Formation of Charge-Transfer Complexes. The Mulliken plot in **Figure 1s** was obtained as follows: To 10 ml solution of bis(N-methylimino-)-1,4-dithiin (10 mM) in dichloromethane, 10 ml solutions of various antharacenes (9-Br, H, Me and 9,10-diMe-anthracene) were added. In each case, λ_{max} for the CT absorption band was determined by subtracting the absorption spectra of pure anthracene and pure 1,4-dithiin solution from that of the mixture. The transition energies ($E_{CT} = hc/\lambda_{max}$) were plotted *versus* the ionization potentials (IP) of the anthracenes according to the Mulliken correlation. For the preparation of the Job plot in **Figure 2s,** the concentration of the starting solutions of the 1,4-dithiin and anthracene in dichloromethane was 10 mM. The absorbance at /$\lambda_{max,CT}$ = 489 nm was measured for various molar fractions of anthracene and 1,4-dithiin, and the absorbance values were plotted *versus* the molar fraction [%] of anthracene.

Table 4. Crystal data and structure refinement for the anthracene/1,4-dithiin complex.

Empirical formula	$C_{24}H_{16}N_2O_4S_2$	
Formula weight	460.51	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.1503(12) Å	α= 90°.
	b = 10.216(2) Å	β= 91.438(4)°.
	c = 13.722(2) Å	γ = 90°.
Volume	1002.0(3) $Å^3$	
Z	2	
Density (calculated)	1.526 g/cm^3	
Absorption coefficient	0.303 mm^{-1}	
F(000)	476	
Crystal size	0.2 x 0.3 x 0.5 mm^3	
Theta range for data collection	2.49 to 35.61°.	
Index ranges	-11<=h<=11, 0<=k<=16, 0<=l<=21	
Reflections collected	12404	
Independent reflections	4363 [R(int) = 0.0312]	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4362 / 0 / 146	

Goodness-of-fit on F^2	1.009
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.1191 [on 3389 reflections]
R indices (all data)	R1 = 0.0619, wR2 = 0.1322
Largest diff. peak and hole	0.725 and -0.293 e.$Å^{-3}$

Table 5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for the anthracene/1,4-dithiin complex. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1A)	88(1)	9276(1)	1223(1)	18(1)
N(1A)	1592(2)	12982(1)	963(1)	21(1)
O(1A)	1480(2)	11752(1)	2380(1)	26(1)
O(2A)	1347(2)	13532(1)	-672(1)	26(1)
C(1A)	1283(2)	11859(1)	1507(1)	19(1)
C(2A)	634(2)	10830(1)	803(1)	17(1)
C(3A)	577(2)	11357(1)	-94(1)	17(1)
C(4A)	1206(2)	12750(1)	-15(1)	19(1)
C(5A)	2157(2)	14242(1)	1365(1)	26(1)
C(1)	5603(2)	10674(1)	852(1)	20(1)
C(2)	6243(2)	11390(2)	1690(1)	25(1)
C(3)	6828(2)	12654(2)	1608(1)	29(1)
C(4)	6806(2)	13294(2)	689(1)	30(1)
C(5)	6195(2)	12647(2)	-131(1)	25(1)
C(6)	5577(2)	11320(1)	-74(1)	20(1)
C(7)	5024(2)	9370(1)	904(1)	22(1)

Table 6. Bond lengths [Å] and angles [°] for the anthracene/1,4-dithiin complex.

S(1A)-C(3A)#1	1.7350(13)
S(1A)-C(2A)	1.7368(13)
N(1A)-C(4A)	1.384(2)
N(1A)-C(1A)	1.389(2)
N(1A)-C(5A)	1.453(2)
O(1A)-C(1A)	1.207(2)
O(2A)-C(4A)	1.211(2)
C(1A)-C(2A)	1.494(2)
C(2A)-C(3A)	1.343(2)
C(3A)-C(4A)	1.496(2)
C(3A)-S(1A)#1	1.7350(13)
C(1)-C(7)	1.397(2)
C(1)-C(2)	1.429(2)
C(1)-C(6)	1.432(2)
C(2)-C(3)	1.362(2)
C(3)-C(4)	1.420(2)
C(4)-C(5)	1.367(2)
C(5)-C(6)	1.429(2)
C(6)-C(7)#2	1.398(2)
C(7)-C(6)#2	1.398(2)
C(3A)#1-S(1A)-C(2A)	95.91(6)

C(4A)-N(1A)-C(1A)	110.43(11)
C(4A)-N(1A)-C(5A)	124.54(12)
C(1A)-N(1A)-C(5A)	124.98(12)
O(1A)-C(1A)-N(1A)	126.27(12)
O(1A)-C(1A)-C(2A)	127.18(13)
N(1A)-C(1A)-C(2A)	106.54(11)
C(3A)-C(2A)-C(1A)	108.22(11)
C(3A)-C(2A)-S(1A)	131.94(10)
C(1A)-C(2A)-S(1A)	119.84(9)
C(2A)-C(3A)-C(4A)	108.20(11)
C(2A)-C(3A)-S(1A)#1	132.14(10)
C(4A)-C(3A)-S(1A)#1	119.65(9)
O(2A)-C(4A)-N(1A)	126.25(12)
O(2A)-C(4A)-C(3A)	127.15(12)
N(1A)-C(4A)-C(3A)	106.61(11)
C(7)-C(1)-C(2)	122.45(13)
C(7)-C(1)-C(6)	119.20(12)
C(2)-C(1)-C(6)	118.35(13)
C(3)-C(2)-C(1)	120.76(14)
C(2)-C(3)-C(4)	120.88(14)
C(5)-C(4)-C(3)	120.30(15)
C(4)-C(5)-C(6)	120.46(14)
C(7)#2-C(6)-C(5)	121.56(13)
C(7)#2-C(6)-C(1)	119.18(13)

C(5)-C(6)-C(1)	119.25(13)
C(1)-C(7)-C(6)#2	121.63(13)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z #2 -x+1,-y+2,-z

Table 7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for the anthracene/1,4-dithiin complex. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1A)	24(1)	18(1)	13(1)	2(1)	-1(1)	-2(1)
N(1A)	26(1)	18(1)	18(1)	-1(1)	-3(1)	-2(1)
O(1A)	36(1)	26(1)	15(1)	-2(1)	-4(1)	-2(1)
O(2A)	33(1)	21(1)	23(1)	6(1)	-2(1)	-4(1)
C(1A)	22(1)	19(1)	17(1)	-1(1)	-1(1)	0(1)
C(2A)	20(1)	17(1)	15(1)	0(1)	-1(1)	-1(1)
C(3A)	19(1)	17(1)	15(1)	2(1)	-1(1)	-1(1)
C(4A)	21(1)	17(1)	19(1)	1(1)	-2(1)	-1(1)
C(5A)	32(1)	18(1)	26(1)	-4(1)	-5(1)	-2(1)
C(1)	19(1)	24(1)	18(1)	-1(1)	0(1)	-1(1)
C(2)	23(1)	33(1)	20(1)	-5(1)	1(1)	-1(1)
C(3)	25(1)	32(1)	29(1)	-11(1)	3(1)	-1(1)
C(4)	27(1)	23(1)	40(1)	-7(1)	5(1)	-2(1)
C(5)	25(1)	23(1)	28(1)	2(1)	3(1)	-2(1)
C(6)	18(1)	23(1)	20(1)	1(1)	0(1)	-2(1)
C(7)	22(1)	26(1)	18(1)	3(1)	0(1)	-1(1)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for the anthracene/1,4-dithiin complex.

	x	y	z	U(iso)
H(5AA)	2276(19)	14175(4)	2077(1)	38
H(5AB)	1213(10)	14902(3)	1191(8)	38
H(5AC)	3364(9)	14497(6)	1100(8)	38
H(2A)	6261(2)	10981(2)	2312(1)	30
H(3A)	7257(2)	13113(2)	2173(1)	35
H(4A)	7218(2)	14175(2)	644(1)	36
H(5A)	6180(2)	13083(2)	-742(1)	30
H(7A)	5040(2)	8941(1)	1519(1)	26

Table 9. Crystal data and structure refinement for the anthracene/1,4-dithiin complex at 29.7% conversion.

Empirical formula	$C_{24}H_{16}N_2O_4S_2$	
Formula weight	460.51	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.1737(4) Å	α= 90°.
	b = 10.2018(5) Å	β= 92.1350(10)°.
	c = 13.7650(7) Å	γ = 90°.
Volume	1006.69(9) $Å^3$	
Z	2	
Density (calculated)	1.519 g/cm^3	
Absorption coefficient	0.302 mm^{-1}	
F(000)	476	
Crystal size	0.2 x 0.3 x 0.5 mm^3	
Theta range for data collection	2.49 to 35.45°.	
Index ranges	-11<=h<=11, 0<=k<=14, 0<=l<=21	
Reflections collected	6955	
Independent reflections	3949 [R(int) = 0.0179]	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	3949 / 94 / 197
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0575, wR2 = 0.1570 [on 3236 reflections]
R indices (all data)	R1 = 0.0680, wR2 = 0.1661
Largest diff. peak and hole	1.093 and -0.647 e.$Å^{-3}$

Table 10. Atomic coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for the anthracene/1,4-dithiin complex at 29.7% conversion.

	x	y	z	U(iso)
S(1A)	5047(2)	739(1)	1204(1)	21(1)
N(1A)	6501(4)	-2988(3)	991(2)	22(1)
C(1A)	6171(4)	-2754(3)	8(2)	21(1)
C(2A)	5558(4)	-1359(3)	-84(2)	18(1)
C(3A)	5586(4)	-823(3)	814(2)	19(1)
C(4A)	6223(4)	-1855(3)	1522(2)	22(1)
O(1A)	6275(3)	-3555(2)	-634(2)	24(1)
O(2A)	6369(4)	-1771(3)	2398(2)	26(1)
C(5A)	7097(6)	-4237(3)	1384(2)	27(1)
C(1)	10600(3)	-685(2)	852(2)	20(1)
C(2)	11235(4)	-1374(4)	1689(3)	23(1)
C(3)	11834(5)	-2666(3)	1610(2)	27(1)
C(4)	11820(5)	-3300(3)	697(3)	29(1)
C(5)	11215(5)	-2646(4)	-118(3)	27(1)
C(6)	10573(4)	-1324(2)	-76(2)	21(1)
C(7)	10025(3)	625(2)	904(2)	23(1)
S(1A')	4943(5)	477(4)	1230(2)	18(1)
N(1A')	6666(12)	-2845(22)	931(16)	28(6)
C(1A')	6609(17)	-2733(15)	-77(11)	24(3)

C(2A')	6779(9)	-1233(8)	-217(6)	15(1)
C(3A')	6785(9)	-624(7)	818(5)	13(1)
C(4A')	6643(18)	-1724(20)	1488(13)	31(4)
O(1A')	6696(12)	-3516(8)	-702(6)	12(2)
O(2A')	6665(13)	-1582(11)	2355(6)	12(2)
C(5A')	6589(17)	-4262(11)	1447(8)	21(2)
S(1A")	4665(5)	-770(4)	-1168(2)	16(1)
N(1A")	3196(8)	2977(10)	-887(6)	5(2)
C(1A")	3646(10)	2668(13)	77(9)	10(3)
C(2A")	4249(9)	1278(12)	144(9)	21(4)
C(3A")	4152(8)	796(9)	-764(7)	12(2)
C(4A")	3473(9)	1871(10)	-1447(7)	5(2)
O(1A")	3577(11)	3400(9)	788(7)	14(2)
O(2A")	3194(9)	1847(9)	-2333(5)	8(2)
C(5A")	2550(12)	4229(10)	-1254(8)	17(2)
C(1')	10078(9)	-1078(8)	972(6)	19(2)
C(2')	11181(12)	-1697(12)	1687(7)	19(2)
C(3')	12153(16)	-2764(12)	1507(10)	32(3)
C(4')	12076(18)	-3335(13)	585(10)	30(4)
C(5')	11049(17)	-2780(14)	-150(10)	23(4)
C(6')	10086(12)	-1625(10)	42(6)	21(2)
C(7')	8809(10)	108(8)	1012(6)	17(1)
C(1")	8855(8)	475(8)	-721(6)	15(1)
C(2")	8853(16)	1294(16)	-1551(11)	42(6)

C(3")	8858(13)	2617(11)	-1449(8)	30(2)
C(4")	8826(13)	3202(11)	-508(8)	27(2)
C(5")	8855(11)	2443(11)	299(8)	18(2)
C(6")	8909(10)	1048(9)	205(6)	16(2)
C(7")	8793(10)	-986(9)	-688(6)	18(2)

Table 11. Bond lengths [Å] and angles [°] for the anthracene/1,4-dithiin complex at 29.7% conversion.

S(1A)-C(2A)#1	1.707(3)
S(1A)-C(3A)	1.730(3)
N(1A)-C(4A)	1.386(4)
N(1A)-C(1A)	1.386(4)
N(1A)-C(5A)	1.443(4)
C(1A)-O(1A)	1.207(4)
C(1A)-C(2A)	1.494(4)
C(2A)-C(3A)	1.351(4)
C(2A)-S(1A)#1	1.707(3)
C(3A)-C(4A)	1.495(4)
C(4A)-O(2A)	1.209(3)
C(1)-C(7)	1.401(3)
C(1)-C(2)	1.411(5)
C(1)-C(6)	1.434(3)
C(2)-C(3)	1.391(5)
C(3)-C(4)	1.412(4)
C(4)-C(5)	1.362(5)
C(5)-C(6)	1.427(5)
C(6)-C(7)#2	1.399(3)
C(7)-C(6)#2	1.399(3)
S(1A')-C(2A")	1.759(13)

S(1A')-C(3A')	1.839(8)
N(1A')-C(1A')	1.39(3)
N(1A')-C(4A')	1.38(3)
N(1A')-C(5A')	1.61(2)
C(1A')-O(1A')	1.18(2)
C(1A')-C(2A')	1.55(2)
C(2A')-C(3A')	1.554(11)
C(2A')-C(7")	1.625(10)
C(2A')-S(1A")	2.023(8)
C(3A')-C(4A')	1.46(2)
C(3A')-C(7')	1.646(10)
C(4A')-O(2A')	1.20(2)
S(1A")-C(3A")	1.735(10)
N(1A")-C(4A")	1.386(14)
N(1A")-C(1A")	1.389(14)
N(1A")-C(5A")	1.443(13)
C(1A")-O(1A")	1.234(14)
C(1A")-C(2A")	1.48(2)
C(2A")-C(3A")	1.342(14)
C(3A")-C(4A")	1.514(13)
C(4A")-O(2A")	1.229(11)
C(1')-C(2')	1.392(13)
C(1')-C(6')	1.397(11)
C(1')-C(7')	1.516(12)

C(2')-C(3')	1.32(2)
C(3')-C(4')	1.40(2)
C(4')-C(5')	1.35(2)
C(5')-C(6')	1.40(2)
C(6')-C(7")	1.492(12)
C(7')-C(6")	1.470(12)
C(1")-C(6")	1.402(10)
C(1")-C(2")	1.42(2)
C(1")-C(7")	1.492(11)
C(2")-C(3")	1.36(2)
C(3")-C(4")	1.427(13)
C(4")-C(5")	1.354(14)
C(5")-C(6")	1.430(13)

C(2A)#1-S(1A)-C(3A)	96.52(13)
C(4A)-N(1A)-C(1A)	110.4(3)
C(4A)-N(1A)-C(5A)	125.8(3)
C(1A)-N(1A)-C(5A)	123.7(3)
O(1A)-C(1A)-N(1A)	125.8(3)
O(1A)-C(1A)-C(2A)	127.5(3)
N(1A)-C(1A)-C(2A)	106.6(3)
C(3A)-C(2A)-C(1A)	108.3(2)
C(3A)-C(2A)-S(1A)#1	132.1(2)
C(1A)-C(2A)-S(1A)#1	119.6(2)

C(2A)-C(3A)-C(4A)	107.8(2)
C(2A)-C(3A)-S(1A)	131.3(2)
C(4A)-C(3A)-S(1A)	120.9(2)
O(2A)-C(4A)-N(1A)	125.2(3)
O(2A)-C(4A)-C(3A)	127.8(3)
N(1A)-C(4A)-C(3A)	106.8(2)
C(7)-C(1)-C(2)	121.4(2)
C(7)-C(1)-C(6)	119.0(2)
C(2)-C(1)-C(6)	119.6(2)
C(3)-C(2)-C(1)	119.9(3)
C(2)-C(3)-C(4)	120.8(3)
C(5)-C(4)-C(3)	120.0(3)
C(4)-C(5)-C(6)	121.5(3)
C(7)#2-C(6)-C(5)	122.6(2)
C(7)#2-C(6)-C(1)	119.2(2)
C(5)-C(6)-C(1)	118.2(2)
C(6)#2-C(7)-C(1)	121.8(2)
C(2A")-S(1A')-C(3A')	101.9(4)
C(1A')-N(1A')-C(4A')	119.2(18)
C(1A')-N(1A')-C(5A')	120.8(17)
C(4A')-N(1A')-C(5A')	119.8(17)
O(1A')-C(1A')-N(1A')	132.3(16)
O(1A')-C(1A')-C(2A')	125.0(12)
N(1A')-C(1A')-C(2A')	101.8(13)

C(1A')-C(2A')-C(3A')	106.3(7)
C(1A')-C(2A')-C(7")	106.1(7)
C(3A')-C(2A')-C(7")	109.4(5)
C(1A')-C(2A')-S(1A")	104.5(6)
C(3A')-C(2A')-S(1A")	118.5(4)
C(7")-C(2A')-S(1A")	111.2(5)
C(4A')-C(3A')-C(2A')	105.8(9)
C(4A')-C(3A')-C(7')	109.2(7)
C(2A')-C(3A')-C(7')	107.6(5)
C(4A')-C(3A')-S(1A')	102.0(7)
C(2A')-C(3A')-S(1A')	123.3(4)
C(7')-C(3A')-S(1A')	108.2(5)
O(2A')-C(4A')-N(1A')	130.8(19)
O(2A')-C(4A')-C(3A')	122.4(16)
N(1A')-C(4A')-C(3A')	106.5(15)
C(3A")-S(1A")-C(2A')	99.8(4)
C(4A")-N(1A")-C(1A")	108.2(9)
C(4A")-N(1A")-C(5A")	125.2(8)
C(1A")-N(1A")-C(5A")	126.5(10)
O(1A")-C(1A")-N(1A")	127.3(12)
O(1A")-C(1A")-C(2A")	123.3(11)
N(1A")-C(1A")-C(2A")	109.5(10)
C(3A")-C(2A")-C(1A")	106.7(10)
C(3A")-C(2A")-S(1A')	128.6(9)

C(1A")-C(2A")-S(1A')	124.7(9)
C(2A")-C(3A")-C(4A")	108.5(9)
C(2A")-C(3A")-S(1A")	129.2(8)
C(4A")-C(3A")-S(1A")	122.3(7)
O(2A")-C(4A")-N(1A")	123.2(10)
O(2A")-C(4A")-C(3A")	129.7(10)
N(1A")-C(4A")-C(3A")	107.1(8)
C(2')-C(1')-C(6')	116.4(8)
C(2')-C(1')-C(7')	131.5(8)
C(6')-C(1')-C(7')	112.1(7)
C(3')-C(2')-C(1')	122.1(10)
C(2')-C(3')-C(4')	120.7(11)
C(5')-C(4')-C(3')	120.5(12)
C(4')-C(5')-C(6')	118.1(12)
C(5')-C(6')-C(1')	122.0(9)
C(5')-C(6')-C(7")	122.8(9)
C(1')-C(6')-C(7")	114.7(8)
C(6")-C(7')-C(1')	116.6(6)
C(6")-C(7')-C(3A')	104.0(6)
C(1')-C(7')-C(3A')	99.2(5)
C(6")-C(1")-C(2")	119.2(9)
C(6")-C(1")-C(7")	112.9(7)
C(2")-C(1")-C(7")	128.0(9)
C(3")-C(2")-C(1")	120.2(12)

C(2")-C(3")-C(4")	120.7(11)
C(5")-C(4")-C(3")	120.3(10)
C(4")-C(5")-C(6")	119.6(9)
C(1")-C(6")-C(5")	119.8(8)
C(1")-C(6")-C(7')	114.4(8)
C(5")-C(6")-C(7')	125.4(8)
C(1")-C(7")-C(6')	116.0(6)
C(1")-C(7")-C(2A')	101.3(6)
C(6')-C(7")-C(2A')	101.8(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z #2 -x+2,-y,-z

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for the anthracene/1,4-dithiin complex at 29.7% conversion.

	x	y	z	U(iso)
H(5AA)	7261(35)	-4169(7)	2092(3)	40
H(5AB)	8284(19)	-4487(13)	1106(15)	40
H(5AC)	6152(18)	-4903(6)	1221(16)	40
H(2A)	11254(4)	-957(4)	2307(3)	28
H(3A)	12257(5)	-3127(3)	2176(2)	32
H(4A)	12232(5)	-4182(3)	652(3)	35
H(5A)	11221(5)	-3081(4)	-728(3)	32
H(7A)	10043(3)	1050(2)	1518(2)	28
H(5AD)	6426(144)	-4944(14)	950(9)	32
H(5AE)	5540(88)	-4288(36)	1883(57)	32
H(5AF)	7756(60)	-4416(44)	1823(61)	32
H(5A1)	2625(140)	4880(26)	-730(21)	26
H(5A2)	1253(49)	4149(26)	-1497(71)	26
H(5A3)	3333(93)	4510(50)	-1784(53)	26
H(2'A)	11236(12)	-1341(12)	2325(7)	23
H(3'A)	12912(16)	-3148(12)	2011(10)	38
H(4'A)	12750(18)	-4118(13)	472(10)	36
H(5'A)	10985(17)	-3165(14)	-778(10)	27
H(7'A)	8897(10)	551(8)	1660(6)	20

H(2"A)	8850(16)	916(16)	-2182(11)	51
H(3"A)	8882(13)	3159(11)	-2009(8)	36
H(4"A)	8786(13)	4129(11)	-448(8)	33
H(5"A)	8838(11)	2835(11)	925(8)	21
H(7"A)	8869(10)	-1388(9)	-1348(6)	22

Table 13. Crystal data and structure refinement for the anthracene/1,4-dithiin complex at 35.2% conversion.

Empirical formula	$C_{24}H_{16}N_2O_4S_2$
Formula weight	460.51
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 7.1857(8) Å α= 90°.
	b = 10.2072(12) Å β= 92.279(2)°.
	c = 13.784(2) Å γ = 90°.
Volume	1010.2(2) $Å^3$
Z	2
Density (calculated)	1.514 g/cm^3
Absorption coefficient	0.301 mm^{-1}
F(000)	476
Crystal size	0.2 x 0.3 x 0.5 mm^3
Theta range for data collection	2.48 to 35.66°.
Index ranges	-11<=h<=11, 0<=k<=16, 0<=l<=22
Reflections collected	13267
Independent reflections	4440 [R(int) = 0.0235]
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	4440 / 94 / 197
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0626, wR2 = 0.1679 [on 3654 reflections]
R indices (all data)	R1 = 0.0731, wR2 = 0.1792
Largest diff. peak and hole	1.146 and -0.986 e.$Å^{-3}$

Table 14. Atomic coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for the anthracene/1,4-dithiin complex at 35.2% conversion.

	x	y	z	U(iso)
S(1A)	5040(2)	742(1)	1204(1)	21(1)
N(1A)	6475(4)	-2986(3)	995(3)	23(1)
C(1A)	6152(5)	-2752(3)	13(2)	22(1)
C(2A)	5544(4)	-1352(3)	-80(2)	19(1)
C(3A)	5579(4)	-820(3)	816(2)	19(1)
C(4A)	6202(4)	-1855(3)	1528(2)	22(1)
O(1A)	6249(4)	-3556(2)	-627(2)	24(1)
O(2A)	6346(4)	-1774(3)	2403(2)	26(1)
C(5A)	7082(6)	-4237(3)	1383(3)	26(1)
C(1)	10602(3)	-688(2)	852(2)	21(1)
C(2)	11231(5)	-1378(5)	1685(4)	25(1)
C(3)	11829(5)	-2669(3)	1612(2)	27(1)
C(4)	11815(6)	-3300(3)	696(3)	29(1)
C(5)	11216(6)	-2650(5)	-126(4)	27(1)
C(6)	10574(4)	-1323(3)	-75(2)	21(1)
C(7)	10023(3)	625(2)	903(2)	24(1)
S(1A')	4928(4)	494(3)	1222(2)	20(1)
N(1A')	6661(11)	-2860(18)	938(14)	26(5)
C(1A')	6608(15)	-2746(13)	-69(10)	24(3)

C(2A')	6776(8)	-1228(6)	-223(5)	18(1)
C(3A')	6780(8)	-607(6)	819(5)	16(1)
C(4A')	6621(15)	-1731(16)	1477(11)	25(4)
O(1A')	6684(10)	-3534(7)	-697(6)	13(1)
O(2A')	6651(11)	-1601(8)	2357(5)	12(2)
C(5A')	6583(14)	-4252(9)	1453(7)	22(2)
S(1A")	4659(4)	-762(3)	-1159(2)	17(1)
N(1A")	3184(7)	2976(8)	-889(6)	7(2)
C(1A")	3629(9)	2682(11)	75(8)	11(2)
C(2A")	4226(8)	1305(9)	143(7)	19(3)
C(3A")	4142(7)	809(8)	-760(7)	15(2)
C(4A")	3462(8)	1879(10)	-1448(7)	9(2)
O(1A")	3561(10)	3406(8)	784(6)	18(2)
O(2A")	3194(8)	1839(8)	-2328(4)	12(1)
C(5A")	2535(10)	4228(8)	-1255(7)	21(2)
C(1')	10068(9)	-1057(7)	963(6)	21(1)
C(2')	11177(12)	-1642(10)	1702(7)	21(2)
C(3')	12181(14)	-2735(10)	1520(9)	31(3)
C(4')	12120(16)	-3316(11)	601(9)	29(3)
C(5')	11057(16)	-2755(13)	-123(10)	27(4)
C(6')	10089(11)	-1616(8)	43(6)	20(1)
C(7')	8803(9)	101(7)	1015(5)	19(1)
C(1")	8842(8)	471(7)	-725(5)	19(1)
C(2")	8831(16)	1270(15)	-1566(11)	45(6)

C(3")	8839(12)	2613(10)	-1458(8)	33(2)
C(4")	8816(13)	3202(9)	-516(7)	31(2)
C(5")	8847(11)	2449(10)	290(8)	23(2)
C(6")	8909(9)	1060(7)	207(5)	17(1)
C(7")	8776(9)	-985(7)	-684(6)	21(1)

Table 15. Bond lengths [Å] and angles [°] for the anthracene/1,4-dithiin complex at 35.2% conversion.

S(1A)-C(2A)#1	1.707(3)
S(1A)-C(3A)	1.731(3)
N(1A)-C(1A)	1.385(5)
N(1A)-C(4A)	1.387(4)
N(1A)-C(5A)	1.446(4)
C(1A)-O(1A)	1.208(4)
C(1A)-C(2A)	1.499(4)
C(2A)-C(3A)	1.349(4)
C(2A)-S(1A)#1	1.707(3)
C(3A)-C(4A)	1.498(4)
C(4A)-O(2A)	1.210(4)
C(1)-C(7)	1.406(3)
C(1)-C(2)	1.406(6)
C(1)-C(6)	1.432(3)
C(2)-C(3)	1.391(6)
C(3)-C(4)	1.417(5)
C(4)-C(5)	1.368(6)
C(5)-C(6)	1.434(5)
C(6)-C(7)#2	1.398(3)
C(7)-C(6)#2	1.398(3)
S(1A')-C(2A")	1.759(11)

S(1A')-C(3A')	1.845(7)
N(1A')-C(4A')	1.37(2)
N(1A')-C(1A')	1.39(2)
N(1A')-C(5A')	1.59(2)
C(1A')-O(1A')	1.18(2)
C(1A')-C(2A')	1.570(15)
C(2A')-C(3A')	1.570(10)
C(2A')-C(7")	1.614(9)
C(2A')-S(1A")	2.012(7)
C(3A')-C(4A')	1.47(2)
C(3A')-C(7')	1.637(9)
C(4A')-O(2A')	1.22(2)
S(1A")-C(3A")	1.740(9)
N(1A")-C(4A")	1.378(13)
N(1A")-C(1A")	1.387(13)
N(1A")-C(5A")	1.444(12)
C(1A")-O(1A")	1.228(12)
C(1A")-C(2A")	1.472(14)
C(2A")-C(3A")	1.343(12)
C(3A")-C(4A")	1.515(12)
C(4A")-O(2A")	1.222(11)
C(1')-C(6')	1.390(10)
C(1')-C(2')	1.402(12)
C(1')-C(7')	1.494(10)

C(2')-C(3')	1.358(14)
C(3')-C(4')	1.397(15)
C(4')-C(5')	1.36(2)
C(5')-C(6')	1.379(14)
C(6')-C(7")	1.495(11)
C(7')-C(6")	1.487(11)
C(1")-C(6")	1.416(10)
C(1")-C(2")	1.42(2)
C(1")-C(7")	1.488(10)
C(2")-C(3")	1.38(2)
C(3")-C(4")	1.432(13)
C(4")-C(5")	1.351(14)
C(5")-C(6")	1.424(12)

C(2A)#1-S(1A)-C(3A)	96.05(14)
C(1A)-N(1A)-C(4A)	110.7(3)
C(1A)-N(1A)-C(5A)	123.4(3)
C(4A)-N(1A)-C(5A)	125.9(3)
O(1A)-C(1A)-N(1A)	125.7(3)
O(1A)-C(1A)-C(2A)	127.6(3)
N(1A)-C(1A)-C(2A)	106.6(3)
C(3A)-C(2A)-C(1A)	108.1(2)
C(3A)-C(2A)-S(1A)#1	132.8(2)
C(1A)-C(2A)-S(1A)#1	119.1(2)

C(2A)-C(3A)-C(4A)	108.1(2)
C(2A)-C(3A)-S(1A)	131.1(2)
C(4A)-C(3A)-S(1A)	120.8(2)
O(2A)-C(4A)-N(1A)	125.3(3)
O(2A)-C(4A)-C(3A)	128.1(3)
N(1A)-C(4A)-C(3A)	106.5(2)
C(7)-C(1)-C(2)	121.5(3)
C(7)-C(1)-C(6)	118.9(2)
C(2)-C(1)-C(6)	119.6(2)
C(3)-C(2)-C(1)	120.4(3)
C(2)-C(3)-C(4)	120.2(3)
C(5)-C(4)-C(3)	120.5(3)
C(4)-C(5)-C(6)	120.6(4)
C(7)#2-C(6)-C(1)	119.4(2)
C(7)#2-C(6)-C(5)	122.0(3)
C(1)-C(6)-C(5)	118.5(3)
C(6)#2-C(7)-C(1)	121.7(2)
C(2A")-S(1A')-C(3A')	102.6(4)
C(4A')-N(1A')-C(1A')	118.0(15)
C(4A')-N(1A')-C(5A')	120.5(15)
C(1A')-N(1A')-C(5A')	121.3(15)
O(1A')-C(1A')-N(1A')	132.2(14)
O(1A')-C(1A')-C(2A')	124.4(11)
N(1A')-C(1A')-C(2A')	102.6(12)

C(1A')-C(2A')-C(3A')	105.8(7)
C(1A')-C(2A')-C(7")	106.2(6)
C(3A')-C(2A')-C(7")	109.2(4)
C(1A')-C(2A')-S(1A")	105.1(6)
C(3A')-C(2A')-S(1A")	117.7(4)
C(7")-C(2A')-S(1A")	111.9(5)
C(4A')-C(3A')-C(2A')	104.6(7)
C(4A')-C(3A')-C(7')	109.5(6)
C(2A')-C(3A')-C(7')	107.4(4)
C(4A')-C(3A')-S(1A')	102.4(6)
C(2A')-C(3A')-S(1A')	123.1(4)
C(7')-C(3A')-S(1A')	109.1(4)
O(2A')-C(4A')-N(1A')	129.0(15)
O(2A')-C(4A')-C(3A')	122.0(13)
N(1A')-C(4A')-C(3A')	108.5(13)
C(3A")-S(1A")-C(2A')	100.4(3)
C(4A")-N(1A")-C(1A")	109.1(8)
C(4A")-N(1A")-C(5A")	125.2(8)
C(1A")-N(1A")-C(5A")	125.7(8)
O(1A")-C(1A")-N(1A")	128.2(11)
O(1A")-C(1A")-C(2A")	122.9(10)
N(1A")-C(1A")-C(2A")	108.9(9)
C(3A")-C(2A")-C(1A")	107.4(8)
C(3A")-C(2A")-S(1A')	127.4(7)

C(1A")-C(2A")-S(1A')	125.2(8)
C(2A")-C(3A")-C(4A")	108.1(8)
C(2A")-C(3A")-S(1A")	129.7(7)
C(4A")-C(3A")-S(1A")	122.3(7)
O(2A")-C(4A")-N(1A")	124.1(9)
O(2A")-C(4A")-C(3A")	129.2(9)
N(1A")-C(4A")-C(3A")	106.6(7)
C(6')-C(1')-C(2')	117.4(7)
C(6')-C(1')-C(7')	113.4(7)
C(2')-C(1')-C(7')	129.1(7)
C(3')-C(2')-C(1')	120.5(9)
C(2')-C(3')-C(4')	121.2(10)
C(5')-C(4')-C(3')	118.9(11)
C(4')-C(5')-C(6')	120.4(12)
C(5')-C(6')-C(1')	121.4(9)
C(5')-C(6')-C(7")	124.1(9)
C(1')-C(6')-C(7")	113.9(6)
C(6")-C(7')-C(1')	115.8(5)
C(6")-C(7')-C(3A')	103.8(5)
C(1')-C(7')-C(3A')	100.4(5)
C(6")-C(1")-C(2")	119.7(8)
C(6")-C(1")-C(7")	112.9(7)
C(2")-C(1")-C(7")	127.3(9)
C(3")-C(2")-C(1")	118.9(12)

C(2")-C(3")-C(4")	121.0(10)
C(5")-C(4")-C(3")	120.4(9)
C(4")-C(5")-C(6")	120.0(9)
C(1")-C(6")-C(5")	119.7(7)
C(1")-C(6")-C(7')	113.5(6)
C(5")-C(6")-C(7')	126.3(7)
C(1")-C(7")-C(6')	115.8(6)
C(1")-C(7")-C(2A')	101.5(5)
C(6')-C(7")-C(2A')	102.6(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z #2 -x+2,-y,-z

Table 16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for the anthracene/1,4-dithiin complex at 35.2% conversion.

	x	y	z	U(iso)
H(5AA)	7367(35)	-4152(7)	2081(4)	38
H(5AB)	8201(22)	-4522(13)	1057(14)	38
H(5AC)	6091(15)	-4886(7)	1273(17)	38
H(2A)	11248(5)	-959(5)	2301(4)	29
H(3A)	12249(5)	-3128(3)	2179(2)	33
H(4A)	12225(6)	-4182(3)	653(3)	35
H(5A)	11226(6)	-3082(5)	-736(4)	33
H(7A)	10039(3)	1050(2)	1517(2)	28
H(5AD)	5917(105)	-4873(23)	1023(26)	33
H(5AE)	5931(106)	-4171(19)	2061(31)	33
H(5AF)	7853(14)	-4569(39)	1592(57)	33
H(5A1)	2864(115)	4913(15)	-781(31)	32
H(5A2)	1179(18)	4200(30)	-1363(64)	32
H(5A3)	3122(100)	4419(43)	-1869(36)	32
H(2'A)	11227(12)	-1270(10)	2334(7)	25
H(3'A)	12939(14)	-3112(10)	2027(9)	37
H(4'A)	12809(16)	-4090(11)	485(9)	35
H(5'A)	10981(16)	-3150(13)	-747(10)	32
H(7'A)	8900(9)	538(7)	1664(5)	23

H(2"A)	8818(16)	886(15)	-2194(11)	54
H(3"A)	8859(12)	3155(10)	-2018(8)	40
H(4"A)	8780(13)	4129(9)	-458(7)	37
H(5"A)	8826(11)	2846(10)	913(8)	27
H(7"A)	8852(9)	-1389(7)	-1342(6)	25

Table 17. Crystal data and structure refinement for the anthracene/1,4-dithiin complex at 80.0% conversion.

Empirical formula	$C_{24}H_{16}N_2O_4S_2$	
Formula weight	460.51	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.2933(4) Å	α= 90°.
	b = 10.1098(5) Å	β= 94.179(11)°.
	c = 13.8243(7) Å	γ = 90°.
Volume	1016.61(9) $Å^3$	
Z	2	
Density (calculated)	1.504 g/cm^3	
Absorption coefficient	0.299 mm^{-1}	
F(000)	476	
Crystal size	0.2 x 0.3 x 0.5 mm^3	
Theta range for data collection	2.50 to 35.68°.	
Index ranges	-11<=h<=11, 0<=k<=16, 0<=l<=22	
Reflections collected	14283	
Independent reflections	4479 [R(int) = 0.0333]	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	4474 / 94 / 197
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0717, wR2 = 0.1673 [on 3131 reflections]
R indices (all data)	R1 = 0.1040, wR2 = 0.1886
Largest diff. peak and hole	0.582 and -0.725 e.$Å^{-3}$

Table 18. Atomic coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for the anthracene/1,4-dithiin complex at 80.0% conversion.

	x	y	z	U(iso)
S(1A)	4953(5)	756(4)	1205(2)	14(1)
N(1A)	6193(11)	-3001(8)	1092(6)	18(2)
C(1A)	6031(16)	-2760(11)	108(8)	23(4)
C(2A)	5502(12)	-1335(9)	-12(7)	13(2)
C(3A)	5461(10)	-830(9)	890(7)	18(2)
C(4A)	5930(15)	-1887(9)	1625(7)	21(2)
O(1A)	6137(11)	-3627(8)	-482(6)	20(2)
O(2A)	5993(12)	-1840(8)	2480(5)	23(2)
C(5A)	6664(19)	-4325(12)	1318(12)	25(3)
C(1)	10535(14)	-720(10)	855(8)	32(2)
C(2)	11161(22)	-1440(18)	1666(13)	63(11)
C(3)	11811(18)	-2705(10)	1590(7)	20(2)
C(4)	11851(18)	-3309(12)	668(9)	24(3)
C(5)	11247(20)	-2597(15)	-139(11)	24(4)
C(6)	10580(19)	-1319(14)	-68(10)	50(4)
C(7)	9874(27)	570(26)	893(21)	96(8)
S(1A')	4918(2)	474(2)	1134(1)	23(1)
N(1A')	6711(7)	-2952(7)	891(5)	22(2)
C(1A')	6623(8)	-2699(5)	-86(4)	20(1)