 = 142.6379 C8-S9-F14 = 109.606
O10-S9-F14 = 137.9145 O11-S9-F14 = 92.6103 S9-C12-F14 = 109.4988
O10-C12-F14 = 140.9785 O11-C12-F14 = 93.8204 S9-F13-F14 = 64.6593
F13-C12-F14 = 109.3699 C8-S9-F15 = 158.6719 O10-S9-F15 = 88.8774
C8-O11-F15 = 101.6385 O11-S9-F15 = 87.8116 O10-O11-F15 = 67.8726
S9-C12-F15 = 109.6997 O10-C12-F15 = 87.8396 O11-C12-F15 = 88.7063
S9-F13-F15 = 64.7471 O11-F15-F13 = 94.2692 F13-C12-F15 = 109.4024
S9-F14-F15 = 64.7264 O11-F15-F14 = 70.9574 F14-C12-F15 = 109.4089
F14-F13-F15 = 60.019 O2-S1-C16 = 97.6058 O3-S1-C16 = 83.0183
C4-S1-C16 = 148.6452 F5-S1-C16 = 139.9337 F6-S1-C16 = 120.6015
F7-S1-C16 = 162.3473 S1-C8-C16 = 115.3824 O2-C8-C16 = 100.756
O3-C8-C16 = 88.1916 S1-C16-S9 = 65.7302 S9-C8-C16 = 115.1257
S1-C16-O10 = 96.4501 O10-C8-C16 = 85.2924 O10-S9-C16 = 81.5574
O11-C8-C16 = 132.4017 O11-S9-C16 = 119.327 O11-O10-C16 = 90.4247
C12-S9-C16 = 131.8851 C12-O10-C16 = 95.1917 F13-S9-C16 = 104.3235
F14-S9-C16 = 127.4717 F15-S9-C16 = 152.0814 S1-C8-C17 = 122.2176
O2-C8-C17 = 123.0723 O3-C8-C17 = 88.7622 S9-C8-C17 = 123.158
O10-C8-C17 = 90.5371 O11-C8-C17 = 119.3865 S1-C16-C17 = 123.0739
C8-C16-C17 = 116.2112 S9-C16-C17 = 124.4118 O10-C16-C17 = 108.4785
S1-C8-F18 = 119.5325 O2-C8-F18 = 139.2565 O3-C8-F18 = 89.9338
S9-C8-F18 = 120.9008 O10-C8-F18 = 95.4301 O11-C8-F18 = 99.5043
S1-C16-F18 = 97.7028 C8-C16-F18 = 84.5664 S9-C16-F18 = 98.6586
O10-C16-F18 = 95.6167 C8-C17-F18 = 82.9629 C16-C17-F18 = 116.2717
S1-C16-C19 = 142.171 C8-C16-C19 = 146.0894 S9-C16-C19 = 143.2377
O10-C16-C19 = 115.6899 C8-C17-C19 = 154.0082 C16-C17-C19 = 120.6981
C8-F18-C19 = 95.1789 F18-C16-C19 = 61.5233 F18-C17-C19 = 123.0274

C8-C17-F20 = 176.3349 C16-C17-F20 = 150.3549 C8-F18-F20 = 123.9704
C16-F18-F20 = 89.7666 F18-C17-F20 = 93.3722 C16-C19-F20 = 149.0315
C17-C19-F20 = 119.6078 F18-C19-F20 = 91.5302 S1-C16-C21 = 145.545
C8-C16-C21 = 176.1289 S9-C16-C21 = 145.3521 O10-C16-C21 = 115.6486
C8-C17-C21 = 123.7655 C16-C17-C21 = 90.4555 F18-C16-C21 = 91.5646
F18-C17-C21 = 153.264 C16-C19-C21 = 90.05 C17-C19-C21 = 119.4735
F18-C19-C21 = 147.5476 C16-C21-F20 = 88.9429 C17-F20-C21 = 60.7813
F18-F20-C21 = 89.7228 F20-C19-C21 = 120.9185 C16-C19-F22 = 119.6665
C17-C19-F22 = 149.0901 F18-C19-F22 = 177.1414 C17-F20-F22 = 90.123
F18-F20-F22 = 119.0643 F20-C19-F22 = 91.3021 C16-C21-F22 = 179.6302
C17-C21-F22 = 150.0425 C19-C21-F22 = 119.7588 F20-C21-F22 = 90.7235
S1-C16-C23 = 129.7741 C8-C16-C23 = 153.7907 S9-C16-C23 = 128.3552
O10-C16-C23 = 108.174 C8-C17-C23 = 93.6381 C17-C16-C23 = 89.9941
F18-C16-C23 = 121.6345 F18-C17-C23 = 176.484 C19-C16-C23 = 60.1168
C17-C19-C23 = 89.4945 F18-C19-C23 = 117.5685 F20-C17-C23 = 90.0269
F20-C19-C23 = 150.8956 C16-C23-C21 = 89.7573 C17-C21-C23 = 89.7903
C19-C21-C23 = 120.0735 F20-C21-C23 = 149.1068 C16-C23-F22 = 119.1576
C17-C23-F22 = 89.4821 C19-F22-C23 = 61.0569 F20-F22-C23 = 90.3665
F22-C21-C23 = 120.167 C16-C21-F24 = 89.6047 C17-C21-F24 = 119.2267
C19-C21-F24 = 149.5085 F20-C21-F24 = 178.4528 C19-F22-F24 = 90.4654
F20-F22-F24 = 119.774 F22-C21-F24 = 90.7303 C16-C23-F24 = 150.1706
C17-C23-F24 = 179.6785 C19-C23-F24 = 150.0171 C21-C23-F24 = 120.072
F22-C23-F24 = 90.6717 S1-C8-C25 = 103.9677 O2-C8-C25 = 79.9627
O3-C8-C25 = 88.5506 S9-C8-C25 = 102.0705 O10-C8-C25 = 81.219
O11-C8-C25 = 132.5287 S1-C16-C25 = 106.4905 C8-C16-C25 = 123.7002
S9-C16-C25 = 104.4628 O10-C16-C25 = 96.0047 C8-C17-C25 = 63.4243
C17-C16-C25 = 120.0813 F18-C8-C25 = 88.302 F18-C16-C25 = 151.7087
F18-C17-C25 = 146.3726 C8-C25-C19 = 89.0898 C19-C16-C25 = 90.2062
C19-C17-C25 = 90.5846 F18-C19-C25 = 87.4217 F20-C17-C25 = 120.2407
F20-C19-C25 = 178.9003 C8-C25-C21 = 119.119 C16-C25-C21 = 89.8977
C21-C17-C25 = 60.342 C19-C21-C25 = 89.8429 F20-C21-C25 = 118.8776
F22-C19-C25 = 89.7438 F22-C21-C25 = 150.398 C8-C25-C23 = 149.2636
C16-C25-C23 = 120.0421 C17-C25-C23 = 90.2434 C19-C23-C25 = 89.6776
C21-C23-C25 = 119.6242 F22-C23-C25 = 149.0246 C8-C25-F24 = 178.5444
C16-C25-F24 = 149.3231 C17-C25-F24 = 119.524 C19-C25-F24 = 89.4552
C21-F24-C25 = 60.9063 F22-F24-C25 = 90.3346 F24-C23-C25 = 120.3035
S1-O2-F26 = 98.3181 O3-O2-F26 = 98.2805 C4-O2-F26 = 132.3882
F7-O2-F26 = 150.5985 S1-C8-F26 = 89.9107 C8-O2-F26 = 62.0816
O3-C8-F26 = 89.6056 S9-C8-F26 = 86.2287 O10-C8-F26 = 78.6769
O11-C8-F26 = 121.206 O2-F26-F13 = 74.2074 C8-F26-F13 = 78.2886
S9-F13-F26 = 71.3355 C12-F13-F26 = 110.4162 F14-F13-F26 = 113.4609
F15-F13-F26 = 133.4534 S1-C16-F26 = 81.7722 O2-F26-C16 = 80.9577
C8-C16-F26 = 93.6743 S9-C16-F26 = 78.9422 O10-C16-F26 = 82.0855
F13-F26-C16 = 105.3417 C17-C8-F26 = 85.4933 C17-C16-F26 = 150.0831
F18-C8-F26 = 116.231 F18-C16-F26 = 177.556 C19-C16-F26 = 120.2243
C21-C16-F26 = 90.1892 O2-F26-C23 = 126.1329 C8-F26-C23 = 92.6028
F13-F26-C23 = 148.504 C16-F26-C23 = 61.2991 C17-C23-F26 = 88.2541
C19-C23-F26 = 118.3864 C21-C23-F26 = 148.3315 F22-C23-F26 = 177.6556
O2-F26-F24 = 139.2291 C8-F26-F24 = 121.7233 F13-F26-F24 = 145.7852
C16-F26-F24 = 90.4202 C21-F24-F26 = 89.7785 F22-F24-F26 = 119.2058
F24-C23-F26 = 91.589 O2-F26-C25 = 104.8083 C8-C25-F26 = 89.5272
F13-F26-C25 = 131.111 C16-C25-F26 = 118.7459 C17-C25-F26 = 148.5223
C19-C25-F26 = 178.1356 C21-C25-F26 = 151.3368 C23-C25-F26 = 121.2051
F24-C25-F26 = 91.9284 O2-S1-Li27 = 150.6512 O3-S1-Li27 = 94.5363
C4-S1-Li27 = 90.482 F5-S1-Li27 = 88.3254 F6-S1-Li27 = 66.3041
F7-S1-Li27 = 116.7511 S1-C8-Li27 = 103.0084 O2-C8-Li27 = 134.4773
O3-C8-Li27 = 94.4639 S1-Li27-S9 = 61.9665 S9-C8-Li27 = 99.3203
O10-C8-Li27 = 96.7938 O10-S9-Li27 = 101.6308 S1-Li27-O11 = 83.477
C8-Li27-O11 = 69.0752 S9-O11-Li27 = 86.7849 O10-O11-Li27 = 93.58
C12-S9-Li27 = 148.4689 C12-O11-Li27 = 120.7885 F13-S9-Li27 = 152.83
F14-S9-Li27 = 118.8845 F15-S9-Li27 = 148.1629 F15-O11-Li27 = 147.1457
S1-C16-Li27 = 63.9898 C16-C8-Li27 = 107.7277 S9-C16-Li27 = 62.123
O10-C16-Li27 = 75.1485 O11-Li27-C16 = 89.2597 S1-Li27-C17 = 80.449
C17-C8-Li27 = 77.3013 S9-Li27-C17 = 82.1804 O11-Li27-C17 = 109.5805
C16-C17-Li27 = 77.5611 S1-Li27-F18 = 101.8286 C8-Li27-F18 = 84.5607
S9-Li27-F18 = 105.5361 O11-Li27-F18 = 126.9488 C16-F18-Li27 = 82.9777
C17-F18-Li27 = 115.0234 C19-C16-Li27 = 103.9478 C19-C17-Li27 = 161.598

C19-F18-Li27 = 143.8353 F20-C17-Li27 = 132.0507 F20-F18-Li27 = 172.1856
C21-C16-Li27 = 133.9486 C21-C17-Li27 = 167.7429 C23-C16-Li27 = 163.8342
C23-C17-Li27 = 137.7971 C25-C8-Li27 = 134.7 C25-C16-Li27 = 165.489
C25-C17-Li27 = 107.6266 F26-C8-Li27 = 162.2083 F26-C16-Li27 = 135.655

Molecular Orbital Coefficients

				111 (LUMO)	112 (NLUMO)	113	114	115
EIGENVALUES --				0.09913	0.15924	0.19747	0.20504	0.21552
1	1	S	1S	-0.00187	0.01557	-0.01434	-0.00565	-0.02377
2			2S	0.00489	-0.04538	0.04506	0.01758	0.06950
3			2PX	-0.00462	0.03189	-0.03322	-0.01322	-0.04548
4			2PY	-0.00095	-0.01988	0.04342	0.01585	0.04706
5			2PZ	0.00692	-0.05429	0.03866	0.01600	0.06935
6			3S	-0.03614	0.26099	-0.20966	-0.08495	-0.40002
7			3PX	0.01739	-0.11672	0.11988	0.04756	0.16979
8			3PY	0.00317	0.07424	-0.16104	-0.05812	-0.17391
9			3PZ	-0.02418	0.19938	-0.14120	-0.05874	-0.25683
10	2	O	1S	0.00062	-0.00175	0.00080	0.00019	0.00131
11			2S	-0.00261	0.01054	-0.00612	-0.00183	-0.00885
12			2PX	-0.02651	0.07580	0.03388	0.00676	-0.04964
13			2PY	0.00777	-0.04848	0.04864	0.01499	0.07834
14			2PZ	0.02209	-0.10019	0.04136	0.02066	0.09632
15	3	O	1S	0.00465	-0.00644	-0.00619	-0.00199	0.00391
16			2S	-0.02623	0.03748	0.03632	0.01181	-0.02619
17			2PX	0.05953	0.02805	-0.12107	-0.03912	-0.04253
18			2PY	-0.01917	0.00412	0.06934	0.02440	0.02992
19			2PZ	-0.01908	0.03009	0.08567	0.03232	0.07652
20	4	C	1S	0.00138	0.02546	-0.04455	-0.01644	-0.04579
21			2S	-0.01947	-0.11786	0.23092	0.08517	0.21479
22			2PX	-0.01189	-0.04100	0.08484	0.03250	0.05796
23			2PY	0.03715	0.15151	-0.25428	-0.09521	-0.25041
24			2PZ	0.00603	-0.00633	0.02777	0.00811	0.01366
25	5	F	1S	0.00438	-0.00497	0.00003	0.00016	0.00914
26			2S	-0.02544	0.02878	0.00158	-0.00034	-0.05337
27			2PX	0.02538	0.02941	-0.05731	-0.02171	-0.04720
28			2PY	0.00257	-0.05160	0.05305	0.02025	0.07624
29			2PZ	-0.02514	0.03752	-0.01767	-0.00695	-0.06992
30	6	F	1S	0.01300	-0.00112	-0.00568	-0.00243	0.00664
31			2S	-0.07588	0.00700	0.03472	0.01477	-0.03944
32			2PX	0.05566	-0.00965	-0.02667	-0.00892	0.02754
33			2PY	0.04926	-0.03429	0.00942	0.00200	0.07042
34			2PZ	-0.00732	0.01419	-0.02653	-0.01031	-0.02271
35	7	F	1S	0.00054	-0.00295	0.00477	0.00182	0.00490
36			2S	-0.00298	0.01659	-0.02689	-0.01029	-0.02776
37			2PX	0.00815	-0.01392	0.03049	0.01161	0.02390
38			2PY	-0.01180	-0.05805	0.09815	0.03687	0.08584
39			2PZ	-0.00464	0.00671	-0.01772	-0.00600	-0.01162
40	8	C	1S	0.01498	-0.00755	-0.07741	-0.03031	-0.09929
41			2S	-0.04628	0.05747	0.42000	0.16428	0.50018
42			2PX	0.01447	0.08097	0.10495	0.04238	0.35775
43			2PY	-0.01428	0.02480	0.16725	0.06415	0.17262
44			2PZ	-0.00100	0.34257	-0.07211	-0.03622	0.07775
45	9	S	1S	0.00583	-0.01644	-0.01010	-0.00419	-0.02762
46			2S	-0.01764	0.04836	0.02876	0.01225	0.08331
47			2PX	-0.00275	0.04113	0.02927	0.01117	0.07170
48			2PY	-0.01121	-0.01176	-0.01761	-0.00513	0.01103
49			2PZ	0.00962	-0.06314	-0.04632	-0.01711	-0.07535
50			3S	0.09229	-0.27163	-0.17726	-0.07037	-0.44049
51			3PX	0.01075	-0.14716	-0.10376	-0.03984	-0.26713
52			3PY	0.03966	0.04204	0.06797	0.01915	-0.04289
53			3PZ	-0.03393	0.23229	0.17052	0.06288	0.28098
54	10	O	1S	-0.00070	0.00529	0.00447	0.00160	-0.00453
55			2S	0.00559	-0.03013	-0.02771	-0.00951	0.02411
56			2PX	-0.00195	0.09529	0.09048	0.02546	0.05708
57			2PY	-0.02214	-0.04439	-0.02945	-0.00609	-0.01872
58			2PZ	0.00186	-0.02618	-0.08695	-0.02478	-0.10371

59	11	O	1S	0.01652	0.01426	0.02080	0.00581	-0.01022
60			2S	-0.08991	-0.08339	-0.12189	-0.03394	0.05926
61			2PX	0.06707	0.10200	0.09119	0.03086	0.00786
62			2PY	0.00958	0.07571	0.11946	0.03468	-0.04786
63			2PZ	0.12425	-0.03456	0.00751	-0.00694	-0.09378
64	12	C	1S	0.01338	-0.03484	-0.01913	-0.00801	-0.06416
65			2S	-0.06337	0.16982	0.09363	0.03941	0.31746
66			2PX	0.06882	-0.19520	-0.11378	-0.04690	-0.34233
67			2PY	0.04565	-0.08492	-0.03725	-0.01691	-0.17094
68			2PZ	0.00796	0.00801	0.01985	0.00718	0.00404
69	13	F	1S	-0.00136	-0.00006	-0.00112	-0.00034	0.00186
70			2S	0.00772	0.00070	0.00670	0.00207	-0.01031
71			2PX	-0.03209	0.03281	0.00448	0.00341	0.07667
72			2PY	-0.00421	0.02781	0.02139	0.00788	0.03452
73			2PZ	0.00036	-0.00463	-0.00536	-0.00216	-0.00644
74	14	F	1S	0.00008	0.00094	0.00001	-0.00004	0.00189
75			2S	-0.00033	-0.00510	0.00009	0.00026	-0.01066
76			2PX	-0.01368	0.04712	0.02525	0.00985	0.07518
77			2PY	-0.01024	0.01882	0.00280	0.00130	0.03357
78			2PZ	-0.00217	-0.00754	-0.00789	-0.00262	-0.00500
79	15	F	1S	-0.00096	0.00582	0.00465	0.00177	0.00859
80			2S	0.00532	-0.03288	-0.02670	-0.01019	-0.04920
81			2PX	-0.01949	0.06441	0.04014	0.01552	0.09405
82			2PY	-0.01786	0.05385	0.03460	0.01365	0.08334
83			2PZ	-0.01128	0.06854	0.05182	0.01965	0.09735
84	16	C	1S	-0.00404	-0.00164	0.01986	0.00791	0.02052
85			2S	0.02414	0.01187	-0.09576	-0.03843	-0.10338
86			2PX	0.00551	0.00546	0.00236	0.00046	0.02654
87			2PY	0.03052	0.01291	-0.10674	-0.04277	-0.13233
88			2PZ	-0.00644	0.40441	-0.26159	-0.06133	0.08833
89	17	C	1S	-0.01445	-0.00656	-0.00958	-0.00399	-0.00408
90			2S	0.06391	0.03399	0.04920	0.02036	0.04438
91			2PX	-0.07087	-0.00563	0.01541	-0.00444	0.14259
92			2PY	0.04512	0.01606	0.01271	0.00511	-0.01880
93			2PZ	0.02106	-0.33177	0.28844	-0.49515	-0.00976
94	18	F	1S	0.02840	0.00371	0.00908	0.00356	-0.02576
95			2S	-0.16692	-0.02169	-0.05693	-0.02251	0.16283
96			2PX	-0.00029	0.00618	0.01643	0.00722	0.07176
97			2PY	-0.06270	0.00271	-0.03171	-0.01083	0.01766
98			2PZ	0.03387	0.02505	-0.18728	0.10053	0.08648
99	19	C	1S	0.00423	0.00139	0.00728	0.00309	0.00694
100			2S	-0.02086	-0.00662	-0.03600	-0.01562	-0.02911
101			2PX	-0.01075	-0.00261	0.00242	0.00307	0.03476
102			2PY	-0.02758	-0.00934	-0.02875	-0.01185	-0.00847
103			2PZ	0.00583	-0.15567	-0.07060	0.58087	-0.05454
104	20	F	1S	0.00154	0.00021	-0.00064	-0.00014	-0.00496
105			2S	-0.00852	-0.00120	0.00363	0.00079	0.02867
106			2PX	-0.01481	-0.00203	0.00983	0.00153	0.04563
107			2PY	-0.00824	0.00058	0.01023	0.00314	0.03751
108			2PZ	-0.00144	0.05006	0.01975	-0.17824	0.01760
109	21	C	1S	-0.00442	-0.00093	-0.00055	-0.00020	0.00537
110			2S	0.02032	0.00437	0.00178	0.00068	-0.02627
111			2PX	-0.01579	-0.00238	-0.00477	-0.00456	0.01902
112			2PY	0.00485	-0.00002	0.00031	0.00050	0.00093
113			2PZ	-0.01690	0.44819	-0.23829	-0.10585	0.08369
114	22	F	1S	0.00084	0.00026	0.00020	0.00006	-0.00148
115			2S	-0.00462	-0.00150	-0.00112	-0.00033	0.00851
116			2PX	0.00508	0.00071	0.00162	0.00146	-0.00398
117			2PY	-0.01444	-0.00406	-0.00254	-0.00079	0.02050
118			2PZ	0.00604	-0.14671	0.07423	0.03240	-0.02547
119	23	C	1S	-0.00173	-0.00170	0.00313	0.00124	0.00081
120			2S	0.00888	0.00779	-0.01464	-0.00566	-0.00472
121			2PX	-0.00010	0.00297	-0.00913	-0.00130	0.00031
122			2PY	0.00386	0.00320	-0.00934	-0.00317	0.00291
123			2PZ	0.00339	-0.19119	0.29396	-0.47817	-0.02866
124	24	F	1S	0.00019	0.00041	-0.00083	-0.00051	-0.00021
125			2S	-0.00105	-0.00226	0.00475	0.00295	0.00126

126		2PX	0.00243	0.00393	-0.00691	-0.00600	-0.00340
127		2PY	-0.00310	-0.00458	0.00936	0.00559	0.00083
128		2PZ	-0.00118	0.06330	-0.09237	0.14858	0.00879
129	25	C 1S	-0.00160	0.00132	-0.00034	0.00035	0.01168
130		2S	0.00842	-0.00699	0.00376	-0.00063	-0.05881
131		2PX	-0.00022	0.01507	-0.01560	-0.01892	0.02752
132		2PY	0.00613	-0.00325	-0.00431	-0.00210	-0.03433
133		2PZ	0.01642	-0.30558	-0.04167	0.57285	-0.05204
134	26	F 1S	0.00040	-0.00008	-0.00168	-0.00082	-0.00206
135		2S	-0.00198	0.00048	0.00992	0.00454	0.01228
136		2PX	0.01052	-0.00180	-0.01860	-0.00333	-0.03181
137		2PY	0.00374	0.00409	-0.00756	-0.00352	-0.00775
138		2PZ	-0.00541	0.10408	0.01397	-0.18341	0.01920
139	27	Li 1S	-0.21306	-0.01803	-0.03257	-0.00862	0.02293
140		2S	0.79360	0.06730	0.09330	0.02139	-0.08346
141		2PX	-0.48033	-0.15167	-0.23771	-0.08722	0.10151
142		2PY	0.31814	0.03182	-0.05397	-0.02966	0.27254
143		2PZ	-0.23161	0.38707	0.65391	0.21042	-0.49768

Total atomic charges:

		1
1	S	0.875386
2	O	-0.492950
3	O	-0.487670
4	C	0.326748
5	F	-0.103658
6	F	-0.118283
7	F	-0.101903
8	C	-0.255920
9	S	0.885808
10	O	-0.477500
11	O	-0.436312
12	C	0.337647
13	F	-0.108785
14	F	-0.120529
15	F	-0.093502
16	C	-0.018417
17	C	0.154833
18	F	-0.069259
19	C	0.112689
20	F	-0.104296
21	C	0.127017
22	F	-0.097495
23	C	0.115691
24	F	-0.100939
25	C	0.145624
26	F	-0.102185
27	Li	0.208158

Sum of Mulliken charges = 0.00000

Cite this work as:
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M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 1998.

X-Crystal and molecular structure of 6c

The study of the titled structure was undertaken to establish its three dimensional structure. Geometries are tabulated below. All Diagrams and calculations were

performed using maXus (MacScience, Japan).

Crystal data

$C_{15}H_6F_{10}O_4S_2$	D_m = 1.86 Mg m^{-3}
M_r = 504.317	Density measured by not measured
Monoclinic	Mo $K\alpha$ radiation
$P2_1/c$	l = 0.71073 Å
a = 18.499 (1) Å	m = 0.42 mm^{-1}
b = 7.9660 (4) Å	T = 298 K
c = 12.3480 (6) Å	Cube
b = 98.503 (2)°	0.9 x 0.5 x 0.4 mm
V = 1799.6 (2) Å^3	Colourless
Z = 4	
D_x = 1.861 Mg m^{-3}	

Data collection

DIP Image plate diffractometer	[$I > 3.00\ \sigma(I)$]
Absorption correction: None	q_{max} = 27.97°
3609 measured reflections	$h = -24 \rightarrow 24$
3437 independent reflections	$k = -10 \rightarrow 0$
3096 observed reflections	$l = 0 \rightarrow 14$

Refinement

Refinement on F	$(\ /s)_{max}$ = 0.0576
R = 0.068	r_{max} = 0.26 eÅ^{-3}
R_w= 0.071	r_{min} = 0.32 eA^{-3}
S = 0.909	Extinction correction: None
3096 reflection	Atomic scattering factors from
290 parameters	D. Waasmaier & A. Kirfel, *Acta Cryst.*
Only coordinates of H atoms refined	**1995**, *A51*, 416–431.
Unit	

Data collection: DIP Image plate. Data reduction: maXus (Mackay *et al.*, 1999). Program(s) used to solve structure: maXus. Program(s) used to refine structure: maXus. Molecular graphics: maXus. Software used to prepare material for publication: maXus.