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Supporting Information

for

Synthesis and highly efficient light-induced rearrangements of diphenylmethylene(2-benzo[*b*]thienyl)fulgides and fulgimides

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X-ray analysis data of 3*Z*, 3*E* and 9*C*

Contents

Table S1. Bond lengths [A] and angles [deg] for **3***Z*.

S-C(13)	1.7406(19)
S-C(6)	1.7622(18)
O(1)-C(1)	1.385(2)
O(1)-C(2)	1.404(2)
O(2)-C(1)	1.202(2)
O(3)-C(2)	1.192(2)
O(4)-C(7)	1.368(2)
O(4)-C(27)	1.441(2)
C(1)-C(4)	1.467(3)
C(2)-C(3)	1.491(3)
C(3)-C(14)	1.356(2)
C(3)-C(4)	1.476(2)
C(4)-C(5)	1.360(2)
C(5)-C(6)	1.433(2)
C(6)-C(7)	1.384(2)
C(7)-C(8)	1.428(2)
C(8)-C(9)	1.404(2)
C(8)-C(13)	1.406(2)
C(9)-C(10)	1.383(2)
C(10)-C(11)	1.399(3)
C(11)-C(12)	1.383(3)
C(12)-C(13)	1.397(2)
C(14)-C(21)	1.496(2)
C(14)-C(15)	1.501(2)
C(15)-C(20)	1.395(2)
C(15)-C(16)	1.398(2)
C(16)-C(17)	1.386(3)
C(17)-C(18)	1.386(3)
C(18)-C(19)	1.393(3)
C(19)-C(20)	1.383(3)
C(21)-C(26)	1.394(2)
C(21)-C(22)	1.394(3)
C(22)-C(23)	1.390(3)
C(23)-C(24)	1.386(3)
C(24)-C(25)	1.386(3)
C(25)-C(26)	1.387(2)
C(13)-S-C(6)	91.59(9)
C(1)-O(1)-C(2)	110.67(14)
C(7)-O(4)-C(27)	114.85(14)
O(2)-C(1)-O(1)	119.25(16)
O(2)-C(1)-C(4)	131.49(18)
O(1)-C(1)-C(4)	109.26(15)
O(3)-C(2)-O(1)	118.90(16)
O(3)-C(2)-C(3)	133.10(17)
O(1)-C(2)-C(3)	107.98(15)
C(14)-C(3)-C(4)	132.17(16)
C(14)-C(3)-C(2)	122.07(16)

C(4)-C(3)-C(2)	105.75(15)
C(5)-C(4)-C(1)	125.19(17)
C(5)-C(4)-C(3)	128.42(17)
C(1)-C(4)-C(3)	106.34(15)
C(4)-C(5)-C(6)	133.77(17)
C(7)-C(6)-C(5)	119.66(16)
C(7)-C(6)-S	110.31(13)
C(5)-C(6)-S	129.99(14)
O(4)-C(7)-C(6)	121.89(16)
O(4)-C(7)-C(8)	123.21(16)
C(6)-C(7)-C(8)	114.85(16)
C(9)-C(8)-C(13)	120.00(16)
C(9)-C(8)-C(7)	129.07(17)
C(13)-C(8)-C(7)	110.88(16)
C(10)-C(9)-C(8)	118.86(17)
C(9)-C(10)-C(11)	120.43(18)
C(12)-C(11)-C(10)	121.68(17)
C(11)-C(12)-C(13)	118.04(17)
C(12)-C(13)-C(8)	120.97(17)
C(12)-C(13)-S	126.64(15)
C(8)-C(13)-S	112.34(13)
C(3)-C(14)-C(21)	123.43(16)
C(3)-C(14)-C(15)	121.68(16)
C(21)-C(14)-C(15)	114.89(15)
C(20)-C(15)-C(16)	119.06(17)
C(20)-C(15)-C(14)	121.17(16)
C(16)-C(15)-C(14)	119.77(16)
C(17)-C(16)-C(15)	120.19(18)
C(16)-C(17)-C(18)	120.41(17)
C(17)-C(18)-C(19)	119.65(17)
C(20)-C(19)-C(18)	120.12(18)
C(19)-C(20)-C(15)	120.51(17)
C(26)-C(21)-C(22)	118.72(17)
C(26)-C(21)-C(14)	119.92(16)
C(22)-C(21)-C(14)	121.31(17)
C(23)-C(22)-C(21)	120.42(18)
C(24)-C(23)-C(22)	120.33(18)
C(25)-C(24)-C(23)	119.54(18)
C(24)-C(25)-C(26)	120.22(18)
C(25)-C(26)-C(21)	120.69(17)

Table S2. Bond lengths [A] and angles [deg] for **3***E*.

S-C(13)	1.7363(16)
S-C(6)	1.7562(15)
O(1)-C(1)	1.3848(18)
O(1)-C(2)	1.4092(18)
O(2)-C(1)	1.1987(18)
O(3)-C(2)	1.1905(18)
O(4)-C(7)	1.3678(16)
O(4)-C(27)	1.4354(18)
C(1)-C(4)	1.480(2)
C(2)-C(3)	1.487(2)
C(3)-C(14)	1.375(2)
C(3)-C(4)	1.461(2)
C(4)-C(5)	1.361(2)
C(5)-C(6)	1.432(2)
C(6)-C(7)	1.375(2)
C(7)-C(8)	1.432(2)
C(8)-C(9)	1.401(2)
C(8)-C(13)	1.4080(19)
C(9)-C(10)	1.382(2)
C(10)-C(11)	1.408(2)
C(11)-C(12)	1.384(2)
C(12)-C(13)	1.398(2)
C(14)-C(15)	1.472(2)
C(14)-C(21)	1.492(2)
C(15)-C(20)	1.399(2)
C(15)-C(16)	1.403(2)
C(16)-C(17)	1.386(2)
C(17)-C(18)	1.388(3)
C(18)-C(19)	1.384(3)
C(19)-C(20)	1.393(2)
C(21)-C(22)	1.393(2)
C(21)-C(26)	1.394(2)
C(22)-C(23)	1.386(2)
C(23)-C(24)	1.384(3)
C(24)-C(25)	1.384(3)
C(25)-C(26)	1.390(2)
C(13)-S-C(6)	91.72(7)
C(1)-O(1)-C(2)	109.83(12)
C(7)-O(4)-C(27)	115.42(11)
O(2)-C(1)-O(1)	120.03(14)
O(2)-C(1)-C(4)	130.81(15)
O(1)-C(1)-C(4)	109.14(12)
O(3)-C(2)-O(1)	118.29(14)
O(3)-C(2)-C(3)	133.00(14)
O(1)-C(2)-C(3)	108.59(12)
C(14)-C(3)-C(4)	132.88(14)
C(14)-C(3)-C(2)	120.87(13)

C(4)-C(3)-C(2)	105.70(12)
C(5)-C(4)-C(3)	137.05(14)
C(5)-C(4)-C(1)	116.34(13)
C(3)-C(4)-C(1)	106.42(13)
C(4)-C(5)-C(6)	129.69(14)
C(7)-C(6)-C(5)	130.02(14)
C(7)-C(6)-S	111.06(11)
C(5)-C(6)-S	118.89(11)
O(4)-C(7)-C(6)	125.45(14)
O(4)-C(7)-C(8)	120.56(13)
C(6)-C(7)-C(8)	113.98(13)
C(9)-C(8)-C(13)	119.56(14)
C(9)-C(8)-C(7)	129.00(13)
C(13)-C(8)-C(7)	111.43(13)
C(10)-C(9)-C(8)	119.27(14
C(9)-C(10)-C(11)	120.56(15)
C(12)-C(11)-C(10)	121.12(15)
C(11)-C(12)-C(13)	118.14(14)
C(12)-C(13)-C(8)	121.35(14)
C(12)-C(13)-S	126.85(12)
C(8)-C(13)-S	111.79(11)
C(3)-C(14)-C(15)	124.38(13)
C(3)-C(14)-C(21)	120.12(13)
C(15)-C(14)-C(21)	115.48(12)
C(20)-C(15)-C(16)	118.60(14)
C(20)-C(15)-C(14)	121.34(14)
C(16)-C(15)-C(14)	120.04(14)
C(17)-C(16)-C(15)	120.65(16)
C(16)-C(17)-C(18)	120.15(17)
C(19)-C(18)-C(17)	119.89(16
C(18)-C(19)-C(20)	120.37(17)
C(19)-C(20)-C(15)	120.32(16)
C(22)-C(21)-C(26)	118.76(14)
C(22)-C(21)-C(14)	120.87(13)
C(26)-C(21)-C(14)	120.32(14)
C(23)-C(22)-C(21)	120.68(15)
C(24)-C(23)-C(22)	120.01(17)
C(25)-C(24)-C(23)	120.05(15)
C(24)-C(25)-C(26)	119.96(16)
C(25)-C(26)-C(21)	120.50(16)

Table S3. Bond lengths [A] and angles [deg] for **9**C.

S-C(13)	1.743(2)
S-C(6)	1.7473(19)
O(1)-C(1)	1.390(2)
O(1)-C(2)	1.411(2)
O(2)-C(1)	1.193(2)
O(3)-C(2)	1.190(2)
O(4)-C(7)	1.373(2)
O(4)-C(27)	1.436(3)
C(1)-C(4)	1.510(3)
C(2)-C(3)	1.473(3)
C(3)-C(14)	1.349(3)
C(3)-C(4)	1.496(3)
C(4)-C(5)	1.535(3)
C(5)-C(6)	1.504(3)
C(5)-C(16)	1.531(3)
C(6)-C(7)	1.363(3)
C(7)-C(8)	1.440(3)
C(8)-C(13)	1.405(3)
C(8)-C(9)	1.410(3)
C(9)-C(10)	1.378(3)
C(10)-C(11)	1.396(4)
C(11)-C(12)	1.383(3)
C(12)-C(13)	1.399(3)
C(14)-C(15)	1.478(3)
C(14)-C(21)	1.490(3)
C(15)-C(20)	1.398(3)
C(15)-C(16)	1.411(3)
C(16)-C(17)	1.390(3)
C(17)-C(18)	1.394(3)
C(18)-C(19)	1.389(3)
C(19)-C(20)	1.393(3)
C(21)-C(26)	1.388(3)
C(21)-C(22)	1.392(3)
C(22)-C(23)	1.389(3)
C(23)-C(24)	1.384(4)
C(24)-C(25)	1.384(4)
C(25)-C(26)	1.394(3)
C(28)-Cl(21)	1.715(7)
C(28)-Cl(11)	1.750(8)
C(28)-Cl(31)	1.751(8)
C(28)-Cl(1)	1.758(2)
C(28)-Cl(3)	1.763(2)
C(28)-Cl(2)	1.776(3)
C(13)-S-C(6)	91.61(10)
C(1)-O(1)-C(2)	111.18(14)
C(7)-O(4)-C(27)	112.58(18)
O(2)-C(1)-O(1)	120.69(17)

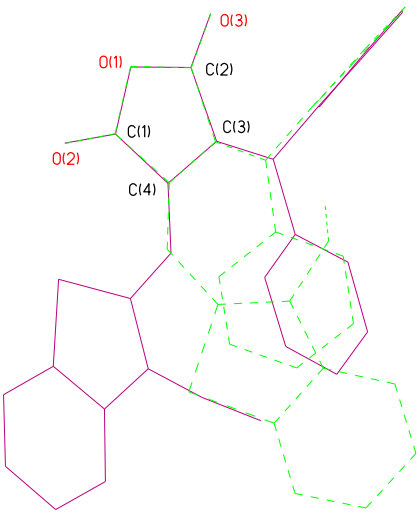
O(2)-C(1)-C(4)	129.77(18)
O(1)-C(1)-C(4)	109.52(16)
O(3)-C(2)-O(1)	119.67(17)
O(3)-C(2)-C(3)	133.11(18)
O(1)-C(2)-C(3)	107.17(15)
C(14)-C(3)-C(2)	128.19(17)
C(14)-C(3)-C(4)	122.76(17)
C(2)-C(3)-C(4)	108.48(16)
C(3)-C(4)-C(1)	102.88(15)
C(3)-C(4)-C(5)	111.77(15)
C(1)-C(4)-C(5)	116.66(16)
C(6)-C(5)-C(16)	111.61(16)
C(6)-C(5)-C(4)	113.97(15)
C(16)-C(5)-C(4)	107.99(15)
C(7)-C(6)-C(5)	124.99(17)
C(7)-C(6)-S	111.49(15)
C(5)-C(6)-S	123.52(14)
C(6)-C(7)-O(4)	122.22(18)
C(6)-C(7)-C(8)	114.19(18)
O(4)-C(7)-C(8)	123.58(17)
C(13)-C(8)-C(9)	119.46(19)
C(13)-C(8)-C(7)	110.96(17)
C(9)-C(8)-C(7)	129.6(2)
C(10)-C(9)-C(8)	118.6(2)
C(9)-C(10)-C(11)	121.2(2)
C(12)-C(11)-C(10)	121.4(2)
C(11)-C(12)-C(13)	117.7(2)
C(12)-C(13)-C(8)	121.56(19)
C(12)-C(13)-S	126.70(17)
C(8)-C(13)-S	111.74(15)
C(3)-C(14)-C(15)	117.65(17)
C(3)-C(14)-C(21)	122.66(17)
C(15)-C(14)-C(21)	119.67(16)
C(20)-C(15)-C(16)	119.08(17)
C(20)-C(15)-C(14)	121.28(17)
C(16)-C(15)-C(14)	119.58(17)
C(17)-C(16)-C(15)	119.63(18)
C(17)-C(16)-C(5)	119.41(17)
C(15)-C(16)-C(5)	120.89(16)
C(16)-C(17)-C(18)	120.65(19)
C(19)-C(18)-C(17)	120.06(18)
C(18)-C(19)-C(20)	119.72(19)
C(19)-C(20)-C(15)	120.85(19)
C(26)-C(21)-C(22)	119.39(19)
C(26)-C(21)-C(14)	120.53(18)
C(22)-C(21)-C(14)	120.09(19)
C(23)-C(22)-C(21)	120.0(2)
C(24)-C(23)-C(22)	120.5(2)
C(25)-C(24)-C(23)	119.7(2)
C(24)-C(25)-C(26)	120.1(2)

C(21)-C(26)-C(25)	120.3(2)
Cl(21)-C(28)-Cl(11)	142.0(7)
Cl(21)-C(28)-Cl(31)	116.8(8)
Cl(11)-C(28)-Cl(31)	101.0(8)
Cl(21)-C(28)-Cl(1)	122.9(5)
Cl(11)-C(28)-Cl(1)	21.8(5)
Cl(31)-C(28)-Cl(1)	119.5(7)
Cl(21)-C(28)-Cl(3)	117.8(4)
Cl(11)-C(28)-Cl(3)	98.1(5)
Cl(31)-C(28)-Cl(3)	22.5(6)
Cl(1)-C(28)-Cl(3)	110.77(13)
Cl(21)-C(28)-Cl(2)	27.0(5)
Cl(11)-C(28)-Cl(2)	131.8(6)
Cl(31)-C(28)-Cl(2)	119.2(7)
Cl(1)-C(28)-Cl(2)	110.09(14)
Cl(3)-C(28)-Cl(2)	108.93(13)

Table S4. Crystal data and structure refinement for **3*Z*, 3*E*** and **9C.**

Compound	**3*Z***	**3*E***	**9C**
Empirical formula	$C_{27}H_{18}O_4S$	$C_{27}H_{18}O_4S$	$C_{27}H_{19}Cl_3O_4S$
Formula weight	438.47	438.47	557.84
Temperature, K	100.0(1)	100.0(1)	100.0(1)
Wavelength, Å	0.71073	0.71073	0.71073
Crystal system, space group	Monoclinic, P $2_1/c$	Triclinic, P -1	Monoclinic, P $2_1/c$
Volume, $Å^3$	2071.31(9)	1060.57(10)	2468.0(9)
Unit cell dimensions, Å and deg.	a = 11.0297(3) α = 90°, b = 7.46108(18) β = 97.289(3)°, c = 25.3750(7) γ = 90°	a = 9.8735(6) α= 69.581(5)°, b = 10.5094(6) β= 87.765(5)°, c =11.2616(6) γ= 75.859(5)°	a = 13.170(3) α = 90°, b = 9.6300(19) β=104.50(3)°, c = 20.100(4) γ = 90°
Z, Calculated density, g/cm^3	4, 1.406	2, 1.373	4, 1.501
Absorption coefficient, mm^{-1}	0.190	0.186	0.491
F(000)	912	456	1144
Crystal size, mm	0.36 x 0.35 x 0.33	0.48 x 0.44 x 0.41	0.50 x 0.15 x 0.05
Theta range for data collection, deg.	3.17 to 26.07	2.85 to 29.07	2.98 to 29.07

Limiting indices	-13<=h<=8, 31<=l<=31, -8<=k<=9	-12<=h<=13, -14<=k<=12, -15<=l<=15	-17<=h<=18, -12<=k<=13, -27<=l<=19
Reflections collected / unique	8306/4088[R(int)=0.0311]	9115 / 5666 [R(int) = 0.0244]	22780 / 6554 [R(int) = 0.0335]
Completeness to theta	26.07° 99.5 %	29.07° 99.9%	29.07 99.4 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	1.000 and 0.9893	1.0000 and 0.9690	1.0000 and 0.92002
Data / restraints / parameters	4088 / 0 / 289	5666 / 0 / 289	6554 / 33 / 335
Goodness-of-fit on F^2	0.986	1.026	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0413, wR2 = 0.0782	R1 = 0.0434, wR2 = 0.0934	R1 = 0.0441, wR2 = 0.1054
R indices (all data)	R1 = 0.0634, wR2 = 0.0852	R1 = 0.0605, wR2 = 0.1044	R1 = 0.0605, wR2 = 0.1134
Largest diff. peak and hole, e.Å $^{-3}$	0.332 and -0.315	0.377 and -0.350	0.710 and -0.792



Scheme S1. The superimposed molecules **3***Z* and **3***E* by the atoms of furan-2,5-dione fragment O(1), O(2), O(3), C(1), C(2), C(3), C(4) (the solid line corresponds to **3***Z*, the dotted line - to **3***E*).

Crystals formed by **3***Z* have a more favorable lattice energy, compared to **3***E*, equal to -51.5 kcal/mol (for a **3***E* crystal, the lattice energy is −43.8 kcal/mol). In the crystal structure of **3***Z* there are contacts between sulfur atoms S...S*: 3.853 (−x, 1−y, −z), 4.411 (−x, −y, −z), 7.461 (−x, −1−y, z and −x, 1−y, −z). In the crystal structure of **3***E* there is a single contact S...S*: 6.892 (2−x, 2−y, −z).