Crystal Data and Structure Refinement for $(C_5Me_5)_2Sr(THF)_2$ (2) and $(C_5Me_5)_2Ba(THF)_2$ (3)

parameter	(2)	(3)
empirical formula	$C_{28}H_{46}O_2Sr$	$C_{28}H_{46}O_2Ba$
formula weight	502.27	551.99
temp, K	193	193
λ(Mo Kα), Å	0.71073	0.71073
crystal system	monoclinic	monoclinic
space group	*C2/c* (No. 15)	*C2/c* (No 15)
a,Å	21.931(4)	22.054(4)
b,Å	20.688(4)	20.556(4)
c,Å	15.877(3)	16.087(3)
α,deg	90	90
β,deg	130.17(3)	129.45(3)
γ,deg	90	90
V (Å^3), Z	5505(2), 8	5631(2), 8
d calc, g/cm^3	1.212	1.302
μ, mm^{-1}	1.979	1.430
F(000)	2144	2288
Crystal Size, mm	0.35 × 0.35 × 0.27	0.50 × 0.50 × 0.40
θ range, deg	2.58-24.98	2.55-24.04
limiting indices	$0 \le h \le 26$	$0 \le h \le 25$
	$0 \le k \le 24$	$0 \le k \le 23$
	$-18 \le l \le 14$	$-18 \le l \le 14$
reflections collected	4231	4220
independent reflections	4010	4133
no. of reflections [F_0>4σ(F)]	2919	3724
refinement method	full-matrix least-squares on F^2	
data/parameters	4010/299	4133/298
goodness-of-fit on F^2	1.033	1.031
final R indices [I >2σ(I)][a]	R_1=0.0686, wR_2=0.1584	R_1=0.0409, wR_2=0.1042
R indices (all data)	R_1=0.1054, wR_2=0.1720	R_1=0.0471, wR_2=0.1076
extinction coefficient	0.0014(3)	none
max/min diff peak, e Å^{-3}	1.365/-1.75	1.012/-1.587

[a] $R_1 = 3\,||F_o|-|F_c||\,/\,3|F_o|$, $wR_2 = \{3[w(F_o^2 - F_c^2)^2]\,/\,3[w(F_o^2)^2]\}^{1/2}$

Using Cyclopentadienyl Precursors by J. Ihanus et al.

complex (2) cm0111130

File: D:\CRYSTAL\SRCPT1B\SR1.CIF 22.2.2001, 15:27:14

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 'Sr'  'Sr'  -1.5307   3.2498
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 '-x, -y, -z'
 'x, -y, z-1/2'
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_atom_sites_solution_secondary    difmap
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Sr1 Sr 0.22579(3) 0.63326(3) 0.74950(5) 0.0318(2) Uani 1 d . . .
C1 C 0.1373(4) 0.7202(4) 0.5642(5) 0.0365(17) Uani 1 d . . .
C2 C 0.1196(4) 0.7428(3) 0.6288(5) 0.0342(16) Uani 1 d . . .
C3 C 0.0736(4) 0.6950(3) 0.6301(5) 0.0345(16) Uani 1 d . . .
C4 C 0.0619(4) 0.6433(3) 0.5622(6) 0.0426(18) Uani 1 d . . .
C5 C 0.1014(4) 0.6584(4) 0.5230(5) 0.046(2) Uani 1 d . . .
C6 C 0.1760(5) 0.7606(5) 0.5299(7) 0.062(3) Uani 1 d . . .
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H6A H 0.1352 0.7746 0.4533 0.094 Uiso 1 calc R . .
H6B H 0.2163 0.7345 0.5364 0.094 Uiso 1 calc R . .
H6C H 0.2016 0.7985 0.5779 0.094 Uiso 1 calc R . .
C7 C 0.1335(5) 0.8097(3) 0.6782(7) 0.057(2) Uani 1 d . . .
H7A H 0.0834 0.8264 0.6566 0.085 Uiso 1 calc R . .
H7B H 0.1528 0.8388 0.6511 0.085 Uiso 1 calc R . .
H7C H 0.1734 0.8069 0.7587 0.085 Uiso 1 calc R . .
C8 C 0.0352(5) 0.7026(5) 0.6813(7) 0.062(2) Uani 1 d . . .
H8A H -0.0165 0.7241 0.6289 0.093 Uiso 1 calc R . .
H8B H 0.0698 0.7287 0.7484 0.093 Uiso 1 calc R . .
H8C H 0.0274 0.6599 0.6997 0.093 Uiso 1 calc R . .
C9 C 0.0126(5) 0.5841(4) 0.5335(7) 0.082(3) Uani 1 d . . .
H9A H -0.0309 0.5824 0.4535 0.123 Uiso 1 calc R . .
H9B H -0.0098 0.5856 0.5706 0.123 Uiso 1 calc R . .
H9C H 0.0461 0.5456 0.5575 0.123 Uiso 1 calc R . .
C10 C 0.0976(6) 0.6195(5) 0.4387(7) 0.090(4) Uani 1 d . . .
H10A H 0.0453 0.6254 0.3656 0.135 Uiso 1 calc R . .
H10B H 0.1056 0.5736 0.4586 0.135 Uiso 1 calc R . .
H10C H 0.1395 0.6342 0.4374 0.135 Uiso 1 calc R . .
C11 C 0.1970(4) 0.5558(3) 0.8714(5) 0.0376(17) Uani 1 d . . .
C12 C 0.2473(4) 0.5179(3) 0.8669(6) 0.0412(18) Uani 1 d . . .
C13 C 0.3229(4) 0.5480(4) 0.9327(5) 0.0414(18) Uani 1 d . . .
C14 C 0.3190(4) 0.6040(4) 0.9775(6) 0.0416(17) Uani 1 d . . .
C15 C 0.2398(4) 0.6087(4) 0.9392(6) 0.0451(18) Uani 1 d . . .
C16 C 0.1144(5) 0.5374(4) 0.8249(7) 0.060(2) Uani 1 d . . .
H16A H 0.1131 0.5324 0.8851 0.090 Uiso 1 calc R . .
H16B H 0.0994 0.4964 0.7849 0.090 Uiso 1 calc R . .
H16C H 0.0768 0.5712 0.7744 0.090 Uiso 1 calc R . .
C17 C 0.2247(6) 0.4518(4) 0.8106(7) 0.068(3) Uani 1 d . . .
H17A H 0.2011 0.4251 0.8342 0.102 Uiso 1 calc R . .
H17B H 0.2725 0.4305 0.8312 0.102 Uiso 1 calc R . .
H17C H 0.1859 0.4575 0.7305 0.102 Uiso 1 calc R . .
C18 C 0.3984(5) 0.5212(4) 0.9587(7) 0.064(3) Uani 1 d . . .
H18A H 0.4430 0.5238 1.0382 0.096 Uiso 1 calc R . .
H18B H 0.4110 0.5466 0.9195 0.096 Uiso 1 calc R . .
H18C H 0.3897 0.4760 0.9349 0.096 Uiso 1 calc R . .
C19 C 0.3862(5) 0.6491(4) 1.0593(6) 0.063(3) Uani 1 d . . .
H19A H 0.3983 0.6455 1.1303 0.094 Uiso 1 calc R . .
H19B H 0.3705 0.6936 1.0322 0.094 Uiso 1 calc R . .
H19C H 0.4336 0.6376 1.0687 0.094 Uiso 1 calc R . .
C20 C 0.2122(6) 0.6584(4) 0.9792(7) 0.065(2) Uani 1 d . . .
H20A H 0.2545 0.6654 1.0586 0.097 Uiso 1 calc R . .
H20B H 0.1641 0.6425 0.9648 0.097 Uiso 1 calc R . .
H20C H 0.2002 0.6993 0.9400 0.097 Uiso 1 calc R . .
O1 O 0.2829(3) 0.5733(3) 0.6687(4) 0.0523(14) Uani 1 d . . .
C21 C 0.3005(7) 0.5059(5) 0.6665(8) 0.095(4) Uani 1 d . . .
H21A H 0.261(3) 0.4876(15) 0.598(5) 0.114 Uiso 1 calc R . .
H21B H 0.3052(7) 0.4822(19) 0.720(4) 0.114 Uiso 1 calc R . .
C22 C 0.3793(7) 0.5093(7) 0.6903(9) 0.106(5) Uani 1 d . . .
H22A H 0.418(4) 0.5066(8) 0.760(6) 0.127 Uiso 1 calc R . .
H22B H 0.3830(8) 0.478(3) 0.658(3) 0.127 Uiso 1 calc R . .
C23 C 0.3792(6) 0.5735(7) 0.6468(9) 0.099(5) Uani 1 d . . .
H23A H 0.3766(6) 0.5690(7) 0.593(5) 0.118 Uiso 1 calc R . .
H23B H 0.420(4) 0.594(2) 0.694(4) 0.118 Uiso 1 calc R . .
C24 C 0.3064(5) 0.6065(5) 0.6150(7) 0.066(3) Uani 1 d . . .
H24A H 0.3174(8) 0.649(3) 0.6367(15) 0.080 Uiso 1 calc R . .
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H24B H 0.266(3) 0.6051(5) 0.540(5) 0.080 Uiso 1 calc R . .
O2 O 0.3464(3) 0.7070(3) 0.8274(4) 0.0529(14) Uani 1 d . . .
C25 C 0.3517(5) 0.7767(4) 0.8345(7) 0.061(2) Uani 1 d . . .
H25A H 0.3783(16) 0.7901(9) 0.905(4) 0.074 Uiso 1 calc R . .
H25B H 0.302(3) 0.7949(12) 0.790(3) 0.074 Uiso 1 calc R . .
C26 C 0.3970(5) 0.7944(5) 0.7960(7) 0.068(3) Uani 1 d . . .
H26A H 0.361(2) 0.8046(8) 0.718(5) 0.081 Uiso 1 calc R . .
H26B H 0.431(2) 0.831(2) 0.836(2) 0.081 Uiso 1 calc R . .
C27 C 0.4453(5) 0.7357(5) 0.8187(7) 0.066(3) Uani 1 d . . .
H27A H 0.497(3) 0.7448(7) 0.866(3) 0.079 Uiso 1 calc R . .
H27B H 0.4327(9) 0.7205(11) 0.756(4) 0.079 Uiso 1 calc R . .
C28 C 0.4247(4) 0.6866(5) 0.8679(7) 0.064(3) Uani 1 d . . .
H28A H 0.4228(5) 0.645(3) 0.8443(15) 0.077 Uiso 1 calc R . .
H28B H 0.461(2) 0.6876(5) 0.944(5) 0.077 Uiso 1 calc R . .

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C1 0.028(4) 0.053(5) 0.028(3) 0.009(3) 0.018(3) 0.005(3)
C2 0.031(4) 0.027(4) 0.031(4) 0.002(3) 0.014(3) 0.001(3)
C3 0.028(4) 0.034(4) 0.036(4) 0.007(3) 0.019(3) 0.004(3)
C4 0.027(3) 0.026(4) 0.045(4) -0.001(3) 0.009(3) -0.004(3)
C5 0.029(4) 0.052(5) 0.027(4) -0.010(3) 0.004(3) 0.013(3)
C6 0.039(4) 0.098(7) 0.051(5) 0.016(5) 0.029(4) -0.003(5)
C7 0.042(4) 0.032(4) 0.062(5) -0.005(4) 0.018(4) -0.003(4)
C8 0.040(4) 0.084(7) 0.070(6) 0.028(5) 0.039(5) 0.016(5)
C9 0.058(6) 0.044(5) 0.069(6) 0.008(5) 0.008(5) -0.017(5)
C10 0.066(6) 0.108(9) 0.045(5) -0.025(5) 0.012(5) 0.031(6)
C11 0.034(4) 0.031(4) 0.033(4) 0.007(3) 0.015(3) 0.003(3)
C12 0.043(4) 0.024(4) 0.037(4) 0.002(3) 0.017(4) -0.001(3)
C13 0.033(4) 0.044(4) 0.029(4) 0.009(3) 0.012(3) 0.012(3)
C14 0.037(4) 0.042(4) 0.034(4) -0.002(3) 0.017(3) 0.000(4)
C15 0.045(4) 0.035(4) 0.048(4) 0.003(3) 0.027(4) 0.002(4)
C16 0.043(5) 0.056(5) 0.063(5) 0.018(4) 0.026(4) -0.006(4)
C17 0.081(7) 0.035(5) 0.062(6) -0.002(4) 0.035(5) 0.002(5)
C18 0.057(5) 0.079(7) 0.060(5) 0.022(5) 0.039(5) 0.036(5)
C19 0.055(5) 0.078(7) 0.036(4) -0.011(4) 0.021(4) -0.020(5)
C20 0.078(6) 0.055(5) 0.073(6) 0.001(5) 0.054(6) 0.004(5)
O1 0.045(3) 0.056(4) 0.050(3) -0.013(3) 0.028(3) 0.005(3)
C21 0.121(10) 0.071(7) 0.054(6) -0.018(5) 0.040(6) 0.025(7)
C22 0.090(9) 0.143(13) 0.064(7) -0.004(7) 0.041(6) 0.070(9)
C23 0.053(6) 0.149(13) 0.086(8) -0.039(8) 0.042(6) 0.008(7)
C24 0.059(5) 0.090(7) 0.060(5) -0.014(5) 0.043(5) 0.002(5)
O2 0.039(3) 0.066(4) 0.048(3) -0.004(3) 0.025(3) -0.014(3)
C25 0.042(5) 0.060(6) 0.066(6) -0.014(4) 0.027(5) -0.006(4)
C26 0.057(6) 0.065(6) 0.064(6) -0.009(5) 0.031(5) -0.028(5)
C27 0.042(5) 0.091(8) 0.061(5) -0.025(5) 0.031(5) -0.029(5)
C28 0.034(4) 0.084(7) 0.048(5) -0.003(5) 0.015(4) 0.004(5)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Sr1 O1 2.612(5) . ?
Sr1 C5 2.827(7) . ?
Sr1 C4 2.832(7) . ?
Sr1 C13 2.848(7) . ?
Sr1 C14 2.847(7) . ?
Sr1 C3 2.864(6) . ?
Sr1 C15 2.869(7) . ?
Sr1 C12 2.873(7) . ?
Sr1 C11 2.878(7) . ?
Sr1 C1 2.880(6) . ?
Sr1 C2 2.912(6) . ?
C1 C2 1.390(9) . ?
C1 C5 1.420(10) . ?
C1 C6 1.521(10) . ?
C2 C3 1.422(9) . ?
C2 C7 1.520(9) . ?
C3 C4 1.420(10) . ?
C3 C8 1.508(10) . ?
C4 C5 1.392(11) . ?
C4 C9 1.496(10) . ?
C5 C10 1.518(11) . ?
C6 H6A 0.9800 . ?
C6 H6B 0.9800 . ?
C6 H6C 0.9800 . ?
C7 H7A 0.9800 . ?
C7 H7B 0.9800 . ?
C7 H7C 0.9800 . ?
C8 H8A 0.9800 . ?
C8 H8B 0.9800 . ?
C8 H8C 0.9800 . ?
C9 H9A 0.9800 . ?
C9 H9B 0.9800 . ?
C9 H9C 0.9800 . ?
C10 H10A 0.9800 . ?
C10 H10B 0.9800 . ?
C10 H10C 0.9800 . ?
C11 C15 1.391(10) . ?
C11 C12 1.393(10) . ?
C11 C16 1.499(10) . ?
C12 C13 1.412(10) . ?
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C12 C17 1.531(10) . ?
C13 C14 1.390(10) . ?
C13 C18 1.530(10) . ?
C14 C15 1.426(10) . ?
C14 C19 1.504(11) . ?
C15 C20 1.524(11) . ?
C16 H16A 0.9800 . ?
C16 H16B 0.9800 . ?
C16 H16C 0.9800 . ?
C17 H17A 0.9800 . ?
C17 H17B 0.9800 . ?
C17 H17C 0.9800 . ?
C18 H18A 0.9800 . ?
C18 H18B 0.9800 . ?
C18 H18C 0.9800 . ?
C19 H19A 0.9800 . ?
C19 H19B 0.9800 . ?
C19 H19C 0.9800 . ?
C20 H20A 0.9800 . ?
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C5 Sr1 C13 152.3(2) . . ?
C4 Sr1 C13 136.4(2) . . ?
O2 Sr1 C14 80.96(19) . . ?
O1 Sr1 C14 110.18(19) . . ?
C5 Sr1 C14 165.7(2) . . ?
C4 Sr1 C14 137.3(2) . . ?
C13 Sr1 C14 28.3(2) . . ?
O2 Sr1 C3 116.80(19) . . ?
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O1 Sr1 C15 132.13(19) . . ?
C5 Sr1 C15 136.9(2) . . ?
C4 Sr1 C15 108.6(2) . . ?
C13 Sr1 C15 46.8(2) . . ?
C14 Sr1 C15 28.9(2) . . ?
C3 Sr1 C15 93.7(2) . . ?
O2 Sr1 C12 119.48(19) . . ?
O1 Sr1 C12 89.6(2) . . ?
C5 Sr1 C12 126.8(2) . . ?
C4 Sr1 C12 107.9(2) . . ?
C13 Sr1 C12 28.6(2) . . ?
C14 Sr1 C12 46.8(2) . . ?
C3 Sr1 C12 115.7(2) . . ?
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