X-Ray data for (*S*,*S*)-6ai. Crystal data and structure refinement.

Identification code	CCDC 1866767	
Empirical formula	$C_{30}H_{37}BO_2S$	
Formula weight	472.52	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 9.5200(2) Å	□= 90°.
	b = 13.4283(4) Å	□= 90°.
	c = 20.6016(6) Å	□ = 90°.
Volume	2633.66 (12) $Å^3$	
Z	4	
Density (calculated)	1.192 Mg/m^3	
Absorption coefficient	0.613 mm^{-1}	
F(000)	1016	
Crystal size	0.51 x 0.37 x 0.26 mm	
Theta range for data collection	2.36 to 28.30°.	
Index ranges	-12<=h<=12, -17<=k<=17, -27<=l<=27	
Reflections collected	49428	
Independent reflections	6522 [R(int) = 0.044]	
Completeness to theta = 28.3°	99.8 %	
Absorption correction	Integration	
Max. and min. transmission	0.746 and 0.700	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6522 / 0 / 314	
Goodness-of-fit on F^2	0.995	
Final R indices [I>2sigma(I)]	R1 = 0.0306, wR2 = 0.0733	
Largest diff. peak and hole	0.2864 and -0.1977 $e.Å^{-3}$	

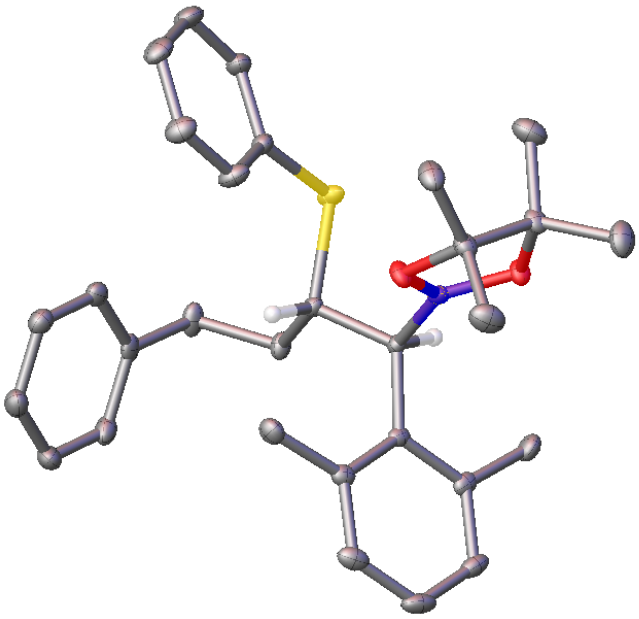

Figure 1. X-ray structure of complex (*S,S*)-**6ai.**

The crystals were obtained directly from recrystallization as yellow needles 0.51 x 0.37 x 0.26 mm in size and mounted using oil (Paratone-N, Exxon) to a thin glass fiver with the (1 0 0) scattering planes roughly normal to the spindle axis. Systematic absences for (*S,S*)-**6ai** were consistent with the space group $P2_12_12_1$. Unit cell dimensions were a = 9.5200(2) Å, b = 13.4283(4) Å, c = 20.6016(6) Å Å, α= 90°, β= 90°, γ = 90°. Integration absorption correction was applied and maximum and minimum transmission factors were 0.746 and 0.700. The 6522 data points were used in the full-matrix least-squares refinement. The structure was solved using charge flipping by using SHELXTL software package.[i] Hydrogen atoms were placed in "idealized" positions and their displacement parameters were fixed to be 20-50 % larger than those of the attached non-hydrogen atoms.

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Refinement. Omit (060), (012), (110), and (014). No restraints nor constraints

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²) for (mo_DD48M_0m)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.37901 (4)	0.65733 (2)	0.510290 (15)	0.01819 (8)
O1	0.23720 (9)	0.50566 (7)	0.63213 (5)	0.0178 (2)
O2	0.26085 (9)	0.65401 (7)	0.68593 (4)	0.01567 (18)
C1	0.68061 (15)	0.25499 (11)	0.43328 (7)	0.0222 (3)
H1	0.67861 (15)	0.18487 (11)	0.42727 (7)	0.0267 (3)*
C2	0.79399 (15)	0.29997 (12)	0.46412 (7)	0.0249 (3)
H2	0.87002 (15)	0.26046 (12)	0.47923 (7)	0.0299 (4)*
C3	0.57054 (15)	0.31367 (10)	0.41143 (7)	0.0196 (3)
H3	0.49225 (15)	0.28347 (10)	0.39069 (7)	0.0235 (3)*
C4	0.79636 (14)	0.40235 (11)	0.47285 (6)	0.0223 (3)
H4	0.87379 (14)	0.43219 (11)	0.49448 (6)	0.0268 (4)*
C5	0.57389 (14)	0.41639 (10)	0.41964 (6)	0.0184 (3)
H5	0.49811 (14)	0.45574 (10)	0.40407 (6)	0.0221 (3)*
C6	0.68678 (14)	0.46234 (10)	0.45037 (6)	0.0175 (3)
C7	0.69006 (16)	0.57360 (10)	0.46128 (6)	0.0218 (3)
H7a	0.78459 (16)	0.59923 (10)	0.45024 (6)	0.0262 (3)*
H7b	0.62146 (16)	0.60587 (10)	0.43193 (6)	0.0262 (3)*
C8	0.65522 (13)	0.60158 (10)	0.53187 (6)	0.0166 (3)
H8a	0.72178 (13)	0.56677 (10)	0.56099 (6)	0.0199 (3)*
H8b	0.67005 (13)	0.67404 (10)	0.53747 (6)	0.0199 (3)*
C9	0.50543 (13)	0.57613 (9)	0.55292 (6)	0.0126 (2)
H9	0.48508 (13)	0.50505 (9)	0.54191 (6)	0.0151 (3)*
C10	0.48308 (12)	0.59231 (9)	0.62662 (6)	0.0117 (2)
H10	0.50946 (12)	0.66330 (9)	0.63478 (6)	0.0140 (3)*
C11	0.57330 (12)	0.53103 (10)	0.67380 (6)	0.0128 (2)
C12	0.58838 (12)	0.42669 (10)	0.66956 (6)	0.0151 (2)
C13	0.63367 (13)	0.58072 (10)	0.72772 (6)	0.0155 (2)
C14	0.52427 (14)	0.36410 (9)	0.61617 (7)	0.0189 (3)
H14a	0.5774 (7)	0.3738 (6)	0.57592 (14)	0.0283 (4)*
H14b	0.5275 (10)	0.29369 (12)	0.6286 (2)	0.0283 (4)*
H14c	0.4264 (4)	0.3843 (5)	0.6094 (3)	0.0283 (4)*
C15	0.62111 (16)	0.69221 (10)	0.73714 (6)	0.0209 (3)
H15a	0.6623 (10)	0.71082 (14)	0.7790 (2)	0.0313 (4)*
H15b	0.6711 (9)	0.72661 (10)	0.7021 (3)	0.0313 (4)*
H15c	0.52178 (17)	0.71134 (15)	0.7364 (5)	0.0313 (4)*
C16	0.66380 (13)	0.37535 (11)	0.71756 (7)	0.0203 (3)
H16	0.67580 (13)	0.30536 (11)	0.71382 (7)	0.0243 (3)*
C17	0.70548 (13)	0.52689 (11)	0.77508 (6)	0.0201 (3)
H17	0.74440 (13)	0.56092 (11)	0.81129 (6)	0.0241 (3)*
C18	0.72103 (14)	0.42472 (12)	0.77025 (7)	0.0231 (3)
H18	0.77048 (14)	0.38884 (12)	0.80276 (7)	0.0277 (3)*
C19	0.27465 (13)	0.57724 (10)	0.46143 (6)	0.0157 (2)
C20	0.24599 (14)	0.47803 (11)	0.47566 (7)	0.0210 (3)
H20	0.28421 (14)	0.44860 (11)	0.51369 (7)	0.0253 (3)*
C21	0.21368 (15)	0.61993 (10)	0.40629 (6)	0.0196 (3)

H21	0.23336 (15)	0.68733 (10)	0.39561 (6)	0.0236 (3)*
C22	0.16154 (15)	0.42156 (11)	0.43446 (7)	0.0233 (3)
H22	0.14605 (15)	0.35308 (11)	0.44354 (7)	0.0279 (3)*
C23	0.12431 (16)	0.56429 (11)	0.36693 (6)	0.0243 (3)
H23	0.07980 (16)	0.59474 (11)	0.33074 (6)	0.0292 (3)*
C24	0.10009 (15)	0.46452 (12)	0.38041 (7)	0.0246 (3)
H24	0.04170 (15)	0.42596 (12)	0.35272 (7)	0.0295 (4)*
C25	0.10955 (13)	0.51575 (10)	0.67193 (6)	0.0173 (2)
C26	−0.01545 (14)	0.48278 (11)	0.63209 (7)	0.0239 (3)
H26a	−0.0159 (7)	0.5186 (6)	0.5906 (2)	0.0359 (4)*
H26b	−0.0092 (6)	0.41101 (19)	0.6240 (5)	0.0359 (4)*
H26c	−0.10220 (15)	0.4974 (8)	0.6559 (2)	0.0359 (4)*
C27	0.12852 (17)	0.44748 (11)	0.73029 (8)	0.0283 (3)
H27a	0.1454 (13)	0.3793 (2)	0.71530 (8)	0.0425 (5)*
H27b	0.2089 (8)	0.4702 (6)	0.7561 (3)	0.0425 (5)*
H27c	0.0435 (5)	0.4491 (7)	0.7571 (3)	0.0425 (5)*
C28	0.11140 (13)	0.62884 (9)	0.68967 (6)	0.0164 (2)
C29	0.03659 (16)	0.69350 (11)	0.63938 (8)	0.0271 (3)
H29a	0.0534 (10)	0.76393 (11)	0.6491 (3)	0.0406 (5)*
H29b	0.0729 (9)	0.6780 (6)	0.59602 (10)	0.0406 (5)*
H29c	−0.0645 (2)	0.6800 (6)	0.6407 (4)	0.0406 (5)*
C30	0.05973 (16)	0.65390 (13)	0.75723 (7)	0.0283 (3)
H30a	0.1188 (8)	0.6203 (7)	0.78943 (7)	0.0424 (5)*
H30b	0.0646 (12)	0.72607 (15)	0.7639 (2)	0.0424 (5)*
H30c	−0.0377 (4)	0.6316 (8)	0.7621 (2)	0.0424 (5)*
B1	0.32321 (15)	0.58392 (11)	0.64725 (7)	0.0136 (3)

Atomic displacement parameters (Å²) for (mo_DD48M_0m)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02331 (15)	0.01365 (14)	0.01761 (14)	−0.00035 (12)	−0.00727 (12)	0.00146 (11)
O1	0.0105 (4)	0.0188 (5)	0.0242 (5)	−0.0003 (3)	0.0029 (4)	−0.0052 (4)
O2	0.0108 (4)	0.0171 (4)	0.0191 (4)	−0.0016 (4)	0.0028 (3)	−0.0042 (4)
C1	0.0269 (7)	0.0200 (7)	0.0198 (6)	0.0034 (5)	0.0012 (6)	−0.0025 (5)
C2	0.0218 (7)	0.0299 (7)	0.0231 (7)	0.0105 (6)	−0.0033 (6)	−0.0061 (6)
C3	0.0199 (6)	0.0234 (7)	0.0155 (6)	−0.0015 (5)	0.0001 (5)	−0.0004 (5)
C4	0.0172 (6)	0.0312 (8)	0.0186 (6)	−0.0005 (5)	0.0016 (5)	−0.0087 (5)
C5	0.0194 (6)	0.0227 (7)	0.0131 (6)	0.0031 (5)	0.0025 (5)	0.0012 (5)
C6	0.0217 (6)	0.0200 (7)	0.0109 (5)	−0.0007 (5)	0.0069 (5)	−0.0017 (5)
C7	0.0298 (7)	0.0196 (7)	0.0161 (6)	−0.0054 (6)	0.0092 (5)	−0.0018 (5)
C8	0.0171 (6)	0.0178 (6)	0.0148 (6)	−0.0039 (5)	0.0038 (5)	−0.0031 (5)
C9	0.0140 (5)	0.0124 (6)	0.0113 (5)	0.0000 (4)	−0.0007 (4)	0.0003 (4)
C10	0.0117 (5)	0.0126 (5)	0.0108 (5)	−0.0003 (4)	−0.0008 (4)	−0.0011 (4)
C11	0.0082 (5)	0.0186 (6)	0.0117 (5)	−0.0003 (4)	0.0016 (4)	0.0019 (5)
C12	0.0113 (5)	0.0178 (6)	0.0162 (6)	−0.0002 (4)	0.0025 (4)	0.0028 (5)
C13	0.0108 (5)	0.0239 (6)	0.0117 (5)	−0.0028 (5)	0.0028 (4)	0.0012 (5)
C14	0.0207 (6)	0.0129 (6)	0.0230 (6)	0.0008 (5)	0.0008 (5)	0.0004 (5)
C15	0.0214 (6)	0.0257 (7)	0.0156 (6)	−0.0025 (6)	−0.0027 (5)	−0.0056 (5)
C16	0.0147 (6)	0.0206 (7)	0.0254 (7)	0.0006 (5)	0.0025 (5)	0.0090 (5)
C17	0.0134 (6)	0.0343 (8)	0.0126 (6)	−0.0043 (5)	−0.0013 (5)	0.0032 (5)
C18	0.0144 (6)	0.0345 (8)	0.0204 (6)	0.0011 (6)	−0.0013 (5)	0.0131 (6)
C19	0.0141 (5)	0.0196 (6)	0.0133 (5)	0.0003 (5)	−0.0017 (5)	−0.0021 (5)
C20	0.0211 (6)	0.0236 (7)	0.0184 (6)	−0.0056 (5)	−0.0069 (5)	0.0038 (5)

C21	0.0218 (6)	0.0207 (6)	0.0163 (6)	0.0035 (5)	−0.0024 (5)	0.0011 (5)
C22	0.0223 (7)	0.0236 (7)	0.0238 (7)	−0.0073 (5)	−0.0057 (5)	0.0023 (6)
C23	0.0245 (7)	0.0323 (8)	0.0162 (6)	0.0021 (6)	−0.0067 (6)	0.0021 (5)
C24	0.0200 (7)	0.0346 (8)	0.0192 (6)	−0.0056 (6)	−0.0057 (5)	−0.0030 (6)
C25	0.0122 (5)	0.0184 (6)	0.0213 (6)	0.0000 (5)	0.0023 (5)	−0.0015 (5)

C26	0.0137 (6)	0.0262 (7)	0.0319 (8)	−0.0025 (5)	0.0006 (5)	−0.0090 (6)
C27	0.0247 (7)	0.0276 (7)	0.0327 (8)	0.0005 (6)	0.0035 (6)	0.0108 (6)
C28	0.0100 (5)	0.0181 (6)	0.0212 (6)	−0.0010 (5)	0.0033 (5)	−0.0022 (5)
C29	0.0209 (7)	0.0227 (7)	0.0376 (8)	0.0038 (6)	0.0001 (6)	0.0057 (6)
C30	0.0226 (7)	0.0332 (8)	0.0290 (7)	−0.0040 (6)	0.0092 (6)	−0.0089 (7)
B1	0.0131 (6)	0.0150 (6)	0.0127 (6)	0.0010 (5)	−0.0021 (5)	0.0014 (5)

Geometric parameters (Å, º) for (mo_DD48M_0m)

S1—C9	1.8462 (12)	C14—H14c	0.9800
S1—C19	1.7767 (13)	C15—H15a	0.9800
O1—C25	1.4722 (15)	C15—H15b	0.9800
O1—B1	1.3681 (17)	C15—H15c	0.9800
O2—C28	1.4644 (15)	C16—H16	0.9500
O2—B1	1.3687 (16)	C16—C18	1.384 (2)
C1—H1	0.9500	C17—H17	0.9500
C1—C2	1.390 (2)	C17—C18	1.384 (2)
C1—C3	1.3863 (19)	C18—H18	0.9500
C2—H2	0.9500	C19—C20	1.3911 (19)
C2—C4	1.387 (2)	C19—C21	1.3986 (17)
C3—H3	0.9500	C20—H20	0.9500
C3—C5	1.3900 (19)	C20—C22	1.3934 (19)
C4—H4	0.9500	C21—H21	0.9500
C4—C6	1.397 (2)	C21—C23	1.3927 (19)
C5—H5	0.9500	C22—H22	0.9500
C5—C6	1.3916 (19)	C22—C24	1.384 (2)
C6—C7	1.5111 (18)	C23—H23	0.9500
C7—H7a	0.9900	C23—C24	1.388 (2)
C7—H7b	0.9900	C24—H24	0.9500
C7—C8	1.5381 (17)	C25—C26	1.5120 (18)
C8—H8a	0.9900	C25—C27	1.5227 (19)
C8—H8b	0.9900	C25—C28	1.5620 (18)
C8—C9	1.5291 (16)	C26—H26a	0.9800
C9—H9	1.0000	C26—H26b	0.9800
C9—C10	1.5486 (16)	C26—H26c	0.9800
C10—H10	1.0000	C27—H27a	0.9800
C10—C11	1.5360 (16)	C27—H27b	0.9800
C10—B1	1.5842 (18)	C27—H27c	0.9800
C11—C12	1.4111 (17)	C28—C29	1.5279 (19)
C11—C13	1.4176 (17)	C28—C30	1.5141 (19)
C12—C14	1.5128 (18)	C29—H29a	0.9800
C12—C16	1.4031 (18)	C29—H29b	0.9800
C13—C15	1.5143 (19)	C29—H29c	0.9800
C13—C17	1.3935 (18)	C30—H30a	0.9800
C14—H14a	0.9800	C30—H30b	0.9800
C14—H14b	0.9800	C30—H30c	0.9800
C19—S1—C9	106.05 (6)	H16—C16—C12	119.37 (8)
B1—O1—C25	107.25 (10)	C18—C16—C12	121.26 (13)
B1—O2—C28	107.06 (10)	C18—C16—H16	119.37 (8)
C2—C1—H1	120.39 (8)	H17—C17—C13	119.45 (8)

C3—C1—H1	120.39 (8)	C18—C17—C13	121.09 (13)
C3—C1—C2	119.23 (13)	C18—C17—H17	119.45 (8)
H2—C2—C1	119.91 (8)	C17—C18—C16	119.31 (12)
C4—C2—C1	120.17 (13)	H18—C18—C16	120.35 (8)
C4—C2—H2	119.91 (9)	H18—C18—C17	120.35 (8)
H3—C3—C1	119.76 (8)	C20—C19—S1	124.75 (10)
C5—C3—C1	120.47 (13)	C21—C19—S1	116.36 (10)
C5—C3—H3	119.76 (8)	C21—C19—C20	118.84 (12)
H4—C4—C2	119.45 (9)	H20—C20—C19	119.80 (7)
C6—C4—C2	121.10 (13)	C22—C20—C19	120.39 (13)
C6—C4—H4	119.45 (8)	C22—C20—H20	119.80 (8)
H5—C5—C3	119.56 (8)	H21—C21—C19	119.78 (8)
C6—C5—C3	120.87 (13)	C23—C21—C19	120.43 (13)
C6—C5—H5	119.56 (8)	C23—C21—H21	119.78 (8)
C5—C6—C4	118.15 (12)	H22—C22—C20	119.76 (8)
C7—C6—C4	120.36 (13)	C24—C22—C20	120.48 (14)
C7—C6—C5	121.47 (13)	C24—C22—H22	119.76 (9)
H7a—C7—C6	109.17 (7)	H23—C23—C21	119.90 (8)
H7b—C7—C6	109.17 (8)	C24—C23—C21	120.20 (12)
H7b—C7—H7a	107.9	C24—C23—H23	119.90 (8)
C8—C7—C6	112.19 (11)	C23—C24—C22	119.56 (13)
C8—C7—H7a	109.17 (7)	H24—C24—C22	120.22 (9)
C8—C7—H7b	109.17 (8)	H24—C24—C23	120.22 (8)
H8a—C8—C7	108.64 (8)	C26—C25—O1	108.69 (10)
H8b—C8—C7	108.64 (7)	C27—C25—O1	106.64 (10)
H8b—C8—H8a	107.6	C27—C25—C26	110.22 (12)
C9—C8—C7	114.49 (11)	C28—C25—O1	102.16 (10)
C9—C8—H8a	108.64 (7)	C28—C25—C26	114.87 (11)
C9—C8—H8b	108.64 (7)	C28—C25—C27	113.53 (11)
C8—C9—S1	109.94 (8)	H26a—C26—C25	109.5
H9—C9—S1	109.25 (4)	H26b—C26—C25	109.5
H9—C9—C8	109.25 (7)	H26b—C26—H26a	109.5
C10—C9—S1	107.10 (8)	H26c—C26—C25	109.5
C10—C9—C8	112.01 (10)	H26c—C26—H26a	109.5
C10—C9—H9	109.25 (6)	H26c—C26—H26b	109.5
H10—C10—C9	105.31 (6)	H27a—C27—C25	109.5
C11—C10—C9	117.94 (10)	H27b—C27—C25	109.5
C11—C10—H10	105.31 (6)	H27b—C27—H27a	109.5
B1—C10—C9	112.64 (10)	H27c—C27—C25	109.5
B1—C10—H10	105.31 (7)	H27c—C27—H27a	109.5
B1—C10—C11	109.23 (9)	H27c—C27—H27b	109.5
C12—C11—C10	123.34 (11)	C25—C28—O2	102.89 (10)
C13—C11—C10	118.06 (11)	C29—C28—O2	106.62 (10)
C13—C11—C12	118.34 (11)	C29—C28—C25	112.87 (11)
C14—C12—C11	123.75 (11)	C30—C28—O2	108.22(11)
C16—C12—C11	119.75 (12)	C30—C28—C25	115.31 (11)
C16—C12—C14	116.48 (12)	C30—C28—C29	110.22 (12)
C15—C13—C11	122.26 (12)	H29a—C29—C28	109.5
C17—C13—C11	120.22 (12)	H29b—C29—C28	109.5
C17—C13—C15	117.50 (12)	H29b—C29—H29a	109.5
H14a—C14—C12	109.5	H29c—C29—C28	109.5
H14b—C14—C12	109.5	H29c—C29—H29a	109.5
H14b—C14—H14a	109.5	H29c—C29—H29b	109.5
H14c—C14—C12	109.5	H30a—C30—C28	109.5

H14c—C14—H14a	109.5	H30b—C30—C28	109.5
H14c—C14—H14b	109.5	H30b—C30—H30a	109.5
H15a—C15—C13	109.5	H30c—C30—C28	109.5
H15b—C15—C13	109.5	H30c—C30—H30a	109.5
H15b—C15—H15a	109.5	H30c—C30—H30b	109.5
H15c—C15—C13	109.5	O2—B1—O1	113.65(11)
H15c—C15—H15a	109.5	C10—B1—O1	124.65(11)
H15c—C15—H15b	109.5	C10—B1—O2	121.60(11)

(i) Sheldrick, G. M. SHELX-97, University of Gottingen, Gottingen, Germany, 1997.