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Table 1. Crystal data and structure refinement for [Tc(CO)3(9S3)]Br.

Compound	[Tc(CO)3(9S3)]Br
Empirical formula	C9 H12 Br O3 S3 Tc
Formula weight	442.28
Temperature	203(2) K
Wavelength	0.70930 A
Crystal system / Spacegroup	Monoclinic/ P21/c
Unit cell dimensions	a = 14.79(2) A alpha = 90 deg. b = 11.691(2) A beta = 94.88(6) deg. c = 16.94(2) A gamma = 90 deg.
Volume	2918(5) A^3
Z	8
Density (calculated)	2.014 Mg/m^3
Absorption coefficient	4.147 mm^-1
F(000)	1728
Crystal size / Colour	0.6 x 0.2 x 0.1 mm / colourless
No. of reflns. (lattice)	25
Theta range (lattice)	8.943 to 13.619 deg.
Theta range for data collection	3.19 to 28.89 deg.
Index ranges	0<=h<=15, -1<=k<=15, -23<=l<=22
Reflections collected	8048
Independent reflections	7128 [R(int) = 0.0314]
Reflections observed	4990
Criterion for observation	>2sigma(I)
Absorption correction	Psi Scan
Max. and min. transmission	0.9993 and 0.9034
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7124 / 0 / 307
Goodness-of-fit on F^2	1.155
Final R indices [I>2sigma(I)]	R1 = 0.0483, wR2 = 0.0779
Largest diff. peak and hole	0.895 and -0.882 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Tc(CO)3(9S3)]Br.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Tc(1)	3767(1)	2159(1)	1827(1)	18(1)
Tc(2)	2839(1)	7506(1)	365(1)	22(1)
Br(1)	1328(1)	2522(1)	-291(1)	31(1)
Br(2)	124(1)	5025(1)	2331(1)	32(1)
S(1)	3791(1)	2706(1)	3223(1)	24(1)
S(2)	2589(1)	795(1)	2127(1)	24(1)
S(3)	2510(1)	3542(1)	1624(1)	19(1)
S(4)	1773(1)	6499(1)	1141(1)	24(1)
S(5)	1792(1)	9119(1)	396(1)	23(1)
S(6)	1850(1)	6883(1)	-788(1)	25(1)
O(1)	3679(3)	1331(5)	107(2)	46(1)
O(2)	5272(3)	419(5)	2236(3)	55(2)
O(3)	5248(3)	3835(4)	1407(3)	41(1)
O(4)	4010(4)	5355(5)	290(3)	62(2)
O(5)	4110(4)	8837(5)	-638(3)	61(2)
O(6)	3916(4)	8238(6)	1904(3)	69(2)
C(1)	3687(4)	1641(5)	740(3)	26(1)
C(2)	4708(4)	1065(6)	2075(3)	31(2)
C(3)	4683(4)	3247(5)	1575(3)	26(1)
C(4)	3580(4)	6152(6)	318(4)	35(2)
C(5)	3640(4)	8335(6)	-265(4)	35(2)
C(6)	3522(4)	7978(6)	1332(4)	38(2)
C(16)	2891(4)	3766(5)	3280(3)	26(1)
C(11)	3290(4)	1444(5)	3644(3)	30(1)
C(12)	2462(5)	969(6)	3180(3)	34(2)
C(13)	1579(4)	1473(5)	1671(3)	25(1)
C(14)	1506(4)	2738(5)	1839(3)	24(1)
C(15)	2674(4)	4421(5)	2510(3)	23(1)
C(26)	1148(4)	7668(5)	1543(3)	30(1)
C(21)	932(4)	5866(5)	419(3)	26(1)
C(22)	1288(4)	5663(5)	-370(3)	30(1)
C(23)	935(4)	7937(5)	-905(3)	32(1)
C(24)	1249(4)	9114(5)	-605(3)	33(2)
C(25)	874(4)	8614(5)	960(3)	26(1)

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Table 3. Bond lengths [A] and angles [deg] for [Tc(CO)3(9S3)]Br.

Tc(1)-C(2)	1.910(7)
Tc(1)-C(1)	1.931(6)
Tc(1)-C(3)	1.933(6)
Tc(1)-S(2)	2.447(2)
Tc(1)-S(1)	2.448(3)
Tc(1)-S(3)	2.465(2)
Tc(2)-C(5)	1.923(7)
Tc(2)-C(6)	1.931(7)
Tc(2)-C(4)	1.931(7)
Tc(2)-S(4)	2.440(2)
Tc(2)-S(5)	2.443(2)
Tc(2)-S(6)	2.448(3)
S(1)-C(11)	1.823(6)
S(1)-C(16)	1.827(6)
S(2)-C(13)	1.805(6)
S(2)-C(12)	1.821(6)
S(3)-C(15)	1.818(6)
S(3)-C(14)	1.820(6)
S(4)-C(26)	1.814(6)
S(4)-C(21)	1.826(6)
S(5)-C(24)	1.813(6)
S(5)-C(25)	1.825(6)
S(6)-C(22)	1.825(6)
S(6)-C(23)	1.829(6)
O(1)-C(1)	1.131(7)
O(2)-C(2)	1.142(7)
O(3)-C(3)	1.137(7)
O(4)-C(4)	1.131(7)
O(5)-C(5)	1.140(7)
O(6)-C(6)	1.129(8)
C(16)-C(15)	1.523(8)
C(11)-C(12)	1.504(9)
C(13)-C(14)	1.511(7)
C(26)-C(25)	1.515(8)
C(21)-C(22)	1.496(8)
C(23)-C(24)	1.525(9)
C(2)-Tc(1)-C(1)	89.1(3)
C(2)-Tc(1)-C(3)	88.7(3)
C(1)-Tc(1)-C(3)	89.0(2)
C(2)-Tc(1)-S(2)	92.1(2)
C(1)-Tc(1)-S(2)	90.4(2)
C(3)-Tc(1)-S(2)	179.0(2)
C(2)-Tc(1)-S(1)	90.7(2)
C(1)-Tc(1)-S(1)	175.9(2)
C(3)-Tc(1)-S(1)	95.1(2)
S(2)-Tc(1)-S(1)	85.52(7)
C(2)-Tc(1)-S(3)	175.0(2)
C(1)-Tc(1)-S(3)	95.1(2)
C(3)-Tc(1)-S(3)	94.1(2)
S(2)-Tc(1)-S(3)	85.10(9)
S(1)-Tc(1)-S(3)	84.95(7)
C(5)-Tc(2)-C(6)	91.4(3)
C(5)-Tc(2)-C(4)	90.6(3)
C(6)-Tc(2)-C(4)	90.6(3)
C(5)-Tc(2)-S(4)	177.8(2)
C(6)-Tc(2)-S(4)	89.8(2)
C(4)-Tc(2)-S(4)	91.3(2)
C(5)-Tc(2)-S(5)	92.5(2)
C(6)-Tc(2)-S(5)	92.8(2)
C(4)-Tc(2)-S(5)	175.3(2)
S(4)-Tc(2)-S(5)	85.51(8)
C(5)-Tc(2)-S(6)	93.5(2)
C(6)-Tc(2)-S(6)	174.6(2)
C(4)-Tc(2)-S(6)	91.5(2)
S(4)-Tc(2)-S(6)	85.24(10)
S(5)-Tc(2)-S(6)	84.85(7)
C(11)-S(1)-C(16)	101.9(3)
C(11)-S(1)-Tc(1)	101.2(2)
C(16)-S(1)-Tc(1)	106.1(2)
C(13)-S(2)-C(12)	102.7(3)
C(13)-S(2)-Tc(1)	101.7(2)
C(12)-S(2)-Tc(1)	105.4(2)
C(15)-S(3)-C(14)	100.4(3)
C(15)-S(3)-Tc(1)	102.1(2)
C(14)-S(3)-Tc(1)	104.6(2)
C(26)-S(4)-C(21)	102.5(3)
C(26)-S(4)-Tc(2)	102.2(2)
C(21)-S(4)-Tc(2)	105.6(2)
C(24)-S(5)-C(25)	101.4(3)
C(24)-S(5)-Tc(2)	102.0(2)
C(25)-S(5)-Tc(2)	105.2(2)
C(22)-S(6)-C(23)	102.2(3)
C(22)-S(6)-Tc(2)	100.6(2)
C(23)-S(6)-Tc(2)	105.8(2)
O(1)-C(1)-Tc(1)	177.1(5)
O(2)-C(2)-Tc(1)	178.8(6)
O(3)-C(3)-Tc(1)	175.9(6)
O(4)-C(4)-Tc(2)	179.5(7)
O(5)-C(5)-Tc(2)	179.2(6)
O(6)-C(6)-Tc(2)	178.8(7)
C(15)-C(16)-S(1)	113.4(4)
C(12)-C(11)-S(1)	115.7(4)
C(11)-C(12)-S(2)	114.0(4)
C(14)-C(13)-S(2)	114.8(4)
C(13)-C(14)-S(3)	113.3(4)

C(16)-C(15)-S(3)	115.2(4)
C(25)-C(26)-S(4)	115.0(4)
C(22)-C(21)-S(4)	113.0(4)
C(21)-C(22)-S(6)	115.4(4)
C(24)-C(23)-S(6)	111.7(4)
C(23)-C(24)-S(5)	114.4(4)
C(26)-C(25)-S(5)	114.1(4)

Symmetry transformations used to generate equivalent atoms:

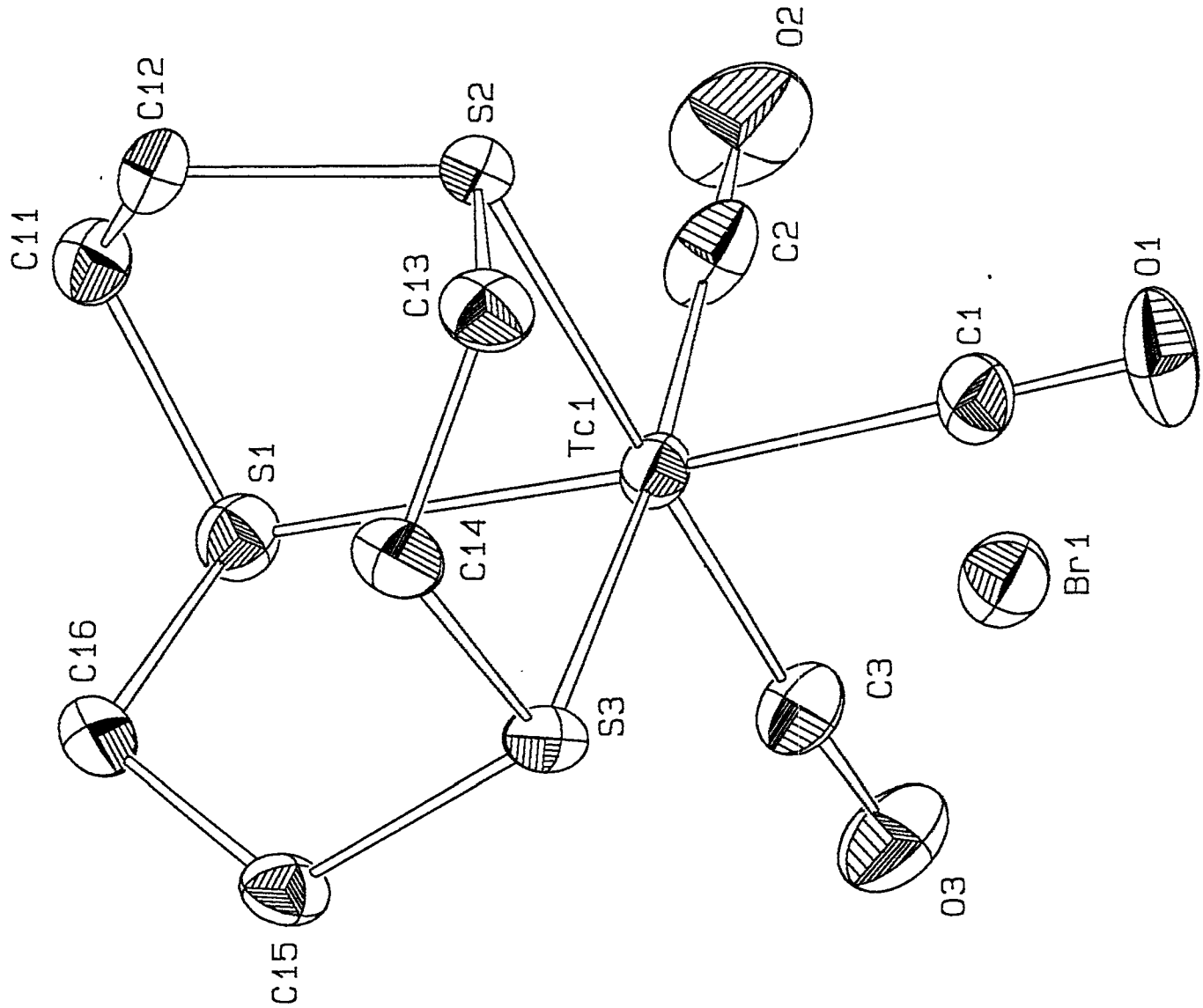
Table 4. Anisotropic displacement parameters (A^2 x 10^3) for [Tc(CO)3(9S3)]Br.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Tc(1)	18(1)	20(1)	18(1)	3(1)	4(1)	3(1)
Tc(2)	19(1)	20(1)	26(1)	0(1)	3(1)	2(1)
Br(1)	28(1)	32(1)	33(1)	3(1)	5(1)	1(1)
Br(2)	36(1)	30(1)	32(1)	4(1)	14(1)	8(1)
S(1)	26(1)	27(1)	20(1)	2(1)	-1(1)	3(1)
S(2)	33(1)	15(1)	25(1)	-1(1)	10(1)	0(1)
S(3)	19(1)	15(1)	23(1)	0(1)	0(1)	0(1)
S(4)	30(1)	20(1)	24(1)	3(1)	5(1)	2(1)
S(5)	26(1)	15(1)	29(1)	-1(1)	3(1)	1(1)
S(6)	31(1)	23(1)	22(1)	-3(1)	6(1)	-1(1)
O(1)	51(3)	66(4)	20(2)	-11(2)	6(2)	6(3)
O(2)	38(3)	56(3)	71(4)	25(3)	12(3)	25(3)
O(3)	35(3)	43(3)	44(3)	10(2)	7(2)	-11(2)
O(4)	64(4)	50(3)	74(4)	8(3)	14(3)	37(3)
O(5)	52(3)	51(3)	86(4)	10(3)	39(3)	-4(3)
O(6)	50(4)	92(5)	60(4)	-31(3)	-29(3)	15(3)
C(1)	18(3)	33(3)	27(3)	6(3)	9(2)	9(3)
C(2)	25(4)	40(4)	29(3)	10(3)	6(3)	-1(3)
C(3)	24(3)	31(3)	23(3)	5(3)	1(2)	-1(3)
C(4)	32(4)	37(4)	38(4)	4(3)	7(3)	13(3)
C(5)	27(4)	27(4)	53(4)	-2(3)	11(3)	-2(3)
C(6)	24(4)	48(4)	42(4)	-3(3)	-3(3)	7(3)
C(16)	33(4)	24(3)	22(3)	-3(2)	5(2)	4(3)
C(11)	44(4)	26(3)	20(3)	4(2)	6(3)	5(3)
C(12)	57(5)	26(3)	22(3)	3(3)	19(3)	-4(3)
C(13)	22(3)	21(3)	32(3)	-4(2)	2(2)	-4(2)
C(14)	15(3)	19(3)	37(3)	-5(2)	6(2)	-2(2)
C(15)	23(3)	17(3)	27(3)	-4(2)	-2(2)	-4(2)
C(26)	37(4)	25(3)	28(3)	-5(3)	11(3)	3(3)
C(21)	29(3)	16(3)	34(3)	3(2)	9(3)	-3(2)
C(22)	33(4)	19(3)	38(3)	-6(3)	5(3)	-8(3)
C(23)	36(4)	33(3)	25(3)	-1(3)	-7(3)	1(3)
C(24)	39(4)	27(3)	32(3)	12(3)	-1(3)	5(3)
C(25)	27(3)	21(3)	30(3)	-8(2)	10(2)	0(3)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Tc(CO)3(9S3)]Br.

	x	y	z	U(eq)
H(16A)	2346(4)	3382(5)	3421(3)	31
H(16B)	3071(4)	4306(5)	3699(3)	31
H(11A)	3748(4)	848(5)	3698(3)	36
H(11B)	3130(4)	1633(5)	4172(3)	36
H(12A)	1953(5)	1475(6)	3243(3)	41
H(12B)	2319(5)	231(6)	3400(3)	41
H(13A)	1561(4)	1365(5)	1102(3)	30
H(13B)	1053(4)	1092(5)	1854(3)	30
H(14A)	1404(4)	2842(5)	2393(3)	28
H(14B)	983(4)	3045(5)	1523(3)	28
H(15A)	3165(4)	4954(5)	2444(3)	27
H(15B)	2128(4)	4867(5)	2557(3)	27
H(26A)	605(4)	7360(5)	1747(3)	36
H(26B)	1518(4)	7997(5)	1987(3)	36
H(21A)	729(4)	5144(5)	624(3)	31
H(21B)	410(4)	6370(5)	349(3)	31
H(22A)	787(4)	5429(5)	-741(3)	36
H(22B)	1715(4)	5031(5)	-318(3)	36
H(23A)	718(4)	7991(5)	-1460(3)	38
H(23B)	434(4)	7684(5)	-614(3)	38
H(24A)	728(4)	9620(5)	-627(3)	39
H(24B)	1671(4)	9419(5)	-960(3)	39
H(25A)	644(4)	9254(5)	1248(3)	31
H(25B)	383(4)	8339(5)	593(3)	31


C11
C12
S2
O2
C13
C2
O1
C1
Tc1
S1
C14
Br1
C16
C3
S3
O3
C15

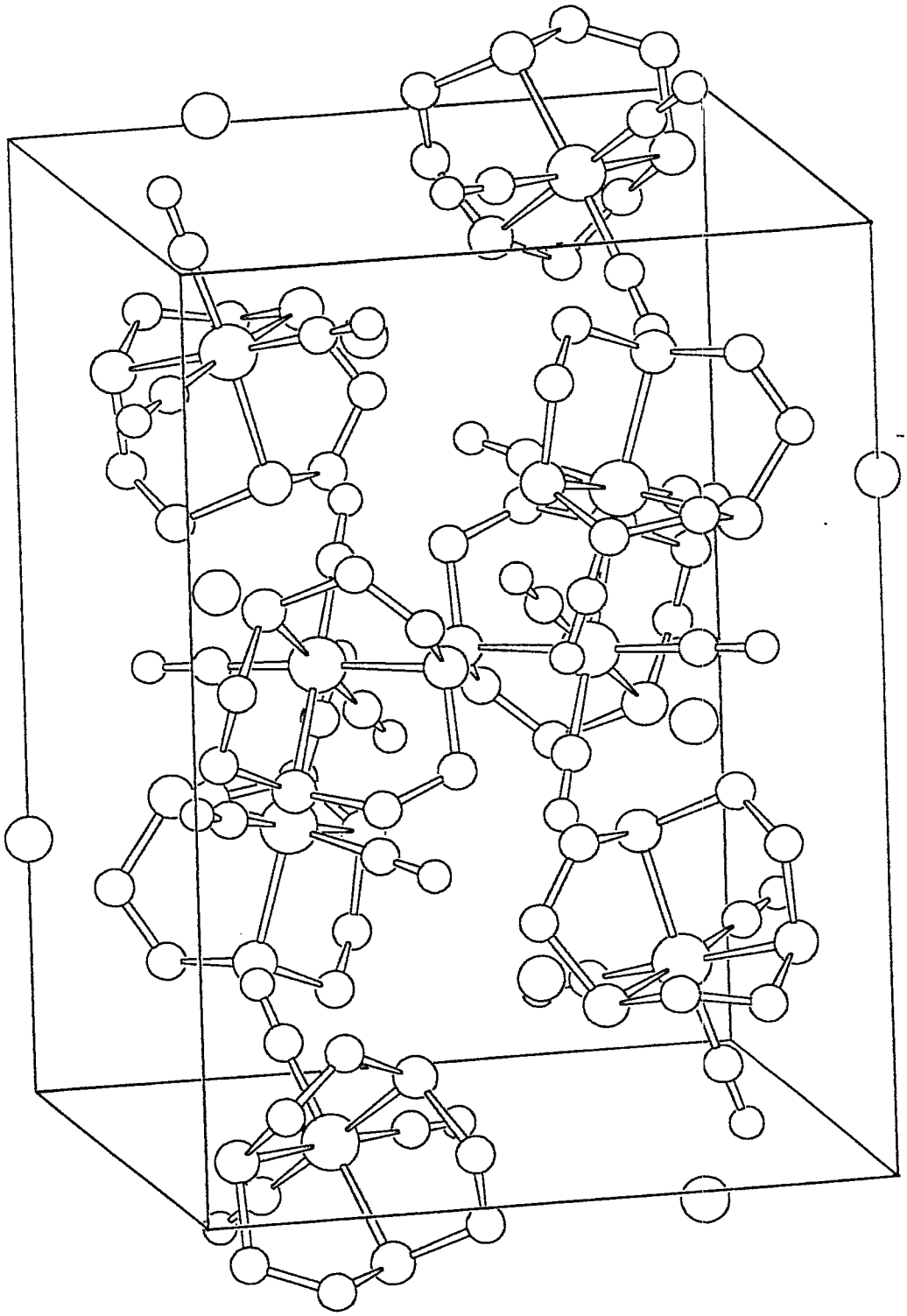

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Table 1 : Crystal data and structure refinement for [Tc2(CO)6(tosylat)2(18-Krone-S6)].

Name	Hexacarbonyl(18-crown-S6-S1,S2,S4,S5)bis(4-toluenedisulfonato-O)ditechnetium(I)
Compound	[Tc2(CO)6(tosylat)2(18-Krone-S6)]
Empirical formula	C32 H38 O12 S8 Tc2
Formula weight	1067.10
Temperature	213(2) K
Wavelength / Radiation	1.54184 A / CuKa
Crystal system / Spacegroup	Monoclinic/ C2/c
Unit cell dimensions	a = 26.073(4)A alpha = 90 deg. b = 9.288(1)A beta = 99.84(1) deg. c = 17.898(3)A gamma = 90 deg.
Volume	4270(1) A^3
Z	4
Density (calculated)	1.660 Mg/m^3
Absorption coefficient	9.396 mm^-1
F(000)	2160
Crystal description	colourless needle
Crystal size	0.5 x 0.2 x 0.1 mm
No. of reflns. (lattice)	25
Theta range (lattice)	14.69 to 27.70 deg.
Theta range for data collection	5.02 to 64.93 deg.
Index ranges	-30<=h<=30, 0<=k<=10, -1<=l<=21
Reflections collected	3927
Independent reflections	3585 [R(int) = 0.0415]
Reflections observed	2654
Criterion for observation	>2sigma(I)
Absorption correction	Psi scan
Max. and min. transmission	0.9984 and 0.7669
Measurement method	omega scans
No. of standard reflections	3
Interval count/time	300/3600
Decay	2.1 %
Structure solution	SHELXS-86 (Sheldrick, 1990)
Structure refinement	SHELXL-93 (Sheldrick, 1993)
Molecular graphics	SCHAKAL (Keller, 1992), ZORTEP (Zsolnai, 1994)
Publication material	SHELXL-93 (Sheldrick, 1993)
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	calc w=1/[s^2^(Fo^2^)+(0.0396P)^2^+15.7433P] where P=(Fo^2^+2Fc^2^)/3
Solution primary	Patterson
Hydrogen treatment	refined
Data / restraints / parameters	3585 / 0 / 319
Final R indices [I>2sigma(I)]	R1 = 0.0401, wR2 = 0.0890
Goodness-of-fit on F^2	1.031
Final R indices (all) R1 / wR2	0.0753 / 0.1028
Largest diff. peak and hole	.582 and -.717 e.A^-3

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (A^2 x 10^3) for [Tc2(CO)6(tosylat)2(18-Krone-S6)]. (U(eq) is defined as one third of the trace of the orthogonalized Uij tensor).

	x	y	z	U(eq)
Tc	.3773(1)	.3354(1)	.1794(1)	31(1)
S(1)	.2977(1)	.4732(2)	.1914(1)	33(1)
C(2)	.2385(2)	.3913(7)	.1403(3)	35(1)
C(3)	.2214(2)	.2735(8)	.1887(3)	33(1)
S(4)	.1530(1)	.2295(2)	.1663(1)	34(1)
C(5)	.1497(3)	.0881(7)	.0955(3)	37(1)
C(6)	.1477(3)	.1495(7)	.0168(3)	35(1)
S(7)	.1258(1)	.0240(2)	-.0595(1)	34(1)
C(8)	.1825(3)	-.0916(8)	-.0555(3)	40(2)
C(9)	.1954(3)	-.1269(7)	-.1316(4)	37(1)
O(11)	.3267(1)	.1826(4)	.1108(2)	30(1)
S(12)	.3217(1)	.0256(2)	.1226(1)	37(1)
O(13)	.2796(2)	-.0290(5)	.0667(3)	55(1)
O(14)	.3194(2)	-.0084(5)	.2006(2)	51(1)
C(21)	.3796(2)	-.0534(6)	.1012(3)	32(1)
C(22)	.3882(2)	-.0515(8)	.0276(4)	43(2)
C(23)	.4326(3)	-.1167(8)	.0098(4)	49(2)
C(24)	.4679(2)	-.1833(8)	.0655(4)	48(2)
C(25)	.4589(2)	-.1828(8)	.1394(4)	47(2)
C(26)	.4146(2)	-.1177(7)	.1580(4)	41(2)
C(27)	.5158(4)	-.2581(18)	.0462(7)	79(3)
O(30)	.4818(2)	.2003(6)	.1596(3)	64(2)
O(40)	.4464(2)	.5547(6)	.2748(3)	56(1)
O(50)	.3768(2)	.1826(7)	.3316(3)	82(2)
C(30)	.4420(2)	.2440(7)	.1666(3)	41(2)
C(40)	.4192(2)	.4752(7)	.2378(3)	38(2)
C(50)	.3766(3)	.2364(8)	.2732(4)	50(2)

Table 3: Full bond lengths [A] and angles [deg] for [Tc2(CO)6(tosylat)2(18-Krone-S6)].

Tc-C(40)	1.891(6)
Tc-C(50)	1.917(7)
Tc-C(30)	1.938(7)
Tc-O(11)	2.171(4)
Tc-S(1)	2.479(2)
Tc-S(7)#1	2.502(2)
S(1)-C(9)#1	1.811(6)
S(1)-C(2)	1.822(6)
C(2)-C(3)	1.510(8)
C(3)-S(4)	1.806(6)
S(4)-C(5)	1.816(7)
C(5)-C(6)	1.513(8)
C(6)-S(7)	1.812(6)
S(7)-C(8)	1.818(6)
S(7)-Tc#1	2.502(2)
C(8)-C(9)	1.494(8)
C(9)-S(1)#1	1.811(6)
O(11)-S(12)	1.483(4)
S(12)-O(14)	1.444(4)
S(12)-O(13)	1.445(4)
S(12)-C(21)	1.777(6)
C(21)-C(22)	1.374(8)
C(21)-C(26)	1.381(8)
C(22)-C(23)	1.391(9)
C(23)-C(24)	1.380(9)
C(24)-C(25)	1.383(9)
C(24)-C(27)	1.519(11)
C(25)-C(26)	1.395(9)
O(30)-C(30)	1.139(7)
O(40)-C(40)	1.153(7)
O(50)-C(50)	1.158(8)

C(40)-Tc-C(50)	86.4(3)
C(40)-Tc-C(30)	86.2(2)
C(50)-Tc-C(30)	91.9(3)
C(40)-Tc-O(11)	177.4(2)
C(50)-Tc-O(11)	94.9(2)
C(30)-Tc-O(11)	95.9(2)
C(40)-Tc-S(1)	90.6(2)
C(50)-Tc-S(1)	92.2(2)
C(30)-Tc-S(1)	174.7(2)
O(11)-Tc-S(1)	87.10(10)
C(40)-Tc-S(7)#1	92.7(2)
C(50)-Tc-S(7)#1	176.3(2)
C(30)-Tc-S(7)#1	91.6(2)
O(11)-Tc-S(7)#1	85.86(10)
S(1)-Tc-S(7)#1	84.23(5)
C(9)#1-S(1)-C(2)	101.2(3)
C(9)#1-S(1)-Tc	100.8(2)
C(2)-S(1)-Tc	113.0(2)
C(3)-C(2)-S(1)	108.8(4)
C(2)-C(3)-S(4)	114.4(4)
C(3)-S(4)-C(5)	104.2(3)
C(6)-C(5)-S(4)	111.5(5)
C(5)-C(6)-S(7)	114.5(5)
C(6)-S(7)-C(8)	101.7(3)
C(6)-S(7)-Tc#1	105.7(2)
C(8)-S(7)-Tc#1	104.4(2)
C(9)-C(8)-S(7)	113.7(4)
C(8)-C(9)-S(1)#1	115.3(5)
S(12)-O(11)-Tc	128.5(2)
O(14)-S(12)-O(13)	116.1(3)
O(14)-S(12)-O(11)	111.9(3)
O(13)-S(12)-O(11)	108.7(3)
O(14)-S(12)-C(21)	107.3(3)
O(13)-S(12)-C(21)	106.2(3)
O(11)-S(12)-C(21)	106.1(2)
C(22)-C(21)-C(26)	121.1(6)
C(22)-C(21)-S(12)	119.1(4)
C(26)-C(21)-S(12)	119.9(4)
C(21)-C(22)-C(23)	119.5(6)
C(24)-C(23)-C(22)	120.5(6)
C(23)-C(24)-C(25)	119.3(6)
C(23)-C(24)-C(27)	120.9(7)
C(25)-C(24)-C(27)	119.8(7)
C(24)-C(25)-C(26)	120.8(6)
C(21)-C(26)-C(25)	118.8(6)
O(30)-C(30)-Tc	174.8(6)
O(40)-C(40)-Tc	176.5(6)
O(50)-C(50)-Tc	176.8(6)

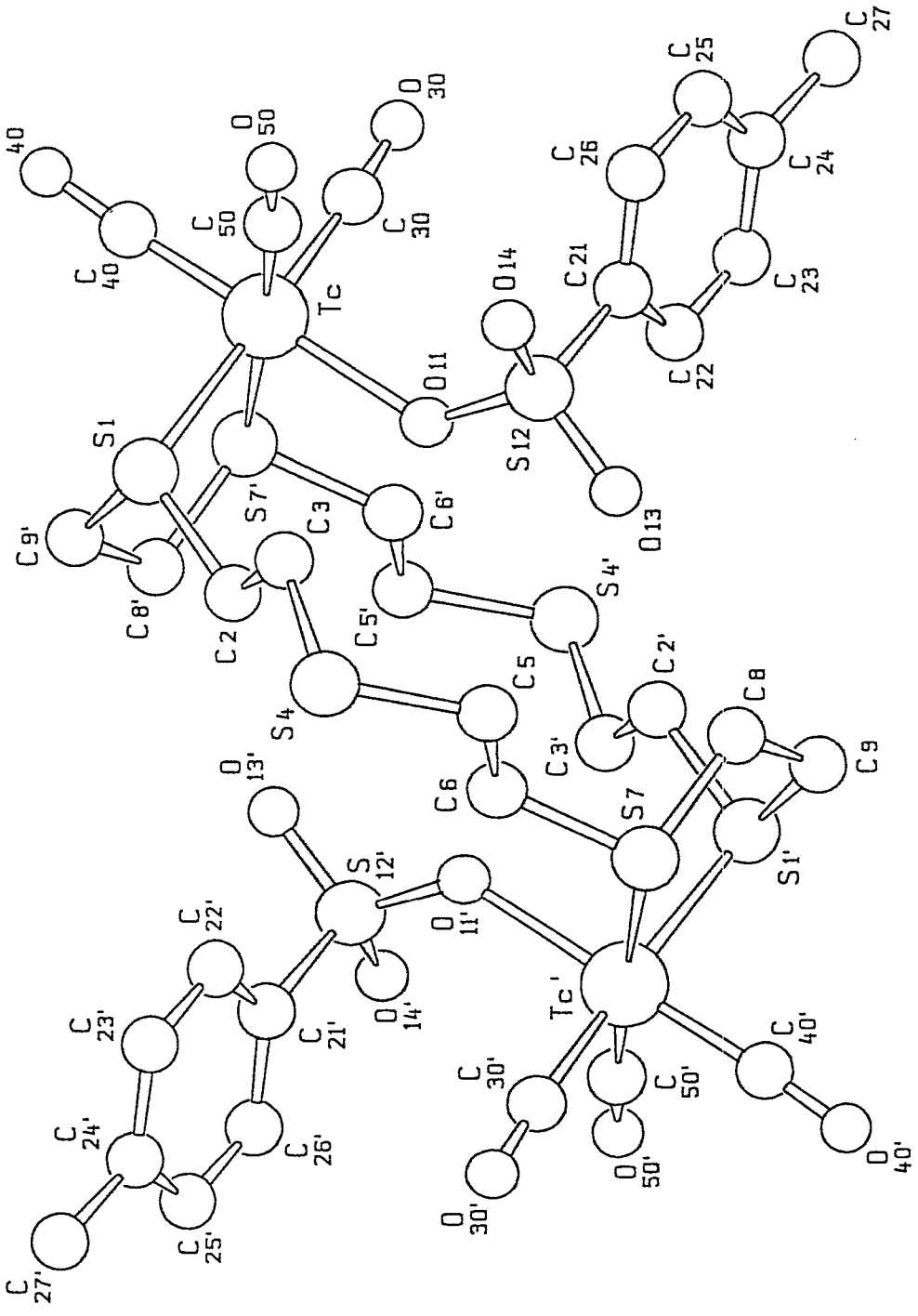
Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y+1/2,-z

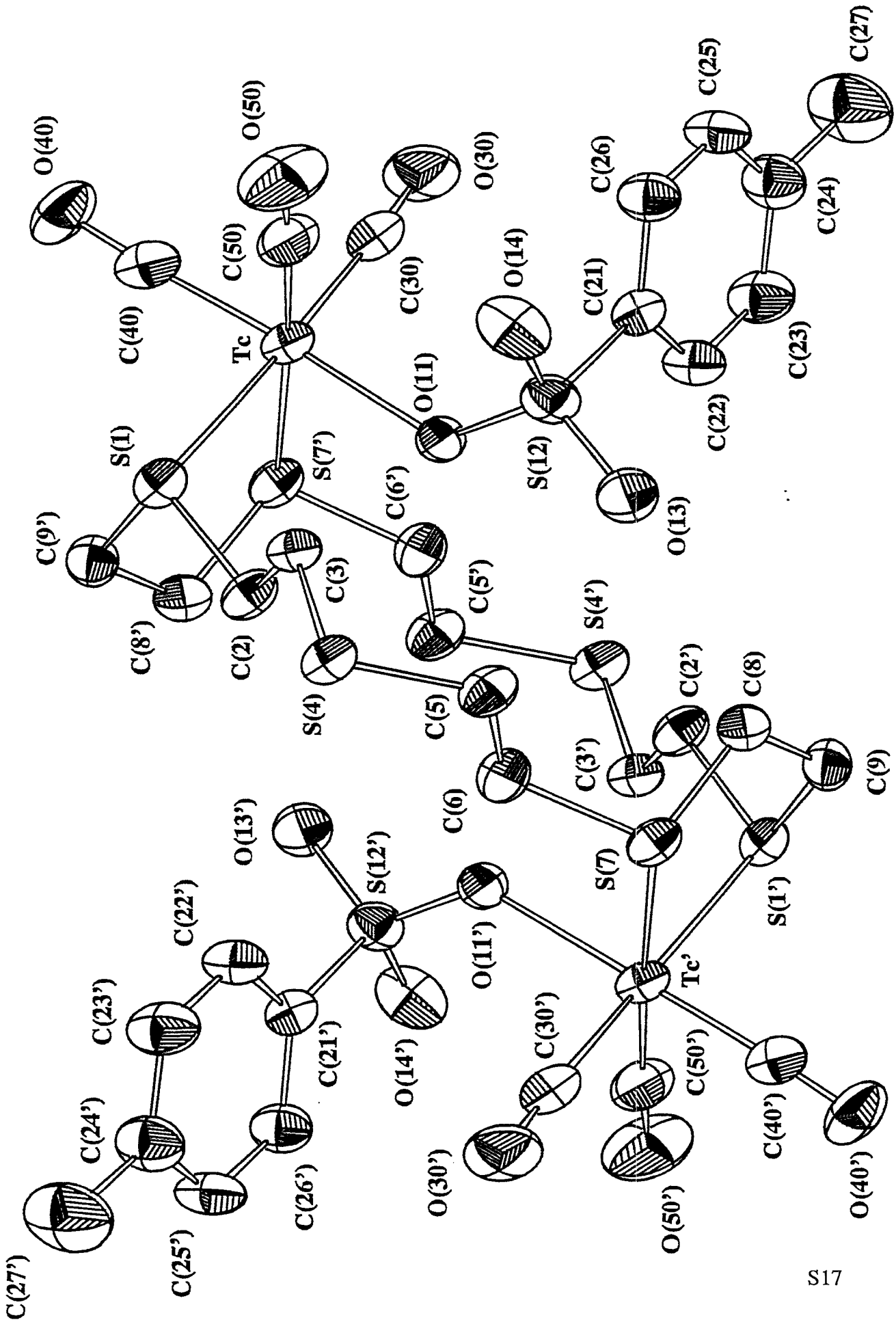
Table 4. Anisotropic displacement parameters (A^2 x 10^3) for [Tc2(CO)6(tosylat)2(18-Krone-S6)]. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

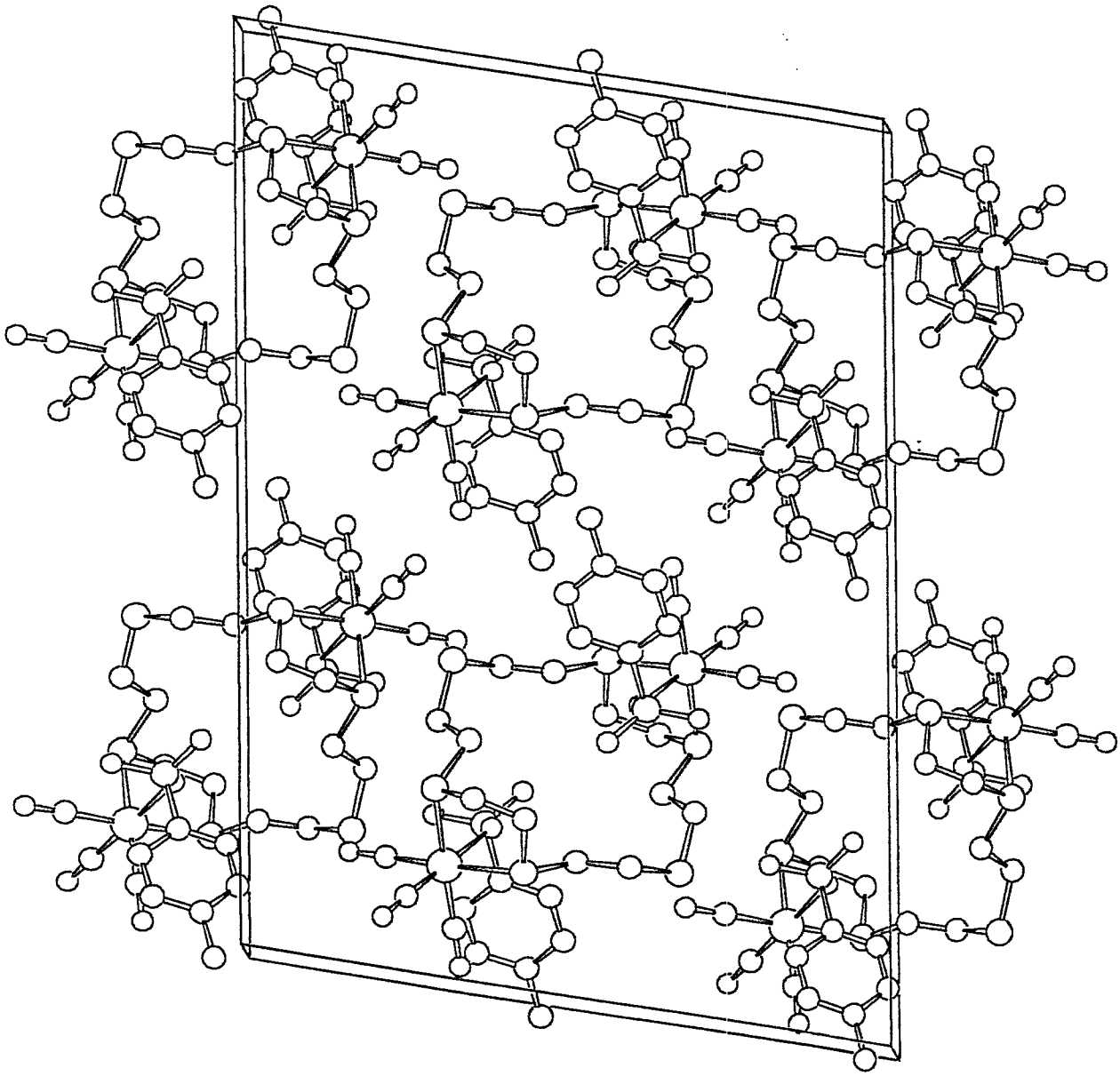
	U11	U22	U33	U23	U13	U12
Tc	26(1)	43(1)	24(1)	0(1)	1(1)	-2(1)
S(1)	29(1)	40(1)	30(1)	-5(1)	6(1)	-4(1)
C(2)	28(3)	49(4)	30(3)	-4(3)	5(2)	-9(3)
C(3)	27(3)	44(4)	27(3)	2(3)	3(2)	2(3)
S(4)	25(1)	51(1)	28(1)	-4(1)	9(1)	-4(1)
C(5)	43(4)	42(4)	25(3)	3(3)	5(3)	-7(3)
C(6)	38(3)	39(4)	31(3)	-4(3)	10(3)	-4(3)
S(7)	32(1)	44(1)	27(1)	-1(1)	5(1)	-8(1)
C(8)	43(4)	41(4)	32(3)	3(3)	-1(3)	4(3)
C(9)	36(3)	34(4)	40(3)	-4(3)	5(3)	0(3)
O(11)	34(2)	26(2)	30(2)	3(2)	3(2)	-2(2)
S(12)	25(1)	39(1)	46(1)	2(1)	6(1)	0(1)
O(13)	26(2)	52(3)	81(3)	-14(3)	-8(2)	-2(2)
O(14)	54(3)	51(3)	52(3)	19(2)	26(2)	7(2)
C(21)	29(3)	38(3)	29(3)	1(3)	3(2)	-4(3)
C(22)	39(3)	51(4)	38(3)	9(3)	-1(3)	6(3)
C(23)	45(4)	72(5)	31(3)	5(3)	9(3)	8(4)
C(24)	38(3)	59(5)	50(4)	3(4)	11(3)	7(3)
C(25)	33(3)	62(5)	43(4)	9(4)	-2(3)	11(3)
C(26)	37(3)	50(4)	35(3)	7(3)	7(3)	3(3)
C(27)	60(6)	108(11)	72(7)	3(7)	24(5)	27(7)
O(30)	32(2)	93(4)	65(3)	-13(3)	3(2)	13(3)
O(40)	33(2)	77(4)	56(3)	-27(3)	4(2)	-14(2)
O(50)	104(5)	96(5)	39(3)	27(3)	-6(3)	-21(4)
C(30)	41(4)	50(4)	31(3)	-5(3)	-2(3)	-6(3)
C(40)	28(3)	61(4)	28(3)	0(3)	8(2)	2(3)
C(50)	48(4)	55(4)	41(4)	-1(3)	-5(3)	-6(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Tc2(CO)6(tosylat)2(18-Krone-S6)].

	x	y	z	U(eq)
H(2A)	2412(23)	3524(65)	854(35)	46(17)
H(2B)	2076(30)	4654(84)	1269(41)	79(25)
H(3A)	2262(22)	2991(63)	2363(34)	36(17)
H(3B)	2412(21)	1860(62)	1881(29)	28(15)
H(5A)	1770(25)	143(72)	1108(34)	50
H(5B)	1204(29)	302(80)	947(39)	68(24)
H(6A)	1790(25)	1809(68)	109(34)	46(19)
H(6B)	1216(22)	2286(64)	84(30)	33(16)
H(8A)	2109(21)	-428(61)	-235(30)	31(15)
H(8B)	1788(23)	-1831(70)	-281(34)	43(18)
H(9A)	2260(22)	-1810(60)	-1256(30)	29(15)
H(9B)	1702(22)	-1804(62)	-1615(31)	32(16)
H(22)	3665(22)	-53(63)	-64(31)	35(17)
H(23)	4390(26)	-1041(72)	-403(38)	57(20)
H(25)	4803(29)	-2262(80)	1794(41)	73(24)
H(26)	4102(23)	-1089(66)	2126(35)	48(18)
H(27A)	5142(36)	-2409(105)	-57(59)	105(36)
H(27B)	5130(43)	-3501(116)	449(61)	118(52)
H(27C)	5411(41)	-2090(121)	725(61)	124(49)


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O(40)
C(40)
Tc
C(50)
O(50)
C(30)
O(30)
O(14)
O(11)
C(21)
C(26)
C(25)
C(24)
C(27)
C(23)
C(22)
S(12)
O(13)
S(1)
S(7')
C(6')
C(9')
C(8')
C(2)
C(3)
C(5')
S(4')
S(4)
C(5)
C(2')
C(8)
C(3')
C(6)
C(9)
S(7)
S(1')
Tc'
O(13')
S(12')
C(22')
C(23')
O(11')
C(24')
C(21')
O(14')
C(30')
C(50')
C(40')
C(27')
C(26')
O(30')
O(50')
O(40')
C(25')



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Table 1 : Crystal data and structure refinement for [Tc2(CO)6(20ane-S6-OH)](O3S(C6H4)CH3)2 x MeOH.

Name	
Compound	[Tc2(CO)6(20ane-S6-OH)](O3S(C6H4)CH3)2 x MeOH
Empirical formula	C35 H46 O14 S8 Tc2
Formula weight	1143.20
Temperature	203(2) K
Wavelength / Radiation	0.71073 A / MoKa
Crystal system / Spacegroup	Monoclinic/ Pc
Unit cell dimensions	a = 25.737(4)A alpha = 90 deg. b = 14.009(1)A beta = 149.56(2) deg. c = 26.479(3)A gamma = 90 deg.
Volume	4836(1) A^3
Z	4
Density (calculated)	1.570 Mg/m^3
Absorption coefficient	0.974 mm^-1
F(000)	2328
Crystal description	colourless plate
Crystal size	0.20 x 0.20 x 0.05 mm
No. of reflns. (lattice)	25
Theta range (lattice)	7.71 to 13.74 deg.
Theta range for data collection	3.02 to 25.00 deg.
Index ranges	-31<=h<=31, -1<=k<=17, -32<=l<=32
Reflections collected	18103
Independent reflections	17032 [R(int) = 0.0471]
Reflections observed	12860
Criterion for observation	>2sigma(I)
Absorption correction	None
Measurement method	omega scans
No. of standard reflections	3
Interval count/time	400/3600
Decay	5.0 %
Structure solution	SHELXS-86 (Sheldrick, 1990)
Structure refinement	SHELXL-93 (Sheldrick, 1993)
Molecular graphics	SCHAKAL (Keller, 1995), ZORTEP (Zsolnai,1997)
Publication material	SHELXL-93 (Sheldrick, 1993)
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	calc w=1/[s^2^(Fo^2^)+(0.1362P)^2^+1.1401P] where P=(Fo^2^+2Fc^2^)/3
Solution primary	Patterson
Hydrogen treatment	riding model
Data / restraints / parameters	16885 / 8 / 1083
Final R indices [I>2sigma(I)]	R1 = 0.0725, wR2 = 0.1792
Goodness-of-fit on F^2	1.040
Final R indices (all) R1 / wR2	0.1152 / 0.2239
Absolute structure parameter	0.44(6)
Extinction coefficient	0.0051(4)
Largest diff. peak and hole	1.685 and -.916 e.A^-3

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (A^2 x 10^3) for [Tc2(CO)6(20ane-S6-OH)](O3S(C6H4)CH3)2 x MeOH. (U(eq) is defined as one third of the trace of the orthogonalized Uij tensor).

	x	y	z	U(eq)
Tc(1)	0.4051(1)	0.7050(1)	0.5262(1)	21(1)
Tc(2)	0.2987(1)	0.7988(1)	0.1917(1)	30(1)
S(1)	0.3043(3)	0.6160(3)	0.3777(3)	49(1)
S(5)	0.2564(3)	0.6735(3)	0.2175(3)	57(1)
S(8)	0.2810(4)	0.6703(4)	0.1150(4)	73(1)
S(11)	0.4815(4)	0.7498(4)	0.3474(4)	66(1)
S(15)	0.5680(3)	0.6684(3)	0.6186(3)	54(1)
S(18)	0.4269(3)	0.5455(3)	0.5819(3)	55(1)
C(2)	0.1769(12)	0.6639(13)	0.2729(13)	64(5)
C(3)	0.1104(13)	0.6375(12)	0.1714(13)	55(4)
C(4)	0.1284(13)	0.6946(17)	0.1387(14)	73(6)
C(6)	0.2349(18)	0.5647(13)	0.1646(19)	85(6)
C(7)	0.2003(15)	0.5871(15)	0.0778(15)	75(5)
C(9)	0.4043(15)	0.6075(13)	0.2176(15)	63(5)
C(10)	0.4968(19)	0.6805(18)	0.3051(19)	95(8)
C(12)	0.5067(15)	0.6586(14)	0.4152(15)	67(5)
C(13)	0.5244(13)	0.7011(12)	0.4831(11)	51(4)
C(14)	0.5536(14)	0.6236(12)	0.5422(13)	55(4)
C(16)	0.6093(12)	0.5653(13)	0.6863(11)	56(4)
C(17)	0.5256(12)	0.4934(12)	0.6249(11)	52(4)
C(19)	0.3094(13)	0.4875(12)	0.4641(13)	64(5)
C(20)	0.2849(13)	0.4969(11)	0.3863(12)	52(4)
O(1)	0.1183(12)	0.5406(12)	0.1644(12)	104(5)
C(101)	0.2858(13)	0.7281(12)	0.4653(12)	54(4)
C(102)	0.3833(14)	0.8276(14)	0.4728(14)	64(5)
C(103)	0.4868(15)	0.7716(14)	0.6445(15)	66(5)
C(104)	0.3212(15)	0.8918(14)	0.2610(13)	63(4)
C(105)	0.1591(20)	0.8320(15)	0.0662(17)	79(6)
C(106)	0.3292(15)	0.8912(16)	0.1689(15)	74(6)
O(101)	0.2184(11)	0.7463(10)	0.4340(11)	78(4)
O(102)	0.3671(13)	0.8951(10)	0.4368(12)	89(4)
O(103)	0.5320(13)	0.8119(11)	0.7126(11)	93(5)
O(104)	0.3324(15)	0.9490(12)	0.3025(13)	107(5)
O(105)	0.0690(11)	0.8588(12)	-0.0139(11)	89(4)
O(106)	0.3458(13)	0.9496(12)	0.1517(12)	97(5)
S(41)	0.5152(3)	0.7648(3)	0.1790(3)	58(1)
O(41)	0.6045(9)	0.7086(11)	0.2616(9)	83(4)
O(42)	0.4323(11)	0.7097(10)	0.0931(10)	97(5)
O(43)	0.4892(13)	0.8208(9)	0.2011(13)	91(5)
C(42)	0.5630(11)	0.9378(12)	0.1771(12)	55(4)
C(41)	0.5451(11)	0.8427(11)	0.1539(11)	52(4)
C(43)	0.5890(15)	1.0005(15)	0.1603(14)	77(6)
C(44)	0.6015(15)	0.9664(16)	0.1229(14)	72(5)
C(45)	0.5850(15)	0.8682(15)	0.1000(13)	74(6)
C(46)	0.5586(16)	0.8063(18)	0.1195(14)	77(6)
C(47)	0.6203(3)	1.0288(3)	0.0909(3)	122(11)
S(51)	0.8877(3)	0.4124(3)	0.3395(3)	70(1)
O(51)	0.7984(3)	0.4748(3)	0.2593(3)	84(4)
O(52)	0.9082(3)	0.3524(3)	0.3128(3)	132(7)
O(53)	0.9794(3)	0.4607(3)	0.4353(3)	120(7)
C(51)	0.8596(3)	0.3300(3)	0.3643(3)	55(4)
C(52)	0.8370(3)	0.2362(3)	0.3366(3)	93(7)
C(53)	0.8193(19)	0.1788(17)	0.3630(19)	84(6)
C(54)	0.8106(16)	0.2135(19)	0.4046(18)	106(10)
C(55)	0.8252(16)	0.3054(20)	0.4266(16)	85(7)
C(56)	0.8557(12)	0.3706(16)	0.4122(12)	74(6)
C(57)	0.7872(19)	0.1415(17)	0.4274(18)	110(9)
Tc(4)	-0.0004(1)	0.1134(1)	-0.0005(1)	22(1)
Tc(3)	0.1158(1)	0.0258(1)	0.3420(1)	26(1)
S(25)	0.1044(3)	0.2094(3)	0.1459(3)	52(1)
S(21)	0.1496(3)	0.1411(3)	0.3021(3)	51(1)
S(38)	0.1328(3)	0.1658(3)	0.4113(3)	57(1)
S(35)	-0.0694(3)	0.0642(3)	0.1873(3)	56(1)
S(31)	-0.1609(3)	0.1536(4)	-0.0893(3)	58(1)
S(28)	-0.0266(3)	0.2677(3)	-0.0646(3)	58(1)
C(24)	0.2294(12)	0.1542(11)	0.2523(11)	48(4)
C(23)	0.2985(13)	0.1786(13)	0.3535(12)	56(4)
C(22)	0.2752(13)	0.1248(11)	0.3830(12)	53(4)
C(40)	0.1617(16)	0.2517(12)	0.3437(16)	72(5)
C(39)	0.1952(15)	0.2459(14)	0.4258(14)	70(5)
C(37)	-0.0004(15)	0.2175(17)	0.3018(15)	79(6)
C(36)	-0.0761(14)	0.1372(14)	0.2373(15)	70(5)
C(34)	-0.1100(14)	0.1502(13)	0.1051(13)	64(4)
C(33)	-0.1158(16)	0.1105(13)	0.0478(16)	71(5)
C(32)	-0.1445(13)	0.1919(14)	-0.0116(13)	63(5)
C(30)	-0.2010(18)	0.2696(24)	-0.1491(21)	142(14)
C(29)	-0.1511(35)	0.3003(27)	-0.1553(46)	301(39)
C(27)	0.0542(26)	0.3541(24)	0.0357(19)	148(14)
C(26)	0.1223(17)	0.3166(15)	0.1235(17)	79(6)
O(21)	0.2944(11)	0.2807(10)	0.3580(11)	79(4)
O(205)	0.1914(11)	0.0689(12)	0.0961(10)	83(4)
O(204)	0.0417(11)	-0.0691(11)	0.0934(10)	82(4)
O(206)	-0.1285(11)	0.0046(12)	-0.1868(10)	87(4)
O(203)	0.0906(13)	-0.1087(11)	0.4111(12)	99(5)
O(201)	0.3426(11)	-0.0321(10)	0.5389(11)	78(4)
O(202)	0.0720(13)	-0.1366(10)	0.2297(12)	94(5)
C(205)	0.1219(13)	0.0882(14)	0.0616(13)	63(5)
C(204)	0.0248(14)	0.0018(14)	0.0569(13)	62(4)
C(206)	-0.0815(14)	0.0434(16)	-0.1167(13)	74(6)
C(203)	0.0983(16)	-0.0609(14)	0.3832(14)	69(5)

C(201)	0.2589(14)	-0.0053(14)	0.4670(13)	61(4)
C(202)	0.0920(14)	-0.0772(14)	0.2761(14)	73(5)
S(61)	0.9541(4)	0.4541(3)	0.1246(4)	67(1)
O(61)	0.9659(11)	0.4386(10)	0.0811(12)	86(4)
O(62)	1.0299(11)	0.5191(11)	0.2067(11)	86(4)
O(63)	0.9530(12)	0.3648(11)	0.1513(13)	108(6)
C(61)	0.8322(15)	0.5066(14)	0.0324(14)	70(5)
C(62)	0.8260(20)	0.5894(15)	0.0565(19)	86(6)
C(63)	0.7262(18)	0.6241(16)	-0.0208(17)	82(6)
C(64)	0.6436(16)	0.5886(14)	-0.1133(16)	69(5)
C(65)	0.6504(14)	0.5041(15)	-0.1375(14)	68(5)
C(66)	0.7474(14)	0.4652(13)	-0.0620(14)	67(5)
C(67)	0.5316(23)	0.6257(18)	-0.1949(21)	113(9)
S(71)	0.4512(4)	0.3617(4)	0.3891(4)	67(1)
O(71)	0.3787(12)	0.2875(12)	0.3125(12)	94(5)
O(72)	0.4504(12)	0.4428(11)	0.3591(13)	97(5)
O(73)	0.4440(13)	0.3850(13)	0.4365(14)	105(5)
C(71)	0.5720(15)	0.3126(13)	0.4830(16)	68(5)
C(72)	0.5901(18)	0.2271(16)	0.4752(17)	78(6)
C(73)	0.6878(25)	0.1923(18)	0.5500(23)	106(9)
C(74)	0.7738(19)	0.2410(21)	0.6363(18)	87(7)
C(75)	0.7582(21)	0.3199(20)	0.6475(18)	103(8)
C(76)	0.6575(21)	0.3607(20)	0.5722(19)	115(10)
C(77)	0.8701(23)	0.2024(24)	0.7084(24)	144(13)
O(200)	0.7573(13)	0.3154(13)	0.1191(14)	42(4)
C(200)	0.7698(21)	0.3752(32)	0.0922(25)	95(17)
O(300)	0.0973(20)	0.4850(27)	0.3635(17)	105(12)
C(300)	0.0387(29)	0.5403(35)	0.3399(26)	89(15)
O(400)	0.2822(27)	0.3572(24)	0.1408(27)	114(11)
C(400)	0.2764(45)	0.2834(32)	0.1080(45)	114(20)
O(500)	0.6468(18)	0.8975(23)	0.3895(19)	90(10)
C(500)	0.6180(35)	0.9748(35)	0.3875(36)	147(29)

Table 3: Full bond lengths [A] and angles [deg] for [Tc2(CO)6(20ane-S6-OH)](O3S(C6H4)CH3)2 x MeOH.

Tc(1)-C(101)	1.90(2)
Tc(1)-C(103)	1.94(2)
Tc(1)-C(102)	1.97(2)
Tc(1)-S(18)	2.460(4)
Tc(1)-S(15)	2.478(4)
Tc(1)-S(1)	2.482(4)
Tc(2)-C(106)	1.86(2)
Tc(2)-C(104)	1.89(2)
Tc(2)-C(105)	1.89(3)
Tc(2)-S(8)	2.446(5)
Tc(2)-S(5)	2.453(5)
Tc(2)-S(11)	2.482(5)
S(1)-C(2)	1.79(2)
S(1)-C(20)	1.81(2)
S(5)-C(6)	1.80(2)
S(5)-C(4)	1.85(2)
S(8)-C(7)	1.76(2)
S(8)-C(9)	1.83(2)
S(11)-C(10)	1.76(2)
S(11)-C(12)	1.81(2)
S(15)-C(16)	1.77(2)
S(15)-C(14)	1.82(2)
S(18)-C(19)	1.81(2)
S(18)-C(17)	1.81(2)
C(2)-C(3)	1.54(2)
C(3)-O(1)	1.41(2)
C(3)-C(4)	1.52(3)
C(6)-C(7)	1.63(3)
C(9)-C(10)	1.60(3)
C(12)-C(13)	1.54(2)
C(13)-C(14)	1.47(2)
C(16)-C(17)	1.50(2)
C(19)-C(20)	1.55(2)
C(101)-O(101)	1.13(2)
C(102)-O(102)	1.14(2)
C(103)-O(103)	1.14(2)
C(104)-O(104)	1.18(2)
C(105)-O(105)	1.24(3)
C(106)-O(106)	1.18(2)
S(41)-O(42)	1.397(13)
S(41)-O(41)	1.420(12)
S(41)-O(43)	1.443(12)
S(41)-C(41)	1.76(2)
C(42)-C(41)	1.37(2)
C(42)-C(43)	1.39(3)
C(41)-C(46)	1.33(2)
C(43)-C(44)	1.37(3)
C(44)-C(45)	1.41(3)
C(44)-C(47)	1.56(2)
C(45)-C(46)	1.44(3)
S(51)-O(52)	1.46
S(51)-O(53)	1.46
S(51)-O(51)	1.46
S(51)-C(51)	1.76
C(51)-C(52)	1.37
C(51)-C(56)	1.47(2)
C(52)-C(53)	1.38(2)
C(53)-C(54)	1.39(4)
C(54)-C(55)	1.33(3)
C(54)-C(57)	1.54(3)
C(55)-C(56)	1.45(3)
Tc(4)-C(204)	1.87(2)
Tc(4)-C(206)	1.93(2)
Tc(4)-C(205)	1.95(2)
Tc(4)-S(28)	2.455(5)
Tc(4)-S(25)	2.466(4)
Tc(4)-S(31)	2.484(4)
Tc(3)-C(202)	1.91(2)
Tc(3)-C(201)	1.92(2)
Tc(3)-C(203)	1.93(2)
Tc(3)-S(38)	2.455(4)
Tc(3)-S(21)	2.463(4)
Tc(3)-S(35)	2.475(5)
S(25)-C(24)	1.81(2)
S(25)-C(26)	1.81(2)
S(21)-C(40)	1.77(2)
S(21)-C(22)	1.77(2)
S(38)-C(39)	1.71(2)
S(38)-C(37)	1.88(2)
S(35)-C(36)	1.80(2)
S(35)-C(34)	1.83(2)
S(31)-C(32)	1.79(2)
S(31)-C(30)	1.84(3)
S(28)-C(29)	1.72(3)
S(28)-C(27)	1.82(3)
C(24)-C(23)	1.50(2)
C(23)-O(21)	1.45(2)
C(23)-C(22)	1.53(2)
C(40)-C(39)	1.50(2)
C(37)-C(36)	1.50(3)
C(34)-C(33)	1.50(2)
C(33)-C(32)	1.52(2)
C(30)-C(29)	1.49(4)
C(27)-C(26)	1.31(3)
O(205)-C(205)	1.13(2)
O(204)-C(204)	1.18(2)
O(206)-C(206)	1.15(2)

O(42)-S(41)-O(43)	111.7(10)
O(41)-S(41)-O(43)	112.1(9)
O(42)-S(41)-C(41)	106.2(9)
O(41)-S(41)-C(41)	105.7(7)
O(43)-S(41)-C(41)	108.7(7)
C(41)-C(42)-C(43)	122.7(17)
C(46)-C(41)-C(42)	119.8(18)
C(46)-C(41)-S(41)	118.6(15)
C(42)-C(41)-S(41)	121.4(12)
C(44)-C(43)-C(42)	119(2)
C(43)-C(44)-C(45)	118.8(19)
C(43)-C(44)-C(47)	125.2(19)
C(45)-C(44)-C(47)	115.6(16)
C(44)-C(45)-C(46)	119(2)
C(41)-C(46)-C(45)	120(2)
O(52)-S(51)-O(53)	112.9
O(52)-S(51)-O(51)	114.3
O(53)-S(51)-O(51)	114.0
O(52)-S(51)-C(51)	103.9
O(53)-S(51)-C(51)	103.0
O(51)-S(51)-C(51)	107.4
C(52)-C(51)-C(56)	121.4(10)
C(52)-C(51)-S(51)	123.5
C(56)-C(51)-S(51)	115.0(10)
C(51)-C(52)-C(53)	117.6(10)
C(52)-C(53)-C(54)	123(2)
C(55)-C(54)-C(53)	121(3)
C(55)-C(54)-C(57)	121(3)
C(53)-C(54)-C(57)	118(2)
C(54)-C(55)-C(56)	120(2)
C(55)-C(56)-C(51)	115.9(18)
C(204)-Tc(4)-C(206)	90.7(9)
C(204)-Tc(4)-C(205)	89.3(9)
C(206)-Tc(4)-C(205)	89.6(8)
C(204)-Tc(4)-S(28)	175.2(6)
C(206)-Tc(4)-S(28)	94.1(7)
C(205)-Tc(4)-S(28)	91.4(6)
C(204)-Tc(4)-S(25)	92.0(5)
C(206)-Tc(4)-S(25)	177.1(6)
C(205)-Tc(4)-S(25)	89.5(5)
S(28)-Tc(4)-S(25)	83.24(14)
C(204)-Tc(4)-S(31)	94.9(6)
C(206)-Tc(4)-S(31)	88.6(6)
C(205)-Tc(4)-S(31)	175.5(6)
S(28)-Tc(4)-S(31)	84.5(2)
S(25)-Tc(4)-S(31)	92.07(15)
C(202)-Tc(3)-C(201)	91.8(8)
C(202)-Tc(3)-C(203)	89.7(9)
C(201)-Tc(3)-C(203)	85.2(8)
C(202)-Tc(3)-S(38)	174.6(5)
C(201)-Tc(3)-S(38)	92.9(6)
C(203)-Tc(3)-S(38)	93.3(6)
C(202)-Tc(3)-S(21)	93.3(7)
C(201)-Tc(3)-S(21)	91.6(5)
C(203)-Tc(3)-S(21)	175.7(6)
S(38)-Tc(3)-S(21)	83.96(14)
C(202)-Tc(3)-S(35)	90.5(5)
C(201)-Tc(3)-S(35)	175.5(5)
C(203)-Tc(3)-S(35)	91.0(6)
S(38)-Tc(3)-S(35)	84.89(15)
S(21)-Tc(3)-S(35)	92.05(14)
C(24)-S(25)-C(26)	104.6(9)
C(24)-S(25)-Tc(4)	106.3(5)
C(26)-S(25)-Tc(4)	100.3(7)
C(40)-S(21)-C(22)	101.7(8)
C(40)-S(21)-Tc(3)	104.2(6)
C(22)-S(21)-Tc(3)	110.3(5)
C(39)-S(38)-C(37)	101.8(10)
C(39)-S(38)-Tc(3)	102.7(6)
C(37)-S(38)-Tc(3)	104.0(6)
C(36)-S(35)-C(34)	100.5(9)
C(36)-S(35)-Tc(3)	100.1(6)
C(34)-S(35)-Tc(3)	114.9(6)
C(32)-S(31)-C(30)	97.2(14)
C(32)-S(31)-Tc(4)	115.4(6)
C(30)-S(31)-Tc(4)	104.8(8)
C(29)-S(28)-C(27)	106(3)
C(29)-S(28)-Tc(4)	105.6(10)
C(27)-S(28)-Tc(4)	106.9(9)
C(23)-C(24)-S(25)	117.6(11)
O(21)-C(23)-C(24)	108.3(14)
O(21)-C(23)-C(22)	110.8(12)
C(24)-C(23)-C(22)	114.7(14)
C(23)-C(22)-S(21)	115.3(12)
C(39)-C(40)-S(21)	115.4(13)
C(40)-C(39)-S(38)	117.1(13)
C(36)-C(37)-S(38)	108.6(15)
C(37)-C(36)-S(35)	114.3(12)
C(33)-C(34)-S(35)	114.5(13)
C(34)-C(33)-C(32)	107.7(15)
C(33)-C(32)-S(31)	112.8(13)
C(29)-C(30)-S(31)	117(2)
C(30)-C(29)-S(28)	121(3)
C(26)-C(27)-S(28)	115(2)
C(27)-C(26)-S(25)	125.6(19)
O(205)-C(205)-Tc(4)	176.6(18)
O(204)-C(204)-Tc(4)	178.9(18)
O(206)-C(206)-Tc(4)	176.6(18)
O(203)-C(203)-Tc(3)	176.6(16)
O(201)-C(201)-Tc(3)	173.8(17)
O(202)-C(202)-Tc(3)	175.3(17)
O(62)-S(61)-O(61)	111.1(9)

O(203)-C(203)	1.14(2)
O(201)-C(201)	1.16(2)
O(202)-C(202)	1.17(2)
S(61)-O(62)	1.431(14)
S(61)-O(61)	1.439(14)
S(61)-O(63)	1.449(15)
S(61)-C(61)	1.77(2)
C(61)-C(66)	1.39(2)
C(61)-C(62)	1.40(3)
C(62)-C(63)	1.40(3)
C(63)-C(64)	1.34(3)
C(64)-C(65)	1.43(3)
C(64)-C(67)	1.58(3)
C(65)-C(66)	1.39(3)
S(71)-O(72)	1.378(14)
S(71)-O(73)	1.453(14)
S(71)-O(71)	1.47(2)
S(71)-C(71)	1.73(2)
C(71)-C(72)	1.36(3)
C(71)-C(76)	1.38(3)
C(72)-C(73)	1.38(3)
C(73)-C(74)	1.37(3)
C(74)-C(75)	1.29(3)
C(74)-C(77)	1.39(3)
C(75)-C(76)	1.45(3)
O(200)-C(200)	1.31(3)
O(300)-C(300)	1.28(3)
O(400)-C(400)	1.27(3)
O(500)-C(500)	1.29(3)

C(101)-Tc(1)-C(103)	89.9(8)
C(101)-Tc(1)-C(102)	89.4(7)
C(103)-Tc(1)-C(102)	88.9(8)
C(101)-Tc(1)-S(18)	91.8(5)
C(103)-Tc(1)-S(18)	95.8(6)
C(102)-Tc(1)-S(18)	175.2(5)
C(101)-Tc(1)-S(15)	174.9(5)
C(103)-Tc(1)-S(15)	87.1(6)
C(102)-Tc(1)-S(15)	94.7(5)
S(18)-Tc(1)-S(15)	84.41(14)
C(101)-Tc(1)-S(1)	91.4(5)
C(103)-Tc(1)-S(1)	178.3(6)
C(102)-Tc(1)-S(1)	92.2(5)
S(18)-Tc(1)-S(1)	83.10(15)
S(15)-Tc(1)-S(1)	91.56(14)
C(106)-Tc(2)-C(104)	88.5(9)
C(106)-Tc(2)-C(105)	87.3(8)
C(104)-Tc(2)-C(105)	93.7(8)
C(106)-Tc(2)-S(8)	94.1(7)
C(104)-Tc(2)-S(8)	175.1(6)
C(105)-Tc(2)-S(8)	90.6(6)
C(106)-Tc(2)-S(5)	178.0(7)
C(104)-Tc(2)-S(5)	93.5(5)
C(105)-Tc(2)-S(5)	92.2(6)
S(8)-Tc(2)-S(5)	84.0(2)
C(106)-Tc(2)-S(11)	90.3(6)
C(104)-Tc(2)-S(11)	91.3(6)
C(105)-Tc(2)-S(11)	174.4(5)
S(8)-Tc(2)-S(11)	84.5(2)
S(5)-Tc(2)-S(11)	89.99(15)
C(2)-S(1)-C(20)	101.8(8)
C(2)-S(1)-Tc(1)	106.4(7)
C(20)-S(1)-Tc(1)	106.7(5)
C(6)-S(5)-C(4)	101.7(11)
C(6)-S(5)-Tc(2)	107.6(6)
C(4)-S(5)-Tc(2)	110.9(7)
C(7)-S(8)-C(9)	102.2(9)
C(7)-S(8)-Tc(2)	103.6(6)
C(9)-S(8)-Tc(2)	106.1(7)
C(10)-S(11)-C(12)	99.0(9)
C(10)-S(11)-Tc(2)	103.8(8)
C(12)-S(11)-Tc(2)	112.9(6)
C(16)-S(15)-C(14)	102.3(8)
C(16)-S(15)-Tc(1)	101.2(6)
C(14)-S(15)-Tc(1)	115.0(6)
C(19)-S(18)-C(17)	104.9(8)
C(19)-S(18)-Tc(1)	101.3(6)
C(17)-S(18)-Tc(1)	102.4(5)
C(3)-C(2)-S(1)	114.1(13)
O(1)-C(3)-C(4)	106.5(16)
O(1)-C(3)-C(2)	113.1(16)
C(4)-C(3)-C(2)	116.5(15)
C(3)-C(4)-S(5)	113.2(13)
C(7)-C(6)-S(5)	111.2(13)
C(6)-C(7)-S(8)	113.1(13)
C(10)-C(9)-S(8)	110.6(12)
C(9)-C(10)-S(11)	113.7(14)
C(13)-C(12)-S(11)	112.2(13)
C(14)-C(13)-C(12)	108.8(14)
C(13)-C(14)-S(15)	110.8(11)
C(17)-C(16)-S(15)	113.6(11)
C(16)-C(17)-S(18)	109.5(12)
C(20)-C(19)-S(18)	114.3(11)
C(19)-C(20)-S(1)	113.9(10)
O(101)-C(101)-Tc(1)	175.3(16)
O(102)-C(102)-Tc(1)	175.6(17)
O(103)-C(103)-Tc(1)	177.6(19)
O(104)-C(104)-Tc(2)	178.0(19)
O(105)-C(105)-Tc(2)	176.4(18)
O(106)-C(106)-Tc(2)	178(2)
O(42)-S(41)-O(41)	111.9(9)

O(62)-S(61)-O(63)	112.5(10)
O(61)-S(61)-O(63)	111.5(10)
O(62)-S(61)-C(61)	107.7(9)
O(61)-S(61)-C(61)	107.7(9)
O(63)-S(61)-C(61)	106.0(8)
C(66)-C(61)-C(62)	123(2)
C(66)-C(61)-S(61)	118.3(16)
C(62)-C(61)-S(61)	118.6(15)
C(63)-C(62)-C(61)	114(2)
C(64)-C(63)-C(62)	124(2)
C(63)-C(64)-C(65)	120.9(18)
C(63)-C(64)-C(67)	121.8(18)
C(65)-C(64)-C(67)	116.3(19)
C(66)-C(65)-C(64)	116.4(18)
C(65)-C(66)-C(61)	120.8(19)
O(72)-S(71)-O(73)	111.2(11)
O(72)-S(71)-O(71)	114.7(11)
O(73)-S(71)-O(71)	113.4(9)
O(72)-S(71)-C(71)	105.8(9)
O(73)-S(71)-C(71)	104.9(10)
O(71)-S(71)-C(71)	105.9(10)
C(72)-C(71)-C(76)	116(2)
C(72)-C(71)-S(71)	123.8(18)
C(76)-C(71)-S(71)	120.2(16)
C(71)-C(72)-C(73)	122(2)
C(74)-C(73)-C(72)	123(2)
C(75)-C(74)-C(73)	116(3)
C(75)-C(74)-C(77)	124(3)
C(73)-C(74)-C(77)	120(3)
C(74)-C(75)-C(76)	124(3)
C(71)-C(76)-C(75)	119(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for [Tc2(CO)6(20ane-S6-OH)](O3S(C6H4)CH3)2 x MeOH. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Tc(1)	26(1)	17(1)	23(1)	-4(1)	21(1)	-3(1)
Tc(2)	35(1)	29(1)	33(1)	9(1)	31(1)	8(1)
S(1)	52(2)	47(2)	55(2)	-4(2)	48(2)	-2(2)
S(5)	51(2)	55(3)	53(2)	7(2)	43(2)	5(2)
S(8)	91(3)	77(3)	75(3)	10(3)	75(3)	16(3)
S(11)	67(3)	73(3)	71(3)	15(2)	61(3)	8(2)
S(15)	54(2)	52(2)	56(2)	-4(2)	48(2)	-5(2)
S(18)	62(2)	50(2)	65(2)	5(2)	56(2)	3(2)
C(2)	46(9)	50(10)	65(10)	8(8)	43(9)	2(8)
C(3)	56(9)	37(9)	61(10)	-14(8)	49(9)	-8(7)
C(4)	41(9)	111(18)	59(11)	29(11)	42(9)	20(10)
C(6)	117(16)	44(10)	153(20)	4(12)	125(18)	6(11)
C(7)	74(12)	76(13)	72(11)	-20(10)	62(11)	-8(10)
C(9)	79(12)	59(11)	89(13)	17(10)	78(12)	15(10)
C(10)	123(18)	103(17)	131(19)	68(16)	120(18)	63(15)
C(12)	72(11)	66(12)	81(12)	3(10)	69(11)	1(9)
C(13)	58(9)	63(11)	40(8)	-4(7)	43(8)	-5(8)
C(14)	71(10)	58(10)	69(10)	-10(8)	65(10)	-10(8)
C(16)	46(8)	67(11)	43(8)	3(8)	36(8)	-2(8)
C(17)	65(9)	51(9)	50(8)	8(7)	51(8)	3(8)
C(19)	62(10)	45(9)	80(12)	7(8)	61(10)	-2(8)
C(20)	66(10)	30(8)	58(9)	-10(7)	53(9)	1(7)
O(1)	87(11)	83(12)	96(11)	-14(9)	72(10)	-14(9)
C(101)	48(9)	56(10)	53(9)	5(8)	43(9)	1(8)
C(102)	62(11)	52(11)	72(11)	-21(9)	57(10)	-18(9)
C(103)	91(13)	62(11)	77(12)	-9(10)	76(12)	-3(10)
C(104)	81(12)	52(10)	61(10)	3(8)	62(10)	-4(9)
C(105)	123(18)	71(13)	93(15)	-29(12)	101(16)	-31(13)
C(106)	71(11)	84(14)	83(12)	42(11)	69(11)	34(10)
O(101)	81(9)	82(10)	90(9)	4(8)	77(9)	16(8)
O(102)	137(13)	51(8)	116(11)	17(8)	115(12)	9(8)
O(103)	125(12)	80(10)	92(10)	-44(9)	96(11)	-40(9)
O(104)	139(14)	82(11)	114(12)	-24(9)	111(12)	-8(10)
O(105)	62(8)	101(12)	67(8)	13(8)	50(8)	18(8)
O(106)	110(11)	93(11)	102(11)	31(9)	93(11)	27(9)
S(41)	57(2)	54(2)	64(3)	1(2)	52(2)	1(2)
O(41)	47(6)	107(11)	65(7)	35(7)	44(6)	11(7)
O(42)	81(10)	63(9)	66(8)	-21(7)	52(8)	-24(7)
O(43)	156(13)	57(8)	171(14)	13(9)	157(13)	14(8)
C(42)	41(8)	56(10)	48(8)	3(7)	36(7)	-1(7)
C(41)	47(8)	52(10)	58(9)	6(8)	45(8)	16(7)
C(43)	78(13)	63(13)	61(11)	3(10)	56(11)	16(10)
C(44)	77(12)	93(16)	60(10)	13(10)	61(11)	2(11)
C(45)	79(13)	66(13)	54(10)	-8(9)	54(11)	-19(10)
C(46)	78(12)	108(17)	65(11)	-1(11)	65(11)	-4(12)
C(47)	102(17)	163(29)	112(18)	15(18)	94(17)	-23(18)
S(51)	60(3)	83(3)	72(3)	3(3)	58(3)	4(3)
O(51)	108(11)	58(8)	99(10)	12(7)	91(10)	6(8)
O(52)	176(17)	106(14)	205(19)	5(14)	178(18)	20(13)
O(53)	61(9)	135(16)	113(12)	11(11)	67(10)	-22(9)
C(51)	41(8)	67(11)	40(8)	-4(8)	32(8)	-8(8)
C(52)	123(19)	78(16)	116(18)	8(14)	109(18)	20(14)
C(53)	107(17)	64(14)	111(17)	-8(12)	98(16)	-12(12)
C(54)	49(11)	72(17)	82(16)	22(13)	39(12)	11(11)
C(55)	81(14)	124(21)	79(13)	41(14)	73(13)	39(14)
C(56)	36(8)	96(15)	34(8)	2(9)	22(8)	14(9)
C(57)	97(17)	77(16)	89(16)	21(13)	70(15)	3(13)
Tc(4)	25(1)	22(1)	23(1)	-2(1)	21(1)	-1(1)
Tc(3)	31(1)	22(1)	28(1)	0(1)	26(1)	-1(1)
S(25)	53(2)	53(3)	49(2)	-1(2)	44(2)	1(2)
S(21)	58(2)	53(2)	57(2)	-4(2)	52(2)	-4(2)
S(38)	63(2)	59(3)	59(2)	-3(2)	54(2)	1(2)
S(35)	58(2)	57(3)	60(2)	-7(2)	51(2)	-6(2)
S(31)	49(2)	69(3)	52(2)	0(2)	43(2)	-3(2)
S(28)	64(3)	55(2)	60(2)	-2(2)	55(2)	-2(2)
C(24)	62(9)	41(9)	59(9)	-17(7)	55(9)	-13(7)
C(23)	57(9)	57(11)	61(10)	6(8)	52(9)	15(8)
C(22)	72(11)	34(8)	54(9)	-11(7)	54(9)	-10(7)
C(40)	91(13)	36(9)	104(14)	-3(9)	87(13)	-16(9)
C(39)	85(13)	73(12)	77(12)	-32(10)	73(12)	-20(10)
C(37)	78(13)	112(18)	77(13)	-31(12)	71(12)	-16(12)
C(36)	59(10)	68(12)	82(12)	-10(10)	60(11)	-8(9)
C(34)	65(10)	59(11)	64(10)	-1(9)	55(10)	8(9)
C(33)	83(13)	58(11)	96(14)	20(10)	81(13)	17(9)
C(32)	40(8)	71(12)	52(9)	6(9)	35(8)	9(8)
C(30)	66(14)	177(30)	117(20)	70(20)	69(15)	9(16)
C(29)	254(44)	145(31)	541(88)	245(47)	348(60)	166(33)
C(27)	177(28)	158(28)	92(18)	-43(18)	114(21)	-87(23)
C(26)	91(14)	64(13)	89(14)	-6(11)	79(13)	-9(11)
O(21)	100(10)	64(8)	102(10)	-22(7)	92(9)	-20(7)
O(205)	81(9)	105(12)	83(9)	14(9)	74(9)	10(9)
O(204)	81(9)	69(9)	75(9)	-5(8)	63(8)	-7(8)
O(206)	83(9)	106(12)	59(8)	-13(8)	59(8)	-11(8)
O(203)	124(12)	98(11)	111(11)	-8(9)	107(11)	-37(9)
O(201)	78(9)	73(9)	89(9)	9(8)	73(9)	7(7)
O(202)	119(12)	56(9)	96(10)	-5(8)	91(10)	14(8)
C(205)	51(10)	77(13)	58(10)	-12(9)	47(9)	4(9)
C(204)	67(11)	60(12)	51(9)	-3(9)	50(9)	-6(9)
C(206)	59(11)	91(15)	48(10)	-25(10)	43(9)	-27(10)
C(203)	88(13)	58(11)	67(11)	-12(9)	68(11)	-17(10)
C(201)	54(10)	67(12)	55(10)	6(9)	46(9)	2(9)

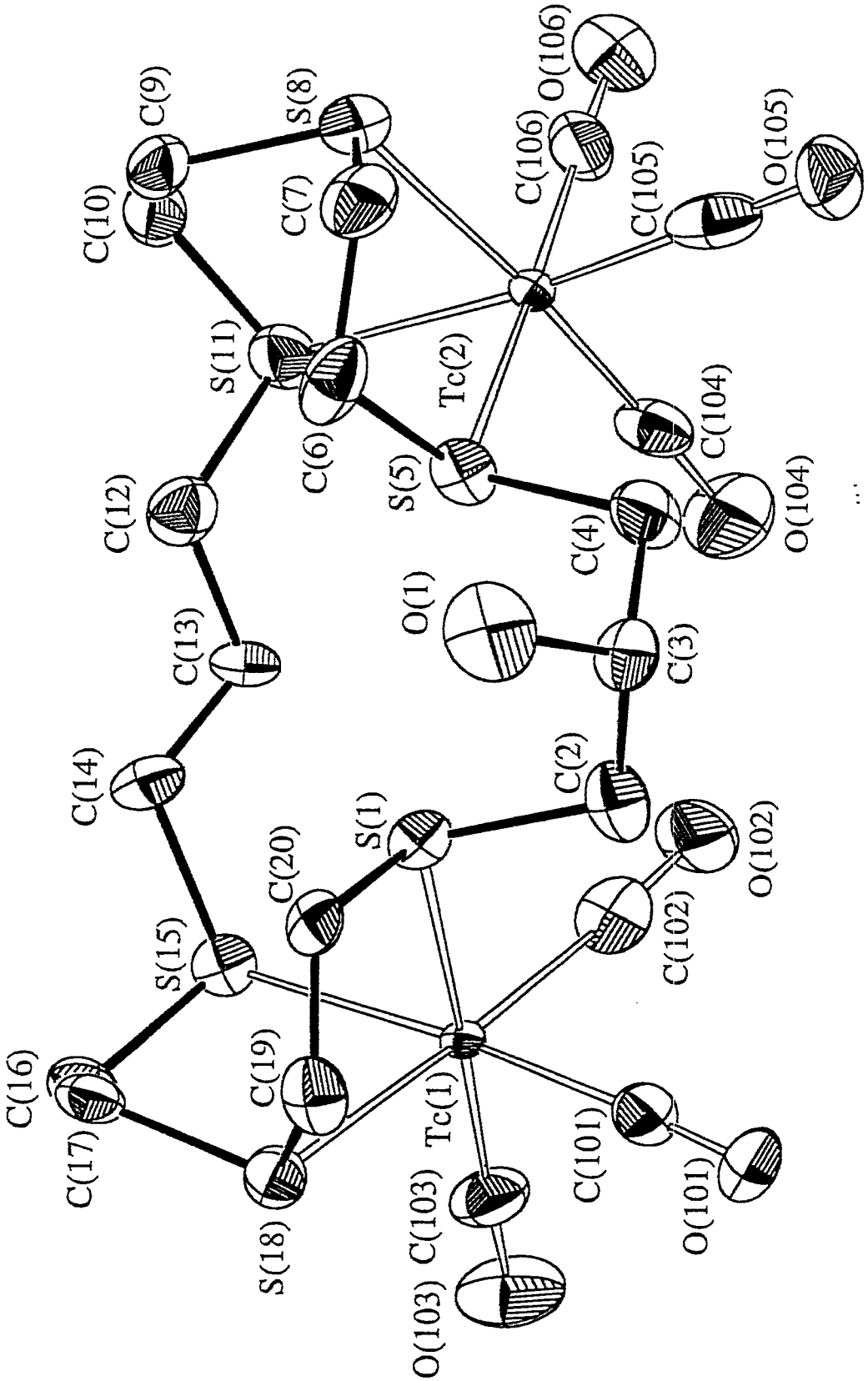
C(202)	52(10)	46(10)	59(10)	2(9)	38(9)	8(8)
S(61)	69(3)	57(3)	81(3)	-1(2)	66(3)	-3(2)
O(61)	94(9)	75(9)	132(12)	1(8)	104(10)	4(7)
O(62)	77(9)	80(10)	79(9)	-20(7)	64(8)	-23(7)
O(63)	83(10)	66(9)	136(14)	29(9)	89(11)	8(8)
C(61)	87(12)	75(13)	68(11)	-15(10)	69(11)	-29(10)
C(62)	112(17)	59(12)	109(17)	-1(12)	98(16)	11(12)
C(63)	96(15)	88(16)	95(15)	19(13)	88(15)	28(13)
C(64)	89(13)	61(11)	83(13)	19(10)	78(13)	22(10)
C(65)	65(11)	82(13)	60(10)	5(9)	55(10)	-5(10)
C(66)	78(12)	53(10)	79(12)	0(9)	69(11)	1(9)
C(67)	185(26)	84(17)	136(20)	50(15)	149(22)	61(17)
S(71)	71(3)	62(3)	87(3)	0(2)	71(3)	0(2)
O(71)	93(10)	113(13)	111(11)	-44(10)	93(10)	-35(9)
O(72)	115(11)	73(10)	135(13)	43(9)	112(12)	30(8)
O(73)	110(11)	130(14)	138(13)	-29(11)	116(12)	-14(10)
C(71)	84(13)	58(11)	97(14)	11(10)	84(13)	11(10)
C(72)	94(15)	86(15)	93(14)	13(12)	87(14)	17(12)
C(73)	177(28)	72(15)	138(23)	40(16)	146(24)	54(18)
C(74)	95(16)	108(19)	83(15)	13(14)	81(15)	2(15)
C(75)	117(19)	107(19)	87(15)	29(13)	88(16)	53(16)
C(76)	116(20)	108(20)	98(17)	-13(15)	89(17)	27(16)
C(77)	108(21)	154(30)	137(25)	50(22)	100(22)	62(21)
O(200)	30(9)	40(10)	55(11)	5(9)	36(9)	2(8)
C(200)	21(13)	186(47)	61(20)	72(26)	33(15)	42(20)
O(300)	70(16)	191(35)	38(12)	44(17)	44(13)	48(20)
C(300)	64(22)	152(44)	49(19)	35(23)	48(19)	53(26)
O(400)	123(26)	105(26)	144(30)	18(22)	120(27)	34(21)
C(400)	173(48)	99(36)	188(51)	-91(36)	173(48)	-83(35)
O(500)	50(13)	136(26)	77(16)	-49(17)	53(14)	-16(15)
C(500)	94(34)	241(78)	112(37)	-112(46)	90(34)	-71(42)

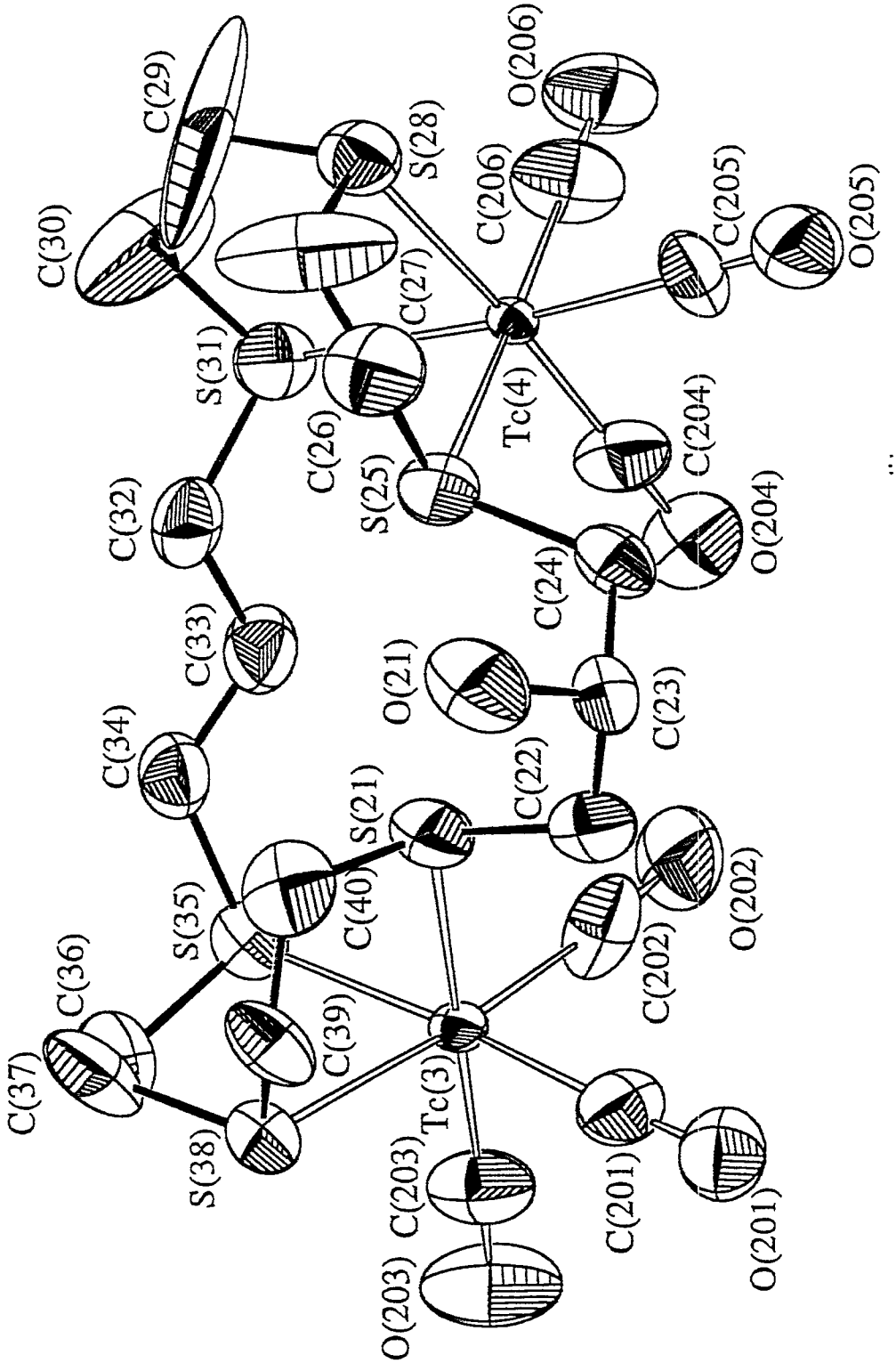
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Tc2(CO)6(20ane-S6-OH)](O3S(C6H4)CH3)2 x MeOH.

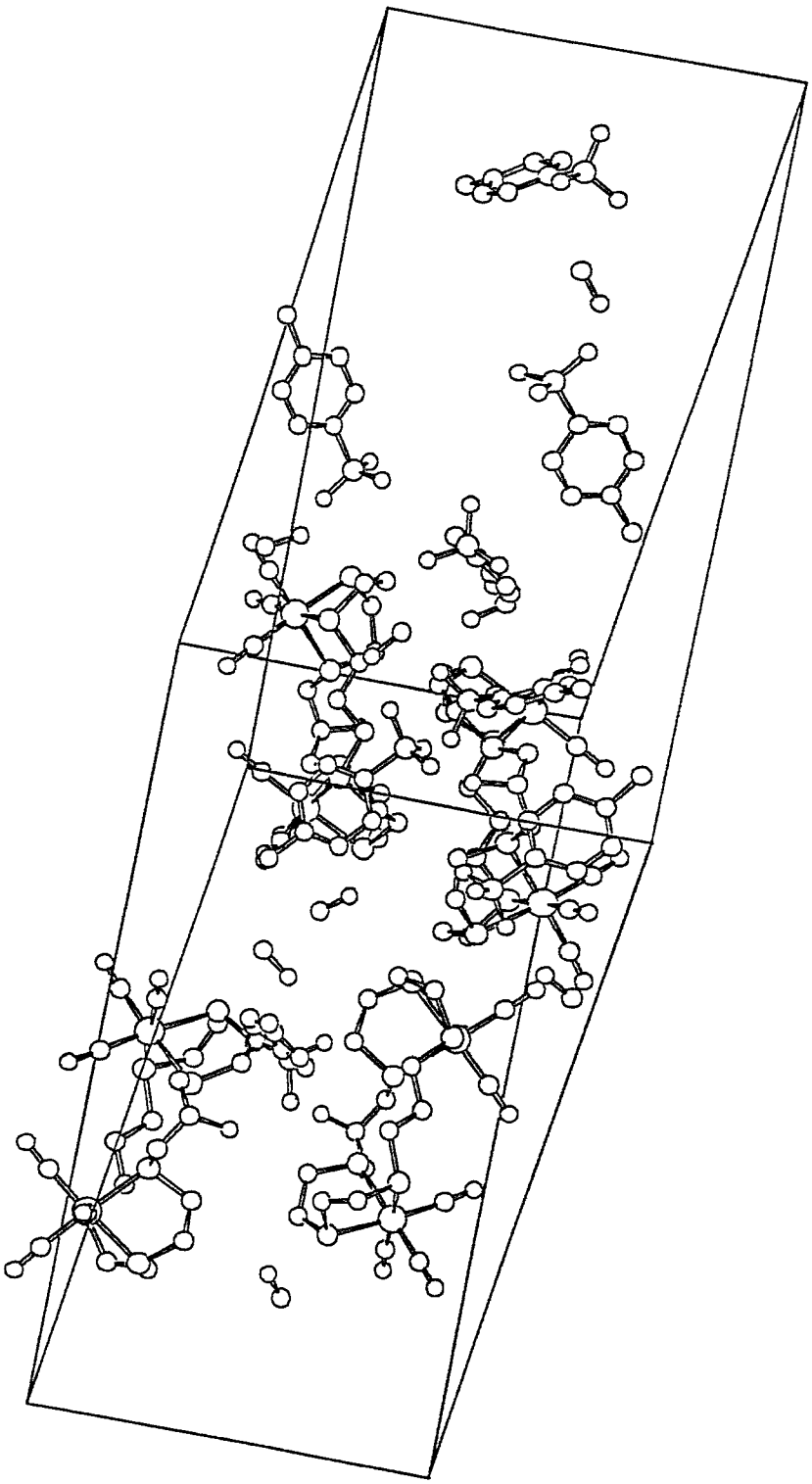
	x	y	z	U(eq)
H(2A)	1429(12)	6408(13)	2751(13)	77
H(2B)	1812(12)	7336(13)	2789(13)	77
H(3)	382(13)	6485(12)	1209(13)	67
H(4A)	1214(13)	7627(17)	1405(14)	88
H(4B)	755(13)	6781(17)	695(14)	88
H(6A)	2980(18)	5266(13)	2173(19)	102
H(6B)	1814(18)	5272(13)	1365(19)	102
H(7A)	1300(15)	6120(15)	191(15)	90
H(7B)	2003(15)	5274(15)	586(15)	90
H(9A)	4045(15)	5580(13)	2439(15)	75
H(9B)	4139(15)	5764(13)	1928(15)	75
H(10A)	5029(19)	7234(18)	2811(19)	114
H(10B)	5609(19)	6443(18)	3614(19)	114
H(12A)	4486(15)	6144(14)	3677(15)	80
H(12B)	5676(15)	6222(14)	4561(15)	80
H(13A)	5789(13)	7492(12)	5274(11)	62
H(13B)	4615(13)	7320(12)	4424(11)	62
H(14A)	6184(14)	5953(12)	5853(13)	66
H(14B)	5010(14)	5737(12)	4974(13)	66
H(16A)	6648(12)	5349(13)	7138(11)	68
H(16B)	6372(12)	5849(13)	7425(11)	68
H(17A)	5540(12)	4366(12)	6651(11)	62
H(17B)	4960(12)	4742(12)	5676(11)	62
H(19A)	3139(13)	4196(12)	4764(13)	77
H(19B)	2524(13)	5147(12)	4357(13)	77
H(20A)	2134(13)	4783(11)	3207(12)	63
H(20B)	3284(13)	4523(11)	4040(12)	63
H(1)	1089(12)	5067(12)	1818(12)	156
H(42)	5575(11)	9615(12)	2056(12)	66
H(43)	5978(15)	10659(15)	1746(14)	92
H(45)	5912(15)	8434(15)	724(13)	89
H(46)	5509(16)	7403(18)	1078(14)	92
H(47A)	6267(3)	9879(3)	669(3)	183
H(47B)	6829(3)	10653(3)	1477(3)	183
H(47C)	5631(3)	10721(3)	382(3)	183
H(52)	8336(3)	2117(3)	3007(3)	111
H(53)	8128(19)	1127(17)	3523(19)	101
H(55)	8157(16)	3285(20)	4516(16)	102
H(56)	8718(12)	4349(16)	4323(12)	88
H(57A)	7790(19)	783(17)	4062(18)	165
H(57B)	7244(19)	1600(17)	3919(18)	165
H(57C)	8434(19)	1410(17)	4985(18)	165
H(24A)	2196(12)	848(11)	2439(11)	58
H(24B)	2652(12)	1709(11)	2509(11)	58
H(23)	3694(13)	1622(13)	4029(12)	67
H(22A)	3245(13)	1452(11)	4501(12)	64
H(22B)	2860(13)	565(11)	3862(12)	64
H(40A)	2111(16)	2911(12)	3667(16)	86
H(40B)	953(16)	2845(12)	2869(16)	86
H(39A)	1876(15)	3094(14)	4345(14)	84
H(39B)	2684(15)	2302(14)	4877(14)	84
H(37A)	-93(15)	2551(17)	3252(15)	95
H(37B)	-114(15)	2597(17)	2636(15)	95
H(36A)	-1454(14)	1638(14)	1819(15)	84
H(36B)	-648(14)	967(14)	2765(15)	84
H(34A)	-1776(14)	1751(13)	577(13)	77
H(34B)	-619(14)	2040(13)	1455(13)	77
H(33A)	-1677(16)	600(13)	28(16)	85
H(33B)	-495(16)	833(13)	937(16)	85
H(32A)	-907(13)	2407(14)	347(13)	76
H(32B)	-2084(13)	2213(14)	-533(13)	76
H(30A)	-2753(18)	2675(24)	-2169(21)	171
H(30B)	-1880(18)	3187(24)	-1126(21)	171
H(29A)	-1539(35)	3702(27)	-1586(46)	361
H(29B)	-1941(35)	2771(27)	-2191(46)	361
H(27A)	904(26)	3924(24)	406(19)	177
H(27B)	102(26)	3974(24)	181(19)	177
H(26A)	1401(17)	3671(15)	1625(17)	95
H(26B)	1838(17)	3054(15)	1546(17)	95
H(21)	3323(11)	2954(10)	4137(11)	118
H(62)	8837(20)	6191(15)	1192(19)	103
H(63)	7166(18)	6760(16)	-68(17)	98
H(65)	5922(14)	4763(15)	-2012(14)	82
H(66)	7561(14)	4103(13)	-746(14)	80
H(67A)	4824(23)	5914(18)	-2568(21)	170
H(67B)	5273(23)	6934(18)	-2059(21)	170
H(67C)	5166(23)	6150(18)	-1721(21)	170
H(72)	5340(18)	1907(16)	4169(17)	93
H(73)	6957(25)	1323(18)	5412(23)	127
H(75)	8157(21)	3529(20)	7081(18)	123
H(76)	6506(21)	4187(20)	5840(19)	138
H(77A)	8632(23)	1433(24)	6839(24)	217
H(77B)	9033(23)	1896(24)	7684(24)	217
H(77C)	9111(23)	2472(24)	7235(24)	217
H(200)	7241(13)	2684(13)	813(14)	63
H(20C)	7259(21)	4303(32)	605(25)	143
H(20D)	7518(21)	3441(32)	456(25)	143
H(20E)	8408(21)	3955(32)	1505(25)	143
H(300)	676(20)	4683(27)	3124(17)	157
H(30C)	142(29)	5070(35)	3491(26)	134
H(30D)	-192(29)	5591(35)	2706(26)	134
H(30E)	768(29)	5966(35)	3819(26)	134

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H(400)	3427(27)	3659(24)	2000(27)	170
H(40C)	2060(45)	2745(32)	382(45)	171
H(40D)	2987(45)	2279(32)	1457(45)	171
H(40E)	3200(45)	2918(32)	1152(45)	171
H(500)	7042(18)	9057(23)	4247(19)	136
H(50A)	5634(35)	9603(35)	3654(36)	220
H(50B)	5933(35)	10199(35)	3419(36)	220
H(50C)	6756(35)	10023(35)	4539(36)	220


C(16)
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S(18)
C(19)
C(20)
S(15)
C(14)
C(13)
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C(10)
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O(101)
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O(103)


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O(202)
C(37)
C(39)
Tc(3)
S(38)
C(203)
C(201)
O(203)
O(201)



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