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Supporting Information For

Near-infared upper phenyl-fused BODIPY as photosensitizer for photothermal-photodynamic therapy

Tao Yu[a†], Dongxiang Zhang[a†], Jie Wang[b†], Changliang Sun[a], Tianfang Cui[a], Zhangrun Xu[b], Xin-Dong Jiang[a,*] and Jianjun Du[c,*]

[a.] Liaoning & Shenyang Key Laboratory of Functional Dye and Pigment, Shenyang University of Chemical Technology, Shenyang, China. E-mail: xdjiang@syuct.edu.cn

[b.]Department of Chemistry, College of Sciences, Northeastern University, Shenyang,China

[c.] State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian, China. E-mail: dujj@dlut.edu.cn

† These three authors contributed equally to this work.

1. Table

Table S1 Spectral data of **BBDP** in different solutions.

BBDP	$\lambda_{abs}/\lambda_{em}$ (nm)	Stokes-shift (nm)	fwhm (nm)	ε[$10^5 \cdot M^{-1} \cdot cm^{-1}$]
DMSO	778/827	49	125.46	2.15
CH_2Cl_2	760/812	52	117.08	1.59
MeOH	754/812	58	106.28	1.72
THF	756/810	54	106.27	2.03
MeCN	754/817	63	110.38	1.73
EtOAc	750/808	60	96.30	1.95
H_2O	774/821	47	164.51	1.29

Note: “fwhm” is an abbreviation for full width at half maxima.

2. Figures

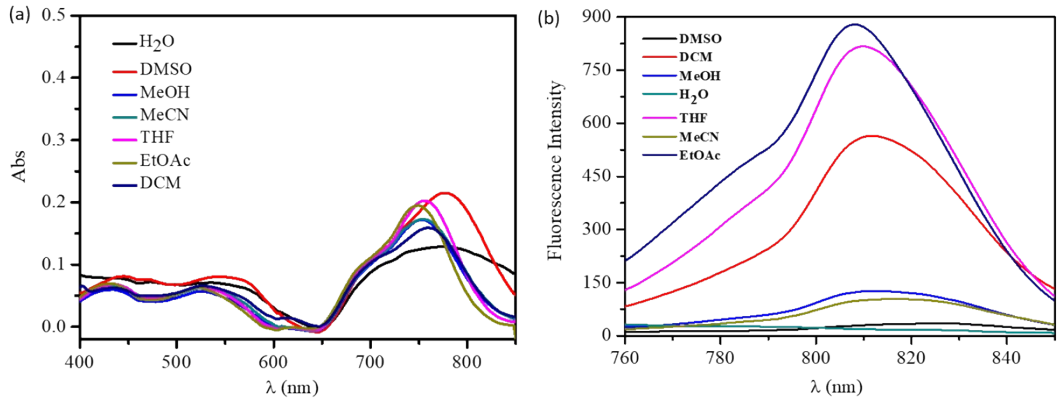


Fig. S1 (a) Absorption spectra and (b) fluorescence spectra in different solvents.

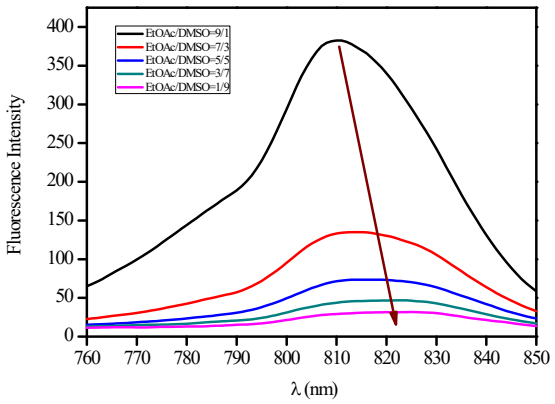


Fig. S2 Absorption spectra at different ratios of ethyl acetate and DMSO from 9:1, 7:3, 5:5, 3:7 to 1:9.

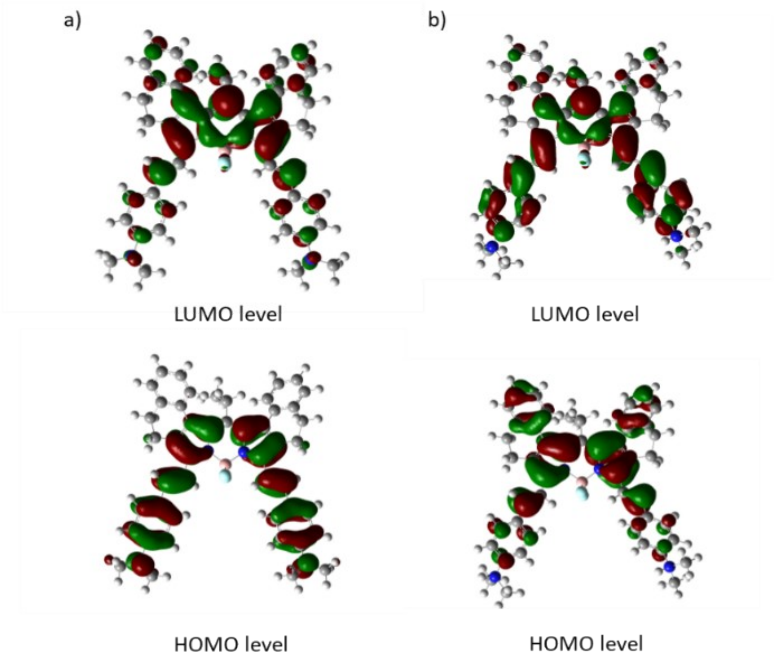


Fig. S3 Frontier molecular orbitals have been performed at the Becke3LYP (B3LYP) level with 6-31+G(d,p) base sites. (a) HOMO/LUMO= -4.67/-2.69 eV, Δ = 1.98 eV for **BBDP**; (b) HOMO/LUMO= -8.92/-6.74 eV, Δ = 2.18 eV for **BBDP-2H**$^{+}$.

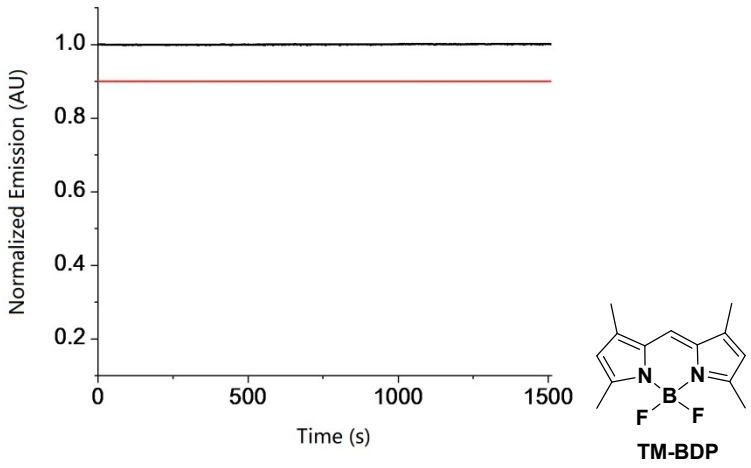


Fig. S4 Fluorescence intensity variations (810 nm for **BBDP**, 540 nm for **TM-BDP**) of 5 μM **BBDP** (black line) and **TM-BDP** (red line) under continuous irradiation with 760 nm for **BBDP**, 470 nm for **TM-BDP** in toluene, and the light power density is 0.5 mW/cm^2, the slit width was 8.0 nm for excitation, and 1 nm for emission. Note: for clarity, the initial normalized intensities are arbitrarily designated as 1.0 and 0.9, respectively.

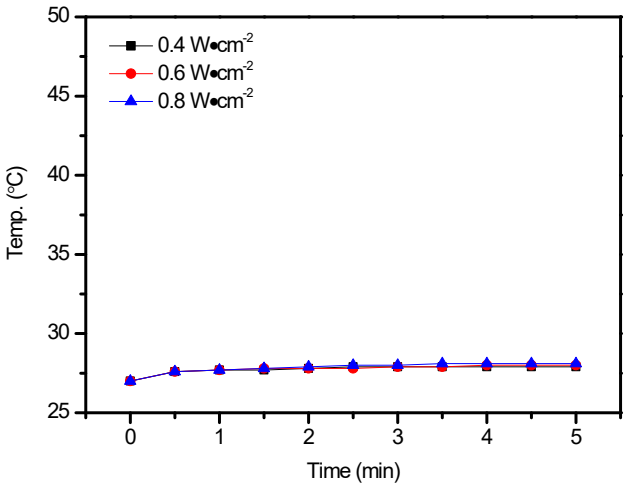


Fig. S5 The temperature of aqueous solution without NPs under different power density (0.4, 0.6, 0.8 W·cm^{-2}) radiation within 5 min.

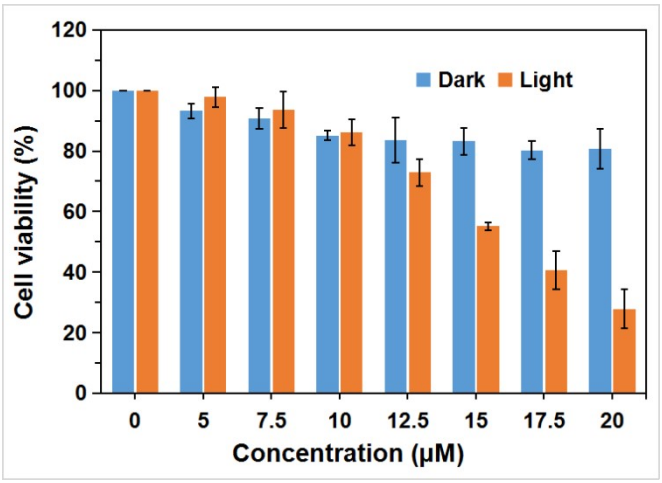


Fig. S6 MTT assay of different concentrations from 0-20 μM with or without light radiation respectively. 635 nm NIR laser (10 mW·cm^{-2}) was applied for 20 min irradiation.

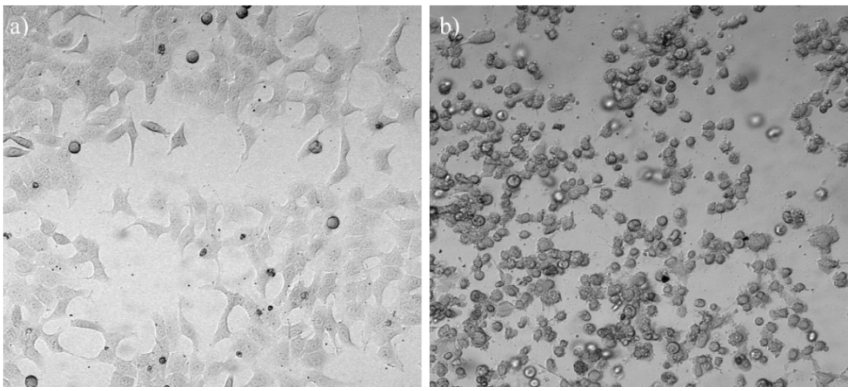
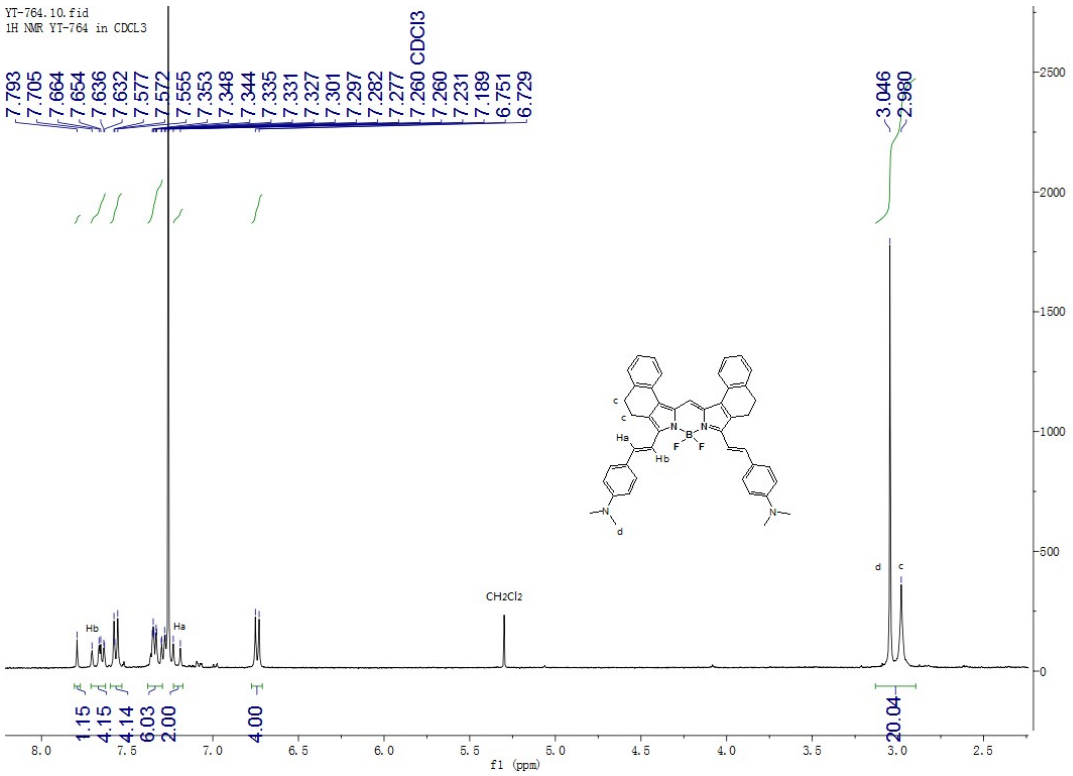
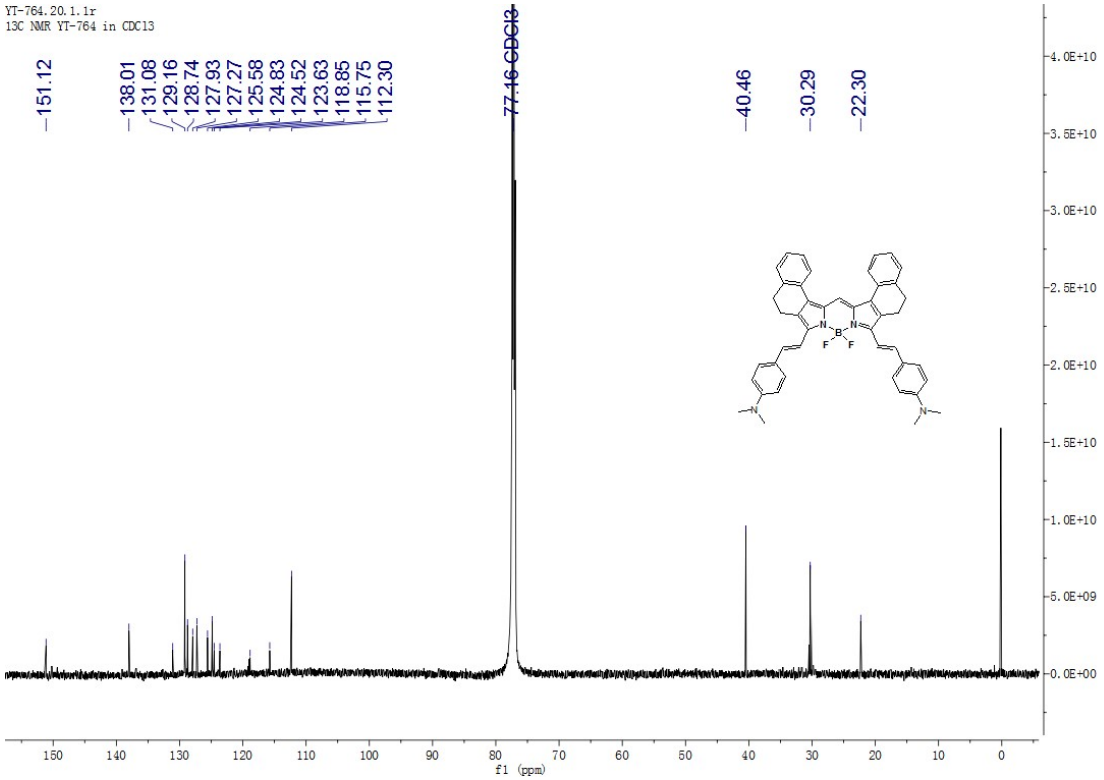


Fig. S7 Bright field photograph of cell. (a) only NPs treated; (b) NPs + light radiation treated.

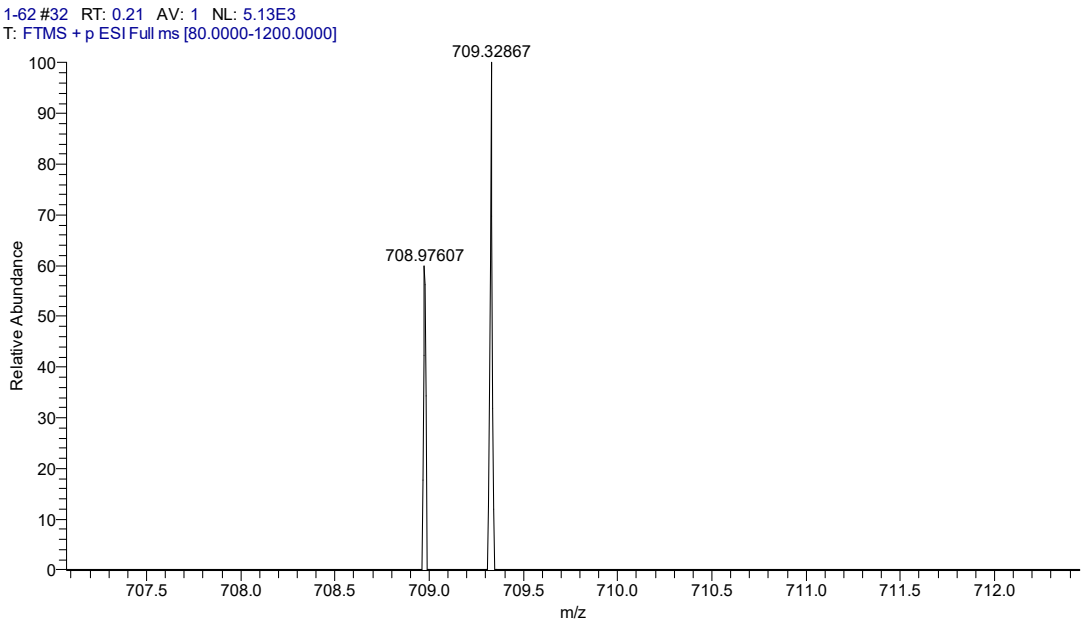
3. NMRand HRMS



^{1}H NMR spectrogram for dye **BBDP**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.68 (d, J = 16 Hz, 2H), 7.64 (d, J = 8.8 Hz, 2H), 7.56 (d, J = 8.8 Hz, 4H), 7.38 – 7.29 (m, 6H), 7.20 (d, J = 16 Hz, 2H), 6.73 (d, J = 8.8 Hz, 4H), 3.05 (s, 12H), 2.98 (s, 8H).



^{13}C NMR spectrogram for dye **BBDP**. ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1, 138.0, 131.1, 129.1, 128.7, 127.9, 127.2, 125.5, 124.8, 124.5, 123.6, 118.8, 115.7, 112.3, 40.4, 30.2, 22.3.



HRMS (ESI) m/z calcd for $C_{45}H_{41}BF_2N_4Na^+$ $(M+Na)^+$ 709.32846, found 709.32867.

4. X-ray data for BBDP

Table 1 Crystal data and structure refinement for YT-2.

Identification code	YT-2
Empirical formula	$C_{45}H_{41}BF_2N_4$
Formula weight	686.63
Temperature/K	170.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.3953(3)
b/Å	23.4385(8)
c/Å	20.7039(7)
α/°	90
β/°	98.181(3)
γ/°	90
Volume/Å^3	3552.2(2)
Z	4
ρ_{calc}g/cm^3	1.284
μ/mm^{-1}	0.653
F(000)	1448.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.728 to 147.84
Index ranges	$-8 \le h \le 8$, $-23 \le k \le 29$, $-25 \le l \le 16$
Reflections collected	14389
Independent reflections	6949 [R_{int} = 0.0830, R_{sigma} = 0.0788]
Data/restraints/parameters	6949/0/473
Goodness-of-fit on F^2	0.980
Final R indexes [I>=2σ (I)]	R_1 = 0.0640, wR_2 = 0.1605
Final R indexes [all data]	R_1 = 0.0866, wR_2 = 0.1778
Largest diff. peak/hole / e Å^{-3}	0.36/-0.33

Crystal structure determination of [YT-2]

Crystal Data for $C_{45}H_{41}BF_2N_4$ (M =686.63 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 7.3953(3) Å, b = 23.4385(8) Å, c = 20.7039(7) Å, β = 98.181(3)°, V = 3552.2(2) Å^3, Z = 4, T = 170.00(10) K, μ(Cu Kα) = 0.653 mm^{-1}, *Dcalc* = 1.284 g/cm^3, 14389 reflections measured (5.728° ≤ 2Θ ≤ 147.84°), 6949 unique (R_{int} = 0.0830, R_{sigma} = 0.0788) which were used in all calculations. The final R_1 was 0.0640 (I >2σ(I)) and wR_2 was 0.1778 (all data).

Refinement model description

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for YT-2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	3998.1(19)	2144.1(6)	7003.5(6)	34.2(3)
F2	7072(2)	2253.3(6)	7207.6(6)	35.6(4)
N1	5644(3)	2224.2(8)	6081.7(8)	23.1(4)
N2	5881(2)	1347.8(8)	6780.4(8)	23.4(4)
N3	3843(3)	5687.3(9)	7725.2(10)	36.7(5)
N4	4943(3)	1742.9(10)	10995.6(10)	43.0(6)
C1	5940(3)	2234.5(9)	5006.4(10)	23.4(5)
C2	6443(3)	2116.2(9)	4361.6(10)	22.9(5)
C3	7723(3)	1707.3(10)	4245.5(11)	27.0(5)
C4	8234(3)	1647.1(10)	3628.4(11)	30.2(5)
C5	7441(4)	1993.5(10)	3124.0(11)	33.0(5)
C6	6167(3)	2401.6(10)	3234.3(11)	31.2(5)
C7	5684(3)	2478.3(10)	3851.6(10)	25.7(5)
C8	4358(3)	2931.1(10)	4000.2(11)	30.9(5)
C9	4973(3)	3228.2(10)	4659.6(10)	27.6(5)
C10	5402(3)	2774.8(9)	5175.1(10)	24.3(5)
C11	5292(3)	2769.6(9)	5852.2(11)	23.9(5)
C12	6021(3)	1885.0(9)	5570.3(10)	23.0(5)
C13	6244(3)	1299.7(9)	5647.5(10)	23.6(5)
C14	6171(3)	1027.8(9)	6236.4(10)	23.3(5)
C15	6268(3)	439.6(9)	6420.7(11)	24.0(5)
C16	6675(3)	-70.1(10)	6057.6(11)	25.5(5)
C17	7501(3)	-60.7(11)	5493.4(11)	32.1(5)
C18	7959(4)	-563.1(11)	5197.7(12)	36.7(6)
C19	7619(3)	-1086.2(11)	5473.7(13)	36.3(6)
C20	6823(3)	-1100.2(10)	6037.7(12)	33.1(6)
C21	6339(3)	-602.3(10)	6336.1(11)	28.5(5)
C22	5362(4)	-625.0(10)	6923.6(12)	33.8(5)
C23	5850(3)	-142.9(10)	7417.7(11)	27.5(5)
C24	5966(3)	412.6(10)	7065.8(10)	24.3(5)
C25	5788(3)	980.2(10)	7292.6(10)	23.1(5)
C26	5558(3)	1197.0(10)	7923.4(10)	26.2(5)
C27	5588(3)	887.5(10)	8475.6(11)	30.6(5)
C28	5354(3)	1114.7(10)	9112.1(11)	28.6(5)
C29	5057(3)	1692.4(10)	9227.3(11)	29.4(5)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for YT-2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C30	4965(3)	1901.5(11)	9842.7(11)	30.6(5)
C31	5096(3)	1533.1(11)	10389.0(11)	31.6(5)
C32	5356(4)	952.7(11)	10273.8(12)	39.0(6)
C33	5508(4)	752.9(11)	9655.6(12)	39.1(6)
C34	5176(4)	2344.0(13)	11136.8(13)	46.1(7)
C35	4888(4)	1360.7(14)	11540.7(12)	48.1(8)
C36	4984(3)	3226.9(10)	6286.9(11)	26.1(5)
C37	4946(3)	3784.6(10)	6127.6(11)	28.9(5)
C38	4710(3)	4262.6(10)	6553.2(11)	27.6(5)
C39	4611(3)	4207.8(10)	7223.7(11)	28.5(5)
C40	4351(3)	4669.1(10)	7610.7(11)	27.4(5)
C41	4147(3)	5226.6(10)	7348.0(12)	29.3(5)
C42	4293(4)	5285.8(11)	6682.0(12)	36.7(6)
C43	4550(4)	4817.4(10)	6301.3(11)	35.3(6)
C44	4101(4)	6260.4(10)	7488.7(13)	38.5(6)
C45	3730(4)	5633.0(11)	8412.5(12)	35.8(6)
B1	5643(4)	2004.5(11)	6789.4(12)	25.2(5)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for YT-2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	41.9(8)	32.3(8)	32.2(7)	6.8(6)	18.5(6)	7.8(6)
F2	47.1(8)	31.0(8)	26.4(7)	-1.0(6)	-2.8(6)	-7.6(6)
N1	30.0(10)	20.7(9)	19.6(9)	-0.1(7)	6.5(7)	1.5(8)
N2	26.9(9)	23.7(10)	20.1(9)	2.0(7)	5.4(7)	-0.1(8)
N3	51.7(13)	23.5(11)	37.1(11)	-3.6(9)	13.7(10)	5.0(10)
N4	55.6(14)	50.9(15)	23.8(11)	-1.8(10)	10.3(10)	3.0(12)
C1	25.0(11)	23.3(11)	22.1(11)	0.5(8)	4.7(9)	1.3(9)
C2	25.7(11)	22.0(11)	21.0(10)	-1.6(8)	3.1(8)	-2.3(9)
C3	31.1(12)	23.1(11)	26.5(11)	0.3(9)	3.1(9)	2.7(9)
C4	33.3(12)	29.6(12)	28.6(12)	-4.4(9)	6.9(10)	4.3(10)
C5	48.2(14)	29.9(13)	22.5(11)	-1.3(9)	10.5(10)	0.5(11)
C6	40.4(13)	28.7(12)	24.5(11)	3.2(9)	4.8(10)	2.2(11)
C7	32.3(12)	22.8(11)	21.8(11)	0.2(8)	3.3(9)	-0.6(9)
C8	37.4(13)	32.8(13)	22.3(11)	4.0(9)	3.5(10)	9.0(11)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for YT-2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C9	33.6(12)	24.8(11)	25.1(11)	3.3(9)	6.1(9)	4.9(10)
C10	28.3(11)	22.5(11)	22.6(11)	1.4(8)	5.9(9)	-0.5(9)
C11	25.5(11)	22.8(11)	23.8(11)	0.6(8)	4.7(9)	0.8(9)
C12	25.1(11)	23.1(11)	21.4(10)	-1.2(8)	5.5(8)	1.3(9)
C13	28.3(11)	23.7(11)	19.5(10)	0.6(8)	5.4(9)	1.4(9)
C14	25.0(11)	22.0(11)	23.6(11)	-1.5(8)	5.5(9)	-1.0(9)
C15	23.2(10)	22.8(11)	25.7(11)	1.7(9)	2.7(9)	-1.4(9)
C16	25.2(11)	24.1(11)	26.0(11)	-1.7(9)	-0.8(9)	0.4(9)
C17	38.2(13)	28.2(13)	29.8(12)	0.3(10)	5.0(10)	1.9(11)
C18	43.8(14)	38.0(14)	29.3(12)	-6.5(10)	8.5(11)	1.6(12)
C19	37.9(14)	28.9(13)	40.8(14)	-8.6(11)	1.3(11)	2.5(11)
C20	32.5(12)	22.6(12)	42.5(14)	-0.4(10)	-0.1(11)	-1.4(10)
C21	28.8(12)	23.5(12)	31.9(12)	-0.4(9)	-0.2(9)	-2.1(9)
C22	39.5(13)	24.0(12)	39.0(13)	4.3(10)	9.4(11)	-4.2(10)
C23	31.0(12)	25.8(12)	26.6(11)	5.6(9)	7.1(9)	0.6(9)
C24	24.8(11)	23.5(11)	24.5(11)	2.9(9)	3.0(9)	-0.6(9)
C25	22.9(10)	25.9(11)	20.7(10)	2.6(8)	3.5(8)	-2.6(9)
C26	28.0(11)	26.8(12)	24.1(11)	1.5(9)	4.3(9)	-0.8(9)
C27	38.3(13)	27.7(12)	25.8(12)	0.6(9)	4.1(10)	-0.8(10)
C28	34.3(12)	29.1(12)	22.2(11)	2.5(9)	3.8(9)	-2.9(10)
C29	31.5(12)	30.6(13)	26.5(12)	7.0(9)	5.8(9)	1.2(10)
C30	33.8(12)	32.4(13)	26.5(12)	1.9(10)	7.9(10)	2.7(10)
C31	33.1(12)	42.3(15)	19.9(11)	1.7(10)	5.6(9)	-1.4(11)
C32	56.2(17)	35.9(14)	24.5(12)	7.6(10)	4.9(11)	-6.6(13)
C33	59.2(17)	29.5(13)	28.7(13)	4.4(10)	6.9(12)	-6.9(12)
C34	47.0(16)	55.6(18)	35.2(14)	-14.6(13)	4.1(12)	6.7(14)
C35	46.3(16)	76(2)	22.6(13)	4.7(13)	7.6(11)	4.3(15)
C36	30.7(11)	25.9(11)	22.9(11)	-2.0(9)	7.6(9)	-0.2(9)
C37	34.6(12)	26.3(12)	26.3(11)	-1.6(9)	6.4(10)	0.1(10)
C38	32.6(12)	23.1(11)	27.8(11)	-1.3(9)	6.3(9)	0.1(10)
C39	35.2(12)	20.0(11)	31.4(12)	2.5(9)	8.4(10)	-2.1(10)
C40	30.9(11)	26.9(12)	25.8(11)	0.4(9)	8.7(9)	-0.1(10)
C41	30.7(12)	24.9(12)	33.3(12)	-2.4(9)	7.5(10)	2.9(10)
C42	54.2(16)	22.7(12)	33.8(13)	4.3(10)	8.2(12)	4.3(11)
C43	53.7(16)	27.9(13)	25.0(12)	3.1(10)	8.1(11)	2.7(11)
C44	45.7(15)	23.6(12)	48.4(15)	-2.7(11)	14.1(12)	3.8(11)
C45	35.4(13)	36.4(14)	36.0(13)	-6.1(11)	6.9(11)	3.1(11)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for YT-2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B1	32.0(13)	23.1(12)	21.0(12)	0.2(10)	5.8(10)	-2.2(11)

Table 4 Bond Lengths for YT-2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	B1	1.392(3)	C14	C15	1.429(3)
F2	B1	1.395(3)	C15	C16	1.465(3)
N1	C11	1.375(3)	C15	C24	1.387(3)
N1	C12	1.384(3)	C16	C17	1.393(3)
N1	B1	1.553(3)	C16	C21	1.411(3)
N2	C14	1.395(3)	C17	C18	1.391(3)
N2	C25	1.375(3)	C18	C19	1.391(4)
N2	B1	1.550(3)	C19	C20	1.381(4)
N3	C41	1.370(3)	C20	C21	1.391(3)
N3	C44	1.452(3)	C21	C22	1.501(3)
N3	C45	1.443(3)	C22	C23	1.533(3)
N4	C31	1.368(3)	C23	C24	1.500(3)
N4	C34	1.444(4)	C24	C25	1.423(3)
N4	C35	1.446(3)	C25	C26	1.434(3)
C1	C2	1.462(3)	C26	C27	1.352(3)
C1	C10	1.387(3)	C27	C28	1.454(3)
C1	C12	1.421(3)	C28	C29	1.398(3)
C2	C3	1.392(3)	C28	C33	1.401(3)
C2	C7	1.408(3)	C29	C30	1.376(3)
C3	C4	1.390(3)	C30	C31	1.415(3)
C4	C5	1.385(3)	C31	C32	1.399(4)
C5	C6	1.384(3)	C32	C33	1.382(4)
C6	C7	1.386(3)	C36	C37	1.347(3)
C7	C8	1.507(3)	C37	C38	1.451(3)
C8	C9	1.542(3)	C38	C39	1.406(3)
C9	C10	1.507(3)	C38	C43	1.400(3)
C10	C11	1.416(3)	C39	C40	1.376(3)
C11	C36	1.439(3)	C40	C41	1.415(3)
C12	C13	1.388(3)	C41	C42	1.405(3)
C13	C14	1.384(3)	C42	C43	1.381(3)

Table 5 Bond Angles for YT-2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	N1	C12	108.57(17)	C18	C17	C16	121.2(2)
C11	N1	B1	127.49(18)	C19	C18	C17	119.7(2)
C12	N1	B1	123.94(18)	C20	C19	C18	119.5(2)
C14	N2	B1	125.06(18)	C19	C20	C21	121.5(2)
C25	N2	C14	108.41(18)	C16	C21	C22	119.7(2)
C25	N2	B1	126.49(18)	C20	C21	C16	119.3(2)
C41	N3	C44	119.8(2)	C20	C21	C22	120.9(2)
C41	N3	C45	122.0(2)	C21	C22	C23	114.8(2)
C45	N3	C44	116.3(2)	C24	C23	C22	109.88(18)
C31	N4	C34	120.9(2)	C15	C24	C23	122.4(2)
C31	N4	C35	120.6(2)	C15	C24	C25	108.06(19)
C34	N4	C35	117.5(2)	C25	C24	C23	129.6(2)
C10	C1	C2	121.5(2)	N2	C25	C24	108.31(18)
C10	C1	C12	107.44(19)	N2	C25	C26	120.4(2)
C12	C1	C2	130.9(2)	C24	C25	C26	131.3(2)
C3	C2	C1	123.8(2)	C27	C26	C25	126.2(2)
C3	C2	C7	119.6(2)	C26	C27	C28	125.5(2)
C7	C2	C1	116.40(19)	C29	C28	C27	123.5(2)
C4	C3	C2	120.6(2)	C29	C28	C33	116.5(2)
C5	C4	C3	119.5(2)	C33	C28	C27	120.0(2)
C6	C5	C4	120.4(2)	C30	C29	C28	122.2(2)
C5	C6	C7	120.8(2)	C29	C30	C31	121.1(2)
C2	C7	C8	118.24(19)	N4	C31	C30	120.6(2)
C6	C7	C2	119.1(2)	N4	C31	C32	122.5(2)
C6	C7	C8	122.7(2)	C32	C31	C30	116.9(2)
C7	C8	C9	112.34(19)	C33	C32	C31	121.2(2)
C10	C9	C8	108.32(18)	C32	C33	C28	122.1(2)
C1	C10	C9	120.29(19)	C37	C36	C11	124.7(2)
C1	C10	C11	107.48(19)	C36	C37	C38	126.9(2)
C11	C10	C9	132.2(2)	C39	C38	C37	123.8(2)
N1	C11	C10	108.40(19)	C43	C38	C37	120.1(2)
N1	C11	C36	121.01(19)	C43	C38	C39	116.1(2)
C10	C11	C36	130.5(2)	C40	C39	C38	122.3(2)
N1	C12	C1	107.93(18)	C39	C40	C41	121.2(2)
N1	C12	C13	120.88(19)	N3	C41	C40	121.7(2)
C13	C12	C1	130.9(2)	N3	C41	C42	121.6(2)
C14	C13	C12	122.5(2)	C42	C41	C40	116.7(2)
N2	C14	C15	108.11(18)	C43	C42	C41	121.2(2)

Table 5 Bond Angles for YT-2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C13	C14	N2	119.57(19)	C42	C43	C38	122.5(2)
C13	C14	C15	132.3(2)	F1	B1	F2	108.87(19)
C14	C15	C16	131.0(2)	F1	B1	N1	109.89(19)
C24	C15	C14	107.0(2)	F1	B1	N2	110.06(19)
C24	C15	C16	122.0(2)	F2	B1	N1	110.18(19)
C17	C16	C15	124.3(2)	F2	B1	N2	110.20(19)
C17	C16	C21	118.7(2)	N2	B1	N1	107.63(18)
C21	C16	C15	116.7(2)				

Table 6 Torsion Angles for YT-2.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C11	C36	C37	167.9(2)	C15	C16	C21	C22	8.4(3)
N1	C12	C13	C14	-2.4(3)	C15	C24	C25	N2	3.3(3)
N2	C14	C15	C16	-175.2(2)	C15	C24	C25	C26	-176.4(2)
N2	C14	C15	C24	2.2(2)	C16	C15	C24	C23	-6.1(3)
N2	C25	C26	C27	-174.5(2)	C16	C15	C24	C25	174.39(19)
N3	C41	C42	C43	-178.2(2)	C16	C17	C18	C19	-1.1(4)
N4	C31	C32	C33	-180.0(3)	C16	C21	C22	C23	-37.5(3)
C1	C2	C3	C4	-175.2(2)	C17	C16	C21	C20	-0.6(3)
C1	C2	C7	C6	177.5(2)	C17	C16	C21	C22	-176.8(2)
C1	C2	C7	C8	-3.2(3)	C17	C18	C19	C20	0.2(4)
C1	C10	C11	N1	-3.8(3)	C18	C19	C20	C21	0.4(4)
C1	C10	C11	C36	172.8(2)	C19	C20	C21	C16	-0.2(3)
C1	C12	C13	C14	-175.7(2)	C19	C20	C21	C22	175.9(2)
C2	C1	C10	C9	11.8(3)	C20	C21	C22	C23	146.4(2)
C2	C1	C10	C11	-171.0(2)	C21	C16	C17	C18	1.3(3)
C2	C1	C12	N1	171.3(2)	C21	C22	C23	C24	42.0(3)
C2	C1	C12	C13	-14.8(4)	C22	C23	C24	C15	-22.0(3)
C2	C3	C4	C5	-0.8(4)	C22	C23	C24	C25	157.3(2)
C2	C7	C8	C9	41.8(3)	C23	C24	C25	N2	-176.2(2)
C3	C2	C7	C6	3.0(3)	C23	C24	C25	C26	4.1(4)
C3	C2	C7	C8	-177.7(2)	C24	C15	C16	C17	-160.3(2)
C3	C4	C5	C6	0.8(4)	C24	C15	C16	C21	14.1(3)
C4	C5	C6	C7	1.2(4)	C24	C25	C26	C27	5.1(4)
C5	C6	C7	C2	-3.1(4)	C25	N2	C14	C13	177.5(2)
C5	C6	C7	C8	177.7(2)	C25	N2	C14	C15	-0.2(2)
C6	C7	C8	C9	-138.9(2)	C25	N2	B1	F1	-54.0(3)

Table 6 Torsion Angles for YT-2.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C7	C2	C3	C4	-1.1(3)	C25	N2	B1	F2	66.1(3)
C7	C8	C9	C10	-51.3(3)	C25	N2	B1	N1	-173.73(19)
C8	C9	C10	C1	26.3(3)	C25	C26	C27	C28	179.9(2)
C8	C9	C10	C11	-150.1(2)	C26	C27	C28	C29	0.2(4)
C9	C10	C11	N1	173.0(2)	C26	C27	C28	C33	-176.7(2)
C9	C10	C11	C36	-10.3(4)	C27	C28	C29	C30	-175.4(2)
C10	C1	C2	C3	149.1(2)	C27	C28	C33	C32	177.8(3)
C10	C1	C2	C7	-25.1(3)	C28	C29	C30	C31	-2.5(4)
C10	C1	C12	N1	-3.6(2)	C29	C28	C33	C32	0.7(4)
C10	C1	C12	C13	170.3(2)	C29	C30	C31	N4	-177.8(2)
C10	C11	C36	C37	-8.3(4)	C29	C30	C31	C32	1.1(4)
C11	N1	C12	C1	1.3(2)	C30	C31	C32	C33	1.1(4)
C11	N1	C12	C13	-173.4(2)	C31	C32	C33	C28	-2.0(4)
C11	N1	B1	F1	53.3(3)	C33	C28	C29	C30	1.6(4)
C11	N1	B1	F2	-66.7(3)	C34	N4	C31	C30	-18.2(4)
C11	N1	B1	N2	173.1(2)	C34	N4	C31	C32	162.9(3)
C11	C36	C37	C38	-177.5(2)	C35	N4	C31	C30	173.6(2)
C12	N1	C11	C10	1.5(3)	C35	N4	C31	C32	-5.4(4)
C12	N1	C11	C36	-175.5(2)	C36	C37	C38	C39	4.7(4)
C12	N1	B1	F1	-127.0(2)	C36	C37	C38	C43	-174.7(2)
C12	N1	B1	F2	113.0(2)	C37	C38	C39	C40	-178.7(2)
C12	N1	B1	N2	-7.2(3)	C37	C38	C43	C42	178.9(2)
C12	C1	C2	C3	-25.2(4)	C38	C39	C40	C41	0.7(4)
C12	C1	C2	C7	160.7(2)	C39	C38	C43	C42	-0.6(4)
C12	C1	C10	C9	-172.8(2)	C39	C40	C41	N3	178.4(2)
C12	C1	C10	C11	4.5(3)	C39	C40	C41	C42	-2.3(4)
C12	C13	C14	N2	-0.6(3)	C40	C41	C42	C43	2.5(4)
C12	C13	C14	C15	176.4(2)	C41	C42	C43	C38	-1.0(4)
C13	C14	C15	C16	7.5(4)	C43	C38	C39	C40	0.8(4)
C13	C14	C15	C24	-175.1(2)	C44	N3	C41	C40	164.3(2)
C14	N2	C25	C24	-1.8(2)	C44	N3	C41	C42	-14.9(4)
C14	N2	C25	C26	177.89(19)	C45	N3	C41	C40	0.6(4)
C14	N2	B1	F1	123.9(2)	C45	N3	C41	C42	-178.6(2)
C14	N2	B1	F2	-116.0(2)	B1	N1	C11	C10	-178.7(2)
C14	N2	B1	N1	4.1(3)	B1	N1	C11	C36	4.3(3)
C14	C15	C16	C17	16.8(4)	B1	N1	C12	C1	-178.5(2)
C14	C15	C16	C21	-168.8(2)	B1	N1	C12	C13	6.9(3)
C14	C15	C24	C23	176.15(19)	B1	N2	C14	C13	-0.7(3)

Table 6 Torsion Angles for YT-2.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C14	C15	C24	C25	-3.3(2)	B1	N2	C14	C15	-178.4(2)
C15	C16	C17	C18	175.7(2)	B1	N2	C25	C24	176.3(2)
C15	C16	C21	C20	-175.4(2)	B1	N2	C25	C26	-4.0(3)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for YT-2.

Atom	*x*	*y*	*z*	U(eq)
H3	8242.12	1472.27	4583.85	32
H4	9100.87	1376.4	3554.69	36
H5	7767.14	1951.78	2709.01	40
H6	5627.13	2626.94	2890.21	37
H8A	3168.6	2758.57	4007.82	37
H8B	4233.96	3214.42	3655.21	37
H9A	6047.66	3459.38	4632.86	33
H9B	4009.04	3475.13	4769.35	33
H13	6450.72	1082.01	5289.68	28
H17	7751.19	288.08	5310.99	38
H18	8489.89	-549.26	4816.98	44
H19	7924.83	-1423.98	5279.95	44
H20	6604.86	-1450.83	6222.42	40
H22A	5636	-986.85	7143.2	41
H22B	4057.01	-614.05	6777.39	41
H23A	4926.7	-116.7	7705.4	33
H23B	7013.45	-224.14	7681.62	33
H26	5368.95	1587.65	7955.54	31
H27	5774.99	496.53	8446.13	37
H29	4917.3	1943.86	8876.3	35
H30	4813.33	2291.2	9900.64	37
H32	5428.75	696.63	10619.62	47
H33	5718.94	366.19	9598.8	47
H34A	6306.97	2472.2	11009.54	69
H34B	5195.81	2406.33	11596.05	69
H34C	4181.12	2553.17	10898.72	69
H35A	4021.94	1061.57	11415.37	72
H35B	4527.86	1568.89	11900.96	72
H35C	6076.34	1198.04	11667.68	72
H36	4796.62	3130.64	6708.18	31

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for YT-2.

Atom	*x*	*y*	*z*	U(eq)
H37	5086.06	3872.46	5699.53	35
H39	4726.61	3846.99	7412.04	34
H40	4308.14	4613.57	8053.01	33
H42	4214.11	5647.08	6494.32	44
H43	4620.71	4872.47	5860.76	42
H44A	5355.42	6310.83	7429.16	58
H44B	3789.63	6533.16	7800.69	58
H44C	3330.57	6316.26	7079.72	58
H45A	2985.23	5309.64	8482.51	54
H45B	3196.31	5972.29	8563.98	54
H45C	4933.39	5581.11	8648.31	54

Experimental

Single crystals of $C_{45}H_{41}BF_2N_4$ **[YT-2]** were **[]**. A suitable crystal was selected and **[]** on a **SuperNova, Dual, Cu at zero, AtlasS2** diffractometer. The crystal was kept at 170.00(10) K during data collection.

5. CheckCIF of BBDP

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) yt-2

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: yt-2

```
Bond precision:   C-C = 0.0031 A          Wavelength=1.54184

Cell:             a=7.3953(3)     b=23.4385(8)        c=20.7039(7)
                  alpha=90        beta=98.181(3)      gamma=90
Temperature:      170 K

                  Calculated                  Reported
Volume            3552.2(2)                   3552.2(2)
Space group       P 21/n                      P 1 21/n 1
Hall group        -P 2yn                      -P 2yn
Moiety formula    C45 H41 B F2 N4             C45 H41 B F2 N4
Sum formula       C45 H41 B F2 N4             C45 H41 B F2 N4
Mr                686.63                      686.63
Dx,g cm-3         1.284                       1.284
Z                 4                           4
Mu (mm-1)         0.653                       0.653
F000              1448.0                      1448.0
F000'             1452.13
h,k,lmax          9,29,25                     8,29,25
Nref              7197                        6949
Tmin,Tmax         0.913,0.937                 0.193,1.000
Tmin'             0.913

Correction method= # Reported T Limits: Tmin=0.193 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.966          Theta(max)= 73.920

R(reflections)= 0.0640( 4926)                 wR2(reflections)=
                                              0.1778( 6949)
S = 0.980                 Npar= 473
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.239 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 9 Report

Alert level G

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 185 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock yt-2 - ellipsoid plot