Table 7. Crystal data and structure refinement for f60628b.

Identification code	f60628b
Empirical formula	C44 H66 Dy2 N6 O2 S2
Formula weight	1100.15
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 10.086(4) A alpha = 90 deg. b = 11.719(4) A beta = 93.451(4) deg. c = 19.487(7) A gamma = 90 deg.
Volume	2299.2(14) A^3
Z, Calculated density	2, 1.589 Mg/m^3
Absorption coefficient	3.357 mm^-1
F(000)	1104
Crystal size	0.12 x 0.10 x 0.08 mm
Theta range for data collection	2.03 to 27.01 deg.
Limiting indices	-12<=h<=12, -9<=k<=14, -24<=l<=23
Reflections collected / unique	11050 / 4978 [R(int) = 0.0473]
Completeness to theta = 27.01	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7750 and 0.6888
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4978 / 0 / 257
Goodness-of-fit on F^2	0.909
Final R indices [I>2sigma(I)]	R1 = 0.0300, wR2 = 0.0607
R indices (all data)	R1 = 0.0431, wR2 = 0.0640
Largest diff. peak and hole	1.123 and -0.626 e.A^-3

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for f60628b.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Dy(1)	5716(1)	4632(1)	1012(1)	38(1)
S(1)	3387(1)	5461(1)	337(1)	43(1)
O(1)	4696(3)	5495(2)	2012(1)	56(1)
N(1)	5862(3)	6571(3)	837(1)	37(1)
N(2)	7641(3)	5736(3)	1343(2)	44(1)
N(3)	7804(3)	7716(3)	1079(2)	51(1)
C(1)	3540(4)	6883(4)	649(2)	46(1)
C(2)	2423(4)	7555(4)	693(2)	61(1)
C(3)	2511(5)	8643(5)	951(2)	75(2)
C(4)	3705(5)	9073(4)	1177(2)	70(1)
C(5)	4847(4)	8433(4)	1143(2)	55(1)
C(6)	4806(4)	7333(3)	874(2)	43(1)

C(7)	7130(3)	6694(3)	1092(2)	38(1)
C(8)	9066(4)	5588(4)	1519(2)	57(1)
C(9)	9284(5)	5152(5)	2247(2)	78(2)
C(10)	9642(5)	4792(5)	1010(3)	96(2)
C(11)	7717(4)	8480(4)	487(2)	54(1)
C(12)	8236(6)	9635(4)	703(3)	94(2)
C(13)	8466(5)	7995(5)	-88(2)	82(2)
C(14)	5382(8)	2371(5)	899(3)	93(2)
C(15)	6639(8)	2507(5)	1139(4)	97(2)
C(16)	6617(7)	2894(5)	1800(4)	96(2)
C(17)	5319(7)	3005(5)	1948(3)	83(2)
C(18)	4574(5)	2695(5)	1389(4)	90(2)
C(19)	5368(5)	6231(5)	2510(2)	78(2)
C(20)	4371(6)	6678(6)	2942(3)	124(3)
C(21)	3084(6)	6391(6)	2601(3)	108(2)
C(22)	3327(4)	5406(5)	2184(2)	70(1)

Table 9. Bond lengths [A] and angles [deg] for f60628b.

Dy(1)-N(1)	2.303(3)
Dy(1)-N(2)	2.389(3)
Dy(1)-O(1)	2.474(3)
Dy(1)-C(15)	2.665(5)
Dy(1)-C(18)	2.669(5)
Dy(1)-C(16)	2.677(5)
Dy(1)-C(14)	2.679(5)
Dy(1)-C(17)	2.686(5)
Dy(1)-S(1)	2.7966(12)
Dy(1)-C(7)	2.806(4)
Dy(1)-S(1)#1	2.8318(13)
S(1)-C(1)	1.778(4)
S(1)-Dy(1)#1	2.8318(13)
O(1)-C(19)	1.437(5)
O(1)-C(22)	1.445(5)
N(1)-C(7)	1.352(4)
N(1)-C(6)	1.396(4)
N(2)-C(7)	1.318(5)
N(2)-C(8)	1.468(5)
N(3)-C(7)	1.377(5)
N(3)-C(11)	1.459(5)
C(1)-C(2)	1.381(5)
C(1)-C(6)	1.425(5)
C(2)-C(3)	1.372(6)
C(3)-C(4)	1.354(7)
C(4)-C(5)	1.380(6)
C(5)-C(6)	1.392(5)
C(8)-C(10)	1.504(6)
C(8)-C(9)	1.513(6)
C(11)-C(13)	1.501(6)
C(11)-C(12)	1.503(6)
C(14)-C(15)	1.334(8)
C(14)-C(18)	1.347(7)
C(15)-C(16)	1.367(8)
C(16)-C(17)	1.364(7)
C(17)-C(18)	1.335(7)
C(19)-C(20)	1.448(6)
C(20)-C(21)	1.462(7)
C(21)-C(22)	1.441(7)
N(1)-Dy(1)-N(2)	56.50(10)
N(1)-Dy(1)-O(1)	75.32(9)
N(2)-Dy(1)-O(1)	86.30(10)
N(1)-Dy(1)-C(15)	155.57(17)
N(2)-Dy(1)-C(15)	102.0(2)
O(1)-Dy(1)-C(15)	117.92(16)
N(1)-Dy(1)-C(18)	155.82(15)
N(2)-Dy(1)-C(18)	138.00(15)
O(1)-Dy(1)-C(18)	85.64(18)
C(15)-Dy(1)-C(18)	48.20(18)
N(1)-Dy(1)-C(16)	144.38(14)
N(2)-Dy(1)-C(16)	90.83(14)
O(1)-Dy(1)-C(16)	90.1(2)
C(15)-Dy(1)-C(16)	29.65(18)

C(18)-Dy(1)-C(16)	48.09(16)
N(1)-Dy(1)-C(14)	166.53(14)
N(2)-Dy(1)-C(14)	130.82(19)
O(1)-Dy(1)-C(14)	114.39(16)
C(15)-Dy(1)-C(14)	28.90(18)
C(18)-Dy(1)-C(14)	29.17(16)
C(16)-Dy(1)-C(14)	48.01(17)
N(1)-Dy(1)-C(17)	144.54(14)
N(2)-Dy(1)-C(17)	110.67(18)
O(1)-Dy(1)-C(17)	70.69(14)
C(15)-Dy(1)-C(17)	48.60(17)
C(18)-Dy(1)-C(17)	28.88(16)
C(16)-Dy(1)-C(17)	29.47(16)
C(14)-Dy(1)-C(17)	47.93(16)
N(1)-Dy(1)-S(1)	69.35(7)
N(2)-Dy(1)-S(1)	125.82(8)
O(1)-Dy(1)-S(1)	81.46(7)
C(15)-Dy(1)-S(1)	130.3(2)
C(18)-Dy(1)-S(1)	93.48(12)
C(16)-Dy(1)-S(1)	141.33(14)
C(14)-Dy(1)-S(1)	101.94(16)
C(17)-Dy(1)-S(1)	114.25(16)
N(1)-Dy(1)-C(7)	28.59(9)
N(2)-Dy(1)-C(7)	27.94(10)
O(1)-Dy(1)-C(7)	80.68(10)
C(15)-Dy(1)-C(7)	128.8(2)
C(18)-Dy(1)-C(7)	160.68(18)
C(16)-Dy(1)-C(7)	118.00(14)
C(14)-Dy(1)-C(7)	156.6(2)
C(17)-Dy(1)-C(7)	132.06(16)
S(1)-Dy(1)-C(7)	97.88(8)
N(1)-Dy(1)-S(1)#1	82.75(7)
N(2)-Dy(1)-S(1)#1	88.36(8)
O(1)-Dy(1)-S(1)#1	156.61(7)
C(15)-Dy(1)-S(1)#1	85.47(15)
C(18)-Dy(1)-S(1)#1	112.97(17)
C(16)-Dy(1)-S(1)#1	112.7(2)
C(14)-Dy(1)-S(1)#1	86.08(14)
C(17)-Dy(1)-S(1)#1	132.20(12)
S(1)-Dy(1)-S(1)#1	83.29(3)
C(7)-Dy(1)-S(1)#1	83.97(7)
C(1)-S(1)-Dy(1)	96.36(13)
C(1)-S(1)-Dy(1)#1	109.13(12)
Dy(1)-S(1)-Dy(1)#1	96.71(3)
C(19)-O(1)-C(22)	107.8(3)
C(19)-O(1)-Dy(1)	125.2(2)
C(22)-O(1)-Dy(1)	127.0(3)
C(7)-N(1)-C(6)	128.4(3)
C(7)-N(1)-Dy(1)	96.8(2)
C(6)-N(1)-Dy(1)	124.6(2)
C(7)-N(2)-C(8)	122.8(3)
C(7)-N(2)-Dy(1)	93.9(2)
C(8)-N(2)-Dy(1)	140.2(3)
C(7)-N(3)-C(11)	122.8(3)
C(2)-C(1)-C(6)	119.3(4)
C(2)-C(1)-S(1)	120.0(3)
C(6)-C(1)-S(1)	120.7(3)
C(3)-C(2)-C(1)	121.2(4)
C(4)-C(3)-C(2)	120.1(4)
C(3)-C(4)-C(5)	120.7(5)
C(4)-C(5)-C(6)	121.0(4)
C(5)-C(6)-N(1)	127.3(4)
C(5)-C(6)-C(1)	117.7(4)
N(1)-C(6)-C(1)	114.8(3)
N(2)-C(7)-N(1)	112.6(3)
N(2)-C(7)-N(3)	124.4(3)
N(1)-C(7)-N(3)	122.9(3)
N(2)-C(7)-Dy(1)	58.1(2)
N(1)-C(7)-Dy(1)	54.59(19)
N(3)-C(7)-Dy(1)	175.7(3)
N(2)-C(8)-C(10)	109.3(4)
N(2)-C(8)-C(9)	110.1(3)
C(10)-C(8)-C(9)	111.7(4)
N(3)-C(11)-C(13)	110.5(4)
N(3)-C(11)-C(12)	109.1(4)

C(13)-C(11)-C(12)	111.6(4)
C(15)-C(14)-C(18)	108.7(5)
C(15)-C(14)-Dy(1)	75.0(3)
C(18)-C(14)-Dy(1)	75.0(3)
C(14)-C(15)-C(16)	107.5(6)
C(14)-C(15)-Dy(1)	76.1(4)
C(16)-C(15)-Dy(1)	75.6(3)
C(17)-C(16)-C(15)	107.5(5)
C(17)-C(16)-Dy(1)	75.6(3)
C(15)-C(16)-Dy(1)	74.7(3)
C(18)-C(17)-C(16)	107.6(5)
C(18)-C(17)-Dy(1)	74.9(3)
C(16)-C(17)-Dy(1)	74.9(3)
C(17)-C(18)-C(14)	108.6(5)
C(17)-C(18)-Dy(1)	76.2(3)
C(14)-C(18)-Dy(1)	75.8(3)
O(1)-C(19)-C(20)	107.1(4)
C(19)-C(20)-C(21)	106.3(5)
C(22)-C(21)-C(20)	105.3(5)
C(21)-C(22)-O(1)	105.7(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z

Table 10. Anisotropic displacement parameters (A^2 x 10^3) for f60628b.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Dy(1)	37(1)	39(1)	38(1)	5(1)	1(1)	-1(1)
S(1)	35(1)	54(1)	42(1)	1(1)	2(1)	1(1)
O(1)	53(2)	69(2)	45(2)	-8(1)	12(1)	-5(2)
N(1)	33(2)	37(2)	40(2)	0(1)	4(1)	5(1)
N(2)	36(2)	46(2)	51(2)	7(2)	0(1)	-1(2)
N(3)	49(2)	45(2)	58(2)	-1(2)	-6(2)	-6(2)
C(1)	49(2)	49(3)	38(2)	-2(2)	3(2)	10(2)
C(2)	40(2)	84(4)	59(3)	-8(3)	-1(2)	19(2)
C(3)	69(3)	83(4)	73(3)	-9(3)	1(3)	42(3)
C(4)	92(4)	52(3)	67(3)	-10(3)	-1(3)	30(3)
C(5)	62(3)	54(3)	49(2)	-8(2)	4(2)	12(2)
C(6)	44(2)	47(3)	38(2)	2(2)	5(2)	8(2)
C(7)	41(2)	40(2)	34(2)	-2(2)	2(2)	1(2)
C(8)	40(2)	57(3)	72(3)	12(2)	-8(2)	-5(2)
C(9)	66(3)	101(4)	65(3)	3(3)	-22(2)	15(3)
C(10)	50(3)	162(6)	75(4)	-11(4)	6(2)	31(3)
C(11)	58(3)	48(3)	55(3)	12(2)	-3(2)	-6(2)
C(12)	122(5)	52(3)	105(4)	13(3)	-10(4)	-21(3)
C(13)	83(4)	91(4)	71(3)	15(3)	10(3)	4(3)
C(14)	167(7)	54(4)	57(4)	11(3)	-10(4)	-41(4)
C(15)	121(5)	40(3)	136(6)	33(4)	58(5)	21(4)
C(16)	105(5)	59(4)	116(5)	43(4)	-62(4)	-16(3)
C(17)	138(6)	61(4)	50(3)	21(3)	19(3)	9(4)
C(18)	71(3)	76(4)	121(5)	53(4)	2(4)	-24(3)
C(19)	77(3)	106(5)	50(3)	-18(3)	4(2)	-16(3)
C(20)	128(5)	143(7)	108(5)	-71(5)	56(4)	-41(5)
C(21)	97(4)	114(6)	119(5)	-31(4)	56(4)	2(4)
C(22)	54(3)	97(4)	61(3)	-8(3)	21(2)	-12(3)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for f60628b.

	x	y	z	U(eq)
H(3A)	8670	7553	1163	61
H(3B)	7554	8124	1441	61
H(2)	1597	7264	544	73

H(3)	1749	9086	971	91
H(4)	3755	9808	1356	84
H(5)	5658	8742	1303	66
H(8)	9503	6332	1488	68
H(9A)	8930	5691	2559	118
H(9B)	10219	5057	2357	118
H(9C)	8843	4432	2288	118
H(10A)	9225	4058	1036	143
H(10B)	10580	4715	1114	143
H(10C)	9487	5094	554	143
H(11)	6780	8558	328	65
H(12A)	7702	9940	1051	141
H(12B)	8199	10137	314	141
H(12C)	9139	9565	884	141
H(13A)	9399	7992	42	122
H(13B)	8305	8454	-493	122
H(13C)	8172	7229	-182	122
H(14)	5109	2098	465	112
H(15)	7392	2364	900	116
H(16)	7353	3054	2095	115
H(17)	5009	3251	2362	99
H(18)	3650	2702	1346	107
H(19A)	5805	6850	2281	93
H(19B)	6034	5806	2784	93
H(20A)	4464	7498	2991	149
H(20B)	4461	6334	3396	149
H(21A)	2442	6215	2937	130
H(21B)	2749	7021	2318	130
H(22A)	2740	5407	1771	84
H(22B)	3185	4709	2437	84