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Table 16A. Crystal data, data collection, structure solution and refinement parameters for **16**.

Empirical formula	$C_{19}H_{24}C_{l2}SZr$
Formula weight	446.56
Temperature	110(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pca2(1)
Unit cell dimensions	a = 16.763(3) A, $\alpha = 90°$
	b = 8.9146(14) A, $\beta = 90°$
	c = 25.051(4) A, $\gamma = 90°$
Volume	3743.6(10) A^3
Z, Calculated density	8, 1.585 Mg/m^3
Absorption coefficient	0.981 mm^{-1}
F(000)	1824
Crystal size	0.4 x 0.2 x 0.1 mm
Theta range for data collection	1.63 to 31.05°
Limiting indices	-24<=h<=24, -12<=k<=10, -36<=l<=36
Reflections collected / unique	33704 / 11837 [R(int) = 0.0427]
Completeness to theta = 31.05	97.6%
Absorption correction	sadabs
Max. and min. transmission	0.56365 and 0.80176
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11806 / 1 / 415
Goodness-of-fit on F^2	0.980
Final R indices [I>2σ(I)]	$R_1 = 0.0522$, $wR_2 = 0.1236$
R indices (all data)	$R_1 = 0.0654$, $wR_2 = 0.1349$
Absolute structure parameter	0.45(4)
Largest diff. peak and hole	3.227 and -1.057 $e.A^{-3}$

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Table 16B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **16**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Zr(1)	2234(1)	-5345(1)	6547(1)	13(1)
Cl(1)	2146(1)	-7798(1)	6120(1)	25(1)
Cl(2)	865(1)	-5264(1)	6885(1)	24(1)
S(1)	2531(1)	-2849(1)	7734(1)	24(1)
C(1)	3477(3)	-4908(5)	7043(2)	18(1)
C(2)	2859(3)	-4440(5)	7398(2)	18(1)
C(3)	1851(3)	-3934(5)	8093(2)	22(1)
C(4)	1864(3)	-5398(5)	7971(2)	19(1)
C(5)	2442(3)	-5736(5)	7573(2)	17(1)
C(6)	2788(2)	-7021(5)	7322(2)	17(1)
C(7)	3429(3)	-6489(5)	7005(2)	17(1)
C(8)	2572(3)	-8632(5)	7418(2)	22(1)
C(9)	4017(3)	-7461(5)	6713(2)	24(1)
C(10)	1615(3)	-3916(5)	5776(2)	17(1)
C(11)	1906(3)	-2842(4)	6148(2)	14(1)
C(12)	2739(3)	-2917(5)	6161(2)	18(1)
C(13)	2982(3)	-4081(5)	5802(2)	17(1)
C(14)	2275(3)	-4661(5)	5556(2)	16(1)
C(15)	758(3)	-4128(5)	5619(2)	20(1)
C(16)	1413(3)	-1678(5)	6437(2)	22(1)
C(17)	3287(3)	-1776(5)	6419(2)	24(1)
C(18)	3822(3)	-4505(5)	5642(2)	22(1)
C(19)	2269(3)	-5737(6)	5098(2)	22(1)
Zr(1')	67(1)	376(1)	4034(1)	14(1)
Cl(1')	-43(1)	2842(1)	4447(1)	30(1)
Cl(2')	-1313(1)	228(2)	3723(1)	27(1)
S(1')	309(1)	-2125(1)	2838(1)	23(1)
C(1')	1285(3)	-89(5)	3515(2)	17(1)
C(2')	658(3)	-519(5)	3165(2)	16(1)
C(3')	-383(3)	-1039(6)	2492(2)	25(1)
C(4')	-372(3)	443(6)	2611(2)	23(1)
C(5')	236(3)	778(5)	3001(2)	19(1)
C(6')	593(3)	2037(5)	3246(2)	16(1)
C(7')	1246(3)	1511(5)	3553(2)	16(1)
C(8')	381(3)	3651(5)	3153(2)	21(1)
C(9')	1837(3)	2463(5)	3848(2)	21(1)
C(10')	589(3)	-2045(5)	4410(2)	17(1)
C(11')	869(3)	-880(5)	4754(2)	18(1)
C(12')	197(3)	-258(5)	5021(2)	16(1)
C(13')	-498(3)	-995(5)	4831(2)	17(1)
C(14')	-243(3)	-2095(4)	4456(2)	15(1)
C(15')	1087(3)	-3197(5)	4139(2)	21(1)

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Table 16B. *(Continued)*

C(16')	1730(3)	-528(5)	4877(2)	23(1)
C(17')	216(3)	850(6)	5476(2)	24(1)
C(18')	-1324(3)	-693(6)	5034(2)	24(1)
C(19')	-785(3)	-3255(5)	4197(2)	23(1)

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Table 16C. Bond lengths [Å] and angles [deg] for **16**.

Zr(1)-Cl(1)	2.4391(13)
Zr(1)-Cl(2)	2.4467(12)
Zr(1)-C(1)	2.457(4)
Zr(1)-C(11)	2.505(4)
Zr(1)-C(2)	2.509(4)
Zr(1)-C(13)	2.514(4)
Zr(1)-C(12)	2.516(5)
Zr(1)-C(7)	2.524(4)
Zr(1)-C(10)	2.535(4)
Zr(1)-C(14)	2.557(4)
Zr(1)-C(5)	2.617(4)
Zr(1)-C(6)	2.620(4)
S(1)-C(2)	1.738(5)
S(1)-C(3)	1.746(5)
C(1)-C(7)	1.415(6)
C(1)-C(2)	1.428(6)
C(2)-C(5)	1.420(6)
C(3)-C(4)	1.340(7)
C(4)-C(5)	1.424(6)
C(5)-C(6)	1.429(6)
C(6)-C(7)	1.418(6)
C(6)-C(8)	1.501(6)
C(7)-C(9)	1.502(6)
C(10)-C(14)	1.405(6)
C(10)-C(11)	1.423(6)
C(10)-C(15)	1.501(6)
C(11)-C(12)	1.398(6)
C(11)-C(16)	1.511(6)
C(12)-C(13)	1.432(6)
C(12)-C(17)	1.515(6)
C(13)-C(14)	1.432(6)
C(13)-C(18)	1.512(6)
C(14)-C(19)	1.495(6)

Zr(1')-Cl(1')	2.4364(13)
Zr(1')-Cl(2')	2.4436(13)
Zr(1')-C(1')	2.456(4)
Zr(1')-C(14')	2.498(4)
Zr(1')-C(10')	2.511(4)
Zr(1')-C(11')	2.513(4)
Zr(1')-C(2')	2.521(4)
Zr(1')-C(7')	2.526(4)
Zr(1')-C(13')	2.525(4)
Zr(1')-C(12')	2.545(4)
Zr(1')-C(6')	2.621(4)
Zr(1')-C(5')	2.627(5)
S(1')-C(3')	1.742(5)
S(1')-C(2')	1.750(4)
C(1')-C(2')	1.422(6)
C(1')-C(7')	1.431(6)
C(2')-C(5')	1.416(6)
C(3')-C(4')	1.354(7)
C(4')-C(5')	1.444(6)
C(5')-C(6')	1.411(6)
C(6')-C(7')	1.418(6)
C(6')-C(8')	1.501(6)
C(7')-C(9')	1.500(6)
C(10')-C(14')	1.400(6)
C(10')-C(11')	1.429(6)
C(10')-C(15')	1.487(6)
C(11')-C(12')	1.422(6)
C(11')-C(16')	1.508(6)
C(12')-C(13')	1.419(6)
C(12')-C(17')	1.509(6)
C(13')-C(14')	1.424(6)
C(13')-C(18')	1.500(6)
C(14')-C(19')	1.522(6)

Cl(1)-Zr(1)-Cl(2)	96.98(4)
Cl(1)-Zr(1)-C(1)	114.51(11)
Cl(2)-Zr(1)-C(1)	128.00(11)
Cl(1)-Zr(1)-C(11)	127.65(10)
Cl(2)-Zr(1)-C(11)	84.61(10)
C(1)-Zr(1)-C(11)	104.26(15)
Cl(1)-Zr(1)-C(2)	133.32(11)
Cl(2)-Zr(1)-C(2)	95.05(12)
C(1)-Zr(1)-C(2)	33.40(15)
C(11)-Zr(1)-C(2)	98.26(14)
C(13)-Zr(1)-C(12)	33.07(14)
Cl(1)-Zr(1)-C(7)	83.37(10)
Cl(2)-Zr(1)-C(7)	126.78(10)

Cl(1)-Zr(1)-C(13)	96.12(11)
Cl(2)-Zr(1)-C(13)	135.32(11)
C(1)-Zr(1)-C(13)	83.19(15)
C(11)-Zr(1)-C(13)	54.17(14)
C(2)-Zr(1)-C(13)	106.2(2)
Cl(1)-Zr(1)-C(12)	128.54(11)
Cl(2)-Zr(1)-C(12)	115.03(10)
C(1)-Zr(1)-C(12)	76.86(15)
C(11)-Zr(1)-C(12)	32.33(14)
C(2)-Zr(1)-C(12)	84.80(15)
C(1)-Zr(1)-C(10)	130.75(14)
C(11)-Zr(1)-C(10)	32.80(13)
C(2)-Zr(1)-C(10)	131.04(15)

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Table 16C. *(Continued 1)*

C(1)-Zr(1)-C(7)	32.98(14)
C(11)-Zr(1)-C(7)	135.66(14)
C(2)-Zr(1)-C(7)	54.00(14)
C(13)-Zr(1)-C(7)	97.06(14)
C(12)-Zr(1)-C(7)	104.78(14)
Cl(1)-Zr(1)-C(10)	95.28(11)
Cl(2)-Zr(1)-C(10)	82.22(10)
C(2)-Zr(1)-C(14)	137.49(15)
C(13)-Zr(1)-C(14)	32.79(14)
C(12)-Zr(1)-C(14)	54.08(14)
C(7)-Zr(1)-C(14)	121.07(14)
C(10)-Zr(1)-C(14)	32.03(14)
Cl(1)-Zr(1)-C(5)	108.60(11)
Cl(2)-Zr(1)-C(5)	77.83(11)
C(1)-Zr(1)-C(5)	53.94(14)
C(11)-Zr(1)-C(5)	122.63(14)
C(2)-Zr(1)-C(5)	32.07(14)
C(13)-Zr(1)-C(6)	128.98(14)
C(12)-Zr(1)-C(6)	130.98(14)
C(7)-Zr(1)-C(6)	31.94(13)
C(10)-Zr(1)-C(6)	174.84(14)
C(14)-Zr(1)-C(6)	147.75(14)
C(5)-Zr(1)-C(6)	31.66(14)
C(2)-S(1)-C(3)	90.2(2)
C(7)-C(1)-C(2)	107.0(4)
C(7)-C(1)-Zr(1)	76.2(2)
C(2)-C(1)-Zr(1)	75.3(3)
C(14)-C(10)-C(11)	107.7(4)
C(14)-C(10)-C(15)	126.3(4)
C(11)-C(10)-C(15)	125.8(4)
C(1)-C(7)-Zr(1)	70.9(2)
C(15)-C(10)-Zr(1)	121.9(3)
C(2)-C(5)-C(4)	112.3(4)
C(2)-C(5)-C(6)	108.5(4)
C(4)-C(5)-C(6)	138.9(4)
C(2)-C(5)-Zr(1)	69.8(2)
C(4)-C(5)-Zr(1)	124.7(3)
C(12)-C(11)-C(10)	109.0(4)
C(12)-C(11)-C(16)	124.7(4)
C(10)-C(11)-C(16)	125.9(4)
C(12)-C(11)-Zr(1)	74.3(2)
C(10)-C(11)-Zr(1)	74.8(2)
C(16)-C(11)-Zr(1)	122.7(3)
C(11)-C(12)-C(13)	107.7(4)
C(11)-C(12)-C(17)	125.6(4)

C(13)-Zr(1)-C(10)	54.13(15)
C(12)-Zr(1)-C(10)	54.08(15)
C(7)-Zr(1)-C(10)	150.97(14)
Cl(1)-Zr(1)-C(14)	77.85(10)
Cl(2)-Zr(1)-C(14)	110.76(11)
C(1)-Zr(1)-C(14)	115.48(14)
C(11)-Zr(1)-C(14)	53.64(13)
C(13)-Zr(1)-C(5)	136.22(15)
C(12)-Zr(1)-C(5)	116.55(14)
C(7)-Zr(1)-C(5)	52.68(14)
C(10)-Zr(1)-C(5)	150.39(14)
C(14)-Zr(1)-C(5)	168.98(14)
Cl(1)-Zr(1)-C(6)	80.49(10)
Cl(2)-Zr(1)-C(6)	95.31(10)
C(1)-Zr(1)-C(6)	54.21(14)
C(11)-Zr(1)-C(6)	151.75(13)
C(2)-Zr(1)-C(6)	53.54(14)
C(6)-C(7)-Zr(1)	77.7(2)
C(9)-C(7)-Zr(1)	122.2(3)
C(3)-C(4)-C(5)	112.2(4)
C(5)-C(2)-C(1)	108.1(4)
C(5)-C(2)-S(1)	111.1(4)
C(1)-C(2)-S(1)	140.3(4)
C(5)-C(2)-Zr(1)	78.2(3)
C(1)-C(2)-Zr(1)	71.3(2)
S(1)-C(2)-Zr(1)	122.8(2)
C(4)-C(3)-S(1)	114.3(3)
C(6)-C(5)-Zr(1)	74.3(2)
C(7)-C(6)-C(5)	106.6(4)
C(7)-C(6)-C(8)	126.3(4)
C(5)-C(6)-C(8)	126.8(4)
C(7)-C(6)-Zr(1)	70.3(2)
C(5)-C(6)-Zr(1)	74.1(2)
C(8)-C(6)-Zr(1)	125.5(3)
C(1)-C(7)-C(6)	109.8(4)
C(1)-C(7)-C(9)	124.7(4)
C(6)-C(7)-C(9)	125.3(4)
C(13)-C(12)-Zr(1)	73.4(3)
C(17)-C(12)-Zr(1)	128.2(3)
C(14)-C(13)-C(12)	107.3(4)
C(14)-C(13)-C(18)	124.4(4)
C(12)-C(13)-C(18)	127.7(4)
C(14)-C(13)-Zr(1)	75.3(2)
C(12)-C(13)-Zr(1)	73.6(2)
C(18)-C(13)-Zr(1)	123.3(3)

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Table 16C. *(Continued 2)*

C(10')-Zr(1')-C(13')	54.46(14)
C(11')-Zr(1')-C(13')	54.37(13)
C(2')-Zr(1')-C(13')	132.61(14)
Cl(1')-Zr(1')-C(6')	80.56(10)
Cl(2')-Zr(1')-C(6')	96.24(10)
C(1')-Zr(1')-C(6')	54.33(14)
C(14')-Zr(1')-C(6')	152.50(13)
C(10')-Zr(1')-C(6')	130.58(14)
C(11')-Zr(1')-C(6')	127.79(14)
C(2')-Zr(1')-C(6')	52.84(13)
C(12')-C(13')-C(18')	124.2(4)
C(13)-C(12)-C(17)	125.6(4)
C(10)-C(14)-C(19)	126.8(4)
C(13)-C(14)-C(19)	124.7(4)
C(10)-C(14)-Zr(1)	73.1(2)
C(13)-C(14)-Zr(1)	71.9(2)
C(19)-C(14)-Zr(1)	126.3(3)
C(7')-Zr(1')-C(6')	31.91(13)
C(13')-Zr(1')-C(6')	174.42(14)
C(12')-Zr(1')-C(6')	145.95(14)
C(6')-Zr(1')-C(5')	31.20(14)
C(3')-S(1')-C(2')	90.0(2)
C(2')-C(1')-C(7')	106.0(4)
C(2')-C(1')-Zr(1')	75.9(3)
C(7')-C(1')-Zr(1')	76.0(2)
C(17')-C(12')-Zr(1')	126.2(3)
C(12')-C(13')-C(14')	107.0(4)
C(14')-C(10')-C(11')	107.4(4)
C(14')-C(10')-C(15')	125.1(4)
C(11')-C(10')-C(15')	126.3(4)
C(14')-C(10')-Zr(1')	73.2(2)
C(11')-C(10')-Zr(1')	73.5(2)
C(1')-Zr(1')-C(14')	104.37(15)
Cl(1')-Zr(1')-C(10')	129.97(10)
Cl(2')-Zr(1')-C(10')	113.74(11)
C(1')-Zr(1')-C(10')	76.33(14)
C(14')-Zr(1')-C(10')	32.45(14)
Cl(1')-Zr(1')-C(11')	97.90(11)
Cl(2')-Zr(1')-C(11')	135.31(11)
C(1')-Zr(1')-C(11')	81.95(14)
C(14')-Zr(1')-C(11')	54.16(14)
C(10')-Zr(1')-C(11')	33.06(14)
C(10')-Zr(1')-C(7')	104.50(14)
C(11')-Zr(1')-C(7')	95.89(14)
C(2')-Zr(1')-C(7')	53.66(14)
Cl(1')-Zr(1')-C(13')	94.14(11)
Cl(2')-Zr(1')-C(13')	82.57(10)
C(1')-Zr(1')-C(13')	130.45(15)
C(14')-Zr(1')-C(13')	32.93(14)

C(2')-Zr(1')-C(12')	137.28(14)
C(7')-Zr(1')-C(12')	119.04(14)
C(13')-Zr(1')-C(12')	32.51(15)
Cl(1')-Zr(1')-C(5')	107.67(11)
Cl(2')-Zr(1')-C(5')	78.20(11)
C(1')-Zr(1')-C(5')	54.00(15)
C(14')-Zr(1')-C(5')	124.02(14)
C(10')-Zr(1')-C(5')	116.65(14)
C(11')-Zr(1')-C(5')	135.2(2)
C(2')-Zr(1')-C(5')	31.85(14)
C(19')-C(14')-Zr(1')	122.9(3)
C(14)-C(10)-Zr(1)	74.8(2)
C(11)-C(10)-Zr(1)	72.4(2)
C(11)-C(12)-Zr(1)	73.4(2)
C(10)-C(14)-C(13)	108.1(4)
Cl(1')-Zr(1')-Cl(2')	96.46(5)
Cl(1')-Zr(1')-C(1')	116.10(11)
C(7')-Zr(1')-C(5')	52.50(14)
C(13')-Zr(1')-C(5')	152.26(15)
C(12')-Zr(1')-C(5')	167.83(15)
C(1')-C(2')-S(1')	139.1(4)
C(5')-C(2')-Zr(1')	78.2(3)
C(1')-C(2')-Zr(1')	70.9(2)
S(1')-C(2')-Zr(1')	122.1(2)
C(4')-C(3')-S(1')	115.1(4)
C(10')-C(14')-Zr(1')	74.3(2)
C(13')-C(14')-Zr(1')	74.6(2)
Cl(1')-Zr(1')-Cl(2')	96.46(5)
Cl(1')-Zr(1')-C(1')	116.10(11)
Cl(2')-Zr(1')-C(1')	127.53(11)
Cl(1')-Zr(1')-C(14')	126.86(10)
Cl(2')-Zr(1')-C(14')	83.71(11)
Cl(1')-Zr(1')-C(2')	133.00(10)
Cl(2')-Zr(1')-C(2')	94.57(11)
C(1')-Zr(1')-C(2')	33.17(14)
C(14')-Zr(1')-C(2')	99.68(14)
C(10')-Zr(1')-C(2')	85.11(13)
C(11')-Zr(1')-C(2')	105.6(2)
Cl(1')-Zr(1')-C(7')	84.29(10)
Cl(2')-Zr(1')-C(7')	127.58(10)
C(1')-Zr(1')-C(7')	33.34(14)
C(14')-Zr(1')-C(7')	135.88(14)
C(7')-Zr(1')-C(13')	149.83(14)
Cl(1')-Zr(1')-C(12')	78.13(11)
Cl(2')-Zr(1')-C(12')	112.24(11)
C(1')-Zr(1')-C(12')	113.91(14)
C(14')-Zr(1')-C(12')	53.90(14)
C(10')-Zr(1')-C(12')	54.23(14)
C(11')-Zr(1')-C(12')	32.65(14)

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Table 16C. *(Continued 3)*

C(3')-C(4')-C(5')	111.1(4)
C(5')-C(2')-C(1')	109.2(4)
C(5')-C(2')-S(1')	111.4(3)
C(6')-C(5')-C(2')	108.2(4)
C(6')-C(5')-C(4')	139.2(5)
C(2')-C(5')-C(4')	112.3(4)
C(6')-C(5')-Zr(1')	74.2(3)
C(2')-C(5')-Zr(1')	70.0(3)
C(4')-C(5')-Zr(1')	124.2(3)
C(5')-C(6')-C(7')	107.5(4)
C(5')-C(6')-C(8')	126.5(4)
C(7')-C(6')-C(8')	125.7(4)
C(5')-C(6')-Zr(1')	74.6(3)
C(10')-C(11')-Zr(1')	73.4(2)
C(16')-C(11')-Zr(1')	124.5(3)
C(13')-C(12')-C(11')	108.2(4)
C(13')-C(12')-C(17')	125.0(4)
C(11')-C(12')-C(17')	126.4(4)
C(13')-C(12')-Zr(1')	73.0(2)
C(11')-C(12')-Zr(1')	72.4(2)

C(15')-C(10')-Zr(1')	128.2(3)
C(12')-C(11')-C(10')	107.9(4)
C(12')-C(11')-C(16')	125.5(4)
C(7')-C(6')-Zr(1')	70.4(2)
C(8')-C(6')-Zr(1')	125.4(3)
C(6')-C(7')-C(1')	109.2(4)
C(6')-C(7')-C(9')	126.2(4)
C(1')-C(7')-C(9')	124.4(4)
C(6')-C(7')-Zr(1')	77.7(2)
C(1')-C(7')-Zr(1')	70.6(2)
C(9')-C(7')-Zr(1')	120.6(3)
C(10')-C(11')-C(16')	126.0(4)
C(12')-C(11')-Zr(1')	74.9(2)
C(14')-C(13')-C(18')	128.6(4)
C(12')-C(13')-Zr(1')	74.5(2)
C(14')-C(13')-Zr(1')	72.5(2)
C(18')-C(13')-Zr(1')	121.8(3)
C(10')-C(14')-C(13')	109.4(4)
C(10')-C(14')-C(19')	125.5(4)
C(13')-C(14')-C(19')	124.7(4)

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Table 16D. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **16**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	12(1)	13(1)	14(1)	1(1)	-1(1)	-1(1)
Cl(1)	41(1)	13(1)	22(1)	-1(1)	-11(1)	-3(1)
Cl(2)	13(1)	36(1)	23(1)	10(1)	2(1)	0(1)
S(1)	29(1)	19(1)	24(1)	-6(1)	-2(1)	2(1)
C(1)	12(2)	20(2)	20(2)	3(2)	-7(2)	-5(2)
C(2)	19(2)	19(2)	16(2)	-3(2)	-4(2)	1(2)
C(3)	19(2)	22(2)	23(2)	-3(2)	-1(2)	2(2)
C(4)	18(2)	23(2)	15(2)	-2(2)	1(2)	-1(2)
C(5)	13(2)	25(2)	14(2)	0(2)	-2(2)	-1(2)
C(6)	15(2)	18(2)	16(2)	3(2)	-4(2)	-1(2)
C(7)	17(2)	16(2)	16(2)	2(2)	-1(2)	-3(2)
C(8)	26(2)	16(2)	24(2)	3(2)	-4(2)	0(2)
C(9)	18(2)	27(2)	26(2)	-3(2)	0(2)	6(2)
C(10)	14(2)	18(2)	18(2)	3(2)	-2(2)	3(2)
C(11)	24(2)	4(2)	13(2)	2(1)	1(2)	-1(2)
C(12)	16(2)	16(2)	21(2)	-2(2)	2(2)	0(2)
C(13)	16(2)	18(2)	17(2)	2(2)	6(2)	0(2)
C(14)	20(2)	12(2)	14(2)	0(2)	0(2)	-1(2)
C(15)	18(2)	24(2)	19(2)	3(2)	-7(2)	4(2)
C(16)	22(2)	14(2)	31(2)	-2(2)	3(2)	3(2)
C(17)	27(2)	17(2)	28(2)	1(2)	2(2)	-6(2)
C(18)	15(2)	28(3)	23(2)	1(2)	6(2)	3(2)
C(19)	26(3)	27(2)	14(2)	-7(2)	1(2)	1(2)
Zr(1')	14(1)	12(1)	15(1)	1(1)	1(1)	1(1)
Cl(1')	51(1)	14(1)	24(1)	0(1)	15(1)	4(1)
Cl(2')	12(1)	40(1)	29(1)	13(1)	-2(1)	0(1)
S(1')	25(1)	19(1)	24(1)	-6(1)	1(1)	-1(1)
C(1')	14(2)	22(2)	14(2)	-1(2)	5(2)	0(2)
C(2')	14(2)	19(2)	14(2)	-3(2)	2(2)	0(2)
C(3')	22(2)	35(3)	19(2)	-4(2)	-1(2)	-1(2)
C(4')	17(2)	37(3)	14(2)	5(2)	-3(2)	0(2)
C(5')	19(2)	21(2)	18(2)	-2(2)	0(2)	1(2)
C(6')	20(2)	13(2)	16(2)	4(2)	-4(2)	-1(2)
C(7')	15(2)	18(2)	15(2)	1(2)	3(1)	-5(2)
C(8')	23(2)	15(2)	24(2)	3(2)	4(2)	4(2)
C(9')	21(2)	22(2)	22(2)	-3(2)	-1(2)	-4(2)
C(10')	18(2)	16(2)	16(2)	1(2)	-3(2)	1(2)
C(11')	15(2)	18(2)	19(2)	2(2)	-3(2)	-2(2)
C(12')	15(2)	20(2)	12(2)	5(2)	-3(1)	3(2)
C(13')	16(2)	15(2)	21(2)	7(2)	4(2)	1(2)
C(14')	26(2)	6(2)	13(2)	2(1)	0(2)	-2(2)
C(15')	22(2)	14(2)	26(2)	-1(2)	1(2)	4(2)

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Table 16D. *(Continued)*

C(16')	18(2)	28(3)	23(2)	0(2)	-5(2)	2(2)
C(17')	27(2)	28(3)	19(2)	-4(2)	-2(2)	1(2)
C(18')	15(2)	30(2)	26(2)	6(2)	4(2)	1(2)
C(19')	23(2)	19(2)	26(2)	-2(2)	-5(2)	-2(2)

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Table 16E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **16**.

Atom	x	y	z	U(eq)
H(1A)	3934(3)	-4276(5)	6920(2)	21
H(3A)	1501(3)	-3522(5)	8353(2)	26
H(4A)	1527(3)	-6125(5)	8132(2)	23
H(8A)	2105(3)	-8684(5)	7652(2)	33
H(8B)	3022(3)	-9147(5)	7588(2)	33
H(8C)	2450(3)	-9118(5)	7077(2)	33
H(9A)	3856(3)	-8514(5)	6744(2)	36
H(9B)	4549(3)	-7330(5)	6869(2)	36
H(9C)	4030(3)	-7173(5)	6335(2)	36
H(15A)	419(3)	-3470(5)	5836(2)	30
H(15B)	603(3)	-5175(5)	5678(2)	30
H(15C)	691(3)	-3877(5)	5241(2)	30
H(16A)	845(3)	-1859(5)	6367(2)	33
H(16B)	1558(3)	-676(5)	6309(2)	33
H(16C)	1514(3)	-1746(5)	6822(2)	33
H(17A)	3843(3)	-2089(5)	6372(2)	36
H(17B)	3165(3)	-1705(5)	6801(2)	36
H(17C)	3206(3)	-795(5)	6251(2)	36
H(18A)	4204(3)	-3964(5)	5867(2)	33
H(18B)	3910(3)	-4239(5)	5267(2)	33
H(18C)	3896(3)	-5588(5)	5689(2)	33
H(19A)	2813(3)	-6088(6)	5029(2)	33
H(19B)	2060(3)	-5234(6)	4780(2)	33
H(19C)	1928(3)	-6596(6)	5186(2)	33
H(1'A)	1745(3)	-731(5)	3627(2)	20
H(3'A)	-742(3)	-1456(6)	2239(2)	31
H(4'A)	-719(3)	1167(6)	2458(2)	27
H(8'A)	722(3)	4292(5)	3374(2)	31
H(8'B)	-179(3)	3817(5)	3249(2)	31
H(8'C)	460(3)	3899(5)	2776(2)	31
H(9'A)	2226(3)	1816(5)	4028(2)	32
H(9'B)	1558(3)	3074(5)	4114(2)	32
H(9'C)	2115(3)	3120(5)	3595(2)	32
H(15D)	1650(3)	-2904(5)	4160(2)	31
H(15E)	927(3)	-3277(5)	3764(2)	31
H(15F)	1013(3)	-4168(5)	4316(2)	31
H(16D)	2076(3)	-1102(5)	4637(2)	34
H(16E)	1846(3)	-801(5)	5248(2)	34
H(16F)	1825(3)	547(5)	4826(2)	34
H(17D)	764(3)	1200(6)	5530(2)	37
H(17E)	24(3)	362(6)	5802(2)	37
H(17F)	-128(3)	1706(6)	5391(2)	37

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Table 16E. *(Continued)*

H(18D)	-1705(3)	-1334(6)	4844(2)	36
H(18E)	-1460(3)	363(6)	4973(2)	36
H(18F)	-1348(3)	-911(6)	5417(2)	36
H(19D)	-1341(3)	-3043(5)	4292(2)	34
H(19E)	-640(3)	-4258(5)	4324(2)	34
H(19F)	-724(3)	-3210(5)	3808(2)	34

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Table 17A. Crystal data, data collection, structure solution and refinement parameters for **17**.

Empirical formula	$C_{19}H_{24}C_{12}SZr$
Formula weight	446.56
Temperature	110(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.644(2) Å, α = 100.396(4)°
	b = 14.207(4) Å, β = 97.017(4)°
	c = 14.786(4) Å, γ = 105.615(4)°
Volume	1887.7(8) Å^3
Z	4
Density (calculated)	1.571 Mg/m^3
Absorption coefficient	0.973 mm^{-1}
F(000)	912
Crystal size	0.1 × 0.2 × 0.3 mm
Theta range for data collection	1.42 to 27.03°
Index ranges	-12<=h<=12, -18<=k<=18, -18<=l<=18
Reflections collected	17801
Independent reflections	8154 [R(int) = 0.0295]
Completeness to theta = 27.03°	98.5 %
Absorption correction	Semi-empirical from equivalents
T_{min}/T_{max}	0.520 / 0.962
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8154 / 0 / 415
Goodness-of-fit on F^2	1.155
Final R indices [for 7739 rfln with I>2σ(I)]	R1 = 0.0785, wR2 = 0.1861
R indices (all data)	R1 = 0.0986, wR2 = 0.1988
Largest diff. peak and hole	2.272 and -0.757 e·Å^{-3}

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Table 17B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **17**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Zr(1)	11731(1)	14151(1)	7374(1)	17(1)
Zr(1')	6634(1)	9211(1)	7623(1)	18(1)
Cl(1)	11996(2)	12494(1)	6810(1)	28(1)
Cl(2)	9727(2)	13572(1)	8189(1)	29(1)
Cl(1')	4370(2)	8768(1)	8241(1)	30(1)
Cl(2')	6399(2)	7534(1)	6729(1)	28(1)
S(1)	12141(2)	15032(1)	10039(1)	29(1)
S(1')	6388(2)	8687(1)	4963(1)	34(1)
C(1)	13773(7)	14188(5)	8718(4)	26(1)
C(2)	13046(7)	14865(5)	9112(4)	25(1)
C(3)	11934(8)	16141(5)	9768(5)	37(2)
C(4)	12523(8)	16393(5)	9046(4)	32(1)
C(5)	13186(7)	15659(4)	8629(4)	25(1)
C(6)	14074(7)	15475(5)	7942(4)	26(1)
C(7)	14432(7)	14590(5)	8020(4)	28(1)
C(8)	15442(7)	14175(6)	7485(5)	37(2)
C(9)	13916(8)	13280(5)	9067(5)	33(2)
C(10)	9572(7)	13974(5)	6108(4)	24(1)
C(11)	10090(7)	14997(5)	6604(4)	26(1)
C(12)	11486(7)	15423(4)	6425(4)	26(1)
C(13)	11871(7)	14650(5)	5836(4)	27(1)
C(14)	10672(7)	13781(5)	5619(4)	27(1)
C(15)	8071(7)	13272(5)	6044(5)	30(1)
C(16)	9236(7)	15553(5)	7173(5)	34(2)
C(17)	12307(8)	16521(5)	6647(5)	36(2)
C(18)	13237(8)	14802(6)	5414(5)	37(2)
C(19)	10544(8)	12846(5)	4924(4)	36(2)
C(1')	4917(7)	9610(5)	6341(4)	26(1)
C(2')	6126(7)	9452(5)	5923(4)	27(1)
C(3')	8267(8)	9334(6)	5257(5)	41(2)
C(4')	8664(8)	10068(5)	6011(4)	32(2)
C(5')	7439(7)	10176(5)	6428(4)	27(1)
C(6')	7036(7)	10817(4)	7142(4)	27(1)
C(7')	5497(7)	10475(5)	7064(4)	26(1)
C(8')	4605(8)	10982(5)	7622(5)	37(2)
C(9')	3325(7)	9048(5)	6012(5)	38(2)
C(10')	8119(7)	8633(5)	8835(4)	26(1)
C(11')	9108(7)	9146(4)	8323(4)	25(1)
C(12')	9179(7)	10167(5)	8531(4)	27(1)
C(13')	8182(7)	10276(5)	9140(4)	29(1)
C(14')	7558(7)	9340(5)	9357(4)	25(1)
C(15')	7819(7)	7552(5)	8887(5)	31(1)
C(16')	10043(7)	8693(5)	7723(5)	32(1)
C(17')	10284(7)	11011(5)	8293(5)	35(2)
C(18')	7962(9)	11257(5)	9612(5)	40(2)
C(19')	6610(8)	9165(5)	10074(4)	34(2)

Table 17C. Bond lengths [Å] and angles [deg] for **17**.

Zr(1)-Cl(2)	2.4359(15)
Zr(1)-Cl(1)	2.4442(16)
Zr(1)-C(6)	2.455(6)
Zr(1)-C(13)	2.509(6)
Zr(1)-C(5)	2.513(6)
Zr(1)-C(11)	2.514(6)
Zr(1)-C(12)	2.521(6)
Zr(1)-C(7)	2.528(6)
Zr(1)-C(10)	2.549(6)
Zr(1)-C(14)	2.573(6)
Zr(1)-C(1)	2.604(6)
Zr(1)-C(2)	2.610(6)
Zr(1')-Cl(1')	2.4407(16)
Zr(1')-Cl(2')	2.4435(16)
Zr(1')-C(6')	2.458(6)
Zr(1')-C(5')	2.498(6)
Zr(1')-C(13')	2.509(6)
Zr(1')-C(11')	2.514(6)
Zr(1')-C(12')	2.532(6)
Zr(1')-C(10')	2.545(6)
Zr(1')-C(7')	2.548(6)
Zr(1')-C(14')	2.567(6)
Zr(1')-C(2')	2.602(6)
Zr(1')-C(1')	2.604(6)
S(1)-C(2)	1.727(6)
S(1)-C(3)	1.750(7)
S(1')-C(2')	1.714(6)
S(1')-C(3')	1.756(8)
C(1)-C(7)	1.406(9)
C(1)-C(2)	1.419(9)
C(1)-C(9)	1.507(9)
C(2)-C(5)	1.425(9)
C(3)-C(4)	1.330(10)

C(4)-C(5)	1.449(9)
C(5)-C(6)	1.439(9)
C(6)-C(7)	1.411(9)
C(7)-C(8)	1.499(9)
C(10)-C(14)	1.413(9)
C(10)-C(11)	1.426(9)
C(10)-C(15)	1.501(9)
C(11)-C(12)	1.399(9)
C(11)-C(16)	1.513(9)
C(12)-C(13)	1.433(9)
C(12)-C(17)	1.502(9)
C(13)-C(14)	1.401(9)
C(13)-C(18)	1.506(9)
C(14)-C(19)	1.492(9)
C(1')-C(7')	1.406(9)
C(1')-C(2')	1.434(9)
C(1')-C(9')	1.499(9)
C(2')-C(5')	1.418(9)
C(3')-C(4')	1.318(10)
C(4')-C(5')	1.428(9)
C(5')-C(6')	1.429(9)
C(6')-C(7')	1.416(9)
C(7')-C(8')	1.494(9)
C(10')-C(14')	1.419(8)
C(10')-C(11')	1.419(9)
C(10')-C(15')	1.503(9)
C(11')-C(12')	1.408(8)
C(11')-C(16')	1.523(9)
C(12')-C(13')	1.414(9)
C(12')-C(17')	1.501(9)
C(13')-C(14')	1.416(9)
C(13')-C(18')	1.522(9)
C(14')-C(19')	1.493(9)

Cl(2)-Zr(1)-Cl(1)	95.56(6)
Cl(2)-Zr(1)-C(6)	129.99(15)
Cl(1)-Zr(1)-C(6)	113.62(16)
Cl(2)-Zr(1)-C(13)	133.86(16)
Cl(1)-Zr(1)-C(13)	94.43(15)
C(6)-Zr(1)-C(13)	85.3(2)
Cl(2)-Zr(1)-C(5)	97.26(15)
Cl(1)-Zr(1)-C(5)	134.38(15)
C(6)-Zr(1)-C(5)	33.7(2)
C(13)-Zr(1)-C(5)	107.1(2)
Cl(2)-Zr(1)-C(11)	85.26(15)
Cl(1)-Zr(1)-C(11)	128.17(15)
C(6)-Zr(1)-C(11)	104.3(2)
C(13)-Zr(1)-C(11)	54.1(2)

C(5)-Zr(1)-C(11)	96.5(2)
Cl(2)-Zr(1)-C(12)	116.42(16)
Cl(1)-Zr(1)-C(12)	127.16(15)
C(6)-Zr(1)-C(12)	77.7(2)
C(13)-Zr(1)-C(12)	33.1(2)
C(5)-Zr(1)-C(12)	84.4(2)
C(11)-Zr(1)-C(12)	32.3(2)
Cl(2)-Zr(1)-C(7)	126.34(15)
Cl(1)-Zr(1)-C(7)	83.07(16)
C(6)-Zr(1)-C(7)	32.8(2)
C(13)-Zr(1)-C(7)	99.5(2)
C(5)-Zr(1)-C(7)	54.4(2)
C(11)-Zr(1)-C(7)	136.0(2)
C(12)-Zr(1)-C(7)	105.8(2)

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Table 17C. *(Continued 1)*

Cl(2)-Zr(1)-C(10)	80.50(15)
Cl(1)-Zr(1)-C(10)	96.15(14)
C(6)-Zr(1)-C(10)	131.4(2)
C(13)-Zr(1)-C(10)	53.7(2)
C(5)-Zr(1)-C(10)	129.1(2)
C(11)-Zr(1)-C(10)	32.7(2)
C(12)-Zr(1)-C(10)	53.8(2)
C(7)-Zr(1)-C(10)	153.1(2)
Cl(2)-Zr(1)-C(14)	108.16(16)
Cl(1)-Zr(1)-C(14)	77.83(14)
C(6)-Zr(1)-C(14)	116.9(2)
C(13)-Zr(1)-C(14)	32.0(2)
C(5)-Zr(1)-C(14)	137.0(2)
C(11)-Zr(1)-C(14)	53.4(2)
C(12)-Zr(1)-C(14)	53.5(2)
C(7)-Zr(1)-C(14)	123.6(2)
C(10)-Zr(1)-C(14)	32.02(19)
Cl(2)-Zr(1)-C(1)	94.77(15)
Cl(1)-Zr(1)-C(1)	81.36(14)
C(6)-Zr(1)-C(1)	54.0(2)
C(13)-Zr(1)-C(1)	131.3(2)
C(5)-Zr(1)-C(1)	54.1(2)
C(11)-Zr(1)-C(1)	150.4(2)
C(12)-Zr(1)-C(1)	131.5(2)
C(7)-Zr(1)-C(1)	31.8(2)
C(10)-Zr(1)-C(1)	174.5(2)
C(14)-Zr(1)-C(1)	150.2(2)
Cl(2)-Zr(1)-C(2)	79.14(14)
Cl(1)-Zr(1)-C(2)	109.99(15)
C(6)-Zr(1)-C(2)	53.54(19)
C(13)-Zr(1)-C(2)	137.6(2)
C(5)-Zr(1)-C(2)	32.24(19)
C(11)-Zr(1)-C(2)	120.9(2)
C(12)-Zr(1)-C(2)	116.3(2)
C(7)-Zr(1)-C(2)	52.3(2)
C(10)-Zr(1)-C(2)	148.13(19)
C(14)-Zr(1)-C(2)	169.1(2)
C(1)-Zr(1)-C(2)	31.58(19)
Cl(1')-Zr(1')-Cl(2')	97.10(6)
Cl(1')-Zr(1')-C(6')	111.69(16)
Cl(2')-Zr(1')-C(6')	130.69(15)
Cl(1')-Zr(1')-C(5')	133.83(15)
Cl(2')-Zr(1')-C(5')	98.31(15)
C(6')-Zr(1')-C(5')	33.5(2)
Cl(1')-Zr(1')-C(13')	95.44(16)
Cl(2')-Zr(1')-C(13')	133.64(16)
C(6')-Zr(1')-C(13')	83.9(2)
C(5')-Zr(1')-C(13')	104.4(2)
Cl(1')-Zr(1')-C(11')	127.21(15)
Cl(2')-Zr(1')-C(11')	83.75(14)
C(6')-Zr(1')-C(11')	106.5(2)
C(5')-Zr(1')-C(11')	97.6(2)
C(13')-Zr(1')-C(11')	53.8(2)
Cl(1')-Zr(1')-C(12')	127.45(15)
Cl(2')-Zr(1')-C(12')	114.60(16)
C(6')-Zr(1')-C(12')	78.7(2)
C(5')-Zr(1')-C(12')	83.6(2)
C(13')-Zr(1')-C(12')	32.6(2)
C(11')-Zr(1')-C(12')	32.40(19)
Cl(1')-Zr(1')-C(10')	95.11(15)
Cl(2')-Zr(1')-C(10')	80.90(15)
C(6')-Zr(1')-C(10')	132.1(2)
C(5')-Zr(1')-C(10')	130.2(2)
C(13')-Zr(1')-C(10')	53.6(2)
C(11')-Zr(1')-C(10')	32.6(2)
C(12')-Zr(1')-C(10')	53.7(2)
Cl(1')-Zr(1')-C(7')	81.77(15)
Cl(2')-Zr(1')-C(7')	126.00(15)
C(6')-Zr(1')-C(7')	32.8(2)
C(5')-Zr(1')-C(7')	54.2(2)
C(13')-Zr(1')-C(7')	99.9(2)
C(11')-Zr(1')-C(7')	138.4(2)
C(12')-Zr(1')-C(7')	107.6(2)
C(10')-Zr(1')-C(7')	153.1(2)
Cl(1')-Zr(1')-C(14')	77.18(15)
Cl(2')-Zr(1')-C(14')	109.43(15)
C(6')-Zr(1')-C(14')	115.3(2)
C(5')-Zr(1')-C(14')	135.6(2)
C(13')-Zr(1')-C(14')	32.4(2)
C(11')-Zr(1')-C(14')	53.7(2)
C(12')-Zr(1')-C(14')	53.7(2)
C(10')-Zr(1')-C(14')	32.23(19)
C(7')-Zr(1')-C(14')	122.5(2)
Cl(1')-Zr(1')-C(2')	111.08(16)
Cl(2')-Zr(1')-C(2')	79.35(14)
C(6')-Zr(1')-C(2')	53.57(19)
C(5')-Zr(1')-C(2')	32.2(2)
C(13')-Zr(1')-C(2')	135.4(2)
C(11')-Zr(1')-C(2')	120.8(2)
C(12')-Zr(1')-C(2')	115.1(2)
C(10')-Zr(1')-C(2')	148.8(2)
C(7')-Zr(1')-C(2')	52.37(19)
C(14')-Zr(1')-C(2')	167.6(2)
Cl(1')-Zr(1')-C(1')	81.43(14)
Cl(2')-Zr(1')-C(1')	94.47(15)
C(6')-Zr(1')-C(1')	54.1(2)

Table 17C. *(Continued 2)*

C(5')-Zr(1')-C(1')	54.2(2)
C(13')-Zr(1')-C(1')	131.5(2)
C(11')-Zr(1')-C(1')	151.3(2)
C(12')-Zr(1')-C(1')	132.3(2)
C(10')-Zr(1')-C(1')	173.9(2)
C(7')-Zr(1')-C(1')	31.6(2)
C(14')-Zr(1')-C(1')	149.5(2)
C(2')-Zr(1')-C(1')	32.0(2)
C(2)-S(1)-C(3)	90.0(3)
C(2')-S(1')-C(3')	88.7(4)
C(7)-C(1)-C(2)	106.6(6)
C(7)-C(1)-C(9)	127.8(6)
C(2)-C(1)-C(9)	125.3(6)
C(7)-C(1)-Zr(1)	71.1(3)
C(2)-C(1)-Zr(1)	74.4(3)
C(9)-C(1)-Zr(1)	124.3(4)
C(1)-C(2)-C(5)	109.9(5)
C(1)-C(2)-S(1)	138.1(5)
C(5)-C(2)-S(1)	111.9(5)
C(1)-C(2)-Zr(1)	74.0(3)
C(5)-C(2)-Zr(1)	70.1(3)
S(1)-C(2)-Zr(1)	123.9(3)
C(4)-C(3)-S(1)	115.1(5)
C(3)-C(4)-C(5)	111.6(6)
C(2)-C(5)-C(6)	105.8(5)
C(2)-C(5)-C(4)	111.3(5)
C(6)-C(5)-C(4)	142.5(6)
C(2)-C(5)-Zr(1)	77.6(3)
C(6)-C(5)-Zr(1)	71.0(3)
C(4)-C(5)-Zr(1)	121.6(4)
C(7)-C(6)-C(5)	108.0(5)
C(7)-C(6)-Zr(1)	76.4(3)
C(5)-C(6)-Zr(1)	75.4(3)
C(6)-C(7)-C(1)	109.6(6)
C(6)-C(7)-C(8)	125.4(6)
C(1)-C(7)-C(8)	124.9(6)
C(6)-C(7)-Zr(1)	70.7(3)
C(1)-C(7)-Zr(1)	77.1(4)
C(8)-C(7)-Zr(1)	121.7(4)
C(14)-C(10)-C(11)	107.4(5)
C(14)-C(10)-C(15)	126.7(6)
C(11)-C(10)-C(15)	125.7(6)
C(14)-C(10)-Zr(1)	74.9(3)
C(11)-C(10)-Zr(1)	72.3(3)
C(15)-C(10)-Zr(1)	123.1(4)
C(12)-C(11)-C(10)	108.5(6)
C(12)-C(11)-C(16)	125.4(6)
C(10)-C(11)-C(16)	125.9(6)
C(12)-C(11)-Zr(1)	74.1(3)
C(10)-C(11)-Zr(1)	75.0(3)
C(16)-C(11)-Zr(1)	120.4(4)
C(11)-C(12)-C(13)	107.5(5)
C(11)-C(12)-C(17)	126.1(6)
C(13)-C(12)-C(17)	125.4(6)
C(11)-C(12)-Zr(1)	73.6(3)
C(13)-C(12)-Zr(1)	73.0(3)
C(17)-C(12)-Zr(1)	127.7(4)
C(14)-C(13)-C(12)	108.0(6)
C(14)-C(13)-C(18)	126.3(6)
C(12)-C(13)-C(18)	125.1(6)
C(14)-C(13)-Zr(1)	76.5(3)
C(12)-C(13)-Zr(1)	73.9(3)
C(18)-C(13)-Zr(1)	122.7(4)
C(13)-C(14)-C(10)	108.5(5)
C(13)-C(14)-C(19)	125.1(6)
C(10)-C(14)-C(19)	126.2(6)
C(13)-C(14)-Zr(1)	71.5(3)
C(10)-C(14)-Zr(1)	73.1(3)
C(19)-C(14)-Zr(1)	125.3(4)
C(7')-C(1')-C(2')	106.3(5)
C(7')-C(1')-C(9')	125.9(6)
C(2')-C(1')-C(9')	127.5(6)
C(7')-C(1')-Zr(1')	72.0(3)
C(2')-C(1')-Zr(1')	73.9(3)
C(9')-C(1')-Zr(1')	124.5(4)
C(5')-C(2')-C(1')	109.3(5)
C(5')-C(2')-S(1')	113.0(5)
C(1')-C(2')-S(1')	137.5(5)
C(5')-C(2')-Zr(1')	69.9(3)
C(1')-C(2')-Zr(1')	74.1(3)
S(1')-C(2')-Zr(1')	124.0(3)
C(4')-C(3')-S(1')	115.6(6)
C(3')-C(4')-C(5')	111.7(6)
C(2')-C(5')-C(4')	111.0(6)
C(2')-C(5')-C(6')	106.7(6)
C(4')-C(5')-C(6')	141.9(6)
C(2')-C(5')-Zr(1')	77.9(3)
C(4')-C(5')-Zr(1')	120.5(4)
C(6')-C(5')-Zr(1')	71.7(3)
C(7')-C(6')-C(5')	108.0(5)
C(7')-C(6')-Zr(1')	77.1(3)
C(5')-C(6')-Zr(1')	74.8(3)
C(1')-C(7')-C(6')	109.5(5)
C(1')-C(7')-C(8')	124.8(6)
C(6')-C(7')-C(8')	125.6(6)
C(1')-C(7')-Zr(1')	76.4(3)

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Table 17C. *(Continued 3)*

C(6')-C(7')-Zr(1')	70.1(3)
C(8')-C(7')-Zr(1')	122.5(4)
C(14')-C(10')-C(11')	108.1(6)
C(14')-C(10')-C(15')	125.6(6)
C(11')-C(10')-C(15')	126.2(6)
C(14')-C(10')-Zr(1')	74.8(3)
C(11')-C(10')-Zr(1')	72.5(3)
C(15')-C(10')-Zr(1')	122.8(4)
C(12')-C(11')-C(10')	108.4(6)
C(12')-C(11')-C(16')	125.4(6)
C(10')-C(11')-C(16')	125.9(6)
C(12')-C(11')-Zr(1')	74.5(3)
C(10')-C(11')-Zr(1')	74.9(4)
C(16')-C(11')-Zr(1')	121.1(4)
C(11')-C(12')-C(13')	107.3(6)
C(11')-C(12')-C(17')	126.4(6)

C(13')-C(12')-C(17')	125.5(6)
C(11')-C(12')-Zr(1')	73.1(3)
C(13')-C(12')-Zr(1')	72.8(3)
C(17')-C(12')-Zr(1')	127.5(4)
C(12')-C(13')-C(14')	109.1(6)
C(12')-C(13')-C(18')	126.4(6)
C(14')-C(13')-C(18')	124.0(6)
C(12')-C(13')-Zr(1')	74.6(3)
C(14')-C(13')-Zr(1')	76.1(3)
C(18')-C(13')-Zr(1')	122.7(4)
C(10')-C(14')-C(13')	107.0(6)
C(10')-C(14')-C(19')	126.9(6)
C(13')-C(14')-C(19')	125.8(6)
C(10')-C(14')-Zr(1')	73.0(3)
C(13')-C(14')-Zr(1')	71.5(3)
C(19')-C(14')-Zr(1')	125.3(4)

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Table 17D. Anisotropic displacement parameters ($Å^2$ x 10^3) for **17**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	14(1)	15(1)	21(1)	7(1)	3(1)	2(1)
Zr(1')	17(1)	15(1)	22(1)	7(1)	2(1)	1(1)
Cl(1)	44(1)	20(1)	21(1)	4(1)	4(1)	8(1)
Cl(2)	25(1)	32(1)	23(1)	5(1)	8(1)	-6(1)
Cl(1')	29(1)	30(1)	23(1)	5(1)	11(1)	-3(1)
Cl(2')	41(1)	16(1)	21(1)	1(1)	7(1)	-1(1)
S(1)	37(1)	30(1)	18(1)	3(1)	8(1)	6(1)
S(1')	44(1)	34(1)	21(1)	3(1)	9(1)	8(1)
C(1)	22(3)	28(3)	22(3)	0(2)	-5(2)	4(2)
C(2)	24(3)	34(3)	14(3)	3(2)	3(2)	6(3)
C(3)	52(4)	23(3)	31(4)	-3(3)	2(3)	13(3)
C(4)	41(4)	22(3)	26(3)	2(2)	2(3)	5(3)
C(5)	23(3)	21(3)	23(3)	1(2)	-1(2)	-1(2)
C(6)	23(3)	28(3)	22(3)	7(2)	3(2)	-2(2)
C(7)	20(3)	34(3)	22(3)	-1(2)	-3(2)	4(3)
C(8)	22(3)	57(5)	30(4)	4(3)	4(3)	12(3)
C(9)	35(4)	35(4)	29(3)	11(3)	2(3)	9(3)
C(10)	22(3)	31(3)	17(3)	1(2)	0(2)	10(3)
C(11)	26(3)	29(3)	26(3)	13(3)	1(2)	11(3)
C(12)	30(3)	23(3)	25(3)	10(2)	2(2)	6(3)
C(13)	33(3)	37(3)	19(3)	11(3)	6(3)	18(3)
C(14)	34(3)	33(3)	16(3)	7(2)	3(2)	14(3)
C(15)	28(3)	26(3)	31(3)	4(3)	-2(3)	5(3)
C(16)	30(4)	36(4)	38(4)	9(3)	5(3)	17(3)
C(17)	39(4)	28(3)	42(4)	15(3)	4(3)	6(3)
C(18)	38(4)	48(4)	30(4)	17(3)	14(3)	11(3)
C(19)	45(4)	40(4)	23(3)	-1(3)	-1(3)	21(3)
C(1')	22(3)	31(3)	28(3)	17(3)	2(2)	10(3)
C(2')	39(4)	29(3)	15(3)	6(2)	2(2)	15(3)
C(3')	41(4)	51(5)	35(4)	18(3)	15(3)	9(4)
C(4')	32(4)	38(4)	27(3)	17(3)	11(3)	6(3)
C(5')	31(3)	30(3)	24(3)	15(3)	7(3)	9(3)
C(6')	34(3)	15(3)	26(3)	7(2)	-3(3)	1(2)
C(7')	35(3)	26(3)	25(3)	10(2)	5(3)	17(3)
C(8')	47(4)	36(4)	38(4)	13(3)	10(3)	25(3)
C(9')	24(3)	41(4)	46(4)	25(3)	-7(3)	-1(3)
C(10')	28(3)	33(3)	21(3)	5(2)	3(2)	14(3)
C(11')	21(3)	22(3)	27(3)	2(2)	-6(2)	6(2)
C(12')	28(3)	27(3)	20(3)	3(2)	-3(2)	3(3)
C(13')	26(3)	30(3)	24(3)	0(3)	-6(2)	5(3)
C(14')	27(3)	34(3)	17(3)	5(2)	2(2)	12(3)
C(15')	31(3)	31(3)	34(4)	15(3)	6(3)	12(3)
C(16')	27(3)	37(4)	34(4)	9(3)	6(3)	12(3)
C(17')	30(4)	31(3)	35(4)	9(3)	-2(3)	-2(3)
C(18')	59(5)	30(4)	26(3)	-5(3)	-3(3)	16(3)
C(19')	40(4)	43(4)	21(3)	10(3)	9(3)	11(3)

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Table 17E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **17**.

Atom	x	y	z	U(eq)
H(3A)	11437	16535	10112	44
H(4A)	12511	16982	8829	38
H(6A)	14366	15878	7511	32
H(8A)	16438	14431	7850	55
H(8B)	15431	14381	6887	55
H(8C)	15116	13441	7370	55
H(9A)	14763	13479	9575	50
H(9B)	14051	12788	8555	50
H(9C)	13028	12980	9299	50
H(15A)	7412	13324	5508	45
H(15B)	7700	13452	6619	45
H(15C)	8121	12583	5964	45
H(16A)	8661	15836	6764	50
H(16B)	9916	16095	7664	50
H(16C)	8576	15088	7459	50
H(17A)	11981	16827	6150	55
H(17B)	13358	16607	6694	55
H(17C)	12118	16846	7243	55
H(18A)	13059	14995	4816	55
H(18B)	13504	14178	5310	55
H(18C)	14038	15334	5840	55
H(19A)	10107	12889	4305	54
H(19B)	9923	12268	5107	54
H(19C)	11519	12765	4905	54
H(3'A)	8952	9166	4897	50
H(4'A)	9644	10475	6247	38
H(6'A)	7687	11375	7591	32
H(8'A)	4275	11439	7285	56
H(8'B)	5202	11363	8229	56
H(8'C)	3752	10477	7719	56
H(9'A)	2915	9334	5525	57
H(9'B)	2804	9104	6538	57
H(9'C)	3216	8341	5756	57
H(15D)	8516	7495	9401	46
H(15E)	7927	7160	8297	46
H(15F)	6820	7295	8999	46
H(16D)	10963	8734	8114	48
H(16E)	10255	9065	7233	48
H(16F)	9513	7989	7434	48
H(17D)	11174	11234	8770	52
H(17E)	9877	11571	8271	52
H(17F)	10522	10780	7682	52
H(18D)	8678	11552	10193	60
H(18E)	6970	11127	9753	60
H(18F)	8097	11723	9193	60

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Table 17E. *(Continued)*

Atom	x	y	z	U(eq)
H(19D)	7226	9260	10682	51
H(19E)	5947	8478	9893	51
H(19F)	6037	9640	10119	51

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Table 20A. Crystal data, data collection, structure solution and refinement parameters for **20**.

Empirical formula	$C_{68}H_{94}Cl_{12}Li_2Zr_4$
Formula weight	1715.60
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 23.849(4) Å, α= 90°.
	b = 14.147(2) Å, β= 91.768(12)°.
	c = 22.314(3) Å, γ = 90°.
Volume	7525.0(19) $Å^3$
Z	4
Density (calculated)	1.514 Mg/m^3
Absorption coefficient	1.003 mm^{-1}
F(000)	3488
Crystal size	0.4 x 0.4 x 0.3 mm^3
Theta range for data collection	2.46 to 28.06°.
Index ranges	-31<=h<=31, -3<=k<=18, -29<=l<=29
Reflections collected	9326
Independent reflections	9117 [R(int) = 0.0238]
Completeness to theta = 28.06°	99.7 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9117 / 0 / 392
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0298, wR2 = 0.0729
R indices (all data)	R1 = 0.0421, wR2 = 0.0765
Largest diff. peak and hole	0.828 and -0.608 $e.Å^{-3}$

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Table 20B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **20**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Zr(1)	1707(1)	3237(1)	1054(1)	19(1)
Zr(2)	2942(1)	4226(1)	1550(1)	21(1)
Cl(1)	2143(1)	3375(1)	2116(1)	25(1)
Cl(2)	2026(1)	4972(1)	1072(1)	26(1)
Cl(3)	1970(1)	1541(1)	1045(1)	26(1)
Cl(4)	1871(1)	3242(1)	-54(1)	26(1)
Cl(5)	3508(1)	2821(1)	1705(1)	37(1)
Cl(6)	3359(1)	4549(1)	553(1)	34(1)
C(1)	840(1)	2866(2)	1606(1)	34(1)
C(2)	853(1)	3863(2)	1532(1)	26(1)
C(3)	780(1)	4053(2)	911(1)	26(1)
C(4)	712(1)	3190(2)	606(1)	31(1)
C(5)	748(1)	2459(2)	1031(1)	36(1)
C(6)	861(1)	2339(3)	2188(2)	58(1)
C(7)	883(1)	4585(2)	2024(1)	44(1)
C(8)	711(1)	5007(2)	619(1)	42(1)
C(9)	551(1)	3085(3)	-47(1)	49(1)
C(10)	632(1)	1432(2)	900(2)	61(1)
C(11)	3158(1)	4835(2)	2586(1)	28(1)
C(12)	2803(1)	5515(2)	2300(1)	26(1)
C(13)	3103(1)	5926(2)	1828(1)	28(1)
C(14)	3647(1)	5515(2)	1832(1)	31(1)
C(15)	3681(1)	4850(2)	2302(1)	30(1)
C(16)	3031(1)	4270(2)	3135(1)	37(1)
C(17)	2241(1)	5820(2)	2508(1)	33(1)
C(18)	2911(1)	6732(2)	1438(1)	38(1)
C(19)	4124(1)	5836(2)	1458(1)	43(1)
C(20)	4199(1)	4342(2)	2520(1)	45(1)
Li(1)	2862(2)	3410(3)	24(2)	36(1)
C(1S)	-1668(1)	4051(2)	714(1)	49(1)
C(2S)	-1198(2)	3466(2)	704(2)	55(1)
C(3S)	-711(1)	3713(3)	1016(2)	56(1)
C(4S)	-680(1)	4532(3)	1323(2)	60(1)
C(5S)	-1125(2)	5126(3)	1333(2)	59(1)
C(6S)	-1616(1)	4887(2)	1037(1)	52(1)
C(7S)	-2209(2)	3807(4)	396(2)	86(2)
C(8S)	382(2)	-2284(3)	1264(2)	65(1)
C(9S)	913(2)	-2360(4)	1068(3)	97(2)
C(10S)	1109(3)	-1716(6)	633(4)	160(4)
C(11S)	727(3)	-1030(5)	442(2)	114(3)
C(12S)	201(3)	-952(4)	651(2)	95(2)
C(13S)	21(2)	-1559(3)	1059(2)	69(1)
C(14S)	142(3)	-2928(4)	1698(3)	104(2)

Table 20C. Bond lengths [Å] and angles [deg] for **20**.

Zr(1)-Cl(3)	2.4804(6)
Zr(1)-C(2)	2.490(2)
Zr(1)-C(1)	2.495(2)
Zr(1)-C(3)	2.506(2)
Zr(1)-Cl(4)	2.5145(6)
Zr(1)-C(5)	2.538(2)
Zr(1)-C(4)	2.546(2)
Zr(1)-Cl(1)	2.5651(7)
Zr(1)-Cl(2)	2.5696(6)
Zr(1)-Zr(2)	3.4148(5)
Zr(1)-Li(1)#1	3.524(4)
Zr(1)-H(1M)	1.92(2)
Zr(2)-Cl(5)	2.4208(7)
Zr(2)-C(11)	2.504(2)
Zr(2)-C(12)	2.504(2)
Zr(2)-Cl(6)	2.5082(7)
Zr(2)-C(13)	2.511(2)
Zr(2)-C(14)	2.546(2)
Zr(2)-C(15)	2.551(2)
Zr(2)-Cl(1)	2.6124(6)
Zr(2)-Cl(2)	2.6249(6)
Zr(2)-Li(1)	3.596(4)
Zr(2)-H(1M)	2.01(2)
Cl(3)-Li(1)#1	2.432(5)
Cl(4)-Li(1)	2.376(4)
Cl(4)-Li(1)#1	2.422(5)
Cl(6)-Li(1)	2.304(4)
C(1)-C(5)	1.418(4)
C(1)-C(2)	1.421(4)
C(1)-C(6)	1.497(4)
C(2)-C(3)	1.417(3)
C(2)-C(7)	1.499(3)
C(3)-C(4)	1.405(3)

C(3)-C(8)	1.505(3)
C(4)-C(5)	1.403(4)
C(4)-C(9)	1.502(3)
C(5)-C(10)	1.507(4)
C(11)-C(15)	1.417(3)
C(11)-C(12)	1.420(3)
C(11)-C(16)	1.501(3)
C(12)-C(13)	1.416(3)
C(12)-C(17)	1.497(3)
C(13)-C(14)	1.421(3)
C(13)-C(18)	1.496(3)
C(14)-C(15)	1.409(4)
C(14)-C(19)	1.501(3)
C(15)-C(20)	1.496(3)
Li(1)-Cl(4)#1	2.422(5)
Li(1)-Cl(3)#1	2.432(5)
Li(1)-Li(1)#1	3.101(9)
Li(1)-Zr(1)#1	3.524(4)
C(1S)-C(6S)	1.388(5)
C(1S)-C(2S)	1.394(5)
C(1S)-C(7S)	1.492(5)
C(2S)-C(3S)	1.381(5)
C(3S)-C(4S)	1.348(5)
C(4S)-C(5S)	1.355(5)
C(5S)-C(6S)	1.369(5)
C(8S)-C(9S)	1.356(6)
C(8S)-C(13S)	1.407(6)
C(8S)-C(14S)	1.459(6)
C(9S)-C(10S)	1.422(10)
C(10S)-C(11S)	1.387(11)
C(11S)-C(12S)	1.356(8)
C(12S)-C(13S)	1.332(6)

Cl(3)-Zr(1)-C(2)	123.90(6)
Cl(3)-Zr(1)-C(1)	90.80(6)
C(2)-Zr(1)-C(1)	33.12(8)
Cl(3)-Zr(1)-C(3)	131.81(5)
C(2)-Zr(1)-C(3)	32.95(7)
C(1)-Zr(1)-C(3)	54.44(8)
Cl(3)-Zr(1)-Cl(4)	87.013(19)
C(2)-Zr(1)-Cl(4)	125.04(5)
C(1)-Zr(1)-Cl(4)	130.00(6)
C(3)-Zr(1)-Cl(4)	92.12(5)
Cl(3)-Zr(1)-C(5)	78.94(6)
C(2)-Zr(1)-C(5)	54.15(8)
C(1)-Zr(1)-C(5)	32.70(9)

C(3)-Zr(1)-C(5)	53.53(8)
Cl(4)-Zr(1)-C(5)	98.59(7)
Cl(3)-Zr(1)-C(4)	101.76(6)
C(2)-Zr(1)-C(4)	54.09(7)
C(1)-Zr(1)-C(4)	54.01(8)
C(3)-Zr(1)-C(4)	32.27(8)
Cl(4)-Zr(1)-C(4)	77.63(6)
C(5)-Zr(1)-C(4)	32.04(8)
Cl(3)-Zr(1)-Cl(1)	89.172(19)
C(2)-Zr(1)-Cl(1)	83.72(5)
C(1)-Zr(1)-Cl(1)	82.99(6)
C(3)-Zr(1)-Cl(1)	114.43(5)
Cl(4)-Zr(1)-Cl(1)	146.805(19)

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Table 20C. *(Continued)*

C(5)-Zr(1)-Cl(1)	112.99(7)
C(4)-Zr(1)-Cl(1)	135.27(6)
Cl(3)-Zr(1)-Cl(2)	148.18(2)
C(2)-Zr(1)-Cl(2)	84.19(6)
C(1)-Zr(1)-Cl(2)	116.25(7)
C(3)-Zr(1)-Cl(2)	79.71(5)
Cl(4)-Zr(1)-Cl(2)	87.559(19)
C(5)-Zr(1)-Cl(2)	132.88(6)
C(4)-Zr(1)-Cl(2)	107.62(6)
Cl(1)-Zr(1)-Cl(2)	78.589(18)
Cl(3)-Zr(1)-Zr(2)	100.566(16)
C(2)-Zr(1)-Zr(2)	115.07(5)
C(1)-Zr(1)-Zr(2)	130.20(6)
C(3)-Zr(1)-Zr(2)	126.99(5)
Cl(4)-Zr(1)-Zr(2)	99.139(18)
C(5)-Zr(1)-Zr(2)	162.22(7)
C(4)-Zr(1)-Zr(2)	157.22(6)
Cl(1)-Zr(1)-Zr(2)	49.334(15)
Cl(2)-Zr(1)-Zr(2)	49.603(12)
Cl(3)-Zr(1)-Li(1)#1	43.61(8)
C(2)-Zr(1)-Li(1)#1	141.90(9)
C(1)-Zr(1)-Li(1)#1	117.49(10)
C(3)-Zr(1)-Li(1)#1	119.48(9)
Cl(4)-Zr(1)-Li(1)#1	43.40(8)
C(5)-Zr(1)-Li(1)#1	88.94(9)
C(4)-Zr(1)-Li(1)#1	90.14(9)
Cl(1)-Zr(1)-Li(1)#1	124.21(8)
Cl(2)-Zr(1)-Li(1)#1	123.34(8)
Zr(2)-Zr(1)-Li(1)#1	103.03(7)
Cl(3)-Zr(1)-H(1M)	79.5(7)
C(2)-Zr(1)-H(1M)	145.6(7)
C(1)-Zr(1)-H(1M)	152.0(7)
C(3)-Zr(1)-H(1M)	146.6(7)
Cl(4)-Zr(1)-H(1M)	76.1(7)
C(5)-Zr(1)-H(1M)	158.0(7)
C(4)-Zr(1)-H(1M)	153.6(7)
Cl(1)-Zr(1)-H(1M)	70.8(7)
Cl(2)-Zr(1)-H(1M)	68.8(7)
Zr(2)-Zr(1)-H(1M)	30.6(7)
Li(1)#1-Zr(1)-H(1M)	72.5(7)
Cl(5)-Zr(2)-C(11)	93.04(6)
Cl(5)-Zr(2)-C(12)	125.98(6)
C(11)-Zr(2)-C(12)	32.94(7)
Cl(5)-Zr(2)-Cl(6)	92.39(2)
C(11)-Zr(2)-Cl(6)	132.88(6)
C(12)-Zr(2)-Cl(6)	121.60(6)
Cl(5)-Zr(2)-C(13)	132.15(6)
C(11)-Zr(2)-C(13)	54.38(8)
C(12)-Zr(2)-C(13)	32.81(7)
Cl(6)-Zr(2)-C(13)	88.97(6)
Cl(5)-Zr(2)-C(14)	101.07(6)
C(11)-Zr(2)-C(14)	53.90(8)
C(12)-Zr(2)-C(14)	54.05(7)
Cl(6)-Zr(2)-C(14)	79.13(6)
C(13)-Zr(2)-C(14)	32.64(8)
Cl(5)-Zr(2)-C(15)	79.60(6)
C(11)-Zr(2)-C(15)	32.55(7)
C(12)-Zr(2)-C(15)	53.99(7)
Cl(6)-Zr(2)-C(15)	103.61(6)
C(13)-Zr(2)-C(15)	53.81(8)
C(14)-Zr(2)-C(15)	32.10(8)
Cl(5)-Zr(2)-Cl(1)	87.99(2)
C(11)-Zr(2)-Cl(1)	81.09(6)
C(12)-Zr(2)-Cl(1)	84.25(5)
Cl(6)-Zr(2)-Cl(1)	145.89(2)
C(13)-Zr(2)-Cl(1)	115.53(6)
C(14)-Zr(2)-Cl(1)	134.20(5)
C(15)-Zr(2)-Cl(1)	109.98(6)
Cl(5)-Zr(2)-Cl(2)	147.34(2)
C(11)-Zr(2)-Cl(2)	112.44(6)
C(12)-Zr(2)-Cl(2)	81.55(5)
Cl(6)-Zr(2)-Cl(2)	85.02(2)
C(13)-Zr(2)-Cl(2)	80.43(6)
C(14)-Zr(2)-Cl(2)	110.31(6)
C(15)-Zr(2)-Cl(2)	132.66(6)
Cl(1)-Zr(2)-Cl(2)	76.76(2)
Cl(5)-Zr(2)-Zr(1)	100.475(19)
C(11)-Zr(2)-Zr(1)	126.20(6)
C(12)-Zr(2)-Zr(1)	112.62(5)
Cl(6)-Zr(2)-Zr(1)	98.539(18)
C(13)-Zr(2)-Zr(1)	126.59(5)
C(14)-Zr(2)-Zr(1)	158.41(6)
C(15)-Zr(2)-Zr(1)	157.84(6)
Cl(1)-Zr(2)-Zr(1)	48.140(14)
Cl(2)-Zr(2)-Zr(1)	48.205(15)
Cl(5)-Zr(2)-Li(1)	83.39(8)
C(11)-Zr(2)-Li(1)	171.02(9)
C(12)-Zr(2)-Li(1)	149.57(9)
Cl(6)-Zr(2)-Li(1)	39.53(7)
C(13)-Zr(2)-Li(1)	122.96(9)

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Table 20C. *(Continued)*

C(14)-Zr(2)-Li(1)	118.62(9)
C(15)-Zr(2)-Li(1)	138.48(9)
Cl(1)-Zr(2)-Li(1)	106.93(7)
Cl(2)-Zr(2)-Li(1)	74.00(7)
Zr(1)-Zr(2)-Li(1)	62.69(7)
Cl(5)-Zr(2)-H(1M)	81.1(7)
C(11)-Zr(2)-H(1M)	149.2(7)
C(12)-Zr(2)-H(1M)	141.6(7)
Cl(6)-Zr(2)-H(1M)	77.8(7)
C(13)-Zr(2)-H(1M)	145.1(7)
C(14)-Zr(2)-H(1M)	156.9(7)
C(15)-Zr(2)-H(1M)	160.7(7)
Cl(1)-Zr(2)-H(1M)	68.6(7)
Cl(2)-Zr(2)-H(1M)	66.5(7)
Zr(1)-Zr(2)-H(1M)	29.1(7)
Li(1)-Zr(2)-H(1M)	38.4(7)
Zr(1)-Cl(1)-Zr(2)	82.526(19)
Zr(1)-Cl(2)-Zr(2)	82.192(18)
Li(1)#1-Cl(3)-Zr(1)	91.68(11)
Li(1)-Cl(4)-Li(1)#1	80.50(16)
Li(1)-Cl(4)-Zr(1)	96.50(11)
Li(1)#1-Cl(4)-Zr(1)	91.09(11)
Li(1)-Cl(6)-Zr(2)	96.61(11)
C(5)-C(1)-C(2)	107.5(2)
C(5)-C(1)-C(6)	125.6(3)
C(2)-C(1)-C(6)	126.6(3)
C(5)-C(1)-Zr(1)	75.32(13)
C(2)-C(1)-Zr(1)	73.25(13)
C(6)-C(1)-Zr(1)	121.82(17)
C(3)-C(2)-C(1)	107.4(2)
C(3)-C(2)-C(7)	126.1(2)
C(1)-C(2)-C(7)	126.3(2)
C(3)-C(2)-Zr(1)	74.15(12)
C(1)-C(2)-Zr(1)	73.63(13)
C(7)-C(2)-Zr(1)	122.38(16)
C(4)-C(3)-C(2)	108.5(2)
C(4)-C(3)-C(8)	124.2(2)
C(2)-C(3)-C(8)	126.9(2)
C(4)-C(3)-Zr(1)	75.44(13)
C(2)-C(3)-Zr(1)	72.90(12)
C(8)-C(3)-Zr(1)	123.48(16)
C(5)-C(4)-C(3)	108.0(2)
C(5)-C(4)-C(9)	126.2(2)
C(3)-C(4)-C(9)	125.2(2)
C(5)-C(4)-Zr(1)	73.66(13)
C(3)-C(4)-Zr(1)	72.30(12)
C(9)-C(4)-Zr(1)	126.23(17)
C(4)-C(5)-C(1)	108.5(2)

C(4)-C(5)-C(10)	124.9(3)
C(1)-C(5)-C(10)	126.2(3)
C(4)-C(5)-Zr(1)	74.29(13)
C(1)-C(5)-Zr(1)	71.97(13)
C(10)-C(5)-Zr(1)	125.56(18)
C(15)-C(11)-C(12)	108.0(2)
C(15)-C(11)-C(16)	125.1(2)
C(12)-C(11)-C(16)	126.6(2)
C(15)-C(11)-Zr(2)	75.56(13)
C(12)-C(11)-Zr(2)	73.54(12)
C(16)-C(11)-Zr(2)	121.96(16)
C(13)-C(12)-C(11)	107.8(2)
C(13)-C(12)-C(17)	126.2(2)
C(11)-C(12)-C(17)	125.7(2)
C(13)-C(12)-Zr(2)	73.86(13)
C(11)-C(12)-Zr(2)	73.53(12)
C(17)-C(12)-Zr(2)	123.72(15)
C(12)-C(13)-C(14)	108.0(2)
C(12)-C(13)-C(18)	126.4(2)
C(14)-C(13)-C(18)	125.3(2)
C(12)-C(13)-Zr(2)	73.33(13)
C(14)-C(13)-Zr(2)	75.05(13)
C(18)-C(13)-Zr(2)	123.01(16)
C(15)-C(14)-C(13)	108.1(2)
C(15)-C(14)-C(19)	126.0(2)
C(13)-C(14)-C(19)	125.4(2)
C(15)-C(14)-Zr(2)	74.14(13)
C(13)-C(14)-Zr(2)	72.31(13)
C(19)-C(14)-Zr(2)	125.77(16)
C(14)-C(15)-C(11)	108.1(2)
C(14)-C(15)-C(20)	126.2(2)
C(11)-C(15)-C(20)	125.2(2)
C(14)-C(15)-Zr(2)	73.75(13)
C(11)-C(15)-Zr(2)	71.89(12)
C(20)-C(15)-Zr(2)	126.44(17)
Cl(6)-Li(1)-Cl(4)	127.02(19)
Cl(6)-Li(1)-Cl(4)#1	122.0(2)
Cl(4)-Li(1)-Cl(4)#1	99.50(16)
Cl(6)-Li(1)-Cl(3)#1	112.61(18)
Cl(4)-Li(1)-Cl(3)#1	97.17(16)
Cl(4)#1-Li(1)-Cl(3)#1	90.21(14)
Cl(6)-Li(1)-Li(1)#1	151.1(3)
Cl(4)-Li(1)-Li(1)#1	50.40(13)
Cl(4)#1-Li(1)-Li(1)#1	49.10(13)
Cl(3)#1-Li(1)-Li(1)#1	95.7(2)
Cl(6)-Li(1)-Zr(1)#1	130.98(17)
Cl(4)-Li(1)-Zr(1)#1	101.20(14)
Cl(4)#1-Li(1)-Zr(1)#1	45.51(7)

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Table 20C. *(Continued)*

Cl(3)#1-Li(1)-Zr(1)#1	44.71(7)
Li(1)#1-Li(1)-Zr(1)#1	66.51(14)
Cl(6)-Li(1)-Zr(2)	43.86(8)
Cl(4)-Li(1)-Zr(2)	97.17(13)
Cl(4)#1-Li(1)-Zr(2)	106.11(15)
Cl(3)#1-Li(1)-Zr(2)	156.11(17)
Li(1)#1-Li(1)-Zr(2)	108.2(2)
Zr(1)#1-Li(1)-Zr(2)	148.27(15)
C(6S)-C(1S)-C(2S)	117.0(3)
C(6S)-C(1S)-C(7S)	120.5(4)
C(2S)-C(1S)-C(7S)	122.5(4)
C(3S)-C(2S)-C(1S)	120.4(3)

C(4S)-C(3S)-C(2S)	120.4(3)
C(3S)-C(4S)-C(5S)	120.7(3)
C(4S)-C(5S)-C(6S)	119.8(4)
C(5S)-C(6S)-C(1S)	121.6(3)
C(9S)-C(8S)-C(13S)	121.4(5)
C(9S)-C(8S)-C(14S)	123.6(5)
C(13S)-C(8S)-C(14S)	115.0(4)
C(8S)-C(9S)-C(10S)	120.0(6)
C(11S)-C(10S)-C(9S)	115.5(6)
C(12S)-C(11S)-C(10S)	123.8(6)
C(13S)-C(12S)-C(11S)	120.3(6)
C(12S)-C(13S)-C(8S)	119.0(5)

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Table 20D. Anisotropic displacement parameters ($Å^2$ x 10^3) for **20**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	18(1)	20(1)	20(1)	0(1)	2(1)	0(1)
Zr(2)	19(1)	22(1)	21(1)	-2(1)	1(1)	-1(1)
Cl(1)	24(1)	29(1)	21(1)	2(1)	1(1)	-2(1)
Cl(2)	26(1)	21(1)	29(1)	1(1)	-2(1)	0(1)
Cl(3)	29(1)	22(1)	28(1)	1(1)	2(1)	2(1)
Cl(4)	26(1)	33(1)	20(1)	2(1)	2(1)	3(1)
Cl(5)	28(1)	30(1)	52(1)	-2(1)	-3(1)	5(1)
Cl(6)	37(1)	39(1)	26(1)	-5(1)	9(1)	-15(1)
C(1)	19(1)	43(1)	39(1)	14(1)	8(1)	3(1)
C(2)	19(1)	35(1)	24(1)	-1(1)	2(1)	6(1)
C(3)	18(1)	32(1)	27(1)	1(1)	-1(1)	1(1)
C(4)	19(1)	42(1)	31(1)	-8(1)	1(1)	-3(1)
C(5)	18(1)	31(1)	58(2)	-4(1)	6(1)	-4(1)
C(6)	34(1)	82(2)	58(2)	43(2)	11(1)	2(2)
C(7)	30(1)	64(2)	37(1)	-20(1)	-1(1)	13(1)
C(8)	31(1)	41(2)	54(2)	15(1)	-6(1)	6(1)
C(9)	31(1)	80(2)	34(1)	-17(1)	-7(1)	-4(1)
C(10)	32(1)	36(2)	115(3)	-9(2)	7(2)	-12(1)
C(11)	32(1)	29(1)	23(1)	-4(1)	-3(1)	-3(1)
C(12)	27(1)	25(1)	25(1)	-6(1)	0(1)	-1(1)
C(13)	32(1)	24(1)	28(1)	-4(1)	0(1)	-4(1)
C(14)	28(1)	35(1)	30(1)	-10(1)	2(1)	-9(1)
C(15)	25(1)	33(1)	33(1)	-7(1)	-5(1)	-2(1)
C(16)	48(2)	38(1)	24(1)	1(1)	-4(1)	-1(1)
C(17)	32(1)	33(1)	33(1)	-10(1)	3(1)	3(1)
C(18)	51(2)	24(1)	39(1)	4(1)	-1(1)	-6(1)
C(19)	36(1)	50(2)	45(2)	-14(1)	11(1)	-19(1)
C(20)	30(1)	57(2)	48(2)	-13(1)	-13(1)	8(1)
Li(1)	33(2)	37(2)	37(2)	-9(2)	4(2)	-4(2)
C(1S)	39(2)	65(2)	42(2)	26(1)	6(1)	-5(1)
C(2S)	66(2)	43(2)	57(2)	9(1)	22(2)	-3(2)
C(3S)	35(2)	66(2)	67(2)	22(2)	17(1)	14(2)
C(4S)	42(2)	85(3)	53(2)	13(2)	3(1)	-7(2)
C(5S)	66(2)	61(2)	51(2)	3(2)	18(2)	-6(2)
C(6S)	47(2)	58(2)	53(2)	26(2)	19(1)	16(2)
C(7S)	66(2)	127(4)	64(2)	38(3)	-15(2)	-29(3)
C(8S)	85(3)	52(2)	57(2)	-20(2)	-1(2)	-12(2)
C(9S)	66(3)	107(4)	118(4)	-72(3)	8(3)	-24(3)
C(10S)	117(5)	197(8)	170(7)	-145(7)	55(5)	-92(6)
C(11S)	156(6)	113(5)	77(3)	-49(3)	56(4)	-84(4)
C(12S)	142(5)	84(3)	60(2)	-23(2)	15(3)	-50(3)
C(13S)	85(3)	63(2)	59(2)	-25(2)	0(2)	-20(2)
C(14S)	132(5)	78(3)	101(4)	-8(3)	14(3)	0(3)

Table 20E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **20**.

Atom	x	y	z	U(eq)
H(1M)	2509(10)	3335(17)	1006(11)	23(6)
H(6A)	480	2266	2334	87
H(6B)	1090	2692	2484	87
H(6C)	1027	1714	2128	87
H(7A)	503	4736	2148	66
H(7B)	1064	5160	1878	66
H(7C)	1102	4332	2366	66
H(8A)	314	5187	611	63
H(8B)	844	4978	208	63
H(8C)	931	5476	849	63
H(9A)	141	3087	-96	73
H(9B)	699	2488	-198	73
H(9C)	707	3612	-273	73
H(10B)	228	1311	919	91
H(10C)	833	1038	1197	91
H(10D)	759	1277	498	91
H(16A)	3146	4629	3494	55
H(16B)	3238	3671	3128	55
H(16C)	2628	4141	3141	55
H(17A)	2288	6334	2799	49
H(17B)	2054	5284	2696	49
H(17C)	2011	6041	2164	49
H(18A)	3016	7331	1631	57
H(18B)	2503	6704	1378	57
H(18C)	3089	6687	1049	57
H(19A)	4330	6341	1668	65
H(19B)	3975	6072	1072	65
H(19C)	4376	5302	1390	65
H(20A)	4408	4744	2806	68
H(20B)	4434	4199	2179	68
H(20C)	4093	3753	2717	68
H(2SA)	-1213	2894	481	66
H(3SA)	-396	3302	1014	67
H(4SA)	-342	4695	1535	72
H(5SA)	-1097	5707	1546	71
H(6SA)	-1927	5303	1052	63
H(7SA)	-2484	4308	462	129
H(7SB)	-2350	3208	552	129
H(7SC)	-2147	3744	-34	129
H(9SA)	1154	-2843	1222	116
H(10A)	1477	-1752	483	192
H(11D)	841	-590	148	137
H(12A)	-39	-463	506	114

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Table 20E. *(Continued)*

Atom	x	y	z	U(eq)
H(13A)	-346	-1502	1210	83
H(14D)	421	-3407	1816	155
H(14E)	-189	-3238	1517	155
H(14F)	33	-2571	2052	155

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Table 21A. Crystal data, data collection, structure solution and refinement parameters for **21**.

Empirical formula	C47 H58 Cl4 S2 Zr2
Formula weight	1011.29
Temperature	110(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 8.536(10)A, α = 86.96(3)°
	b = 8.644(8)A, β = 79.14(3)°
	c = 17.563(16)A, γ = 61.21(3)°
Volume	1114.4(19) A^3
Z, Calculated density	1, 1.507 Mg/m^3
Absorption coefficient	0.834 mm^{-1}
F(000)	520
Crystal size	0.30 x 0.25 x 0.20 mm
Theta range for data collection	1.18 to 29.25°
Limiting indices	-11<=h<=11, -11<=k<=10, -23<=l<=23
Reflections collected / unique	9288 / 5889 [R(int) = 0.0510]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.845 and 0.596
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5839 / 0 / 272
Goodness-of-fit on F^2	0.948
Final R indices [I>2σ(I)]	R_1 = 0.0610, wR_2 = 0.1450
R indices (all data)	R_1 = 0.0830, wR_2 = 0.1756
Largest diff. peak and hole	1.840 and -1.407 $e.A^{-3}$

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Table 21B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **21**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Zr(1)	8430(1)	7442(1)	2307(1)	19(1)
Cl(1)	8470(2)	9856(1)	2933(1)	28(1)
Cl(2)	11608(1)	5428(1)	2304(1)	23(1)
S(1)	12483(1)	5048(1)	220(1)	24(1)
C(1)	10286(5)	5007(5)	400(2)	20(1)
C(2)	9009(5)	6738(5)	849(2)	20(1)
C(3)	7103(5)	7682(5)	1126(2)	21(1)
C(4)	6653(6)	9423(5)	1339(2)	25(1)
C(5)	8279(6)	9534(5)	1200(2)	29(1)
C(6)	9690(6)	7912(5)	890(2)	23(1)
C(7)	11574(7)	7315(6)	501(3)	40(1)
C(8)	10605(6)	3344(5)	837(2)	23(1)
C(9)	12627(8)	7947(8)	677(5)	61(2)
C(10)	4808(7)	10961(6)	1611(3)	36(1)
C(11)	7713(6)	6596(6)	3659(2)	25(1)
C(12)	6054(6)	7995(5)	3497(2)	23(1)
C(13)	5532(6)	7369(5)	2921(2)	23(1)
C(14)	6883(5)	5596(5)	2707(2)	22(1)
C(15)	8216(6)	5104(5)	3179(2)	25(1)
C(16)	8716(7)	6638(7)	4270(2)	36(1)
C(17)	4932(7)	9734(6)	3937(3)	36(1)
C(18)	3706(6)	8251(6)	2693(3)	31(1)
C(19)	6651(6)	4373(5)	2221(3)	29(1)
C(20)	9742(6)	3301(6)	3222(3)	33(1)
C(1S)	3340(14)	6618(12)	4929(5)	80(3)
C(2S)	4080(12)	5198(11)	4382(4)	79(3)
C(3S)	5663(12)	3667(9)	4462(4)	71(3)
C(4S)	1468(24)	8465(22)	4874(9)	64(4)

Table 21C. Bond lengths [Å] and angles [deg] for **21**.

Zr(1)-Cl(2)	2.416(3)
Zr(1)-Cl(1)	2.427(2)
Zr(1)-C(3)	2.498(4)
Zr(1)-C(11)	2.500(4)
Zr(1)-C(4)	2.507(4)
Zr(1)-C(12)	2.508(4)
Zr(1)-C(14)	2.519(4)
Zr(1)-C(15)	2.526(4)
Zr(1)-C(13)	2.535(5)
Zr(1)-C(5)	2.562(4)
C(4)-C(5)	1.412(7)
C(4)-C(10)	1.498(6)
C(5)-C(6)	1.386(6)
C(6)-C(7)	1.464(6)
C(7)-C(9)	1.341(8)
C(11)-C(15)	1.416(6)
C(11)-C(12)	1.419(6)
C(11)-C(16)	1.505(6)
C(12)-C(13)	1.406(6)
C(12)-C(17)	1.493(6)

Zr(1)-C(2)	2.563(4)
Zr(1)-C(6)	2.611(4)
S(1)-C(7)	1.783(5)
S(1)-C(1)	1.859(5)
C(1)-C(2)	1.509(5)
C(1)-C(8)	1.521(5)
C(1)-C(1)#1	1.576(8)
C(2)-C(6)	1.402(6)
C(2)-C(3)	1.419(6)
C(3)-C(4)	1.415(6)
C(13)-C(14)	1.420(6)
C(13)-C(18)	1.493(6)
C(14)-C(15)	1.419(6)
C(14)-C(19)	1.499(6)
C(15)-C(20)	1.484(6)
C(1S)-C(2S)	1.405(10)
C(1S)-C(3S)#2	1.429(13)
C(1S)-C(4S)	1.64(2)
C(2S)-C(3S)	1.388(13)
C(3S)-C(1S)#2	1.429(13)

Cl(2)-Zr(1)-Cl(1)	93.79(8)
Cl(2)-Zr(1)-C(3)	120.58(10)
Cl(1)-Zr(1)-C(3)	125.11(10)
Cl(2)-Zr(1)-C(11)	88.53(12)
Cl(1)-Zr(1)-C(11)	84.84(12)
C(3)-Zr(1)-C(11)	132.35(15)
Cl(2)-Zr(1)-C(4)	135.10(10)
Cl(1)-Zr(1)-C(4)	92.43(12)
C(3)-Zr(1)-C(4)	32.84(13)
C(11)-Zr(1)-C(4)	136.34(15)
C(12)-Zr(1)-C(14)	54.24(14)
Cl(2)-Zr(1)-C(15)	78.95(11)
Cl(1)-Zr(1)-C(15)	116.46(12)
C(3)-Zr(1)-C(15)	111.56(15)
C(11)-Zr(1)-C(15)	32.71(14)
C(4)-Zr(1)-C(15)	135.5(2)
C(12)-Zr(1)-C(15)	54.31(13)
C(14)-Zr(1)-C(15)	32.68(14)
Cl(2)-Zr(1)-C(13)	132.80(11)
Cl(1)-Zr(1)-C(13)	108.05(10)
C(4)-Zr(1)-C(5)	32.3(2)
C(12)-Zr(1)-C(5)	127.29(14)
C(14)-Zr(1)-C(5)	133.4(2)
C(15)-Zr(1)-C(5)	165.1(2)
C(13)-Zr(1)-C(5)	118.05(15)
Cl(2)-Zr(1)-C(2)	88.80(10)

Cl(2)-Zr(1)-C(12)	121.23(12)
Cl(1)-Zr(1)-C(12)	80.07(11)
C(3)-Zr(1)-C(12)	109.5(2)
C(11)-Zr(1)-C(12)	32.92(14)
C(4)-Zr(1)-C(12)	103.7(2)
Cl(2)-Zr(1)-C(14)	104.17(12)
Cl(1)-Zr(1)-C(14)	133.92(10)
C(3)-Zr(1)-C(14)	80.89(14)
C(11)-Zr(1)-C(14)	54.25(13)
C(4)-Zr(1)-C(14)	103.0(2)
C(3)-Zr(1)-C(13)	80.06(15)
C(11)-Zr(1)-C(13)	53.92(14)
C(4)-Zr(1)-C(13)	86.4(2)
C(12)-Zr(1)-C(13)	32.36(14)
C(14)-Zr(1)-C(13)	32.64(13)
C(15)-Zr(1)-C(13)	53.91(13)
Cl(2)-Zr(1)-C(5)	107.22(12)
Cl(1)-Zr(1)-C(5)	77.14(12)
C(3)-Zr(1)-C(5)	53.60(15)
C(11)-Zr(1)-C(5)	156.62(14)
C(12)-Zr(1)-C(2)	139.64(15)
C(14)-Zr(1)-C(2)	95.10(13)
C(15)-Zr(1)-C(2)	115.14(14)
C(13)-Zr(1)-C(2)	107.64(14)
C(5)-Zr(1)-C(2)	52.71(13)
Cl(2)-Zr(1)-C(6)	82.65(12)

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Table 21C. *(Continued)*

Cl(1)-Zr(1)-C(2)	127.84(9)
C(3)-Zr(1)-C(2)	32.53(13)
C(11)-Zr(1)-C(2)	147.32(13)
C(4)-Zr(1)-C(2)	53.64(13)
C(12)-Zr(1)-C(6)	156.02(14)
C(14)-Zr(1)-C(6)	126.51(13)
C(15)-Zr(1)-C(6)	142.21(13)
C(13)-Zr(1)-C(6)	132.57(14)
C(5)-Zr(1)-C(6)	31.06(13)
C(2)-Zr(1)-C(6)	31.42(13)
C(7)-S(1)-C(1)	97.0(2)
C(2)-C(1)-C(8)	116.1(3)
C(2)-C(1)-C(1)#1	110.6(4)
C(8)-C(1)-C(1)#1	111.8(4)
C(4)-C(3)-Zr(1)	73.9(2)
C(2)-C(3)-Zr(1)	76.2(2)
C(5)-C(4)-C(3)	107.7(4)
C(5)-C(4)-C(10)	123.8(4)
C(3)-C(4)-C(10)	128.4(4)
C(5)-C(4)-Zr(1)	76.0(2)
C(3)-C(4)-Zr(1)	73.2(2)
C(10)-C(4)-Zr(1)	119.9(3)
C(6)-C(5)-C(4)	108.0(4)
C(6)-C(5)-Zr(1)	76.4(2)
C(15)-C(11)-C(12)	108.3(4)
C(15)-C(11)-C(16)	125.4(4)
C(12)-C(11)-C(16)	126.2(4)
C(15)-C(11)-Zr(1)	74.7(2)
C(12)-C(11)-Zr(1)	73.9(2)
C(16)-C(11)-Zr(1)	120.5(3)
C(13)-C(12)-C(11)	107.8(4)
C(13)-C(12)-C(17)	125.7(4)
C(11)-C(12)-C(17)	126.0(4)
C(13)-C(12)-Zr(1)	74.9(2)
C(13)-C(14)-C(19)	124.1(4)
C(15)-C(14)-Zr(1)	74.0(2)
C(13)-C(14)-Zr(1)	74.3(2)
C(19)-C(14)-Zr(1)	129.3(3)
C(11)-C(15)-C(14)	107.6(4)
C(11)-C(15)-C(20)	126.1(4)
C(14)-C(15)-C(20)	126.0(4)
C(11)-C(15)-Zr(1)	72.6(2)

Cl(1)-Zr(1)-C(6)	97.34(11)
C(3)-Zr(1)-C(6)	52.71(15)
C(11)-Zr(1)-C(6)	171.03(14)
C(4)-Zr(1)-C(6)	52.45(15)
C(2)-C(1)-S(1)	102.1(3)
C(8)-C(1)-S(1)	106.4(3)
C(1)#1-C(1)-S(1)	109.2(3)
C(6)-C(2)-C(3)	107.2(3)
C(6)-C(2)-C(1)	116.6(3)
C(3)-C(2)-C(1)	134.8(4)
C(6)-C(2)-Zr(1)	76.2(2)
C(3)-C(2)-Zr(1)	71.2(2)
C(1)-C(2)-Zr(1)	128.7(2)
C(4)-C(3)-C(2)	107.7(4)
C(4)-C(5)-Zr(1)	71.7(2)
C(5)-C(6)-C(2)	109.4(4)
C(5)-C(6)-C(7)	133.3(4)
C(2)-C(6)-C(7)	116.4(4)
C(5)-C(6)-Zr(1)	72.5(2)
C(2)-C(6)-Zr(1)	72.4(2)
C(7)-C(6)-Zr(1)	129.4(3)
C(9)-C(7)-C(6)	124.2(5)
C(9)-C(7)-S(1)	121.6(4)
C(6)-C(7)-S(1)	106.0(3)
C(11)-C(12)-Zr(1)	73.2(2)
C(17)-C(12)-Zr(1)	124.1(3)
C(12)-C(13)-C(14)	108.4(4)
C(12)-C(13)-C(18)	126.0(4)
C(14)-C(13)-C(18)	124.5(4)
C(12)-C(13)-Zr(1)	72.8(2)
C(14)-C(13)-Zr(1)	73.0(2)
C(18)-C(13)-Zr(1)	129.9(3)
C(15)-C(14)-C(13)	107.8(4)
C(15)-C(14)-C(19)	126.4(4)
C(14)-C(15)-Zr(1)	73.4(2)
C(20)-C(15)-Zr(1)	124.7(3)
C(2S)-C(1S)-C(3S)#2	115.0(9)
C(2S)-C(1S)-C(4S)	122.6(11)
C(3S)#2-C(1S)-C(4S)	122.4(8)
C(3S)-C(2S)-C(1S)	119.9(9)
C(2S)-C(3S)-C(1S)#2	125.1(7)

Table 21D. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **21**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	21(1)	10(1)	22(1)	0(1)	-4(1)	-5(1)
Cl(1)	40(1)	17(1)	30(1)	-2(1)	-5(1)	-15(1)
Cl(2)	20(1)	18(1)	28(1)	1(1)	-6(1)	-6(1)
S(1)	24(1)	17(1)	26(1)	-4(1)	-2(1)	-7(1)
C(1)	22(2)	14(2)	25(2)	-2(1)	-6(2)	-8(1)
C(2)	25(2)	12(2)	18(2)	-1(1)	-4(1)	-5(1)
C(3)	21(2)	15(2)	17(2)	-1(1)	-6(1)	0(1)
C(4)	31(2)	12(2)	19(2)	2(1)	-7(2)	0(2)
C(5)	43(3)	12(2)	23(2)	2(2)	-3(2)	-9(2)
C(6)	32(2)	16(2)	19(2)	-1(1)	3(2)	-11(2)
C(7)	40(3)	25(2)	51(3)	-16(2)	19(2)	-21(2)
C(8)	29(2)	10(2)	25(2)	0(1)	-7(2)	-6(2)
C(9)	24(3)	38(3)	117(6)	-41(3)	-5(3)	-10(2)
C(10)	35(3)	17(2)	35(2)	0(2)	-9(2)	6(2)
C(11)	30(2)	27(2)	21(2)	5(2)	-5(2)	-17(2)
C(12)	24(2)	18(2)	23(2)	-3(2)	3(2)	-9(2)
C(13)	26(2)	18(2)	27(2)	1(2)	-6(2)	-11(2)
C(14)	23(2)	14(2)	27(2)	1(2)	-4(2)	-8(2)
C(15)	25(2)	17(2)	30(2)	9(2)	-5(2)	-10(2)
C(16)	50(3)	39(3)	27(2)	11(2)	-17(2)	-26(2)
C(17)	39(3)	28(2)	39(2)	-13(2)	2(2)	-16(2)
C(18)	19(2)	24(2)	44(2)	-5(2)	-5(2)	-4(2)
C(19)	33(2)	16(2)	39(2)	-5(2)	-3(2)	-13(2)
C(20)	33(2)	18(2)	50(3)	12(2)	-14(2)	-12(2)
C(1S)	111(7)	81(5)	65(4)	-20(4)	40(5)	-76(5)
C(2S)	110(7)	76(5)	68(4)	-26(4)	43(4)	-75(5)
C(3S)	102(6)	53(4)	66(4)	-30(3)	42(4)	-60(4)

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Table 21E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **21**.

Atom	x	y	z	U(eq)
H(3)	6214(5)	7272(5)	1072(2)	25
H(5)	8365(6)	10642(5)	1233(2)	35
H(8A)	9545(18)	3162(22)	874(15)	34
H(8B)	10786(41)	3473(16)	1360(6)	34
H(8C)	11688(24)	2326(8)	559(9)	34
H(10C)	4671(19)	11982(15)	1302(14)	54
H(10B)	4675(19)	11253(30)	2159(6)	54
H(10A)	3873(7)	10653(17)	1549(19)	54
H(16C)	8251(35)	6287(47)	4764(6)	54
H(16B)	8532(40)	7838(12)	4333(15)	54
H(16A)	10017(10)	5818(35)	4111(10)	54
H(7C)	3985(31)	9679(16)	4333(14)	54
H(17B)	4362(39)	10660(10)	3578(4)	54
H(17A)	5711(11)	10003(23)	4187(17)	54
H(18C)	3008(17)	7664(27)	2930(15)	47
H(18B)	3857(6)	8170(38)	2127(3)	47
H(18A)	3055(18)	9496(12)	2872(16)	47
H(19C)	5627(29)	4209(35)	2485(9)	44
H(19B)	7765(17)	3229(15)	2143(16)	44
H(91A)	6411(45)	4882(21)	1716(8)	44
H(20C)	9369(17)	2693(17)	3645(13)	50
H(20B)	10794(16)	3382(6)	3319(19)	50
H(20A)	10071(31)	2637(16)	2730(8)	50
H(1S)	2335(14)	7699(12)	4889(5)	80
H(2S)	3498(12)	5286(11)	3959(4)	95
H(3S)	6119(12)	2736(9)	4082(4)	85
H(4SA)	174(273)	8732(231)	5003(90)	97
H(4SB)	2406(272)	7696(263)	4798(110)	97
H(4SC)	1105(242)	9705(268)	5232(89)	97
H(91)	12069(80)	9043(82)	888(31)	43(15)
H(92)	13631(85)	7749(78)	377(30)	42(16)

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Table 24A. Crystal data, data collection, structure solution and refinement parameters for **24**.

Empirical formula	$C_{22}H_{28}S_2Si$
Formula weight	384.65
Temperature	110(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\bar{1}$
Unit cell dimensions	a = 8.7053(9) Å, α = 98.354(2)°
	b = 10.5026(10) Å, β = 102.703(2)°
	c = 12.2813(12) Å, γ = 106.605(2)°
Volume	1023.35(18) $Å^3$
Z	2
Density (calculated)	1.248 Mg/m^3
Absorption coefficient	0.321 mm^{-1}
F(000)	412
Crystal size	0.4 x 0.3 x 0.3 mm^3
Theta range for data collection	1.74 to 30.02°.
Index ranges	-12<=h<=12, -14<=k<=8, -17<=l<=17
Reflections collected	8503
Independent reflections	5847 [R(int) = 0.0138]
Completeness to theta = 30.02°	97.8 %
Absorption correction	Sadabs program
Max. and min. transmission	0.876 and 0.985
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5847 / 0 / 334
Goodness-of-fit on F^2	1.100
Final R indices for 4885 reflections with [I>2σ(I)]	R_1 = 0.0499, wR_2 = 0.1376
R indices (all data)	R_1 = 0.0574, wR_2 = 0.1477
Largest diff. peak and hole	1.277 and -0.351 $e.Å^{-3}$

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Table 24B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **24**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Si(1)	-2060(1)	983(1)	-1652(1)	19(1)
S(1)	-4802(1)	-3147(1)	-4924(1)	30(1)
C(1)	-3637(2)	701(2)	-3108(1)	21(1)
C(2)	-4125(2)	-734(2)	-3793(1)	21(1)
C(3)	-5806(2)	-1467(2)	-3832(1)	23(1)
C(4)	-6468(2)	-506(2)	-3266(1)	26(1)
C(5)	-5297(2)	729(2)	-2898(1)	24(1)
C(6)	-3400(2)	-1500(2)	-4367(1)	25(1)
C(7)	-6370(2)	-2799(2)	-4401(1)	28(1)
C(8)	-5495(2)	1993(2)	-2303(2)	30(1)
C(9)	-1729(2)	-1125(2)	-4595(2)	32(1)
C(10)	-7996(3)	-3879(2)	-4566(2)	37(1)
C(11)	-428(2)	176(2)	-1710(2)	26(1)
C(12)	-3267(2)	157(2)	-714(1)	25(1)
S(1')	1062(1)	3658(1)	2373(1)	22(1)
C(1')	-904(2)	2904(2)	-1060(1)	19(1)
C(2')	-129(2)	3210(1)	214(1)	19(1)
C(3')	1650(2)	3556(1)	441(1)	19(1)
C(4')	2053(2)	3605(2)	-648(1)	21(1)
C(5')	636(2)	3297(1)	-1498(1)	21(1)
C(6')	-652(2)	3240(2)	1184(1)	21(1)
C(7')	2492(2)	3807(2)	1568(1)	21(1)
C(8')	520(2)	3272(2)	-2734(1)	26(1)
C(9')	-2365(2)	3025(2)	1325(1)	25(1)
C(10')	4312(2)	4122(2)	2111(1)	25(1)

Table 24C. Bond lengths [Å] and angles [deg] for **24**.

Si(1)-C(11)	1.8603(17)
Si(1)-C(12)	1.8669(16)
Si(1)-C(1)	1.9241(15)
Si(1)-C(1')	1.9239(15)
S(1)-C(7)	1.7356(18)
S(1)-C(6)	1.7418(16)
C(1)-C(2)	1.506(2)
C(1)-C(5)	1.530(2)
C(2)-C(6)	1.365(2)
C(2)-C(3)	1.432(2)
C(2')-C(6')	1.3649(19)
C(2')-C(3')	1.4380(19)
C(3')-C(7')	1.363(2)
C(3')-C(4')	1.459(2)

C(3)-C(7)	1.363(2)
C(3)-C(4)	1.463(2)
C(4)-C(5)	1.340(2)
C(5)-C(8)	1.493(2)
C(6)-C(9)	1.494(2)
C(7)-C(10)	1.490(2)
S(1')-C(7')	1.7397(14)
S(1')-C(6')	1.7416(15)
C(1')-C(2')	1.507(2)
C(1')-C(5')	1.5238(19)
C(4')-C(5')	1.350(2)
C(5')-C(8')	1.495(2)
C(6')-C(9')	1.496(2)
C(7')-C(10')	1.496(2)

C(11)-Si(1)-C(12)	106.47(8)
C(11)-Si(1)-C(1)	114.26(7)
C(12)-Si(1)-C(1)	106.66(7)
C(11)-Si(1)-C(1')	106.35(7)
C(12)-Si(1)-C(1')	113.76(7)
C(1)-Si(1)-C(1')	109.48(7)
C(7)-S(1)-C(6)	94.01(8)
C(2)-C(1)-C(5)	101.28(12)
C(2)-C(1)-Si(1)	111.44(10)
C(5)-C(1)-Si(1)	108.45(10)
C(2)-C(6)-C(9)	130.88(15)
C(2)-C(6)-S(1)	109.22(12)
C(9)-C(6)-S(1)	119.86(12)
C(3)-C(7)-C(10)	129.88(17)
C(3)-C(7)-S(1)	108.68(12)
C(10)-C(7)-S(1)	121.41(14)
C(7')-S(1')-C(6')	94.01(7)
C(2')-C(1')-C(5')	101.51(11)
C(2')-C(1')-Si(1)	110.99(10)
C(5')-C(1')-Si(1)	108.26(9)
C(2')-C(6')-C(9')	129.83(14)
C(2')-C(6')-S(1')	109.45(11)
C(9')-C(6')-S(1')	120.68(11)

C(6)-C(2)-C(3)	113.31(14)
C(6)-C(2)-C(1)	137.24(14)
C(3)-C(2)-C(1)	109.45(13)
C(7)-C(3)-C(2)	114.76(14)
C(7)-C(3)-C(4)	137.67(15)
C(2)-C(3)-C(4)	107.50(13)
C(5)-C(4)-C(3)	109.71(14)
C(4)-C(5)-C(8)	126.22(15)
C(4)-C(5)-C(1)	111.58(14)
C(8)-C(5)-C(1)	122.14(14)
C(6')-C(2')-C(3')	113.08(13)
C(6')-C(2')-C(1')	137.64(13)
C(3')-C(2')-C(1')	109.27(12)
C(7')-C(3')-C(2')	114.85(12)
C(7')-C(3')-C(4')	137.52(13)
C(2')-C(3')-C(4')	107.53(12)
C(5')-C(4')-C(3')	109.59(12)
C(4')-C(5')-C(8')	126.12(13)
C(4')-C(5')-C(1')	111.55(12)
C(8')-C(5')-C(1')	122.28(13)
C(3')-C(7')-C(10')	129.65(13)
C(3')-C(7')-S(1')	108.58(11)
C(10')-C(7')-S(1')	121.75(11)

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Table 24D. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **24**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	21(1)	15(1)	18(1)	2(1)	4(1)	3(1)
S(1)	44(1)	19(1)	22(1)	-1(1)	10(1)	4(1)
C(1)	23(1)	17(1)	21(1)	3(1)	6(1)	4(1)
C(2)	24(1)	18(1)	18(1)	3(1)	5(1)	3(1)
C(3)	26(1)	22(1)	18(1)	4(1)	4(1)	2(1)
C(4)	21(1)	30(1)	23(1)	5(1)	4(1)	6(1)
C(5)	25(1)	25(1)	21(1)	4(1)	4(1)	10(1)
C(6)	32(1)	21(1)	19(1)	1(1)	8(1)	6(1)
C(7)	31(1)	26(1)	19(1)	3(1)	6(1)	0(1)
C(8)	32(1)	29(1)	31(1)	3(1)	8(1)	16(1)
C(9)	35(1)	33(1)	29(1)	2(1)	15(1)	12(1)
C(10)	38(1)	30(1)	25(1)	3(1)	3(1)	-11(1)
C(11)	29(1)	19(1)	32(1)	4(1)	9(1)	8(1)
C(12)	27(1)	22(1)	25(1)	6(1)	7(1)	3(1)
S(1')	25(1)	21(1)	18(1)	1(1)	6(1)	7(1)
C(1')	20(1)	17(1)	19(1)	2(1)	6(1)	5(1)
C(2')	20(1)	15(1)	18(1)	1(1)	5(1)	4(1)
C(3')	21(1)	16(1)	21(1)	2(1)	7(1)	5(1)
C(4')	22(1)	17(1)	24(1)	3(1)	10(1)	5(1)
C(5')	26(1)	15(1)	22(1)	4(1)	10(1)	5(1)
C(6')	22(1)	17(1)	21(1)	0(1)	7(1)	4(1)
C(7')	21(1)	18(1)	22(1)	1(1)	6(1)	6(1)
C(8')	32(1)	24(1)	22(1)	6(1)	10(1)	8(1)
C(9')	24(1)	27(1)	25(1)	1(1)	11(1)	6(1)
C(10')	22(1)	25(1)	25(1)	1(1)	2(1)	7(1)

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Table 24E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **24**.

Atom	x	y	z	U(eq)
H(1)	-3260(30)	1370(20)	-3510(20)	42(6)
H(4)	-7562	-723	-3174	31
H(8A)	-4760(30)	2320(20)	-1530(20)	36(6)
H(8B)	-5150(30)	2700(30)	-2660(20)	41(6)
H(8C)	-6540(40)	1910(30)	-2180(30)	60(8)
H(9A)	-920(30)	-1420(30)	-4140(20)	52(7)
H(9B)	-1760(30)	-1430(30)	-5360(30)	61(8)
H(9C)	-1170(30)	-140(30)	-4370(20)	44(6)
H(10C)	-8430(40)	-4370(30)	-5420(30)	64(8)
H(10A)	-7900(30)	-4470(30)	-4100(20)	62(8)
H(10B)	-8810(40)	-3510(30)	-4400(20)	53(7)
H(11C)	130(20)	430(20)	-2237(17)	25(5)
H(11B)	-950(30)	-780(30)	-1930(20)	42(6)
H(11C)	310(30)	420(20)	-1010(20)	34(6)
H(12A)	-4150(20)	479(19)	-672(16)	18(4)
H(12B)	-2520(30)	360(30)	40(20)	48(7)
H(12C)	-3750(30)	-790(30)	-1110(20)	49(7)
H(1')	-1610(30)	3360(20)	-1285(18)	30(5)
H(4')	3250(30)	3880(20)	-643(18)	29(5)
H(8'A)	1650(30)	3600(20)	-2871(19)	37(6)
H(8'B)	-70(30)	2360(30)	-3210(20)	47(7)
H(8'C)	-70(30)	3810(20)	-3006(19)	37(6)
H(9'A)	-3180(30)	2910(20)	620(20)	38(6)
H(9'B)	-2880(30)	2170(30)	1448(19)	38(6)
H(9'C)	-2340(30)	3720(30)	1900(20)	41(6)
H(10D)	4530(30)	3380(30)	2320(20)	39(6)
H(10E)	4970(30)	4400(30)	1570(20)	48(7)
H(10F)	4710(40)	4820(30)	2810(30)	64(8)