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Supporting Information

Note Concerning Use of the SHELXTL-Plus Refinement Program.[1,2] This note is intended for the benefit of editors and referees who may not yet be familiar with the features of the new crystal structure refinement program SHELXTL-Plus and the new International Union of Crystallography CIF archive format.

CIF (S.R. Hall, F.H. Allen and I.D. Brown, *Acta Crystallogr.* **1991**, *A47*, 655-685) is an extremely flexible format for deposition of crystallographic data and is already the method of choice for the transmission of data to the Cambridge (organic) and Inorganic structural databases. At the end of a structure refinement with SHELXTL-Plus two archive files are produced: *.cif contains the crystal data, atomic coordinates, bond lengths etc., and *.fcf contains observed and calculated structure factors, both in CIF format. The .fcf file requires no further processing but the .cif file must be edited by the user to include items such as the crystal color that even the most sophisticated program cannot deduce from the diffraction data; this editing takes the form of replacing a question mark with the appropriate information. With a little practice it is perfectly possible for humans to read CIF files, but SHELX users are encouraged to use the program CIFTAB (supplied with SHELXTL-Plus) to produce more tasteful tables of crystal data, bonds and angles, structure factors etc. for referees.

All refinements with SHELXTL-Plus are performed with F-squared rather than F. This enables ALL data to be used rather than only data with F greater than a specified threshold, with the result that the experimental information is more fully exploited. For weakly scattering crystals this can appreciably improve the precision of the structure determination. However the R-index:

$$\omega R2 = (\Sigma [w(Fo^2-Fc^2)^2] / \Sigma [wFo^4])^{1/2}$$

that (in the absence of restraints) is minimized during the refinement is for statistical reasons about twice as large as the conventional index R1 (based on F):

$$R1 = \Sigma \, | \, |Fo| - |Fc| \, | / \Sigma |Fo|$$

and to make it worse an R-index based on ALL data is inevitably larger than one based only on data with F greater than a given threshold. Note that wR2 should not be confused with 'wR' or 'Rw' (both usually based on F). Since weighting schemes for F-squared and F refinements are quite different, it may not even be possible to calculate a meaningful Rw if the structure has been refined against F-squared.

For comparison with other (older) structures it is however very desirable to quote a conventional R-index (i.e. R1) calculated with a threshold of $F^2 > 2\sigma(F^2)$ [that effectively corresponds to $F > 4\sigma(F)$]. R1 also has the advantage that it is relatively insensitive to manipulation of the weighting scheme.

Some very observant referees have drawn authors' attention to the fact that they had not fixed any coordinates to define the origin in polar space groups. This is because SHELXTL-Plus automatically uses the mathematically superior 'polar axis restraints' proposed by H.D. Flack and D. Schwarzenbach (*Acta Crystallogr.* **1988**, *A44* , 499-506) that restrains a suitable weighted sum of atomic coordinates to be constant. Similarly the Flack 'racemic twinning parameter' is always estimated by the program where appropriate and reported in the .cif file (but not used in the calculation of F^2 unless specified by the user), so that it is unlikely that the user will fail to notice when it is necessary to determine the correct 'absolute structure' (H.D. Flack, *Acta Crystallogr.* **1983**, *A39*, 876-881).

SHELXL-93 uses scattering factors and absorption coefficients from the new Volume C of International Tables for Crystallography (1992), so there will be small discrepancies with values of μ etc. calculated by programs that still use older values.

SHELXL-93 estimates esds in bond lengths, angles and torsion angles from the full covariance matrix. The contributions of the cell esds are also included rigorously, except that the (usually unknown) correlations between the cell parameters are ignored unless defined by the crystal symmetry (e.g. the error in a cubic cell dimension affects the esd of a bond length but not of an angle). The esds in the equations of least-squares planes and in the distances of atoms from such planes are also calculated from the full matrix, but the (small) contributions of the cell esds

to these esds involve some approximations. Thus there will be discrepancies with esds calculated for checking purposes by programs that do not have access to the full covariance matrix.

References for X-Ray Material:

1) G.M. Sheldrick, *Acta Crystallogr.* **1990**, *A46*, 467-473.

2) SHELXTL-Plus V5.0, Siemens Industrial Automation, Inc., Madison, WI.

Table S1. Bond lengths for Bu_2Ph_2Tth.

atom	atom	[Å]	atom	atom	[Å]
S(1)	C(7)	1.724(8)	S(3)	C(26)	1.735(7)
S(1)	C(10)	1.730(7)	S(3)	C(23)	1.739(8)
S(2)	C(11)	1.725(7)	S(2)	C(22)	1.729(7)
C(7)	C(8)	1.358(10)	C(25)	C(26)	1.337(10)
C(8)	C(9)	1.401(10)	C(24)	C(25)	1.423(9)
C(9)	C(10)	1.356(10)	C(23)	C(24)	1.357(10)
C(10)	C(11)	1.468(10)	C(22)	C(23)	1.444(9)
C(11)	C(12)	1.362(10)	C(21)	C(22)	1.390(10)
C(12)	C(13)	1.552(10)	C(20)	C(21)	1.545(10)
C(13)	C(14)	1.490(11)	C(19)	C(20)	1.481(12)
C(14)	C(15)	1.529(11)	C(18)	C(19)	1.567(12)
C(15)	C(16)	1.510(14)	C(17)	C(18)	1.470(14)
C(1)	C(6)	1.372(10)	C(27)	C(32)	1.382(10)
C(1)	C(2)	1.389(11)	C(31)	C(32)	1.383(11)
C(2)	C(3)	1.359(12)	C(30)	C(31)	1.381(13)
C(3)	C(4)	1.353(12)	C(29)	C(30)	1.351(14)
C(4)	C(5)	1.380(11)	C(28)	C(29)	1.374(11)
C(5)	C(6)	1.370(10)	C(27)	C(28)	1.400(10)
C(6)	C(7)	1.478(9)	C(26)	C(27)	1.464(9)
C(12)	C(21)	1.439(9)			

Table S2. Bond angles [°] for Bu_2Ph_2Tth.

atom	atom	atom	[°]	atom	atom	atom	[°]
C(7)	S(1)	C(10)	93.2(3)	C(16)	C(15)	C(14)	111.4(9)
C(11)	S(2)	C(22)	92.2(3)	C(17)	C(18)	C(19)	113.9(11)
C(26)	S(3)	C(23)	93.1(3)	C(20)	C(19)	C(18)	110.0(10)
C(6)	C(1)	C(2)	120.7(8)	C(19)	C(20)	C(21)	112.0(8)
C(3)	C(2)	C(1)	119.7(8)	C(22)	C(21)	C(12)	112.0(7)
C(4)	C(3)	C(2)	119.7(8)	C(22)	C(21)	C(20)	124.2(6)
C(3)	C(4)	C(5)	121.3(9)	C(12)	C(21)	C(20)	123.6(7)
C(6)	C(5)	C(4)	119.8(8)	C(21)	C(22)	C(23)	132.1(7)
C(5)	C(6)	C(1)	118.8(7)	C(21)	C(22)	S(2)	111.0(5)
C(5)	C(6)	C(7)	120.8(7)	C(23)	C(22)	S(2)	116.1(5)
C(1)	C(6)	C(7)	120.4(7)	C(24)	C(23)	C(22)	127.6(7)
C(8)	C(7)	C(6)	129.5(7)	C(24)	C(23)	S(3)	108.8(5)
C(8)	C(7)	S(1)	109.6(5)	C(22)	C(23)	S(3)	123.5(5)
C(6)	C(7)	S(1)	120.9(5)	C(23)	C(24)	C(25)	114.2(7)
C(7)	C(8)	C(9)	113.6(7)	C(26)	C(25)	C(24)	114.0(6)
C(10)	C(9)	C(8)	114.6(7)	C(25)	C(26)	C(27)	129.3(6)
C(9)	C(10)	C(11)	128.5(6)	C(25)	C(26)	S(3)	109.9(5)
C(9)	C(10)	S(1)	109.0(5)	C(27)	C(26)	S(3)	120.9(5)
C(11)	C(10)	S(1)	122.5(5)	C(32)	C(27)	C(28)	117.8(7)
C(12)	C(11)	C(10)	131.6(6)	C(32)	C(27)	C(26)	122.2(7)
C(12)	C(11)	S(2)	111.9(5)	C(28)	C(27)	C(26)	120.1(7)
C(10)	C(11)	S(2)	116.1(5)	C(29)	C(28)	C(27)	120.7(8)
C(11)	C(12)	C(21)	112.8(7)	C(30)	C(29)	C(28)	120.3(9)
C(11)	C(12)	C(13)	124.0(7)	C(29)	C(30)	C(31)	121.0(9)
C(21)	C(12)	C(13)	122.9(7)	C(30)	C(31)	C(32)	118.9(9)

Table S2 (cont). Bond angles [°] for Bu_2Ph_2Tth.

atom	atom	atom	[°]	atom	atom	atom	[°]
C(14)	C(13)	C(12)	113.0(8)	C(27)	C(32)	C(31)	121.3(8)
C(13)	C(14)	C(15)	111.1(9)				

Table S3. Anisotropic displacement parameters [$Å^2 \times 10^3$] for Bu_2Ph_2Tth. Anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$.

	U11	U22	U33	U23	U13	U12
S(1)	78(1)	48(1)	59(1)	2(1)	14(1)	3(1)
S(2)	54(1)	54(1)	78(1)	13(1)	11(1)	4(1)
S(3)	86(1)	54(1)	69(1)	8(1)	30(1)	10(1)
C(1)	80(5)	66(5)	60(5)	8(4)	6(4)	3(4)
C(2)	73(5)	79(6)	80(6)	18(5)	7(5)	-8(4)
C(3)	81(5)	59(5)	90(7)	20(5)	-12(5)	7(4)
C(4)	94(6)	59(5)	89(7)	9(5)	11(5)	12(5)
C(5)	78(5)	64(5)	63(5)	7(4)	14(4)	9(4)
C(6)	48(4)	57(4)	58(4)	12(3)	-7(3)	5(3)
C(7)	48(4)	47(4)	65(4)	0(3)	-8(3)	-1(3)
C(8)	55(4)	63(4)	60(5)	16(4)	19(4)	6(3)
C(9)	68(5)	48(4)	70(5)	3(4)	13(4)	10(4)
C(10)	61(4)	46(4)	53(4)	5(3)	6(3)	4(3)
C(11)	65(4)	51(4)	59(4)	-1(4)	3(4)	0(3)
C(12)	72(5)	59(5)	77(5)	3(4)	10(4)	6(4)
C(13)	79(6)	74(5)	82(6)	1(5)	-2(5)	3(5)
C(14)	95(7)	79(6)	88(7)	4(5)	12(5)	-3(5)
C(15)	82(7)	93(7)	142(11)	-19(8)	-12(7)	41(6)
C(16)	110(9)	99(7)	167(12)	-33(9)	1(9)	46(7)
C(17)	212(16)	96(9)	144(12)	2(9)	96(13)	-19(9)
C(18)	111(9)	120(9)	96(8)	26(8)	42(8)	-10(7)
C(19)	142(10)	79(7)	86(7)	-1(6)	-10(7)	0(7)
C(20)	69(5)	74(6)	85(6)	0(5)	-9(5)	11(4)
C(21)	69(5)	53(4)	71(5)	3(4)	14(4)	-1(4)

Table S3 (cont). Anisotropic displacement parameters [$Å^2 \times 10^3$] for Bu_2Ph_2Tth. Anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$.

	U11	U22	U33	U23	U13	U12
C(22)	66(4)	47(4)	55(4)	-2(3)	11(4)	-1(3)
C(23)	57(4)	51(4)	59(4)	-3(3)	3(4)	4(3)
C(24)	65(5)	53(4)	60(4)	10(3)	11(4)	-4(4)
C(25)	70(5)	46(4)	60(5)	-3(3)	6(4)	9(3)
C(26)	51(4)	52(4)	49(4)	-2(3)	-1(3)	-6(3)
C(27)	53(4)	48(4)	60(4)	7(3)	-10(4)	-3(3)
C(28)	77(5)	65(5)	67(6)	7(4)	0(4)	0(4)
C(29)	92(6)	55(5)	101(8)	15(5)	-8(6)	1(4)
C(30)	93(7)	80(6)	91(7)	25(6)	-13(6)	-18(6)
C(31)	68(5)	104(7)	58(5)	22(5)	7(4)	-28(5)
C(32)	67(5)	65(5)	53(5)	10(4)	-3(4)	-18(4)

Table S4. Torsion angles [°] for Bu_2Ph_2Tth.

atom	atom	atom	atom	[°]	atom	atom	atom	atom	[°]
C(1)	C(2)	C(3)	C(4)	1.5(13)	C(11)	C(12)	C(21)	C(22)	2.0(10)
C(2)	C(3)	C(4)	C(5)	-0.2(13)	C(13)	C(12)	C(21)	C(22)	176.3(8)
C(3)	C(4)	C(5)	C(6)	-0.9(14)	C(11)	C(12)	C(21)	C(20)	-174.2(8)
C(4)	C(5)	C(6)	C(1)	0.5(12)	C(13)	C(12)	C(21)	C(20)	0.0(12)
C(6)	C(1)	C(2)	C(3)	-1.9(12)	C(19)	C(20)	C(21)	C(22)	92.6(11)
C(4)	C(5)	C(6)	C(7)	-179.9(7)	C(19)	C(20)	C(21)	C(12)	-91.5(11)
C(2)	C(1)	C(6)	C(5)	0.8(11)	C(12)	C(21)	C(22)	C(23)	-172.4(8)
C(2)	C(1)	C(6)	C(7)	-178.8(7)	C(20)	C(21)	C(22)	C(23)	4(2)
C(5)	C(6)	C(7)	C(8)	-178.5(8)	C(12)	C(21)	C(22)	S(2)	-3.1(9)
C(1)	C(6)	C(7)	C(8)	1.1(11)	C(20)	C(21)	C(22)	S(2)	173.1(6)
C(5)	C(6)	C(7)	S(1)	1.0(10)	C(11)	S(2)	C(22)	C(21)	2.7(6)
C(1)	C(6)	C(7)	S(1)	-179.4(6)	C(11)	S(2)	C(22)	C(23)	173.9(6)
C(10)	S(1)	C(7)	C(8)	-2.1(6)	C(21)	C(22)	C(23)	C(24)	148.7(9)
C(10)	S(1)	C(7)	C(6)	178.3(6)	S(2)	C(22)	C(23)	C(24)	-20.2(11)
C(6)	C(7)	C(8)	C(9)	-177.6(7)	C(21)	C(22)	C(23)	S(3)	-30.9(13)
S(1)	C(7)	C(8)	C(9)	2.9(8)	S(2)	C(22)	C(23)	S(3)	160.3(4)
C(7)	C(8)	C(9)	C(10)	-2.4(10)	C(26)	S(3)	C(23)	C(24)	-0.5(6)
C(8)	C(9)	C(10)	C(11)	-178.3(7)	C(26)	S(3)	C(23)	C(22)	179.1(7)
C(8)	C(9)	C(10)	S(1)	0.7(9)	C(22)	C(23)	C(24)	C(25)	-179.2(7)
C(7)	S(1)	C(10)	C(9)	0.8(6)	S(3)	C(23)	C(24)	C(25)	0.4(8)
C(7)	S(1)	C(10)	C(11)	179.9(6)	C(23)	C(24)	C(25)	C(26)	0.0(10)
C(9)	C(10)	C(11)	C(12)	-142.6(9)	C(24)	C(25)	C(26)	C(27)	179.0(7)
S(1)	C(10)	C(11)	C(12)	38.5(12)	C(24)	C(25)	C(26)	S(3)	-0.4(8)
C(9)	C(10)	C(11)	S(2)	29.2(11)	C(23)	S(3)	C(26)	C(25)	0.5(6)
S(1)	C(10)	C(11)	S(2)	-149.6(5)	C(23)	S(3)	C(26)	C(27)	-178.9(6)

Table S4. Torsion angles [°] for Bu_2Ph_2Tth.

atom	atom	atom	atom	[°]	atom	atom	atom	atom	[°]
C(22)	S(2)	C(11)	C(12)	-1.6(7)	C(25)	C(26)	C(27)	C(32)	171.5(7)
C(22)	S(2)	C(11)	C(10)	-175.0(6)	S(3)	C(26)	C(27)	C(32)	-9.3(9)
C(10)	C(11)	C(12)	C(21)	172.2(8)	C(25)	C(26)	C(27)	C(28)	-8.9(11)
S(2)	C(11)	C(12)	C(21)	0.0(9)	S(3)	C(26)	C(27)	C(28)	170.4(6)
C(10)	C(11)	C(12)	C(13)	-2.0(14)	C(32)	C(27)	C(28)	C(29)	0.2(11)
S(2)	C(11)	C(12)	C(13)	-174.1(7)	C(26)	C(27)	C(28)	C(29)	-179.4(7)
C(11)	C(12)	C(13)	C(14)	-95.2(10)	C(27)	C(28)	C(29)	C(30)	0.0(13)
C(21)	C(12)	C(13)	C(14)	91.3(10)	C(28)	C(29)	C(30)	C(31)	0.6(14)
C(12)	C(13)	C(14)	C(15)	177.5(9)	C(29)	C(30)	C(31)	C(32)	-1.5(14)
C(13)	C(14)	C(15)	C(16)	179.2(11)	C(28)	C(27)	C(32)	C(31)	-1.2(11)
C(17)	C(18)	C(19)	C(20)	78(2)	C(26)	C(27)	C(32)	C(31)	178.5(7)
C(18)	C(19)	C(20)	C(21)	177.6(8)	C(30)	C(31)	C(32)	C(27)	1.8(12)

Table S5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$ x 10^3] for Bu_2Ph_2Tth.

	x	y	z	U(eq)
H(1)	1919(5)	4235(3)	-3417(15)	86(28)
H(2)	1930(5)	4969(3)	-4348(17)	58(20)
H(3)	1231(5)	5461(3)	-2051(17)	79(24)
H(4)	588(6)	5230(3)	1216(17)	68(23)
H(5)	618(5)	4506(2)	2248(15)	51(18)
H(8)	1982(4)	3519(2)	-2300(14)	76(23)
H(9)	1720(5)	2823(2)	-516(14)	85(27)
H(13A)	-707(6)	3165(3)	3564(16)	81(26)
H(13B)	-1221(6)	2827(3)	5047(16)	85(27)
H(14A)	-109(6)	3463(3)	6875(17)	113(35)
H(14B)	-662(6)	3135(3)	8326(17)	227(75)
H(15A)	-1402(7)	3787(4)	5496(23)	120(44)
H(15B)	-1958(7)	3456(4)	6916(23)	124(42)
H(16A)	-1878(8)	4120(4)	8829(28)	58(18)
H(16B)	-859(8)	4090(4)	8858(28)	593(276)
H(16C)	-1415(8)	3759(4)	10277(28)	398(173)
H(17A)	-1973(13)	1445(4)	12157(30)	227(80)
H(17B)	-955(13)	1459(4)	12310(30)	438(212)
H(17C)	-1410(13)	1377(4)	9967(30)	111(37)
H(18A)	-1521(8)	2152(4)	12403(22)	175(60)
H(18B)	-1976(8)	2071(4)	10062(22)	120(44)
H(19A)	-596(8)	2490(4)	9907(17)	147(46)
H(19B)	-121(8)	2045(4)	10347(17)	164(54)
H(20A)	-1226(5)	2195(3)	6641(15)	52(19)

Table S5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$ x 10^3] for Bu_2Ph_2Tth.

	x	y	z	U(eq)
H(20B)	-715(5)	1760(3)	7063(15)	108(33)
H(24)	1915(5)	1415(2)	3405(13)	51(18)
H(25)	2099(5)	685(2)	4951(13)	30(14)
H(28)	1877(5)	30(2)	6701(15)	48(18)
H(29)	1783(6)	-598(3)	8810(18)	94(28)
H(30)	1110(7)	-594(3)	12245(19)	101(31)
H(31)	483(5)	36(3)	13637(16)	42(15)
H(32)	603(5)	675(3)	11582(13)	61(22)

Table S6. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $[Bu_2Ph_2Tth]PF_6$ at 106 K. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
S(1A)	294(1)	8252(1)	10454(2)	24(1)	1
S(2A)	1178(1)	7341(1)	7683(2)	22(1)	1
S(3A)	2114(1)	8223(1)	5131(2)	23(1)	1
C(1A)	-514(2)	7152(3)	12610(6)	28(1)	1
C(2A)	-826(2)	7253(3)	13506(7)	32(1)	1
C(3A)	-928(2)	7885(3)	13969(7)	35(2)	1
C(4A)	-713(2)	8427(3)	13492(7)	35(2)	1
C(5A)	-402(2)	8335(3)	12599(6)	28(1)	1
C(6A)	-296(1)	7697(3)	12095(6)	28(1)	1
C(7A)	29(1)	7591(2)	11156(6)	25(1)	1
C(8A)	175(2)	6993(2)	10623(6)	24(1)	1
C(9A)	488(1)	7060(2)	9705(6)	22(1)	1
C(10A)	591(1)	7728(3)	9447(6)	24(1)	1
C(11A)	903(1)	7945(2)	8557(6)	21(1)	1
C(12A)	1042(1)	8590(2)	8246(6)	24(1)	1
C(13A)	861(2)	9224(3)	8768(7)	34(1)	1
C(14A)	1030(2)	9469(3)	10332(7)	47(2)	0.71
C(15A)	905(3)	10214(5)	10579(14)	54(3)	0.71
C(16A)	468(3)	10301(4)	10548(13)	58(3)	0.71
C(33A)	1030(2)	9469(3)	10332(7)	47(2)	0.29
C(34A)	776(7)	9925(10)	11263(24)	46(6)	0.29
C(35A)	816(9)	10542(11)	10275(33)	57(8)	0.29
C(17A)	1981(2)	10138(4)	4554(9)	61(2)	1

Table S6. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $[Bu_2Ph_2Tth]PF_6$ at 106 K. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
C(18A)	1560(2)	10163(3)	4898(9)	50(2)	1
C(19A)	1396(2)	9482(3)	5310(7)	39(2)	1
C(20A)	1566(1)	9212(3)	6846(6)	28(1)	1
C(21A)	1369(1)	8578(2)	7359(6)	26(1)	1
C(22A)	1480(1)	7929(2)	6927(6)	24(1)	1
C(23A)	1788(1)	7707(2)	6022(6)	22(1)	1
C(24A)	1866(1)	7047(2)	5652(6)	23(1)	1
C(25A)	2172(1)	6964(3)	4706(6)	24(1)	1
C(26A)	2341(1)	7560(3)	4288(6)	23(1)	1
C(27A)	2670(1)	7658(3)	3317(6)	26(1)	1
C(28A)	2871(2)	7108(3)	2754(6)	29(1)	1
C(29A)	3184(2)	7195(3)	1830(7)	36(2)	1
C(30A)	3310(2)	7835(3)	1492(6)	34(1)	1
C(31A)	3121(2)	8380(3)	2052(7)	34(2)	1
C(32A)	2802(1)	8298(3)	2969(6)	31(1)	1
S(1B)	2192(1)	6723(1)	-427(2)	28(1)	1
S(2B)	1313(1)	7646(1)	2340(2)	22(1)	1
S(3B)	381(1)	6755(1)	4907(2)	25(1)	1
C(1B)	3009(2)	7790(3)	-2574(7)	37(2)	1
C(2B)	3318(2)	7685(3)	-3517(7)	38(2)	1
C(3B)	3412(2)	7045(3)	-3966(7)	43(2)	1
C(4B)	3189(2)	6514(3)	-3515(6)	35(2)	1
C(5B)	2877(2)	6607(3)	-2582(6)	34(2)	1

Table S6. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $[Bu_2Ph_2Tth]PF_6$ at 106 K. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
C(6B)	2782(1)	7256(3)	-2122(6)	26(1)	1
C(7B)	2459(2)	7371(3)	-1139(6)	27(1)	1
C(8B)	2323(2)	7971(3)	-616(6)	27(1)	1
C(9B)	2009(2)	7907(3)	331(6)	29(1)	1
C(10B)	1898(1)	7255(2)	563(6)	22(1)	1
C(11B)	1587(1)	7046(2)	1447(6)	22(1)	1
C(12B)	1445(1)	6402(2)	1776(6)	24(1)	1
C(13B)	1621(1)	5761(3)	1234(6)	30(1)	1
C(14B)	1448(2)	5528(3)	-324(9)	62(2)	0.68
C(15B)	1570(4)	4768(6)	-515(14)	61(4)	0.68
C(16B)	1997(4)	4717(6)	-649(12)	70(4)	0.68
C(33B)	1448(2)	5528(3)	-324(9)	62(2)	0.32
C(34B)	1668(6)	4999(9)	-1190(22)	41(5)	0.32
C(35B)	1475(11)	4402(12)	-419(40)	105(12)	0.32
C(17B)	536(2)	4830(4)	5582(10)	65(2)	1
C(18B)	949(2)	4823(3)	5152(9)	53(2)	1
C(19B)	1108(2)	5516(3)	4731(7)	41(2)	1
C(20B)	926(2)	5783(3)	3178(7)	32(1)	1
C(21B)	1121(1)	6407(2)	2669(6)	26(1)	1
C(22B)	1008(1)	7058(2)	3089(6)	22(1)	1
C(23B)	703(1)	7282(2)	4010(6)	23(1)	1
C(24B)	617(1)	7943(2)	4385(6)	22(1)	1
C(25B)	309(2)	8014(3)	5314(6)	26(1)	1

Table S6. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $[Bu_2Ph_2Tth]PF_6$ at 106 K. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
C(26B)	142(1)	7405(2)	5718(6)	21(1)	1
C(27B)	-186(1)	7304(2)	6685(5)	22(1)	1
C(28B)	-390(2)	7842(3)	7272(6)	27(1)	1
C(29B)	-702(2)	7745(3)	8158(6)	32(1)	1
C(30B)	-816(2)	7107(3)	8537(6)	32(1)	1
C(31B)	-613(2)	6567(3)	7980(6)	29(1)	1
C(32B)	-301(2)	6660(3)	7092(6)	26(1)	1
P(1)	2459(1)	4967(1)	4941(2)	34(1)	1
F(1A)	2181(1)	4881(2)	3424(6)	87(2)	1
F(1B)	2743(1)	4433(2)	4248(5)	64(1)	1
F(1C)	2741(1)	5052(2)	6417(5)	66(1)	1
F(1D)	2173(1)	5500(2)	5629(6)	65(1)	1
F(1E)	2235(1)	4380(2)	5759(5)	54(1)	1
F(1F)	2681(1)	5556(2)	4104(4)	51(1)	1
P(2)	0	5000	0	28(1)	1
F(2A)	214(1)	4883(2)	1641(4)	49(1)	1
F(2B)	319(1)	5540(2)	-416(4)	44(1)	1
F(2C)	263(1)	4434(2)	-733(4)	43(1)	1
P(3)	0	0	5000	27(1)	1
F(3A)	275(1)	-509(2)	4175(4)	48(1)	1
F(3B)	318(1)	96(2)	6353(5)	68(1)	1
F(3C)	177(1)	597(2)	4064(5)	53(1)	1

Table S7. Bond lengths [Å] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	(Å)	atom	atom	(Å)
S(1A)	C(10A)	1.739(5)	S(1B)	C(7B)	1.731(5)
S(1A)	C(7A)	1.742(5)	S(1B)	C(10B)	1.733(5)
S(2A)	C(22A)	1.728(5)	S(2B)	C(22B)	1.733(5)
S(2A)	C(11A)	1.741(5)	S(2B)	C(11B)	1.742(5)
S(3A)	C(26A)	1.731(5)	S(3B)	C(26B)	1.718(5)
S(3A)	C(23A)	1.741(5)	S(3B)	C(23B)	1.750(5)
C(1A)	C(2A)	1.374(7)	C(1B)	C(2B)	1.391(7)
C(1A)	C(6A)	1.416(7)	C(1B)	C(6B)	1.398(8)
C(2A)	C(3A)	1.388(8)	C(2B)	C(3B)	1.392(8)
C(3A)	C(4A)	1.397(8)	C(3B)	C(4B)	1.385(8)
C(4A)	C(5A)	1.366(7)	C(4B)	C(5B)	1.393(7)
C(5A)	C(6A)	1.414(7)	C(5B)	C(6B)	1.411(7)
C(6A)	C(7A)	1.433(7)	C(6B)	C(7B)	1.456(7)
C(7A)	C(8A)	1.395(7)	C(7B)	C(8B)	1.382(7)
C(8A)	C(9A)	1.379(7)	C(8B)	C(9B)	1.397(7)
C(9A)	C(10A)	1.414(7)	C(9B)	C(10B)	1.388(7)
C(10A)	C(11A)	1.423(7)	C(10B)	C(11B)	1.413(7)
C(11A)	C(12A)	1.418(7)	C(11B)	C(12B)	1.422(7)
C(12A)	C(21A)	1.397(7)	C(12B)	C(21B)	1.391(7)
C(12A)	C(13A)	1.502(7)	C(12B)	C(13B)	1.515(6)
C(13A)	C(33A)	1.529(7)	C(13B)	C(33B)	1.523(8)
C(13A)	C(14A)	1.529(7)	C(13B)	C(14B)	1.523(8)
C(14A)	C(15A)	1.582(11)	C(14B)	C(15B)	1.600(13)
C(15A)	C(16A)	1.517(14)	C(15B)	C(16B)	1.49(2)
C(33A)	C(34A)	1.53(2)	C(33B)	C(34B)	1.53(2)

Table S7. Bond lengths [Å] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	(Å)	atom	atom	(Å)
C(34A)	C(35A)	1.52(3)	C(34B)	C(35B)	1.54(3)
C(17A)	C(18A)	1.500(9)	C(17B)	C(18B)	1.492(9)
C(18A)	C(19A)	1.533(8)	C(18B)	C(19B)	1.551(8)
C(19A)	C(20A)	1.528(7)	C(19B)	C(20B)	1.552(7)
C(20A)	C(21A)	1.525(7)	C(20B)	C(21B)	1.502(7)
C(21A)	C(22A)	1.421(7)	C(21B)	C(22B)	1.423(7)
C(22A)	C(23A)	1.425(7)	C(22B)	C(23B)	1.423(7)
C(23A)	C(24A)	1.398(7)	C(23B)	C(24B)	1.407(7)
C(24A)	C(25A)	1.379(7)	C(24B)	C(25B)	1.373(7)
C(25A)	C(26A)	1.392(7)	C(25B)	C(26B)	1.408(7)
C(26A)	C(27A)	1.459(7)	C(26B)	C(27B)	1.455(7)
C(27A)	C(32A)	1.406(7)	C(27B)	C(28B)	1.404(7)
C(27A)	C(28A)	1.409(7)	C(27B)	C(32B)	1.410(7)
C(28A)	C(29A)	1.386(7)	C(28B)	C(29B)	1.365(7)
C(29A)	C(30A)	1.399(8)	C(29B)	C(30B)	1.390(8)
C(30A)	C(31A)	1.380(8)	C(30B)	C(31B)	1.394(8)
C(31A)	C(32A)	1.399(7)	C(31B)	C(32B)	1.365(7)
P(1)	F(1C)	1.577(4)	P(1)	F(1D)	1.598(4)
P(1)	F(1B)	1.593(4)	P(1)	F(1E)	1.597(4)
P(1)	F(1A)	1.597(4)	P(1)	F(1F)	1.607(4)
P(2)	F(2A)	1.586(3)	P(2)	F(2B)	1.603(3)
P(2)	F(2A)[1]	1.586(3)	P(2)	F(2C)	1.609(3)
P(2)	F(2B)[1]	1.603(3)	P(2)	F(2C)[1]	1.609(3)
P(3)	F(3B)[2]	1.577(4)	P(3)	F(3C)	1.591(3)
P(3)	F(3B)	1.577(4)	P(3)	F(3A)	1.591(3)

Table S7. Bond lengths [Å] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	(Å)	atom	atom	(Å)
P(3)	F(3C)^2	1.591(3)	P(3)	F(3A)^2	1.591(3)

Symmetry transformations used to generate equivalent atoms: 1) -x,-y+1,-z; 2) -x,-y,-z+1

Table S8. Bond angles [°] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	atom	angle (°)	atom	atom	atom	angle (°)
C(1A)	C(2A)	C(3A)	121.1(5)	C(1A)	C(6A)	C(7A)	120.4(5)
C(2A)	C(3A)	C(4A)	119.2(5)	C(8A)	C(7A)	C(6A)	128.4(5)
C(5A)	C(4A)	C(3A)	120.3(5)	C(8A)	C(7A)	S(1A)	109.9(4)
C(4A)	C(5A)	C(6A)	121.4(5)	C(6A)	C(7A)	S(1A)	121.6(4)
C(5A)	C(6A)	C(1A)	117.4(5)	C(9A)	C(8A)	C(7A)	114.4(4)
C(5A)	C(6A)	C(7A)	122.2(5)	C(8A)	C(9A)	C(10A)	113.3(5)
C(10A)	S(1A)	C(7A)	92.5(2)	C(26A)	S(3A)	C(23A)	92.4(2)
C(22A)	S(2A)	C(11A)	92.1(2)	C(2A)	C(1A)	C(6A)	120.5(5)
C(9A)	C(10A)	C(11A)	125.7(5)	C(12A)	C(13A)	C(14A)	113.4(5)
C(9A)	C(10A)	S(1A)	109.8(4)	C(13A)	C(14A)	C(15A)	109.4(6)
C(11A)	C(10A)	S(1A)	124.4(4)	C(16A)	C(15A)	C(14A)	112.7(8)
C(12A)	C(11A)	C(10A)	131.2(4)	C(34A)	C(33A)	C(13A)	117.3(9)
C(12A)	C(11A)	S(2A)	111.2(4)	C(35A)	C(34A)	C(33A)	97(2)
C(10A)	C(11A)	S(2A)	117.6(4)	C(17A)	C(18A)	C(19A)	112.9(6)
C(21A)	C(12A)	C(11A)	112.3(4)	C(20A)	C(19A)	C(18A)	113.1(5)
C(21A)	C(12A)	C(13A)	122.6(5)	C(21A)	C(20A)	C(19A)	113.3(4)
C(11A)	C(12A)	C(13A)	125.1(5)	C(12A)	C(21A)	C(22A)	113.4(4)
C(12A)	C(13A)	C(33A)	113.4(5)	C(12A)	C(21A)	C(20A)	122.0(4)
C(24A)	C(23A)	S(3A)	109.3(4)	C(22A)	C(21A)	C(20A)	124.5(5)
C(22A)	C(23A)	S(3A)	124.9(4)	C(21A)	C(22A)	C(23A)	130.8(5)
C(25A)	C(24A)	C(23A)	114.5(5)	C(21A)	C(22A)	S(2A)	110.9(4)
C(24A)	C(25A)	C(26A)	113.2(5)	C(23A)	C(22A)	S(2A)	118.3(4)
C(25A)	C(26A)	C(27A)	128.0(5)	C(24A)	C(23A)	C(22A)	125.7(5)
C(25A)	C(26A)	S(3A)	110.6(4)	C(32A)	C(27A)	C(28A)	118.6(5)
C(27A)	C(26A)	S(3A)	121.3(4)	C(32A)	C(27A)	C(26A)	121.2(5)

Table S8. Bond angles [°] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	atom	angle (°)	atom	atom	atom	angle (°)
C(28A)	C(29A)	C(30A)	119.9(5)	C(28A)	C(27A)	C(26A)	120.2(5)
C(31A)	C(30A)	C(29A)	120.2(5)	C(29A)	C(28A)	C(27A)	120.7(5)
C(30A)	C(31A)	C(32A)	120.4(5)	C(31A)	C(32A)	C(27A)	120.1(5)
C(7B)	S(1B)	C(10B)	92.5(2)	C(5B)	C(6B)	C(7B)	120.4(5)
C(22B)	S(2B)	C(11B)	92.5(2)	C(8B)	C(7B)	C(6B)	127.8(5)
C(26B)	S(3B)	C(23B)	92.6(2)	C(8B)	C(7B)	S(1B)	110.5(4)
C(2B)	C(1B)	C(6B)	120.2(6)	C(6B)	C(7B)	S(1B)	121.7(4)
C(1B)	C(2B)	C(3B)	120.0(6)	C(7B)	C(8B)	C(9B)	113.3(5)
C(4B)	C(3B)	C(2B)	119.9(6)	C(10B)	C(9B)	C(8B)	113.7(5)
C(3B)	C(4B)	C(5B)	121.1(6)	C(9B)	C(10B)	C(11B)	125.8(5)
C(4B)	C(5B)	C(6B)	119.0(5)	C(9B)	C(10B)	S(1B)	109.9(4)
C(1B)	C(6B)	C(5B)	119.7(5)	C(11B)	C(10B)	S(1B)	124.3(4)
C(1B)	C(6B)	C(7B)	119.8(5)	C(10B)	C(11B)	C(12B)	131.3(4)
C(11B)	C(12B)	C(13B)	124.7(4)	C(10B)	C(11B)	S(2B)	118.5(4)
C(12B)	C(13B)	C(33B)	113.1(4)	C(12B)	C(11B)	S(2B)	110.2(3)
C(12B)	C(13B)	C(14B)	113.1(4)	C(13B)	C(14B)	C(15B)	107.0(6)
C(13B)	C(33B)	C(34B)	117.8(9)	C(16B)	C(15B)	C(14B)	110.0(9)
C(33B)	C(34B)	C(35B)	96(2)	C(21B)	C(12B)	C(11B)	113.6(4)
C(17B)	C(18B)	C(19B)	113.9(6)	C(21B)	C(12B)	C(13B)	121.6(5)
C(20B)	C(19B)	C(18B)	112.6(5)	C(21B)	C(20B)	C(19B)	112.2(4)
C(12B)	C(21B)	C(22B)	112.7(4)	C(23B)	C(22B)	C(21B)	130.9(5)
C(12B)	C(21B)	C(20B)	122.8(5)	C(23B)	C(22B)	S(2B)	118.1(4)
C(22B)	C(21B)	C(20B)	124.5(5)	C(21B)	C(22B)	S(2B)	110.9(4)
C(24B)	C(23B)	C(22B)	126.8(5)	C(28B)	C(27B)	C(32B)	117.9(5)
C(24B)	C(23B)	S(3B)	109.1(4)	C(28B)	C(27B)	C(26B)	121.3(4)

Table S8. Bond angles [°] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	atom	angle (°)	atom	atom	atom	angle (°)
C(22B)	C(23B)	S(3B)	124.1(4)	C(32B)	C(27B)	C(26B)	120.8(5)
C(25B)	C(24B)	C(23B)	114.4(4)	C(29B)	C(28B)	C(27B)	121.2(5)
C(24B)	C(25B)	C(26B)	113.2(5)	C(28B)	C(29B)	C(30B)	120.3(5)
C(25B)	C(26B)	C(27B)	127.3(5)	C(29B)	C(30B)	C(31B)	119.3(5)
C(25B)	C(26B)	S(3B)	110.7(4)	C(32B)	C(31B)	C(30B)	120.7(5)
C(27B)	C(26B)	S(3B)	122.0(4)	C(31B)	C(32B)	C(27B)	120.5(5)
F(1C)	P(1)	F(1B)	90.8(2)	F(2B)[1]	P(2)	F(2C)	90.8(2)
F(1C)	P(1)	F(1A)	178.9(3)	F(2B)	P(2)	F(2C)	89.2(2)
F(1B)	P(1)	F(1A)	88.5(3)	F(2A)	P(2)	F(2C)[1]	90.0(2)
F(1C)	P(1)	F(1D)	89.5(2)	F(2A)[1]	P(2)	F(2C)[1]	90.0(2)
F(1B)	P(1)	F(1D)	179.7(2)	F(2B)[1]	P(2)	F(2C)[1]	89.2(2)
F(1A)	P(1)	F(1D)	91.2(3)	F(2B)	P(2)	F(2C)[1]	90.8(2)
F(1C)	P(1)	F(1E)	90.8(2)	F(2C)	P(2)	F(2C)[1]	180.0
F(1B)	P(1)	F(1E)	89.2(2)	F(3B)[2]	P(3)	F(3B)	180.0
F(1A)	P(1)	F(1E)	90.0(3)	F(3B)[2]	P(3)	F(3C)[2]	90.9(2)
F(1D)	P(1)	F(1E)	90.6(2)	F(3B)	P(3)	F(3C)[2]	89.1(2)
F(1C)	P(1)	F(1F)	89.8(2)	F(3B)[2]	P(3)	F(3C)	89.1(2)
F(1B)	P(1)	F(1F)	90.8(2)	F(3B)	P(3)	F(3C)	90.9(2)
F(1A)	P(1)	F(1F)	89.4(2)	F(3C)[2]	P(3)	F(3C)	180.0
F(1D)	P(1)	F(1F)	89.3(2)	F(3B)[2]	P(3)	F(3A)	89.8(2)
F(1E)	P(1)	F(1F)	179.4(2)	F(3B)	P(3)	F(3A)	90.2(2)
F(2A)	P(2)	F(2A)[1]	180.0	F(3C)[2]	P(3)	F(3A)	89.6(2)
F(2A)	P(2)	F(2B)[1]	89.6(2)	F(3C)	P(3)	F(3A)	90.4(2)
F(2A)[1]	P(2)	F(2B)[1]	90.4(2)	F(3B)[2]	P(3)	F(3A)[2]	90.2(2)
F(2A)	P(2)	F(2B)	90.4(2)	F(3B)	P(3)	F(3A)[2]	89.8(2)

Table S8. Bond angles [°] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	atom	angle (°)	atom	atom	atom	angle (°)
F(2A)[1]	P(2)	F(2B)	89.6(2)	F(3C)[2]	P(3)	F(3A)[2]	90.5(2)
F(2B)[1]	P(2)	F(2B)	180.0	F(3C)	P(3)	F(3A)[2]	89.5(2)
F(2A)	P(2)	F(2C)	90.0(2)	F(3A)	P(3)	F(3A)[2]	180.0
F(2A)[1]	P(2)	F(2C)	90.0(2)				

Symmetry transformations used to generate equivalent atoms:

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

Table S9. Anisotropic displacement parameters [$Å^2$ x 10^3] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

Anisotropic displacement factor exponent is: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

atom	U11	U22	U33	U23	U13	U12
S(1A)	18(1)	24(1)	31(1)	0(1)	4(1)	1(1)
S(2A)	19(1)	19(1)	28(1)	-2(1)	-1(1)	1(1)
S(3A)	18(1)	22(1)	31(1)	-1(1)	5(1)	0(1)
C(1A)	25(3)	25(3)	32(3)	14(2)	-8(3)	-3(2)
C(2A)	26(3)	36(3)	34(3)	5(3)	-4(3)	-6(3)
C(3A)	18(3)	49(4)	38(4)	2(3)	1(3)	-4(3)
C(4A)	18(3)	40(4)	48(4)	-8(3)	-2(3)	1(2)
C(5A)	26(3)	23(3)	35(3)	-2(2)	-4(3)	-4(2)
C(6A)	17(3)	32(3)	33(3)	3(3)	-7(2)	-5(2)
C(7A)	12(3)	22(3)	39(4)	6(2)	-12(2)	-3(2)
C(8A)	28(3)	19(3)	25(3)	2(2)	-3(2)	-5(2)
C(9A)	18(3)	20(3)	27(3)	2(2)	-7(2)	1(2)
C(10A)	19(3)	27(3)	24(3)	1(2)	-5(2)	2(2)
C(11A)	15(3)	23(3)	24(3)	-4(2)	-5(2)	5(2)
C(12A)	14(3)	24(3)	33(3)	-1(2)	-2(2)	-1(2)
C(13A)	34(3)	22(3)	47(4)	0(3)	9(3)	-2(2)
C(14A)	40(4)	55(4)	48(4)	-29(3)	-4(3)	7(3)
C(15A)	85(9)	31(7)	46(7)	-4(5)	1(6)	14(6)
C(16A)	83(8)	27(5)	67(7)	2(5)	38(6)	27(5)
C(33A)	40(4)	55(4)	48(4)	-29(3)	-4(3)	7(3)
C(34A)	47(9)	39(9)	52(9)	-4(8)	3(8)	-2(8)
C(35A)	70(15)	40(14)	62(14)	1(12)	0(12)	-3(12)
C(17A)	82(6)	49(5)	55(5)	4(4)	24(4)	-27(4)
C(18A)	65(5)	35(4)	51(4)	8(3)	10(4)	-8(3)

Table S9. Anisotropic displacement parameters [$Å^2 \times 10^3$] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

Anisotropic displacement factor exponent is: $-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

atom	U11	U22	U33	U23	U13	U12
C(19A)	37(4)	28(3)	51(4)	8(3)	2(3)	-2(3)
C(20A)	19(3)	26(3)	39(3)	-9(3)	1(2)	1(2)
C(21A)	23(3)	20(3)	34(3)	-1(2)	-4(3)	-2(2)
C(22A)	22(3)	23(3)	28(3)	-4(2)	-2(2)	-2(2)
C(23A)	22(3)	24(3)	20(3)	-2(2)	-2(2)	0(2)
C(24A)	18(3)	22(3)	29(3)	1(2)	-1(2)	3(2)
C(25A)	22(3)	21(3)	29(3)	0(2)	0(2)	2(2)
C(26A)	13(2)	29(3)	28(3)	-1(2)	-3(2)	3(2)
C(27A)	12(3)	28(3)	37(4)	2(3)	-9(2)	1(2)
C(28A)	25(3)	36(4)	25(3)	1(2)	2(2)	-3(2)
C(29A)	31(3)	38(4)	38(4)	-1(3)	-5(3)	11(3)
C(30A)	19(3)	52(4)	30(3)	1(3)	4(3)	1(3)
C(31A)	20(3)	35(4)	46(4)	4(3)	-2(3)	-5(2)
C(32A)	18(3)	38(4)	37(4)	0(3)	1(3)	2(2)
S(1B)	20(1)	28(1)	38(1)	0(1)	1(1)	1(1)
S(2B)	21(1)	21(1)	23(1)	1(1)	2(1)	-1(1)
S(3B)	20(1)	20(1)	35(1)	0(1)	-1(1)	-2(1)
C(1B)	24(3)	44(4)	41(4)	2(3)	-6(3)	0(3)
C(2B)	14(3)	71(5)	29(3)	3(3)	4(3)	-1(3)
C(3B)	20(3)	73(5)	35(4)	-1(3)	1(3)	-1(3)
C(4B)	23(3)	54(4)	30(3)	-9(3)	4(3)	4(3)
C(5B)	21(3)	47(4)	33(4)	-4(3)	4(3)	-2(3)
C(6B)	17(3)	44(4)	16(3)	1(2)	1(2)	-1(2)
C(7B)	27(3)	35(3)	18(3)	2(2)	1(2)	-3(2)

Table S9. Anisotropic displacement parameters [$Å^2 \times 10^3$] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

Anisotropic displacement factor exponent is: $-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

atom	U11	U22	U33	U23	U13	U12
C(8B)	26(3)	34(3)	21(3)	1(2)	3(2)	-8(2)
C(9B)	21(3)	35(3)	29(3)	-5(3)	-2(3)	0(2)
C(10B)	17(3)	23(3)	25(3)	-4(2)	-2(2)	3(2)
C(11B)	18(3)	24(3)	23(3)	-2(2)	-1(2)	4(2)
C(12B)	16(3)	26(3)	29(3)	-3(2)	1(2)	1(2)
C(13B)	16(3)	21(3)	53(4)	-8(3)	-3(3)	7(2)
C(14B)	50(4)	49(5)	84(6)	-36(4)	-24(4)	15(3)
C(15B)	91(10)	55(9)	37(7)	8(6)	4(7)	-19(7)
C(16B)	110(10)	67(8)	34(6)	0(6)	12(6)	30(7)
C(33B)	50(4)	49(5)	84(6)	-36(4)	-24(4)	15(3)
C(34B)	48(9)	41(9)	35(8)	-21(7)	8(7)	15(7)
C(35B)	142(20)	78(17)	94(18)	19(15)	0(15)	-6(16)
C(17B)	82(6)	53(5)	61(5)	4(4)	28(5)	-20(4)
C(18B)	56(5)	36(4)	67(5)	14(4)	-4(4)	-6(3)
C(19B)	29(3)	34(4)	59(4)	3(3)	-3(3)	-1(3)
C(20B)	22(3)	25(3)	48(4)	-1(3)	8(3)	-1(2)
C(21B)	22(3)	21(3)	35(3)	-1(2)	-8(3)	-1(2)
C(22B)	17(3)	27(3)	22(3)	2(2)	-6(2)	-1(2)
C(23B)	20(3)	24(3)	24(3)	-1(2)	-4(2)	-3(2)
C(24B)	22(3)	18(3)	25(3)	2(2)	-6(2)	-7(2)
C(25B)	37(3)	17(3)	24(3)	5(2)	-6(3)	-1(2)
C(26B)	20(3)	21(3)	20(3)	4(2)	-6(2)	1(2)
C(27B)	27(3)	27(3)	11(3)	2(2)	-3(2)	-2(2)
C(28B)	34(3)	24(3)	22(3)	0(2)	1(2)	-1(2)

Table S9. Anisotropic displacement parameters [$Å^2 \times 10^3$] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

Anisotropic displacement factor exponent is: $-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

atom	U11	U22	U33	U23	U13	U12
C(29B)	29(3)	37(4)	29(3)	-3(3)	3(3)	7(3)
C(30B)	21(3)	50(4)	27(3)	5(3)	7(3)	-9(3)
C(31B)	29(3)	36(3)	22(3)	2(2)	0(3)	-2(3)
C(32B)	24(3)	24(3)	29(3)	4(2)	-2(2)	-3(2)
P(1)	39(1)	20(1)	42(1)	1(1)	2(1)	5(1)
F(1A)	106(4)	61(3)	90(4)	7(3)	-54(3)	-15(3)
F(1B)	91(3)	24(2)	82(3)	4(2)	45(3)	11(2)
F(1C)	72(3)	57(3)	67(3)	0(2)	-27(2)	12(2)
F(1D)	53(2)	27(2)	117(4)	7(2)	38(2)	12(2)
F(1E)	65(3)	24(2)	75(3)	2(2)	35(2)	2(2)
F(1F)	67(3)	26(2)	61(3)	4(2)	28(2)	4(2)
P(2)	28(1)	22(1)	33(1)	2(1)	5(1)	-3(1)
F(2A)	57(2)	46(2)	41(2)	2(2)	-6(2)	5(2)
F(2B)	40(2)	25(2)	69(3)	-1(2)	22(2)	-14(2)
F(2C)	47(2)	27(2)	57(2)	-2(2)	15(2)	-1(2)
P(3)	28(1)	20(1)	34(1)	2(1)	5(1)	2(1)
F(3A)	58(2)	26(2)	62(2)	6(2)	33(2)	13(2)
F(3B)	69(3)	48(3)	82(3)	-4(2)	-34(2)	-2(2)
F(3C)	67(3)	25(2)	69(3)	12(2)	32(2)	7(2)

Table S10. Torsion angles [°] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	atom	atom	angle(°)	atom	atom	atom	atom	angle(°)
C(6A)	C(1A)	C(2A)	C(3A)	2.1(8)	C(1A)	C(6A)	C(7A)	C(8A)	0.3(8)
C(1A)	C(2A)	C(3A)	C(4A)	1.0(9)	C(5A)	C(6A)	C(7A)	S(1A)	4.8(7)
C(2A)	C(3A)	C(4A)	C(5A)	0.9(9)	C(1A)	C(6A)	C(7A)	S(1A)	178.0(4)
C(3A)	C(4A)	C(5A)	C(6A)	1.9(9)	C(10A)	S(1A)	C(7A)	C(8A)	0.5(4)
C(4A)	C(5A)	C(6A)	C(1A)	2.8(8)	C(10A)	S(1A)	C(7A)	C(6A)	177.5(4)
C(4A)	C(5A)	C(6A)	C(7A)	179.9(5)	C(6A)	C(7A)	C(8A)	C(9A)	178.5(5)
C(2A)	C(1A)	C(6A)	C(5A)	2.8(8)	S(1A)	C(7A)	C(8A)	C(9A)	0.7(6)
C(2A)	C(1A)	C(6A)	C(7A)	179.8(5)	C(7A)	C(8A)	C(9A)	C(10A)	1.9(7)
C(5A)	C(6A)	C(7A)	C(8A)	177.6(5)	C(8A)	C(9A)	C(10A)	C(11A)	179.6(5)
C(7A)	S(1A)	C(10A)	C(9A)	1.5(4)	C(8A)	C(9A)	C(10A)	S(1A)	2.2(6)
C(7A)	S(1A)	C(10A)	C(11A)	179.0(4)	C(22A)	S(2A)	C(11A)	C(12A)	0.7(4)
C(9A)	C(10A)	C(11A)	C(12A)	178.1(5)	C(22A)	S(2A)	C(11A)	C(10A)	178.5(4)
S(1A)	C(10A)	C(11A)	C(12A)	1.0(8)	C(10A)	C(11A)	C(12A)	C(21A)	177.4(5)
C(9A)	C(10A)	C(11A)	S(2A)	0.9(7)	S(2A)	C(11A)	C(12A)	C(21A)	1.7(6)
S(1A)	C(10A)	C(11A)	S(2A)	178.0(3)	C(10A)	C(11A)	C(12A)	C(13A)	3.7(9)
S(2A)	C(11A)	C(12A)	C(13A)	177.3(4)	C(12A)	C(13A)	C(14A)	C(15A)	165.5(6)
C(21A)	C(12A)	C(13A)	C(33A)	89.7(7)	C(33A)	C(13A)	C(14A)	C(15A)	0(100)
C(11A)	C(12A)	C(13A)	C(33A)	91.4(7)	C(13A)	C(14A)	C(15A)	C(16A)	59.6(10)
C(21A)	C(12A)	C(13A)	C(14A)	89.7(7)	C(12A)	C(13A)	C(33A)	C(34A)	156.3(11)
C(11A)	C(12A)	C(13A)	C(14A)	91.4(7)	C(14A)	C(13A)	C(33A)	C(34A)	0(100)
C(13A)	C(33A)	C(34A)	C(35A)	74(2)	C(19A)	C(20A)	C(21A)	C(22A)	88.0(6)
C(17A)	C(18A)	C(19A)	C(20A)	67.4(8)	C(12A)	C(21A)	C(22A)	C(23A)	179.1(5)
C(18A)	C(19A)	C(20A)	C(21A)	172.8(5)	C(20A)	C(21A)	C(22A)	C(23A)	2.5(9)
C(11A)	C(12A)	C(21A)	C(22A)	2.0(6)	C(12A)	C(21A)	C(22A)	S(2A)	1.4(6)
C(13A)	C(12A)	C(21A)	C(22A)	177.0(5)	C(20A)	C(21A)	C(22A)	S(2A)	178.0(4)

Table S10. Torsion angles [°] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	atom	atom	angle(°)	atom	atom	atom	atom	angle(°)
C(11A)	C(12A)	C(21A)	C(20A)	178.7(5)	C(11A)	S(2A)	C(22A)	C(21A)	0.4(4)
C(13A)	C(12A)	C(21A)	C(20A)	0.3(8)	C(11A)	S(2A)	C(22A)	C(23A)	179.9(4)
C(19A)	C(20A)	C(21A)	C(12A)	88.3(6)	C(21A)	C(22A)	C(23A)	C(24A)	179.0(5)
S(2A)	C(22A)	C(23A)	C(24A)	1.5(7)	C(23A)	S(3A)	C(26A)	C(25A)	0.8(4)
C(21A)	C(22A)	C(23A)	S(3A)	2.1(8)	C(23A)	S(3A)	C(26A)	C(27A)	179.4(4)
S(2A)	C(22A)	C(23A)	S(3A)	178.4(3)	C(25A)	C(26A)	C(27A)	C(32A)	178.4(5)
C(26A)	S(3A)	C(23A)	C(24A)	0.4(4)	S(3A)	C(26A)	C(27A)	C(32A)	3.2(7)
C(26A)	S(3A)	C(23A)	C(22A)	177.0(5)	C(25A)	C(26A)	C(27A)	C(28A)	3.9(8)
C(22A)	C(23A)	C(24A)	C(25A)	177.4(5)	S(3A)	C(26A)	C(27A)	C(28A)	174.5(4)
S(3A)	C(23A)	C(24A)	C(25A)	0.1(6)	C(32A)	C(27A)	C(28A)	C(29A)	2.3(8)
C(23A)	C(24A)	C(25A)	C(26A)	0.7(7)	C(26A)	C(27A)	C(28A)	C(29A)	180.0(5)
C(24A)	C(25A)	C(26A)	C(27A)	179.5(5)	C(27A)	C(28A)	C(29A)	C(30A)	2.2(8)
C(24A)	C(25A)	C(26A)	S(3A)	1.0(6)	C(28A)	C(29A)	C(30A)	C(31A)	1.3(8)
C(29A)	C(30A)	C(31A)	C(32A)	0.4(8)	C(28A)	C(27A)	C(32A)	C(31A)	1.4(8)
C(30A)	C(31A)	C(32A)	C(27A)	0.5(8)	C(26A)	C(27A)	C(32A)	C(31A)	179.1(5)
C(6B)	C(1B)	C(2B)	C(3B)	2.4(9)	C(1B)	C(6B)	C(7B)	S(1B)	175.1(4)
C(1B)	C(2B)	C(3B)	C(4B)	2.1(9)	C(5B)	C(6B)	C(7B)	S(1B)	2.9(7)
C(2B)	C(3B)	C(4B)	C(5B)	1.6(9)	C(10B)	S(1B)	C(7B)	C(8B)	0.3(4)
C(3B)	C(4B)	C(5B)	C(6B)	1.3(9)	C(10B)	S(1B)	C(7B)	C(6B)	179.1(4)
C(2B)	C(1B)	C(6B)	C(5B)	2.2(8)	C(6B)	C(7B)	C(8B)	C(9B)	179.2(5)
C(2B)	C(1B)	C(6B)	C(7B)	179.8(5)	S(1B)	C(7B)	C(8B)	C(9B)	0.4(6)
C(4B)	C(5B)	C(6B)	C(1B)	1.6(8)	C(7B)	C(8B)	C(9B)	C(10B)	0.4(7)
C(4B)	C(5B)	C(6B)	C(7B)	179.6(5)	C(8B)	C(9B)	C(10B)	C(11B)	179.1(5)
C(1B)	C(6B)	C(7B)	C(8B)	3.6(8)	C(8B)	C(9B)	C(10B)	S(1B)	0.1(6)
C(5B)	C(6B)	C(7B)	C(8B)	178.5(5)	C(7B)	S(1B)	C(10B)	C(9B)	0.1(4)

Table S10. Torsion angles [°] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	atom	atom	angle(°)	atom	atom	atom	atom	angle(°)
C(7B)	S(1B)	C(10B)	C(11B)	178.9(5)	S(2B)	C(11B)	C(12B)	C(13B)	177.9(4)
C(9B)	C(10B)	C(11B)	C(12B)	179.8(5)	C(21B)	C(12B)	C(13B)	C(33B)	89.8(7)
S(1B)	C(10B)	C(11B)	C(12B)	1.4(8)	C(11B)	C(12B)	C(13B)	C(33B)	90.4(7)
C(9B)	C(10B)	C(11B)	S(2B)	0.1(7)	C(21B)	C(12B)	C(13B)	C(14B)	89.8(7)
S(1B)	C(10B)	C(11B)	S(2B)	178.7(3)	C(11B)	C(12B)	C(13B)	C(14B)	90.4(7)
C(22B)	S(2B)	C(11B)	C(10B)	178.6(4)	C(12B)	C(13B)	C(14B)	C(15B)	164.5(7)
C(22B)	S(2B)	C(11B)	C(12B)	1.6(4)	C(33B)	C(13B)	C(14B)	C(15B)	0(100)
C(10B)	C(11B)	C(12B)	C(21B)	178.2(5)	C(13B)	C(14B)	C(15B)	C(16B)	66.6(10)
S(2B)	C(11B)	C(12B)	C(21B)	2.0(6)	C(12B)	C(13B)	C(33B)	C(34B)	164.3(11)
C(10B)	C(11B)	C(12B)	C(13B)	2.0(9)	C(14B)	C(13B)	C(33B)	C(34B)	0(100)
C(13B)	C(33B)	C(34B)	C(35B)	88(2)	C(20B)	C(21B)	C(22B)	C(23B)	0.8(9)
C(17B)	C(18B)	C(19B)	C(20B)	69.7(8)	C(12B)	C(21B)	C(22B)	S(2B)	0.2(6)
C(18B)	C(19B)	C(20B)	C(21B)	172.0(5)	C(20B)	C(21B)	C(22B)	S(2B)	177.7(4)
C(11B)	C(12B)	C(21B)	C(22B)	1.4(6)	C(11B)	S(2B)	C(22B)	C(23B)	179.5(4)
C(13B)	C(12B)	C(21B)	C(22B)	178.4(4)	C(11B)	S(2B)	C(22B)	C(21B)	0.8(4)
C(11B)	C(12B)	C(21B)	C(20B)	179.0(5)	C(21B)	C(22B)	C(23B)	C(24B)	178.9(5)
C(13B)	C(12B)	C(21B)	C(20B)	0.9(8)	S(2B)	C(22B)	C(23B)	C(24B)	0.4(7)
C(19B)	C(20B)	C(21B)	C(12B)	88.0(6)	C(21B)	C(22B)	C(23B)	S(3B)	0.7(8)
C(19B)	C(20B)	C(21B)	C(22B)	89.3(6)	S(2B)	C(22B)	C(23B)	S(3B)	177.7(3)
C(12B)	C(21B)	C(22B)	C(23B)	178.3(5)	C(26B)	S(3B)	C(23B)	C(24B)	0.7(4)
S(3B)	C(23B)	C(24B)	C(25B)	0.8(6)	C(26B)	S(3B)	C(23B)	C(22B)	179.1(4)
C(23B)	C(24B)	C(25B)	C(26B)	0.5(7)	C(22B)	C(23B)	C(24B)	C(25B)	179.1(5)
C(24B)	C(25B)	C(26B)	C(27B)	179.8(5)	C(32B)	C(27B)	C(28B)	C(29B)	2.6(8)
C(24B)	C(25B)	C(26B)	S(3B)	0.0(6)	C(26B)	C(27B)	C(28B)	C(29B)	179.0(5)
C(23B)	S(3B)	C(26B)	C(25B)	0.4(4)	C(27B)	C(28B)	C(29B)	C(30B)	1.9(8)

Table S10. Torsion angles [°] for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

atom	atom	atom	atom	angle(°)	atom	atom	atom	atom	angle(°)
C(23B)	S(3B)	C(26B)	C(27B)	179.8(4)	C(28B)	C(29B)	C(30B)	C(31B)	1.1(8)
C(25B)	C(26B)	C(27B)	C(28B)	3.6(8)	C(29B)	C(30B)	C(31B)	C(32B)	1.1(8)
S(3B)	C(26B)	C(27B)	C(28B)	176.6(4)	C(30B)	C(31B)	C(32B)	C(27B)	1.8(8)
C(25B)	C(26B)	C(27B)	C(32B)	174.8(5)	C(28B)	C(27B)	C(32B)	C(31B)	2.5(8)
S(3B)	C(26B)	C(27B)	C(32B)	5.0(7)	C(26B)	C(27B)	C(32B)	C(31B)	179.0(5)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

	x	y	z	U(eq)
H(1AA)	-444(2)	6714(3)	12334(6)	56(20)
H(2AA)	-974(2)	6883(3)	13814(7)	59(20)
H(3AA)	-1142(2)	7948(3)	14602(7)	77(24)
H(4AA)	-783(2)	8862(3)	13790(7)	72(23)
H(5AA)	-254(2)	8708(3)	12310(6)	54(19)
H(8AA)	68(2)	6575(2)	10870(6)	47(18)
H(9AA)	620(1)	6694(2)	9288(6)	46(18)
H(13A)	579(2)	9155(3)	8838(7)	41
H(13B)	899(2)	9571(3)	7981(7)	41
H(14A)	1316(2)	9437(3)	10364(7)	57
H(14B)	934(2)	9189(3)	11171(7)	57
H(15A)	1018(3)	10372(5)	11586(14)	65
H(15B)	1011(3)	10492(5)	9758(14)	65
H(16A)	406(3)	10769(4)	10702(13)	69
H(16B)	361(3)	10036(4)	11375(13)	69
H(16C)	355(3)	10153(4)	9546(13)	69
H(33A)	1097(7)	9076(10)	10977(24)	57
H(33B)	1275(7)	9706(10)	10154(24)	57
H(34A)	505(7)	9768(10)	11274(24)	55
H(34B)	883(7)	9990(10)	12336(24)	55
H(35A)	667(9)	10905(11)	10707(33)	69
H(35B)	717(9)	10450(11)	9217(33)	69
H(35C)	1090(9)	10669(11)	10265(33)	69
H(17A)	2070(2)	10584(4)	4299(9)	58(20)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

	x	y	z	U(eq)
H(17B)	2016(2)	9842(4)	3675(9)	84(26)
H(17C)	2132(2)	9972(4)	5462(9)	121(37)
H(18A)	1410(2)	10340(3)	3984(9)	83(27)
H(18B)	1526(2)	10471(3)	5770(9)	46(18)
H(19A)	1111(2)	9518(3)	5364(7)	65(21)
H(19B)	1450(2)	9165(3)	4477(7)	64(22)
H(20A)	1846(1)	9122(3)	6747(6)	72(22)
H(20B)	1542(1)	9554(3)	7655(6)	37(16)
H(24A)	1720(1)	6686(2)	6022(6)	32(15)
H(25A)	2259(1)	6543(3)	4373(6)	19(13)
H(28A)	2791(2)	6672(3)	3010(6)	97(29)
H(29A)	3311(2)	6821(3)	1426(7)	21(13)
H(30A)	3528(2)	7895(3)	876(6)	27(15)
H(31A)	3207(2)	8813(3)	1813(7)	32(15)
H(32A)	2674(1)	8676(3)	3357(6)	37(16)
H(1BA)	2952(2)	8225(3)	-2236(7)	27(15)
H(2BA)	3465(2)	8051(3)	-3854(7)	83(26)
H(3BA)	3628(2)	6972(3)	-4582(7)	80(25)
H(4BA)	3251(2)	6080(3)	-3848(6)	53(19)
H(5BA)	2729(2)	6240(3)	-2260(6)	21(13)
H(8BA)	2433(2)	8386(3)	-873(6)	40(16)
H(9BA)	1884(2)	8275(3)	774(6)	33(16)
H(13C)	1582(1)	5412(3)	2015(6)	36
H(13D)	1904(1)	5823(3)	1156(6)	36

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

	x	y	z	U(eq)
H(14C)	1548(2)	5798(3)	-1169(9)	74
H(14D)	1162(2)	5569(3)	-358(9)	74
H(15C)	1492(4)	4511(6)	392(14)	73
H(15D)	1435(4)	4579(6)	-1450(14)	73
H(16D)	2070(4)	4251(6)	-762(12)	84
H(16E)	2130(4)	4900(6)	282(12)	84
H(16F)	2073(4)	4967(6)	-1557(12)	84
H(33C)	1417(6)	5920(9)	-1006(22)	74
H(33D)	1184(6)	5355(9)	-162(22)	74
H(34C)	1951(6)	5017(9)	-958(22)	49
H(34D)	1611(6)	5014(9)	-2321(22)	49
H(35D)	1580(11)	3990(12)	-827(40)	126
H(35E)	1194(11)	4418(12)	-643(40)	126
H(35F)	1530(11)	4421(12)	701(40)	126
H(17D)	455(2)	4378(4)	5833(10)	89(27)
H(17E)	372(2)	4998(4)	4712(10)	60(22)
H(17F)	509(2)	5117(4)	6484(10)	61(21)
H(18C)	974(2)	4523(3)	4259(9)	115(35)
H(18D)	1111(2)	4641(3)	6028(9)	70(23)
H(19C)	1054(2)	5832(3)	5567(7)	0(10)
H(19D)	1393(2)	5488(3)	4660(7)	29(14)
H(20C)	947(2)	5440(3)	2370(7)	35(15)
H(20D)	647(2)	5873(3)	3296(7)	16(12)
H(24B)	761(1)	8309(2)	4025(6)	43(17)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Bu_2Ph_2Tth]PF_6$ at 106 K.

	x	y	z	U(eq)
H(25B)	218(2)	8431(3)	5651(6)	33(15)
H(28B)	-311(2)	8281(3)	7049(6)	20(13)
H(29B)	-841(2)	8116(3)	8518(6)	49(18)
H(30B)	-1029(2)	7040(3)	9169(6)	23(14)
H(31B)	-692(2)	6130(3)	8221(6)	45(18)
H(32B)	-162(2)	6287(3)	6746(6)	96(28)

Table S12. X-Ray Powder Diffraction Data for $[Bu_2Ph_2Tth]PF_6$.

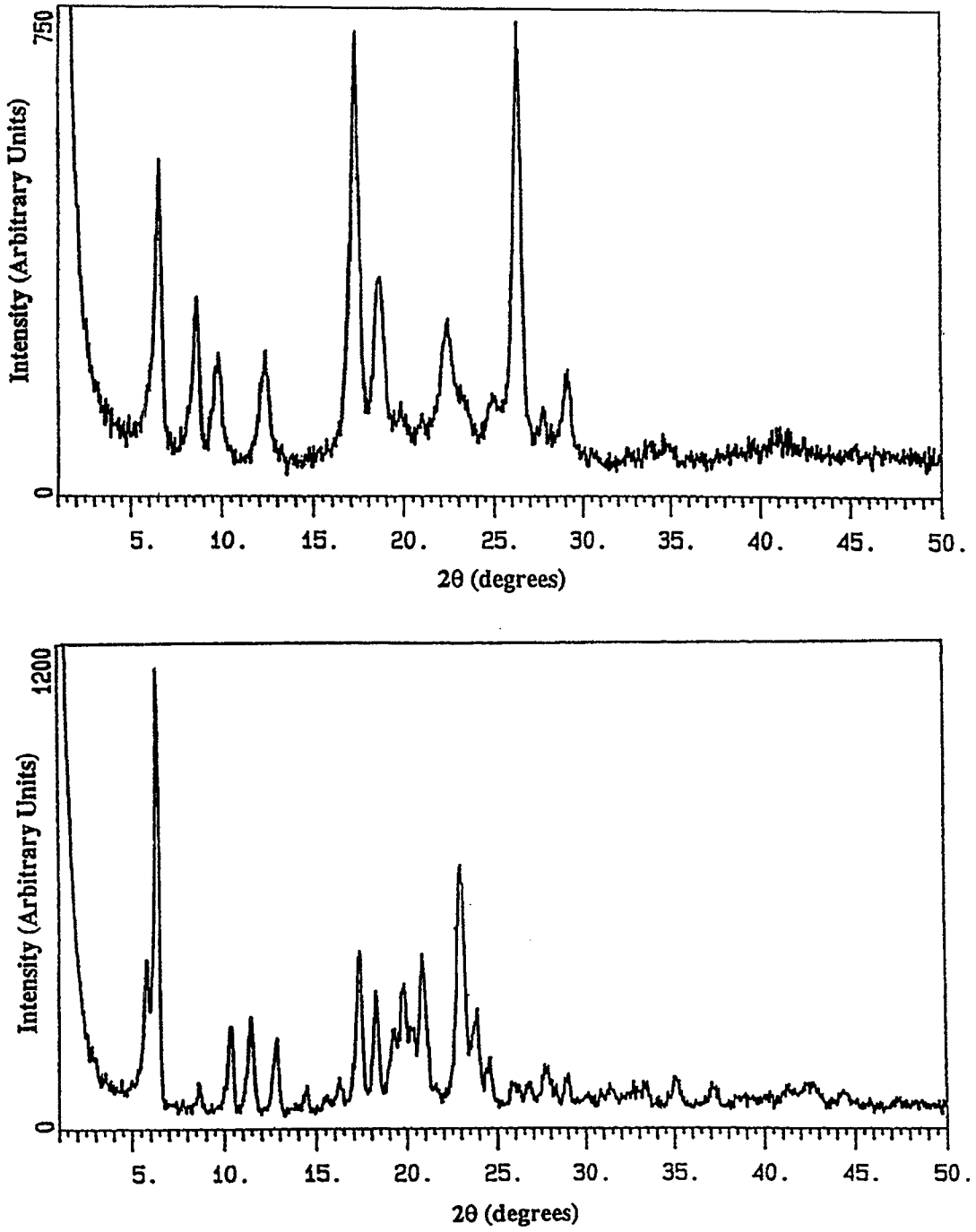
observed		calculated[a]	
2θ (°)	d (Å)	d (Å)	Miller Indices
6.60	13.382	13.568	(110)
8.60	10.214	10.311	(020)
9.85	8.972	9.008	(200)
12.35	7.161	7.155	(111)
		7.241	($\bar{1}$11)
17.25	5.137	5.156	(040)
		5.107	(131)
18.60	4.767	4.733	(311)
19.85	4.469	4.475	(240)
22.40	3.966	3.973	($\bar{2}$41)
		3.944	(241)
24.95	3.566	3.579	(222)
		3.552	($\bar{1}$32)
		3.532	(132)
26.40	3.373	3.392	(312)
27.75	3.212	3.277	(042)
29.15	3.061	3.063	(402)
		3.066	(242)
		3.093	($\bar{2}$42)
		3.075	(332)

a. Calculated from the crystal structure of $[Bu_2Ph_2Tth]PF_6$ as outlined in the text.

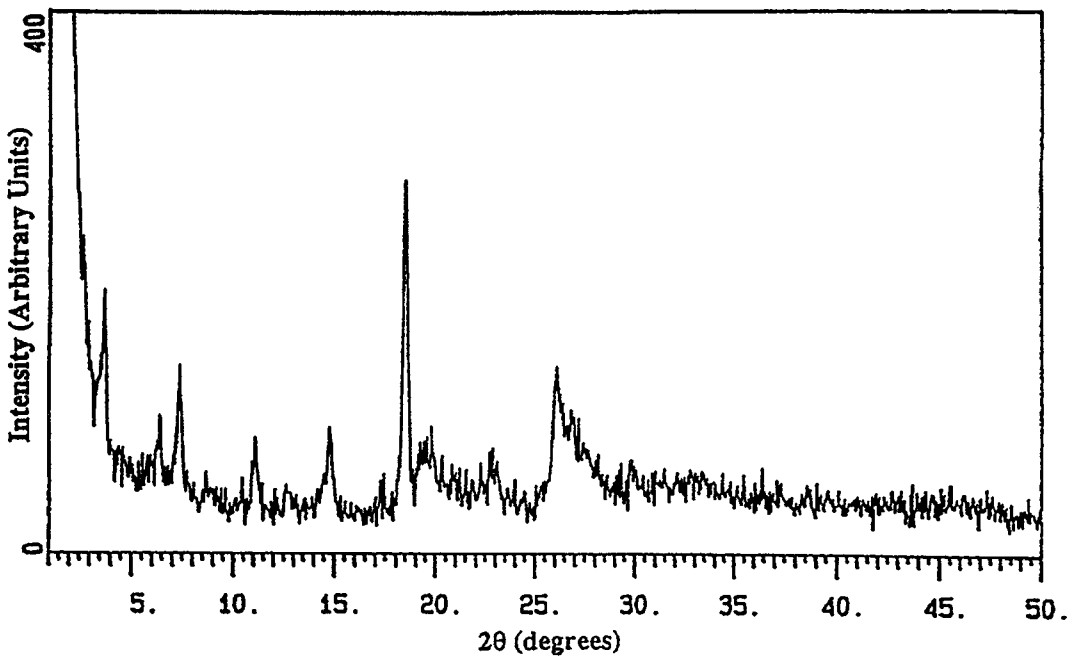
Table S13. X-Ray Powder Diffraction Data for Bu_2Ph_2Tth.

observed		calculated[a]	
2θ , (°)	d (Å)	d (Å)	Miller Indices
5.85	15.094	15.338	(020)
6.40	13.799	13.735	(110)
8.70	10.156	10.225	(030)
10.40	8.499	8.512	(130)
11.55	7.655	7.681	(200)
		7.669	(040)
12.90	6.857	6.868	(220)
		6.861	(140)
14.55	6.080	6.141	(230)
		6.135	(050)
16.35	5.417	5.427	(240)
		5.415	(111)
17.40	5.093	5.113	(060)
		5.051	(310)
18.30	4.844	4.845	(131)
		4.851	(160)
		4.857	(320)
19.35	4.584	4.578	(330)
19.85	4.469	4.470	(141)
20.95	4.237	4.256	(260)
		4.252	(231)
23.05	3.855	3.840	(400)
		3.835	(311)
		3.811	(410)
23.95	3.713	3.725	(420)
		3.719	(251)
24.60	3.616	3.618	(360)

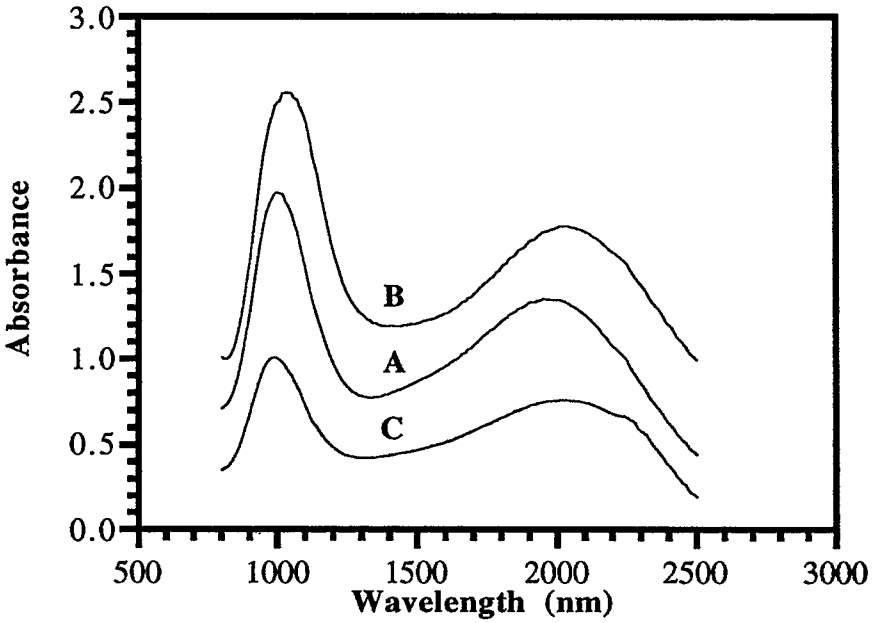
a. Calculated from the crystal structure of Bu_2Ph_2Tth as outlined in the text.



Supporting Figure 1. (Top) X-ray powder diffraction pattern recorded for a sample of electrocrystallized $[Bu_2Ph_2Tth]PF_6$. The diffraction pattern is identical for chemically synthesized samples. (Bottom) X-ray powder diffraction pattern recorded for a sample of Bu_2Ph_2Tth.



Supporting Figure 2. X-ray powder diffraction pattern recorded for a sample of Bu_2Ph_2Tth after doping with I_2 for 20 hours.



Supporting Figure 3. Room temperature vis-NIR-IR spectra for the (A) 5 wt%, (B) 10 wt%, and (C) 15 wt% $[Bu_2Ph_2Tth]PF_6$ / PMMA films.