Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

ELECTRONIC SUPPLEMENTARY INFORMATION FOR:

Structure, Photophysics, and Photooxidation of Crowded Diethynyltetracenes

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Supplemental Figures

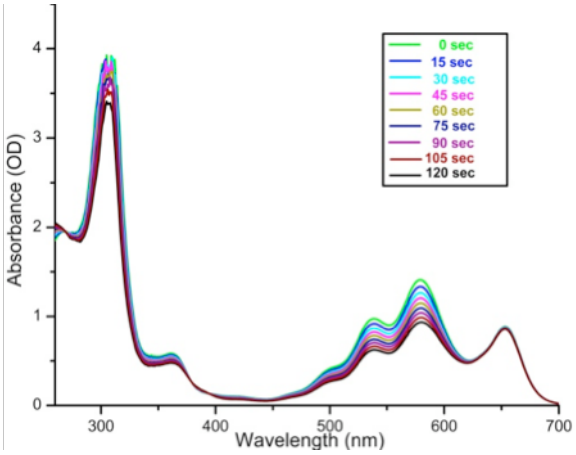

Figure S1. UV/vis response of **1T** to $^1O_2$ photosensization with methylene blue (λ_{max} = 654 nm) in $CHCl_3$.

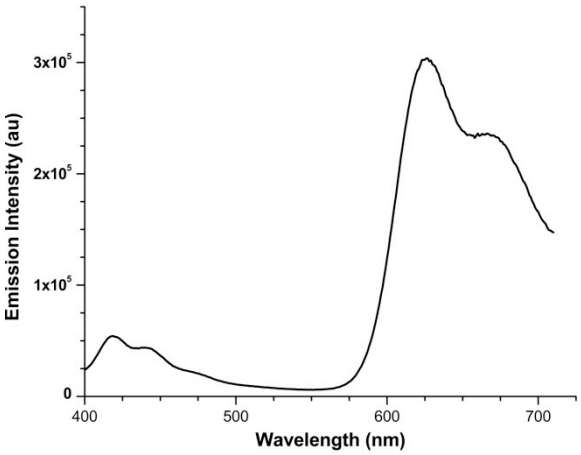

Figure S2. Emission spectrum of 20% (w/w) **2T** in a matrix of poly(9, 9-di-*n*-dodecylfluorenyl-2, 7-diyl) (λ_{excit}=369nm).

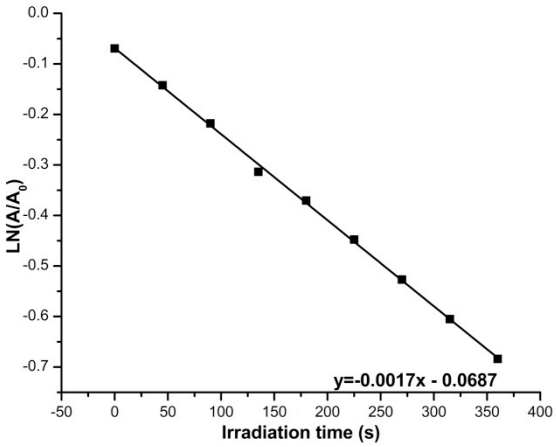

Figure S3. First order kinetics of reaction of **4T** during irradiation of methylene blue in $CHCl_3$.

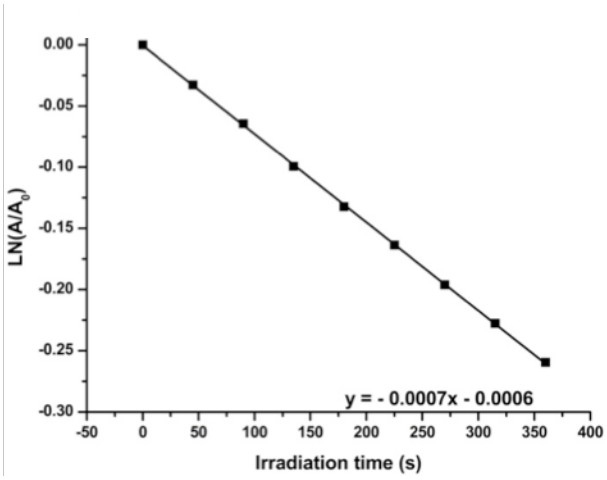

Figure S4. First order kinetics of reaction of **3D** during irradiation of methylene blue in $CHCl_3$.

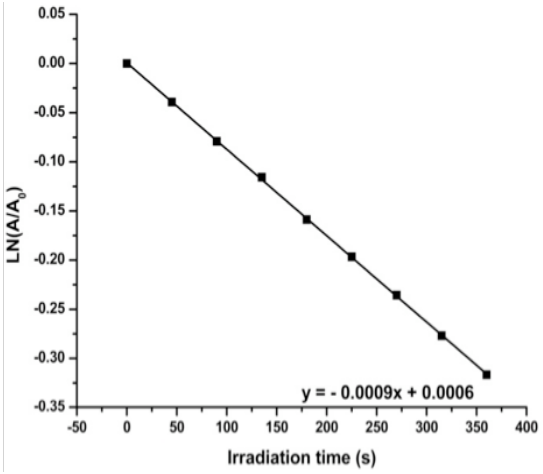

Figure S5. First order kinetics of reaction of **4D** during irradiation of methylene blue in $CHCl_3$.

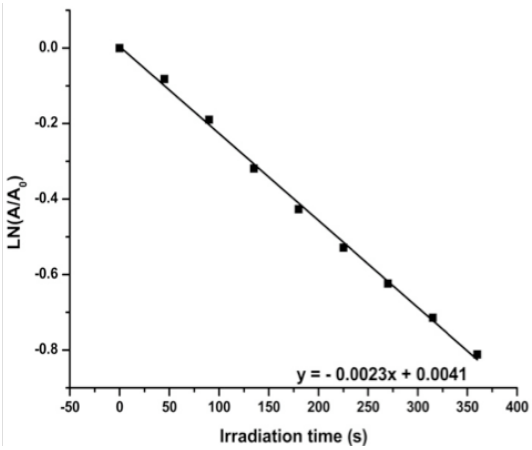

Figure S6. First order kinetics of reaction of **4P** during irradiation of methylene blue in $CHCl_3$.

Xray Crystallography.

Low-temperature diffraction data were collected on a Bruker-AXS X8 Kappa Duo diffractometer coupled to a Smart Apex2 CCD detector with Mo Kα radiation (λ = 0.71073 Å) from an *IμS* micro-source), performing φ-and ω-scans. The structures were solved by direct methods using SHELXS[1] and refined against F^2 on all data by full-matrix least squares with SHELXL-97[2] following established refinement strategies[3]. All non-hydrogen atoms were refined anisotropically; all hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups). Both structures were deposited with the Cambridge Crystallographic Data Centre and the corresponding deposition numbers are CCDC 853371 and CCDC 853372, respectively. Details of the data quality, refinement statistics, bond distances and -angles as well as other parameters are listed in tables 1 to 10.

Table 1. Crystal data and structure refinement for ST2.

Identification code	ST2	
Empirical formula	$C_{48}H_{32}O_2$	
Formula weight	640.74	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.0225(15) Å	α= 101.509(7)°.
	b = 11.456(3) Å	β= 96.474(7)°.
	c = 22.004(6) Å	γ = 104.936(5)°.
Volume	1650.7(7) Å^3	
Z	2	
Density (calculated)	1.289 Mg/m^3	
Absorption coefficient	0.077 mm^{-1}	
F(000)	672	
Crystal size	0.30 x 0.20 x 0.01 mm^3	
Theta range for data collection	1.89 to 30.55°.	
Index ranges	-10<=h<=10, -16<=k<=16, -31<=l<=30	
Reflections collected	60686	
Independent reflections	9944 [R_{int} = 0.0505]	
Completeness to theta = 30.55°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9996 and 0.9772	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9944 / 0 / 453	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2σ(I)]	R1 = 0.0551, wR2 = 0.1310	
R indices (all data)	R1 = 0.0977, wR2 = 0.1535	
Largest diff. peak and hole	0.384 and -0.250 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for st2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(8)	4196(2)	1362(1)	2219(1)	20(1)
C(13)	4447(2)	3939(1)	2417(1)	22(1)
O(2)	9746(2)	-3862(1)	-210(1)	32(1)
C(9)	3098(2)	1920(1)	2665(1)	19(1)
C(11)	5393(2)	2118(1)	1883(1)	20(1)
C(12)	5488(2)	3382(1)	1969(1)	21(1)
C(43)	6622(2)	1654(1)	1431(1)	20(1)
C(5)	1642(2)	-144(2)	2872(1)	21(1)
C(6)	2707(2)	-693(1)	2433(1)	20(1)
C(7)	3966(2)	49(1)	2112(1)	20(1)
C(14)	3292(2)	3218(1)	2765(1)	21(1)
C(10)	1833(2)	1142(1)	2983(1)	20(1)
C(19)	654(2)	1576(2)	3419(1)	23(1)
C(28)	4931(2)	-593(2)	1673(1)	22(1)
C(30)	6603(2)	-1992(1)	932(1)	22(1)
O(1)	-5891(2)	1795(1)	5462(1)	35(1)
C(32)	9657(2)	-2473(2)	712(1)	26(1)
C(16)	6751(2)	5386(2)	1709(1)	29(1)
C(48)	5981(2)	1414(2)	784(1)	24(1)
C(1)	2415(2)	-2011(2)	2316(1)	24(1)
C(37)	2343(2)	3885(2)	3245(1)	23(1)
C(29)	5611(2)	-1281(2)	1331(1)	23(1)
C(31)	8662(2)	-1823(2)	1100(1)	24(1)
C(35)	5581(2)	-2843(2)	373(1)	24(1)
C(17)	5752(2)	5937(2)	2160(1)	29(1)
C(18)	4649(2)	5246(2)	2503(1)	26(1)
C(33)	8623(2)	-3294(2)	149(1)	25(1)
C(2)	1175(2)	-2729(2)	2616(1)	26(1)
C(4)	372(2)	-940(2)	3183(1)	26(1)
C(44)	8538(2)	1611(2)	1652(1)	24(1)
C(15)	6640(2)	4158(2)	1621(1)	26(1)
C(20)	-462(2)	1677(2)	3793(1)	25(1)
C(34)	6560(2)	-3490(2)	-22(1)	25(1)
C(45)	9792(2)	1347(2)	1228(1)	27(1)
C(21)	-1794(2)	1743(2)	4237(1)	24(1)
C(24)	-4489(2)	1750(2)	5080(1)	27(1)
C(3)	152(3)	-2184(2)	3060(1)	28(1)
C(25)	-2706(3)	1472(2)	5244(1)	29(1)
C(46)	9147(3)	1123(2)	589(1)	28(1)
C(23)	-4932(3)	2010(2)	4501(1)	31(1)
C(42)	3335(3)	4354(2)	3866(1)	31(1)
C(38)	522(3)	4119(2)	3075(1)	28(1)
C(26)	-1374(3)	1475(2)	4821(1)	29(1)
C(47)	7232(3)	1140(2)	363(1)	27(1)
C(22)	-3600(3)	2014(2)	4084(1)	30(1)
C(39)	-330(3)	4750(2)	3525(1)	34(1)
C(36)	8753(3)	-4644(2)	-809(1)	36(1)
C(41)	2477(3)	4987(2)	4315(1)	39(1)
C(40)	638(3)	5174(2)	4147(1)	41(1)
C(27)	-5381(3)	1671(2)	6087(1)	41(1)

Table 3. Bond lengths [Å] and angles [°] for st2.

C(8)-C(11)	1.423(2)	C(44)-H(44)	0.9500
C(8)-C(7)	1.439(2)	C(15)-H(15)	0.9500
C(8)-C(9)	1.462(2)	C(20)-C(21)	1.432(2)
C(13)-C(14)	1.404(2)	C(34)-H(34)	0.9500
C(13)-C(12)	1.437(2)	C(45)-C(46)	1.378(3)
C(13)-C(18)	1.439(2)	C(45)-H(45)	0.9500
O(2)-C(33)	1.3671(19)	C(21)-C(26)	1.396(2)
O(2)-C(36)	1.424(2)	C(21)-C(22)	1.403(2)
C(9)-C(14)	1.427(2)	C(24)-C(23)	1.384(2)
C(9)-C(10)	1.434(2)	C(24)-C(25)	1.396(2)
C(11)-C(12)	1.406(2)	C(3)-H(3)	0.9500
C(11)-C(43)	1.495(2)	C(25)-C(26)	1.391(2)
C(12)-C(15)	1.439(2)	C(25)-H(25)	0.9500
C(43)-C(48)	1.393(2)	C(46)-C(47)	1.386(2)
C(43)-C(44)	1.395(2)	C(46)-H(46)	0.9500
C(5)-C(10)	1.413(2)	C(23)-C(22)	1.382(2)
C(5)-C(6)	1.432(2)	C(23)-H(23)	0.9500
C(5)-C(4)	1.436(2)	C(42)-C(41)	1.393(3)
C(6)-C(7)	1.413(2)	C(42)-H(42)	0.9500
C(6)-C(1)	1.436(2)	C(38)-C(39)	1.389(2)
C(7)-C(28)	1.434(2)	C(38)-H(38)	0.9500
C(14)-C(37)	1.498(2)	C(26)-H(26)	0.9500
C(10)-C(19)	1.432(2)	C(47)-H(47)	0.9500
C(19)-C(20)	1.208(2)	C(22)-H(22)	0.9500
C(28)-C(29)	1.205(2)	C(39)-C(40)	1.389(3)
C(30)-C(35)	1.393(2)	C(39)-H(39)	0.9500
C(30)-C(31)	1.404(2)	C(36)-H(36A)	0.9800
C(30)-C(29)	1.438(2)	C(36)-H(36B)	0.9800
O(1)-C(24)	1.3704(19)	C(36)-H(36C)	0.9800
O(1)-C(27)	1.425(2)	C(41)-C(40)	1.384(3)
C(32)-C(31)	1.385(2)	C(41)-H(41)	0.9500
C(32)-C(33)	1.389(2)	C(40)-H(40)	0.9500
C(32)-H(32)	0.9500	C(27)-H(27A)	0.9800
C(16)-C(15)	1.362(2)	C(27)-H(27B)	0.9800
C(16)-C(17)	1.418(2)	C(27)-H(27C)	0.9800
C(16)-H(16)	0.9500		
C(48)-C(47)	1.392(2)	C(11)-C(8)-C(7)	121.67(13)
C(48)-H(48)	0.9500	C(11)-C(8)-C(9)	119.35(13)
C(1)-C(2)	1.360(2)	C(7)-C(8)-C(9)	118.93(13)
C(1)-H(1)	0.9500	C(14)-C(13)-C(12)	120.25(14)
C(37)-C(42)	1.393(2)	C(14)-C(13)-C(18)	121.54(14)
C(37)-C(38)	1.399(2)	C(12)-C(13)-C(18)	118.21(14)
C(31)-H(31)	0.9500	C(33)-O(2)-C(36)	116.95(14)
C(35)-C(34)	1.385(2)	C(14)-C(9)-C(10)	121.79(13)
C(35)-H(35)	0.9500	C(14)-C(9)-C(8)	119.22(13)
C(17)-C(18)	1.360(2)	C(10)-C(9)-C(8)	118.98(13)
C(17)-H(17)	0.9500	C(12)-C(11)-C(8)	120.31(14)
C(18)-H(18)	0.9500	C(12)-C(11)-C(43)	115.87(13)
C(33)-C(34)	1.402(2)	C(8)-C(11)-C(43)	123.82(13)
C(2)-C(3)	1.415(2)	C(11)-C(12)-C(13)	120.41(13)
C(2)-H(2)	0.9500	C(11)-C(12)-C(15)	121.44(14)
C(4)-C(3)	1.360(2)	C(13)-C(12)-C(15)	118.14(14)
C(4)-H(4)	0.9500	C(48)-C(43)-C(44)	118.97(14)
C(44)-C(45)	1.396(2)	C(48)-C(43)-C(11)	120.44(13)

C(44)-C(43)-C(11)	120.07(14)	C(3)-C(4)-C(5)	121.38(15)
C(10)-C(5)-C(6)	120.12(13)	C(3)-C(4)-H(4)	119.3
C(10)-C(5)-C(4)	121.78(14)	C(5)-C(4)-H(4)	119.3
C(6)-C(5)-C(4)	118.10(14)	C(43)-C(44)-C(45)	120.08(15)
C(7)-C(6)-C(5)	120.28(14)	C(43)-C(44)-H(44)	120.0
C(7)-C(6)-C(1)	121.29(14)	C(45)-C(44)-H(44)	120.0
C(5)-C(6)-C(1)	118.41(14)	C(16)-C(15)-C(12)	121.51(15)
C(6)-C(7)-C(28)	115.93(14)	C(16)-C(15)-H(15)	119.2
C(6)-C(7)-C(8)	120.74(13)	C(12)-C(15)-H(15)	119.2
C(28)-C(7)-C(8)	123.31(13)	C(19)-C(20)-C(21)	177.61(18)
C(13)-C(14)-C(9)	120.36(14)	C(35)-C(34)-C(33)	119.19(15)
C(13)-C(14)-C(37)	116.77(14)	C(35)-C(34)-H(34)	120.4
C(9)-C(14)-C(37)	122.85(13)	C(33)-C(34)-H(34)	120.4
C(5)-C(10)-C(19)	115.02(13)	C(46)-C(45)-C(44)	120.36(15)
C(5)-C(10)-C(9)	120.95(14)	C(46)-C(45)-H(45)	119.8
C(19)-C(10)-C(9)	124.02(14)	C(44)-C(45)-H(45)	119.8
C(20)-C(19)-C(10)	165.80(17)	C(26)-C(21)-C(22)	118.48(15)
C(29)-C(28)-C(7)	170.73(16)	C(26)-C(21)-C(20)	120.68(15)
C(35)-C(30)-C(31)	118.48(14)	C(22)-C(21)-C(20)	120.75(15)
C(35)-C(30)-C(29)	121.75(15)	O(1)-C(24)-C(23)	115.57(15)
C(31)-C(30)-C(29)	119.76(15)	O(1)-C(24)-C(25)	124.11(16)
C(24)-O(1)-C(27)	116.90(14)	C(23)-C(24)-C(25)	120.33(15)
C(31)-C(32)-C(33)	120.09(15)	C(4)-C(3)-C(2)	120.49(15)
C(31)-C(32)-H(32)	120.0	C(4)-C(3)-H(3)	119.8
C(33)-C(32)-H(32)	120.0	C(2)-C(3)-H(3)	119.8
C(15)-C(16)-C(17)	120.17(15)	C(26)-C(25)-C(24)	119.09(16)
C(15)-C(16)-H(16)	119.9	C(26)-C(25)-H(25)	120.5
C(17)-C(16)-H(16)	119.9	C(24)-C(25)-H(25)	120.5
C(47)-C(48)-C(43)	120.67(15)	C(45)-C(46)-C(47)	120.08(15)
C(47)-C(48)-H(48)	119.7	C(45)-C(46)-H(46)	120.0
C(43)-C(48)-H(48)	119.7	C(47)-C(46)-H(46)	120.0
C(2)-C(1)-C(6)	121.32(15)	C(22)-C(23)-C(24)	120.32(16)
C(2)-C(1)-H(1)	119.3	C(22)-C(23)-H(23)	119.8
C(6)-C(1)-H(1)	119.3	C(24)-C(23)-H(23)	119.8
C(42)-C(37)-C(38)	118.70(15)	C(37)-C(42)-C(41)	120.54(18)
C(42)-C(37)-C(14)	120.01(15)	C(37)-C(42)-H(42)	119.7
C(38)-C(37)-C(14)	121.15(15)	C(41)-C(42)-H(42)	119.7
C(28)-C(29)-C(30)	174.03(17)	C(39)-C(38)-C(37)	120.51(17)
C(32)-C(31)-C(30)	120.63(16)	C(39)-C(38)-H(38)	119.7
C(32)-C(31)-H(31)	119.7	C(37)-C(38)-H(38)	119.7
C(30)-C(31)-H(31)	119.7	C(25)-C(26)-C(21)	121.25(15)
C(34)-C(35)-C(30)	121.46(15)	C(25)-C(26)-H(26)	119.4
C(34)-C(35)-H(35)	119.3	C(21)-C(26)-H(26)	119.4
C(30)-C(35)-H(35)	119.3	C(46)-C(47)-C(48)	119.81(16)
C(18)-C(17)-C(16)	120.66(15)	C(46)-C(47)-H(47)	120.1
C(18)-C(17)-H(17)	119.7	C(48)-C(47)-H(47)	120.1
C(16)-C(17)-H(17)	119.7	C(23)-C(22)-C(21)	120.53(16)
C(17)-C(18)-C(13)	121.28(15)	C(23)-C(22)-H(22)	119.7
C(17)-C(18)-H(18)	119.4	C(21)-C(22)-H(22)	119.7
C(13)-C(18)-H(18)	119.4	C(38)-C(39)-C(40)	120.21(18)
O(2)-C(33)-C(32)	115.74(15)	C(38)-C(39)-H(39)	119.9
O(2)-C(33)-C(34)	124.15(16)	C(40)-C(39)-H(39)	119.9
C(32)-C(33)-C(34)	120.11(15)	O(2)-C(36)-H(36A)	109.5
C(1)-C(2)-C(3)	120.29(15)	O(2)-C(36)-H(36B)	109.5
C(1)-C(2)-H(2)	119.9	H(36A)-C(36)-H(36B)	109.5
C(3)-C(2)-H(2)	119.9	O(2)-C(36)-H(36C)	109.5

H(36A)-C(36)-H(36C)	109.5	C(39)-C(40)-H(40)	120.2
H(36B)-C(36)-H(36C)	109.5	O(1)-C(27)-H(27A)	109.5
C(40)-C(41)-C(42)	120.29(19)	O(1)-C(27)-H(27B)	109.5
C(40)-C(41)-H(41)	119.9	H(27A)-C(27)-H(27B)	109.5
C(42)-C(41)-H(41)	119.9	O(1)-C(27)-H(27C)	109.5
C(41)-C(40)-C(39)	119.64(17)	H(27A)-C(27)-H(27C)	109.5
C(41)-C(40)-H(40)	120.2	H(27B)-C(27)-H(27C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for st2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(8)	21(1)	18(1)	22(1)	5(1)	3(1)	9(1)
C(13)	22(1)	18(1)	26(1)	6(1)	3(1)	8(1)
O(2)	35(1)	28(1)	40(1)	8(1)	18(1)	17(1)
C(9)	21(1)	18(1)	21(1)	6(1)	4(1)	8(1)
C(11)	20(1)	19(1)	22(1)	6(1)	4(1)	8(1)
C(12)	21(1)	18(1)	26(1)	8(1)	4(1)	8(1)
C(43)	22(1)	16(1)	27(1)	8(1)	8(1)	7(1)
C(5)	22(1)	21(1)	22(1)	8(1)	3(1)	7(1)
C(6)	22(1)	18(1)	22(1)	7(1)	4(1)	8(1)
C(7)	21(1)	19(1)	23(1)	7(1)	4(1)	9(1)
C(14)	23(1)	18(1)	23(1)	5(1)	4(1)	9(1)
C(10)	22(1)	19(1)	20(1)	5(1)	3(1)	8(1)
C(19)	27(1)	20(1)	25(1)	7(1)	5(1)	9(1)
C(28)	24(1)	18(1)	27(1)	9(1)	5(1)	7(1)
C(30)	27(1)	17(1)	26(1)	10(1)	9(1)	10(1)
O(1)	30(1)	44(1)	33(1)	9(1)	13(1)	13(1)
C(32)	23(1)	26(1)	34(1)	13(1)	7(1)	10(1)
C(16)	26(1)	24(1)	40(1)	15(1)	10(1)	8(1)
C(48)	26(1)	21(1)	29(1)	9(1)	6(1)	9(1)
C(1)	27(1)	19(1)	28(1)	8(1)	5(1)	10(1)
C(37)	29(1)	16(1)	28(1)	6(1)	9(1)	10(1)
C(29)	27(1)	18(1)	27(1)	9(1)	6(1)	8(1)
C(31)	27(1)	18(1)	30(1)	8(1)	6(1)	8(1)
C(35)	24(1)	21(1)	30(1)	9(1)	7(1)	9(1)
C(17)	28(1)	17(1)	44(1)	10(1)	7(1)	10(1)
C(18)	26(1)	19(1)	34(1)	6(1)	6(1)	10(1)
C(33)	31(1)	21(1)	32(1)	12(1)	16(1)	15(1)
C(2)	28(1)	19(1)	35(1)	12(1)	6(1)	8(1)
C(4)	27(1)	26(1)	30(1)	11(1)	11(1)	10(1)
C(44)	25(1)	21(1)	27(1)	7(1)	5(1)	9(1)
C(15)	25(1)	20(1)	35(1)	11(1)	9(1)	8(1)
C(20)	28(1)	24(1)	26(1)	8(1)	6(1)	10(1)
C(34)	32(1)	20(1)	24(1)	6(1)	8(1)	9(1)
C(45)	23(1)	23(1)	39(1)	9(1)	7(1)	9(1)
C(21)	28(1)	22(1)	25(1)	5(1)	8(1)	9(1)
C(24)	27(1)	27(1)	29(1)	4(1)	10(1)	8(1)
C(3)	29(1)	25(1)	36(1)	14(1)	11(1)	8(1)
C(25)	33(1)	33(1)	26(1)	10(1)	8(1)	12(1)
C(46)	33(1)	22(1)	36(1)	10(1)	16(1)	11(1)
C(23)	26(1)	36(1)	33(1)	8(1)	7(1)	13(1)
C(42)	38(1)	25(1)	30(1)	4(1)	5(1)	10(1)
C(38)	31(1)	22(1)	35(1)	9(1)	10(1)	12(1)
C(26)	29(1)	33(1)	31(1)	10(1)	8(1)	16(1)
C(47)	35(1)	23(1)	26(1)	9(1)	9(1)	10(1)
C(22)	30(1)	36(1)	28(1)	10(1)	6(1)	14(1)
C(39)	38(1)	23(1)	51(1)	13(1)	21(1)	17(1)
C(36)	46(1)	29(1)	38(1)	8(1)	23(1)	14(1)
C(41)	57(1)	27(1)	31(1)	1(1)	10(1)	11(1)
C(40)	58(1)	26(1)	45(1)	7(1)	28(1)	18(1)
C(27)	39(1)	57(1)	30(1)	12(1)	16(1)	14(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for st2.

	x	y	z	U(eq)
H(32)	11048	-2356	832	32
H(16)	7500	5875	1467	34
H(48)	4677	1438	629	29
H(1)	3102	-2389	2023	28
H(31)	9380	-1258	1483	29
H(35)	4180	-2983	260	28
H(17)	5854	6797	2223	34
H(18)	3999	5634	2805	31
H(2)	994	-3601	2528	32
H(4)	-330	-591	3481	31
H(44)	8990	1761	2092	29
H(15)	7339	3805	1323	31
H(34)	5844	-4060	-404	30
H(45)	11098	1321	1380	33
H(3)	-694	-2690	3273	34
H(25)	-2406	1284	5638	35
H(46)	10015	957	303	34
H(23)	-6157	2187	4390	37
H(42)	4607	4241	3984	37
H(38)	-137	3845	2649	33
H(26)	-155	1291	4931	35
H(47)	6776	966	-77	32
H(22)	-3911	2202	3689	36
H(39)	-1579	4891	3406	41
H(36A)	7614	-5295	-755	54
H(36B)	9688	-5028	-1012	54
H(36C)	8274	-4148	-1073	54
H(41)	3157	5292	4739	47
H(40)	42	5589	4456	49
H(27A)	-5218	841	6071	62
H(27B)	-6448	1781	6324	62
H(27C)	-4124	2304	6295	62

Table 6. Crystal data and structure refinement for 4T.

Identification code	4T	
Empirical formula	$C_{52}H_{60}Si_2$	
Formula weight	741.18	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 9.5021(8) Å	α= 90°.
	b = 18.5086(15) Å	β= 90°.
	c = 24.385(2) Å	γ = 90°.
Volume	4288.6(6) Å^3	
Z	4	
Density (calculated)	1.148 Mg/m^3	
Absorption coefficient	0.117 mm^{-1}	
F(000)	1600	
Crystal size	0.23 x 0.17 x 0.09 mm^3	
Theta range for data collection	1.38 to 30.53°.	
Index ranges	-13<=h<=13, -26<=k<=26, -34<=l<=34	
Reflections collected	92146	
Independent reflections	13123 [R_{int} = 0.0605]	
Completeness to theta = 30.53°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9895 and 0.9736	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13123 / 0 / 499	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2σ(I)]	R1 = 0.0364, wR2 = 0.0831	
R indices (all data)	R1 = 0.0460, wR2 = 0.0889	
Absolute structure parameter	0.01(6)	
Largest diff. peak and hole	0.299 and -0.198 e.Å^{-3}	

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 4t. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	12503(1)	7853(1)	2178(1)	14(1)
Si(2)	2914(1)	10495(1)	4330(1)	14(1)
C(12)	7874(1)	9055(1)	2811(1)	14(1)
C(7)	9230(1)	7953(1)	4004(1)	15(1)
C(10)	8007(1)	9157(1)	4558(1)	14(1)
C(11)	8729(1)	8574(1)	3112(1)	14(1)
C(6)	8810(1)	8647(1)	4850(1)	15(1)
C(9)	7803(1)	9073(1)	3983(1)	13(1)
C(8)	8594(1)	8522(1)	3697(1)	13(1)
C(48)	6564(1)	9777(1)	5288(1)	17(1)
C(5)	9325(1)	8010(1)	4577(1)	15(1)
C(47)	7514(1)	9816(1)	4854(1)	14(1)
C(41)	9637(1)	7268(1)	3727(1)	16(1)
C(22)	4636(1)	10175(1)	4083(1)	16(1)
C(19)	9856(1)	8226(1)	2824(1)	16(1)
C(13)	6865(1)	9495(1)	3093(1)	14(1)
C(2)	9826(2)	8214(1)	5708(1)	21(1)
C(35)	3214(1)	11348(1)	4742(1)	17(1)
C(17)	6015(1)	9948(1)	2216(1)	19(1)
C(42)	11001(1)	6985(1)	3742(1)	17(1)
C(26)	12134(1)	7156(1)	1634(1)	20(1)
C(16)	7046(1)	9529(1)	1938(1)	19(1)
C(14)	6841(1)	9506(1)	3671(1)	14(1)
C(4)	9959(2)	7454(1)	4906(1)	19(1)
C(1)	9142(1)	8739(1)	5420(1)	18(1)
C(32)	1746(1)	10664(1)	3717(1)	19(1)
C(20)	10863(2)	8035(1)	2556(1)	18(1)
C(38)	2117(1)	9751(1)	4765(1)	18(1)
C(18)	5925(1)	9932(1)	2774(1)	17(1)
C(46)	8587(2)	6876(1)	3460(1)	20(1)
C(49)	6198(1)	10393(1)	5584(1)	21(1)
C(15)	7945(1)	9099(1)	2224(1)	18(1)
C(34)	1358(2)	9973(1)	3404(1)	32(1)
C(40)	2607(2)	8995(1)	4586(1)	29(1)
C(52)	8091(1)	10486(1)	4720(1)	18(1)
C(33)	2360(2)	11224(1)	3317(1)	27(1)
C(27)	11758(2)	6421(1)	1886(1)	31(1)
C(29)	13824(2)	7517(1)	2693(1)	21(1)
C(28)	10982(2)	7398(1)	1235(1)	27(1)
C(21)	5714(1)	9898(1)	3927(1)	15(1)
C(50)	6785(2)	11055(1)	5450(1)	23(1)
C(37)	1824(2)	11744(1)	4858(1)	22(1)
C(3)	10210(2)	7553(1)	5449(1)	21(1)
C(43)	11295(2)	6325(1)	3494(1)	22(1)
C(23)	13131(2)	8734(1)	1869(1)	20(1)
C(45)	8884(2)	6216(1)	3212(1)	24(1)
C(39)	2384(2)	9840(1)	5381(1)	29(1)
C(25)	11935(2)	9257(1)	1718(1)	33(1)
C(44)	10242(2)	5942(1)	3230(1)	24(1)
C(31)	14103(2)	8081(1)	3142(1)	33(1)
C(36)	4300(2)	11872(1)	4497(1)	25(1)

C(51)	7735(2)	11102(1)	5017(1)	23(1)
C(24)	14107(2)	8612(1)	1376(1)	28(1)
C(30)	15206(2)	7277(1)	2427(1)	50(1)

Table 8. Bond lengths [Å] and angles [°] for 4t.

Si(1)-C(20)	1.8423(14)	C(32)-C(34)	1.534(2)
Si(1)-C(29)	1.8819(14)	C(32)-C(33)	1.538(2)
Si(1)-C(26)	1.8836(14)	C(32)-H(32)	1.0000
Si(1)-C(23)	1.8923(15)	C(38)-C(39)	1.532(2)
Si(2)-C(22)	1.8413(14)	C(38)-C(40)	1.5375(19)
Si(2)-C(32)	1.8880(14)	C(38)-H(38)	1.0000
Si(2)-C(35)	1.8930(14)	C(18)-H(18)	0.9500
Si(2)-C(38)	1.8960(14)	C(46)-C(45)	1.3917(19)
C(12)-C(11)	1.4103(17)	C(46)-H(46)	0.9500
C(12)-C(13)	1.4335(17)	C(49)-C(50)	1.385(2)
C(12)-C(15)	1.4355(18)	C(49)-H(49)	0.9500
C(7)-C(5)	1.4051(18)	C(15)-H(15)	0.9500
C(7)-C(8)	1.4258(18)	C(34)-H(34A)	0.9800
C(7)-C(41)	1.4873(18)	C(34)-H(34B)	0.9800
C(10)-C(6)	1.4073(17)	C(34)-H(34C)	0.9800
C(10)-C(9)	1.4234(17)	C(40)-H(40A)	0.9800
C(10)-C(47)	1.4913(17)	C(40)-H(40B)	0.9800
C(11)-C(8)	1.4346(17)	C(40)-H(40C)	0.9800
C(11)-C(19)	1.4347(17)	C(52)-C(51)	1.3915(19)
C(6)-C(1)	1.4370(18)	C(52)-H(52)	0.9500
C(6)-C(5)	1.4398(17)	C(33)-H(33A)	0.9800
C(9)-C(14)	1.4344(17)	C(33)-H(33B)	0.9800
C(9)-C(8)	1.4472(17)	C(33)-H(33C)	0.9800
C(48)-C(49)	1.3934(19)	C(27)-H(27A)	0.9800
C(48)-C(47)	1.3936(18)	C(27)-H(27B)	0.9800
C(48)-H(48)	0.9500	C(27)-H(27C)	0.9800
C(5)-C(4)	1.4355(18)	C(29)-C(30)	1.532(2)
C(47)-C(52)	1.3944(18)	C(29)-C(31)	1.534(2)
C(41)-C(46)	1.3949(19)	C(29)-H(29)	1.0000
C(41)-C(42)	1.3983(18)	C(28)-H(28A)	0.9800
C(22)-C(21)	1.2080(18)	C(28)-H(28B)	0.9800
C(19)-C(20)	1.2109(19)	C(28)-H(28C)	0.9800
C(13)-C(14)	1.4108(17)	C(50)-C(51)	1.393(2)
C(13)-C(18)	1.4331(18)	C(50)-H(50)	0.9500
C(2)-C(1)	1.3641(19)	C(37)-H(37A)	0.9800
C(2)-C(3)	1.424(2)	C(37)-H(37B)	0.9800
C(2)-H(2)	0.9500	C(37)-H(37C)	0.9800
C(35)-C(36)	1.5365(19)	C(3)-H(3)	0.9500
C(35)-C(37)	1.5377(18)	C(43)-C(44)	1.384(2)
C(35)-H(35)	1.0000	C(43)-H(43)	0.9500
C(17)-C(18)	1.365(2)	C(23)-C(24)	1.534(2)
C(17)-C(16)	1.4220(19)	C(23)-C(25)	1.537(2)
C(17)-H(17)	0.9500	C(23)-H(23)	1.0000
C(42)-C(43)	1.3934(19)	C(45)-C(44)	1.387(2)
C(42)-H(42)	0.9500	C(45)-H(45)	0.9500
C(26)-C(28)	1.530(2)	C(39)-H(39A)	0.9800
C(26)-C(27)	1.535(2)	C(39)-H(39B)	0.9800
C(26)-H(26)	1.0000	C(39)-H(39C)	0.9800
C(16)-C(15)	1.3606(19)	C(25)-H(25A)	0.9800
C(16)-H(16)	0.9500	C(25)-H(25B)	0.9800
C(14)-C(21)	1.4354(17)	C(25)-H(25C)	0.9800
C(4)-C(3)	1.359(2)	C(44)-H(44)	0.9500
C(4)-H(4)	0.9500	C(31)-H(31A)	0.9800
C(1)-H(1)	0.9500	C(31)-H(31B)	0.9800

C(31)-H(31C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(51)-H(51)	0.9500
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800

C(20)-Si(1)-C(29)	106.84(6)
C(20)-Si(1)-C(26)	108.70(6)
C(29)-Si(1)-C(26)	111.63(6)
C(20)-Si(1)-C(23)	107.93(6)
C(29)-Si(1)-C(23)	109.86(7)
C(26)-Si(1)-C(23)	111.68(6)
C(22)-Si(2)-C(32)	108.49(6)
C(22)-Si(2)-C(35)	107.88(6)
C(32)-Si(2)-C(35)	111.72(6)
C(22)-Si(2)-C(38)	107.73(6)
C(32)-Si(2)-C(38)	109.21(6)
C(35)-Si(2)-C(38)	111.67(6)
C(11)-C(12)-C(13)	119.61(11)
C(11)-C(12)-C(15)	121.88(11)
C(13)-C(12)-C(15)	118.47(11)
C(5)-C(7)-C(8)	119.63(11)
C(5)-C(7)-C(41)	119.91(11)
C(8)-C(7)-C(41)	120.07(11)
C(6)-C(10)-C(9)	119.85(11)
C(6)-C(10)-C(47)	118.34(11)
C(9)-C(10)-C(47)	121.50(11)
C(12)-C(11)-C(8)	120.59(11)
C(12)-C(11)-C(19)	117.26(11)
C(8)-C(11)-C(19)	121.55(12)
C(10)-C(6)-C(1)	121.91(12)
C(10)-C(6)-C(5)	120.05(12)
C(1)-C(6)-C(5)	118.04(11)
C(10)-C(9)-C(14)	123.24(11)
C(10)-C(9)-C(8)	118.82(11)
C(14)-C(9)-C(8)	117.94(11)
C(7)-C(8)-C(11)	122.28(11)
C(7)-C(8)-C(9)	119.15(11)
C(11)-C(8)-C(9)	118.56(11)
C(49)-C(48)-C(47)	120.86(13)
C(49)-C(48)-H(48)	119.6
C(47)-C(48)-H(48)	119.6
C(7)-C(5)-C(4)	121.95(12)
C(7)-C(5)-C(6)	119.92(12)
C(4)-C(5)-C(6)	118.11(12)
C(48)-C(47)-C(52)	118.53(12)
C(48)-C(47)-C(10)	121.87(11)
C(52)-C(47)-C(10)	119.43(11)
C(46)-C(41)-C(42)	118.73(12)
C(46)-C(41)-C(7)	118.00(12)
C(42)-C(41)-C(7)	123.21(12)
C(21)-C(22)-Si(2)	173.52(12)
C(20)-C(19)-C(11)	170.21(14)
C(14)-C(13)-C(18)	121.56(12)
C(14)-C(13)-C(12)	119.85(11)
C(18)-C(13)-C(12)	118.57(11)
C(1)-C(2)-C(3)	120.41(13)
C(1)-C(2)-H(2)	119.8
C(3)-C(2)-H(2)	119.8
C(36)-C(35)-C(37)	110.32(11)
C(36)-C(35)-Si(2)	114.96(10)
C(37)-C(35)-Si(2)	111.52(9)
C(36)-C(35)-H(35)	106.5
C(37)-C(35)-H(35)	106.5
Si(2)-C(35)-H(35)	106.5
C(18)-C(17)-C(16)	120.49(12)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(43)-C(42)-C(41)	120.16(13)
C(43)-C(42)-H(42)	119.9
C(41)-C(42)-H(42)	119.9
C(28)-C(26)-C(27)	110.39(12)
C(28)-C(26)-Si(1)	112.29(10)
C(27)-C(26)-Si(1)	111.58(10)
C(28)-C(26)-H(26)	107.4
C(27)-C(26)-H(26)	107.4
Si(1)-C(26)-H(26)	107.4
C(15)-C(16)-C(17)	120.45(12)
C(15)-C(16)-H(16)	119.8
C(17)-C(16)-H(16)	119.8
C(13)-C(14)-C(9)	120.83(11)
C(13)-C(14)-C(21)	116.96(11)
C(9)-C(14)-C(21)	121.80(11)
C(3)-C(4)-C(5)	121.47(12)
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-H(4)	119.3
C(2)-C(1)-C(6)	121.20(13)
C(2)-C(1)-H(1)	119.4
C(6)-C(1)-H(1)	119.4
C(34)-C(32)-C(33)	109.80(13)
C(34)-C(32)-Si(2)	113.33(10)
C(33)-C(32)-Si(2)	113.02(10)
C(34)-C(32)-H(32)	106.7
C(33)-C(32)-H(32)	106.7
Si(2)-C(32)-H(32)	106.7
C(19)-C(20)-Si(1)	172.67(12)
C(39)-C(38)-C(40)	109.04(12)
C(39)-C(38)-Si(2)	113.79(10)
C(40)-C(38)-Si(2)	112.39(10)
C(39)-C(38)-H(38)	107.1
C(40)-C(38)-H(38)	107.1
Si(2)-C(38)-H(38)	107.1
C(17)-C(18)-C(13)	120.91(12)
C(17)-C(18)-H(18)	119.5
C(13)-C(18)-H(18)	119.5
C(45)-C(46)-C(41)	120.94(13)

C(45)-C(46)-H(46)	119.5	H(37B)-C(37)-H(37C)	109.5
C(41)-C(46)-H(46)	119.5	C(4)-C(3)-C(2)	120.19(13)
C(50)-C(49)-C(48)	120.11(13)	C(4)-C(3)-H(3)	119.9
C(50)-C(49)-H(49)	119.9	C(2)-C(3)-H(3)	119.9
C(48)-C(49)-H(49)	119.9	C(44)-C(43)-C(42)	120.43(13)
C(16)-C(15)-C(12)	121.04(12)	C(44)-C(43)-H(43)	119.8
C(16)-C(15)-H(15)	119.5	C(42)-C(43)-H(43)	119.8
C(12)-C(15)-H(15)	119.5	C(24)-C(23)-C(25)	110.63(12)
C(32)-C(34)-H(34A)	109.5	C(24)-C(23)-Si(1)	112.06(10)
C(32)-C(34)-H(34B)	109.5	C(25)-C(23)-Si(1)	113.89(11)
H(34A)-C(34)-H(34B)	109.5	C(24)-C(23)-H(23)	106.6
C(32)-C(34)-H(34C)	109.5	C(25)-C(23)-H(23)	106.6
H(34A)-C(34)-H(34C)	109.5	Si(1)-C(23)-H(23)	106.6
H(34B)-C(34)-H(34C)	109.5	C(44)-C(45)-C(46)	119.75(14)
C(38)-C(40)-H(40A)	109.5	C(44)-C(45)-H(45)	120.1
C(38)-C(40)-H(40B)	109.5	C(46)-C(45)-H(45)	120.1
H(40A)-C(40)-H(40B)	109.5	C(38)-C(39)-H(39A)	109.5
C(38)-C(40)-H(40C)	109.5	C(38)-C(39)-H(39B)	109.5
H(40A)-C(40)-H(40C)	109.5	H(39A)-C(39)-H(39B)	109.5
H(40B)-C(40)-H(40C)	109.5	C(38)-C(39)-H(39C)	109.5
C(51)-C(52)-C(47)	120.81(12)	H(39A)-C(39)-H(39C)	109.5
C(51)-C(52)-H(52)	119.6	H(39B)-C(39)-H(39C)	109.5
C(47)-C(52)-H(52)	119.6	C(23)-C(25)-H(25A)	109.5
C(32)-C(33)-H(33A)	109.5	C(23)-C(25)-H(25B)	109.5
C(32)-C(33)-H(33B)	109.5	H(25A)-C(25)-H(25B)	109.5
H(33A)-C(33)-H(33B)	109.5	C(23)-C(25)-H(25C)	109.5
C(32)-C(33)-H(33C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(33A)-C(33)-H(33C)	109.5	H(25B)-C(25)-H(25C)	109.5
H(33B)-C(33)-H(33C)	109.5	C(43)-C(44)-C(45)	119.98(13)
C(26)-C(27)-H(27A)	109.5	C(43)-C(44)-H(44)	120.0
C(26)-C(27)-H(27B)	109.5	C(45)-C(44)-H(44)	120.0
H(27A)-C(27)-H(27B)	109.5	C(29)-C(31)-H(31A)	109.5
C(26)-C(27)-H(27C)	109.5	C(29)-C(31)-H(31B)	109.5
H(27A)-C(27)-H(27C)	109.5	H(31A)-C(31)-H(31B)	109.5
H(27B)-C(27)-H(27C)	109.5	C(29)-C(31)-H(31C)	109.5
C(30)-C(29)-C(31)	110.58(15)	H(31A)-C(31)-H(31C)	109.5
C(30)-C(29)-Si(1)	112.64(11)	H(31B)-C(31)-H(31C)	109.5
C(31)-C(29)-Si(1)	111.56(10)	C(35)-C(36)-H(36A)	109.5
C(30)-C(29)-H(29)	107.3	C(35)-C(36)-H(36B)	109.5
C(31)-C(29)-H(29)	107.3	H(36A)-C(36)-H(36B)	109.5
Si(1)-C(29)-H(29)	107.3	C(35)-C(36)-H(36C)	109.5
C(26)-C(28)-H(28A)	109.5	H(36A)-C(36)-H(36C)	109.5
C(26)-C(28)-H(28B)	109.5	H(36B)-C(36)-H(36C)	109.5
H(28A)-C(28)-H(28B)	109.5	C(52)-C(51)-C(50)	120.05(13)
C(26)-C(28)-H(28C)	109.5	C(52)-C(51)-H(51)	120.0
H(28A)-C(28)-H(28C)	109.5	C(50)-C(51)-H(51)	120.0
H(28B)-C(28)-H(28C)	109.5	C(23)-C(24)-H(24A)	109.5
C(22)-C(21)-C(14)	169.95(14)	C(23)-C(24)-H(24B)	109.5
C(49)-C(50)-C(51)	119.64(13)	H(24A)-C(24)-H(24B)	109.5
C(49)-C(50)-H(50)	120.2	C(23)-C(24)-H(24C)	109.5
C(51)-C(50)-H(50)	120.2	H(24A)-C(24)-H(24C)	109.5
C(35)-C(37)-H(37A)	109.5	H(24B)-C(24)-H(24C)	109.5
C(35)-C(37)-H(37B)	109.5	C(29)-C(30)-H(30A)	109.5
H(37A)-C(37)-H(37B)	109.5	C(29)-C(30)-H(30B)	109.5
C(35)-C(37)-H(37C)	109.5	H(30A)-C(30)-H(30B)	109.5
H(37A)-C(37)-H(37C)	109.5	C(29)-C(30)-H(30C)	109.5

H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 9 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 4t. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	13(1)	17(1)	13(1)	-2(1)	1(1)	2(1)
Si(2)	11(1)	15(1)	16(1)	-1(1)	1(1)	1(1)
C(12)	13(1)	14(1)	15(1)	-1(1)	2(1)	-1(1)
C(7)	14(1)	14(1)	17(1)	0(1)	2(1)	0(1)
C(10)	12(1)	13(1)	15(1)	0(1)	2(1)	0(1)
C(11)	14(1)	14(1)	15(1)	-1(1)	2(1)	0(1)
C(6)	14(1)	14(1)	16(1)	1(1)	1(1)	0(1)
C(9)	11(1)	13(1)	15(1)	0(1)	3(1)	0(1)
C(8)	12(1)	13(1)	15(1)	-1(1)	2(1)	0(1)
C(48)	17(1)	19(1)	15(1)	0(1)	0(1)	0(1)
C(5)	15(1)	15(1)	16(1)	1(1)	2(1)	0(1)
C(47)	13(1)	15(1)	14(1)	-1(1)	-1(1)	3(1)
C(41)	19(1)	13(1)	15(1)	2(1)	3(1)	2(1)
C(22)	16(1)	17(1)	16(1)	0(1)	0(1)	1(1)
C(19)	18(1)	15(1)	15(1)	1(1)	1(1)	1(1)
C(13)	13(1)	13(1)	16(1)	0(1)	2(1)	-1(1)
C(2)	25(1)	24(1)	15(1)	1(1)	-2(1)	1(1)
C(35)	14(1)	18(1)	20(1)	-2(1)	-1(1)	2(1)
C(17)	18(1)	22(1)	18(1)	3(1)	-2(1)	1(1)
C(42)	19(1)	16(1)	17(1)	1(1)	1(1)	2(1)
C(26)	18(1)	24(1)	19(1)	-6(1)	0(1)	1(1)
C(16)	19(1)	23(1)	14(1)	2(1)	0(1)	-1(1)
C(14)	12(1)	14(1)	14(1)	-1(1)	1(1)	0(1)
C(4)	23(1)	14(1)	20(1)	1(1)	2(1)	2(1)
C(1)	18(1)	18(1)	16(1)	-1(1)	2(1)	1(1)
C(32)	14(1)	23(1)	19(1)	0(1)	-2(1)	1(1)
C(20)	21(1)	18(1)	15(1)	0(1)	1(1)	2(1)
C(38)	15(1)	19(1)	21(1)	0(1)	2(1)	0(1)
C(18)	16(1)	17(1)	18(1)	-1(1)	1(1)	1(1)
C(46)	21(1)	18(1)	20(1)	1(1)	0(1)	0(1)
C(49)	18(1)	28(1)	16(1)	-5(1)	0(1)	5(1)
C(15)	17(1)	20(1)	16(1)	-1(1)	2(1)	0(1)
C(34)	37(1)	33(1)	28(1)	-6(1)	-11(1)	-4(1)
C(40)	31(1)	17(1)	38(1)	2(1)	9(1)	0(1)
C(52)	17(1)	18(1)	19(1)	0(1)	2(1)	-1(1)
C(33)	27(1)	32(1)	22(1)	7(1)	-1(1)	1(1)
C(27)	40(1)	20(1)	32(1)	-5(1)	-9(1)	2(1)
C(29)	19(1)	24(1)	19(1)	0(1)	-3(1)	2(1)
C(28)	26(1)	34(1)	20(1)	-2(1)	-6(1)	-4(1)
C(21)	15(1)	16(1)	14(1)	1(1)	-1(1)	-1(1)
C(50)	24(1)	23(1)	23(1)	-9(1)	-4(1)	6(1)
C(37)	19(1)	22(1)	26(1)	-5(1)	0(1)	6(1)
C(3)	26(1)	20(1)	18(1)	5(1)	1(1)	4(1)
C(43)	27(1)	19(1)	20(1)	4(1)	4(1)	9(1)
C(23)	24(1)	21(1)	16(1)	0(1)	-1(1)	-1(1)
C(45)	32(1)	16(1)	22(1)	-1(1)	-2(1)	-3(1)
C(39)	34(1)	32(1)	21(1)	5(1)	2(1)	-9(1)
C(25)	40(1)	25(1)	34(1)	11(1)	9(1)	10(1)
C(44)	38(1)	14(1)	20(1)	-2(1)	1(1)	6(1)
C(31)	46(1)	30(1)	22(1)	3(1)	-13(1)	-8(1)
C(36)	22(1)	20(1)	32(1)	-3(1)	1(1)	-5(1)

C(51)	22(1)	16(1)	30(1)	-3(1)	-2(1)	-1(1)
C(24)	24(1)	36(1)	22(1)	3(1)	5(1)	-5(1)
C(30)	27(1)	85(2)	37(1)	0(1)	-6(1)	26(1)

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

	x	y	z	U(eq)
H(48)	6161	9324	5383	20
H(2)	10047	8289	6084	26
H(35)	3594	11192	5105	21
H(17)	5385	10242	2012	23
H(42)	11729	7245	3923	21
H(26)	13017	7090	1417	24
H(16)	7107	9550	1549	22
H(4)	10209	7008	4740	23
H(1)	8880	9174	5601	21
H(32)	847	10871	3860	22
H(38)	1075	9770	4709	22
H(18)	5228	10213	2955	20
H(46)	7656	7063	3446	24
H(49)	5545	10359	5878	25
H(15)	8631	8824	2032	21
H(34A)	700	10091	3108	49
H(34B)	915	9629	3656	49
H(34C)	2211	9757	3249	49
H(40A)	3630	8959	4628	43
H(40B)	2355	8916	4201	43
H(40C)	2149	8629	4815	43
H(52)	8735	10523	4424	21
H(33A)	3255	11046	3170	41
H(33B)	2520	11681	3511	41
H(33C)	1697	11304	3015	41
H(27A)	10881	6464	2095	46
H(27B)	12517	6265	2132	46
H(27C)	11636	6063	1594	46
H(29)	13405	7084	2876	25
H(28A)	10814	7016	965	40
H(28B)	11284	7839	1047	40
H(28C)	10113	7493	1439	40
H(50)	6540	11475	5653	28
H(37A)	1991	12135	5122	33
H(37B)	1139	11403	5011	33
H(37C)	1455	11948	4516	33
H(3)	10643	7180	5657	26
H(43)	12224	6136	3505	27
H(23)	13707	8980	2157	24
H(45)	8160	5953	3032	28
H(39A)	1904	9454	5582	43
H(39B)	2022	10310	5502	43
H(39C)	3398	9815	5453	43
H(25A)	12336	9711	1582	50
H(25B)	11362	9355	2044	50
H(25C)	11345	9040	1433	50
H(44)	10450	5492	3061	29
H(31A)	14745	7878	3416	49
H(31B)	13213	8213	3318	49
H(31C)	14529	8512	2978	49

H(36A)	3914	12092	4164	37
H(36B)	5162	11607	4407	37
H(36C)	4515	12251	4765	37
H(51)	8141	11555	4924	27
H(24A)	13580	8380	1080	41
H(24B)	14893	8301	1486	41
H(24C)	14473	9078	1249	41
H(30A)	15709	7700	2286	74
H(30B)	15004	6945	2124	74
H(30C)	15792	7031	2701	74

References

[1] Sheldrick, G. M. (1990). *Acta Cryst*. **A46**, 467-473.
[2] Sheldrick, G. M. (2008). *Acta Cryst*. **A64**, 112-122.
[3] Müller, P. (2009). *Crystallography Reviews*, **15**, 57-83.