Supplementary information

Synthesis and characterization of phenanthroimidazole derivatives for applications in organic electroluminescent devices

Ying Zhang,[a,b] Shiu-Lun Lai,[b] Qing-Xiao Tong,[a,c,*] Mei-Yee Chan,[d] Tsz-Wai Ng,[b] Zhi-Chun Wen,[a] Guo-Qiang Zhang,[a] Shuit-Tong Lee,[b] Hoi-Lun Kwong[e] and Chun-Sing Lee[b,*]

[a] *Department of Chemistry, Shantou University, Guangdong 515063, China*

[b] *Center of Super-Diamond and Advanced Films (COSDAF) and Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, China*

[c] *Jiangsu Key Lab. for Carbon-Based Funct. Mater. & Devices, Soochow Univ., China*

[d] *Department of Chemistry, The University of Hong Kong, Hong Kong SAR, China*

[e] *Dept of Biology and Chemistry, City University of Hong Kong, Hong Kong SAR, China*

Table 1: Crystal data and structure refinement for compounds reported here

Parameters	**1N-TPI**	**2N-TPI**	**Ph-TPI**	**Py-TPI**
Formula	$C_{39}H_{30}N_2S$	$C_{39}H_{30}N_2S$	$C_{35}H_{28}N_2S$	$C_{45}H_{32}N_2S$
M_r	558.71	558.71	508.65	632.79
Temp (*K*)	298(2)	298(2)	298(2)	298(2)
Cryst system	Triclinic	Monoclinic	Triclinic	Orthorhombic
Space group	*P-1*	*P2(1)/c*	*P-1*	*P2(1)/n*
a (Å)	9.4051(8)	16.2930(18)	9.2496(15)	12.311(2)
b (Å)	11.1593(10)	13.6939(15)	10.8416(17)	12.000(2)
c (Å)	14.8250(13)	13.5127(15)	14.733(2)	21.848(4)
α (deg)	106.3580(10)	90	97.111(3)	90
β (deg)	97.9750(10)	97.737(2)	108.074(2)	90
γ (deg)	101.6110(10)	90	97.119(3)	90
V(Å^3)	1430.5(2)	2987.4(6)	1372.9(4)	3227.7(11)
Z	2	4	2	4
D_{calcd}(g cm^{-3})	1.297	1.242	1.230	1.302
μ (mm^{-1})	0.145	0.139	0.144	0.137
Reflcns collcd	10113	16973	9660	22161
Unique reflcns	4959	5231	4759	5688
R_{int}	0.0197	0.0398	0.0212	0.0247
R1[I>2σ(I)][a]	0.0427	0.0554	0.0456	0.0385
*w*R2[I>2σ(I)][a]	0.1212	0.1328	0.1235	0.1025
R1(all data)	0.0497	0.0848	0.0533	0.0442
*w*R2(all data)	0.1326	0.1519	0.1300	0.1067
GOOF	1.071	1.093	1.027	1.054

[a] $R_1=\sum(||F_0|-|F_c||)/\sum|F_0|$; $wR_2=[\sum_w(F_0^2-F_c^2)^2/\sum w(F_0^2)^2]^{1/2}$

Table 2: Bond lengths (Å) and bond angles (°) for compounds reported here

Compounds	Bond lengths (Å)				Bond angles (°)			
1N-TPI	S(1)-C(12)	1.7221(17)	C(21)-C(33)	1.402(3)	C(12)-S(1)-C(11)	92.67(8)	C(20)-C(12)-S(1)	110.22(13)
	S(1)-C(11)	1.7269(16)	C(22)-C(33)	1.355(3)	C(3)-N(1)-C(4)	105.93(13)	C(1)-C(12)-S(1)	119.05(12)
	N(1)-C(3)	1.382(2)	C(23)-C(34)	1.371(3)	C(3)-N(1)-C(5)	125.84(13)	C(25)-C(13)-C(8)	117.04(17)
	N(1)-C(4)	1.396(2)	C(24)-C(38)	1.368(3)	C(4)-N(1)-C(5)	125.53(13)	C(25)-C(13)-C(10)	122.65(17)
	N(1)-C(5)	1.443(2)	C(25)-C(31)	1.370(3)	C(3)-N(2)-C(2)	105.24(13)	C(8)-C(13)-C(10)	120.31(15)
	N(2)-C(3)	1.319(2)	C(27)-C(32)	1.365(3)	C(21)-C(1)-C(7)	119.29(15)	C(16)-C(14)-C(17)	116.83(16)
	N(2)-C(2)	1.375(2)	C(28)-C(37)	1.523(3)	C(21)-C(1)-C(12)	119.24(15)	C(16)-C(14)-C(28)	123.23(17)
	C(1)-C(21)	1.366(2)	C(28)-C(39)	1.526(3)	C(7)-C(1)-C(12)	121.46(15)	C(17)-C(14)-C(28)	119.88(17)
	C(1)-C(7)	1.430(2)	C(28)-C(36)	1.535(3)	N(2)-C(2)-C(4)	111.11(14)	C(29)-C(15)-C(22)	121.42(17)
	C(1)-C(12)	1.485(2)	C(29)-C(35)	1.347(3)	N(2)-C(2)-C(8)	127.22(15)	C(29)-C(15)-C(7)	119.37(17)
	C(2)-C(4)	1.377(2)	C(30)-C(31)	1.381(3)	C(4)-C(2)-C(8)	121.67(15)	C(22)-C(15)-C(7)	119.20(16)
	C(2)-C(8)	1.433(2)	C(32)-C(34)	1.385(3)	N(2)-C(3)-N(1)	112.34(14)	C(14)-C(16)-C(18)	121.61(17)
	C(3)-C(11)	1.455(2)	C(35)-C(38)	1.396(3)	N(2)-C(3)-C(11)	121.63(14)	C(6)-C(17)-C(14)	122.19(16)
	C(4)-C(9)	1.433(2)			N(1)-C(3)-C(11)	125.95(14)	C(5)-C(18)-C(16)	119.83(16)
	C(5)-C(18)	1.375(2)			C(2)-C(4)-N(1)	105.38(13)	C(30)-C(19)-C(8)	120.65(18)
	C(5)-C(6)	1.379(2)			C(2)-C(4)-C(9)	123.03(15)	C(12)-C(20)-C(26)	113.86(16)
	C(6)-C(17)	1.378(2)			N(1)-C(4)-C(9)	131.31(15)	C(1)-C(21)-C(33)	121.55(17)
	C(7)-C(24)	1.409(2)			C(18)-C(5)-C(6)	120.16(15)	C(33)-C(22)-C(15)	120.89(17)
	C(7)-C(15)	1.422(2)			C(18)-C(5)-N(1)	122.02(14)	C(34)-C(23)-C(9)	120.72(19)
	C(8)-C(19)	1.399(2)			C(6)-C(5)-N(1)	117.82(14)	C(38)-C(24)-C(7)	120.30(19)
	C(8)-C(13)	1.410(2)			C(17)-C(6)-C(5)	119.38(16)	C(31)-C(25)-C(13)	121.88(19)
	C(9)-C(23)	1.409(2)			C(24)-C(7)-C(15)	118.17(16)	C(11)-C(26)-C(20)	113.06(15)
	C(9)-C(10)	1.418(2)			C(24)-C(7)-C(1)	123.01(16)	C(32)-C(27)-C(10)	121.78(19)
	C(10)-C(27)	1.403(2)			C(15)-C(7)-C(1)	118.80(15)	C(37)-C(28)-C(39)	111.1(2)
	C(10)-C(13)	1.467(3)			C(19)-C(8)-C(13)	120.26(16)	C(37)-C(28)-C(14)	107.72(15)
	C(11)-C(26)	1.367(2)			C(19)-C(8)-C(2)	122.41(16)	C(39)-C(28)-C(14)	110.84(17)
	C(12)-C(20)	1.359(2)			C(13)-C(8)-C(2)	117.32(15)	C(37)-C(28)-C(36)	108.17(18)
	C(13)-C(25)	1.408(3)			C(23)-C(9)-C(10)	119.20(16)	C(39)-C(28)-C(36)	107.15(19)
	C(14)-C(16)	1.387(3)			C(23)-C(9)-C(4)	124.67(16)	C(14)-C(28)-C(36)	111.86(18)
	C(14)-C(17)	1.397(3)			C(10)-C(9)-C(4)	115.99(15)	C(35)-C(29)-C(15)	120.94(19)
	C(14)-C(28)	1.529(2)			C(27)-C(10)-C(9)	117.86(17)	C(19)-C(30)-C(31)	119.81(19)
	C(15)-C(29)	1.409(3)			C(27)-C(10)-C(13)	121.08(17)	C(25)-C(31)-C(30)	120.32(18)
	C(15)-C(22)	1.410(3)			C(9)-C(10)-C(13)	121.05(15)	C(27)-C(32)-C(34)	120.21(19)
	C(16)-C(18)	1.387(3)			C(26)-C(11)-C(3)	134.02(15)	C(22)-C(33)-C(21)	120.21(18)
	C(19)-C(30)	1.375(3)			C(26)-C(11)-S(1)	110.18(12)	C(23)-C(34)-C(32)	120.18(19)
	C(20)-C(26)	1.410(2)			C(3)-C(11)-S(1)	115.80(12)	C(29)-C(35)-C(38)	120.10(19)
					C(20)-C(12)-C(1)	130.65(16)	C(24)-C(38)-C(35)	121.1(2)

Compounds	Bond lengths (Å)				Bond angles (°)			
2N-TPI	S(1)-C(2)	1.727(2)	C(21)-C(38)	1.535(4)	C(2)-S(1)-C(12)	92.41(11)	C(7)-C(14)-C(21)	122.8(2)
	S(1)-C(12)	1.727(2)	C(23)-C(33)	1.413(4)	C(6)-N(2)-C(1)	105.21(19)	C(22)-C(14)-C(21)	120.4(2)
	N(2)-C(6)	1.322(3)	C(23)-C(25)	1.415(3)	C(6)-N(1)-C(10)	106.28(17)	C(29)-C(15)-C(13)	119.4(2)
	N(2)-C(1)	1.373(3)	C(24)-C(25)	1.354(3)	C(6)-N(1)-C(8)	125.6(2)	C(29)-C(15)-C(10)	125.0(2)
	N(1)-C(6)	1.379(3)	C(26)-C(32)	1.357(4)	C(10)-N(1)-C(8)	127.59(18)	C(13)-C(15)-C(10)	115.6(2)
	N(1)-C(10)	1.391(3)	C(27)-C(36)	1.383(4)	N(2)-C(1)-C(10)	111.1(2)	C(12)-C(16)-C(4)	113.6(2)
	N(1)-C(8)	1.439(3)	C(28)-C(29)	1.374(4)	N(2)-C(1)-C(3)	127.3(2)	C(27)-C(17)-C(3)	121.0(3)
	C(1)-C(10)	1.376(3)	C(28)-C(32)	1.387(4)	C(10)-C(1)-C(3)	121.6(2)	C(9)-C(18)-C(23)	118.5(2)
	C(1)-C(3)	1.429(3)	C(30)-C(35)	1.352(4)	C(4)-C(2)-C(5)	129.1(2)	C(9)-C(18)-C(30)	123.0(2)
	C(2)-C(4)	1.360(3)	C(31)-C(36)	1.374(4)	C(4)-C(2)-S(1)	110.18(18)	C(23)-C(18)-C(30)	118.5(2)
	C(2)-C(5)	1.466(3)	C(33)-C(39)	1.355(4)	C(5)-C(2)-S(1)	120.70(16)	C(22)-C(19)-C(8)	119.4(2)
	C(3)-C(17)	1.403(3)	C(35)-C(39)	1.389(4)	C(17)-C(3)-C(20)	120.0(2)	C(3)-C(20)-C(31)	117.3(3)
	C(3)-C(20)	1.409(3)			C(17)-C(3)-C(1)	122.4(2)	C(3)-C(20)-C(13)	120.5(2)
	C(4)-C(16)	1.402(3)			C(20)-C(3)-C(1)	117.5(2)	C(31)-C(20)-C(13)	122.2(3)
	C(5)-C(9)	1.369(3)			C(2)-C(4)-C(16)	113.7(2)	C(34)-C(21)-C(14)	112.7(2)
	C(5)-C(24)	1.413(3)			C(9)-C(5)-C(24)	117.9(2)	C(34)-C(21)-C(37)	108.1(2)
	C(6)-C(12)	1.448(3)			C(9)-C(5)-C(2)	122.4(2)	C(14)-C(21)-C(37)	110.6(2)
	C(7)-C(11)	1.379(3)			C(24)-C(5)-C(2)	119.6(2)	C(34)-C(21)-C(38)	109.0(2)
	C(7)-C(14)	1.385(3)			N(2)-C(6)-N(1)	112.0(2)	C(14)-C(21)-C(38)	107.7(2)
	C(8)-C(11)	1.373(3)			N(2)-C(6)-C(12)	123.0(2)	C(37)-C(21)-C(38)	108.6(3)
	C(8)-C(19)	1.374(3)			N(1)-C(6)-C(12)	125.0(2)	C(19)-C(22)-C(14)	122.4(2)
	C(9)-C(18)	1.405(3)			C(11)-C(7)-C(14)	121.7(2)	C(18)-C(23)-C(33)	117.9(3)
	C(10)-C(15)	1.431(3)			C(11)-C(8)-C(19)	120.0(2)	C(18)-C(23)-C(25)	118.1(2)
	C(12)-C(16)	1.361(3)			C(11)-C(8)-N(1)	120.5(2)	C(33)-C(23)-C(25)	124.0(3)
	C(13)-C(26)	1.403(4)			C(19)-C(8)-N(1)	119.4(2)	C(25)-C(24)-C(5)	120.6(2)
	C(13)-C(15)	1.425(3)			C(5)-C(9)-C(18)	122.9(2)	C(24)-C(25)-C(23)	122.0(2)
	C(13)-C(20)	1.462(3)			C(1)-C(10)-N(1)	105.35(19)	C(32)-C(26)-C(13)	122.8(3)
	C(14)-C(22)	1.390(3)			C(1)-C(10)-C(15)	123.6(2)	C(17)-C(27)-C(36)	119.9(3)
	C(14)-C(21)	1.526(3)			N(1)-C(10)-C(15)	131.1(2)	C(29)-C(28)-C(32)	119.8(3)
	C(15)-C(29)	1.410(3)			C(8)-C(11)-C(7)	119.8(2)	C(28)-C(29)-C(15)	120.8(3)
	C(17)-C(27)	1.353(4)			C(16)-C(12)-C(6)	133.4(2)	C(35)-C(30)-C(18)	121.5(3)
	C(18)-C(23)	1.408(3)			C(16)-C(12)-S(1)	110.15(18)	C(36)-C(31)-C(20)	121.0(3)
	C(18)-C(30)	1.411(3)			C(6)-C(12)-S(1)	116.38(16)	C(26)-C(32)-C(28)	120.2(3)
	C(19)-C(22)	1.372(3)			C(26)-C(13)-C(15)	116.9(3)	C(39)-C(33)-C(23)	121.9(3)
	C(20)-C(31)	1.412(3)			C(26)-C(13)-C(20)	121.8(3)	C(30)-C(35)-C(39)	120.3(3)
	C(21)-C(34)	1.525(4)			C(15)-C(13)-C(20)	121.2(2)	C(31)-C(36)-C(27)	120.7(3)
	C(21)-C(37)	1.531(4)			C(7)-C(14)-C(22)	116.7(2)	C(33)-C(39)-C(35)	119.8(3)

Compounds	Bond lengths (Å)				Bond angles (°)			
Ph-TPI	S(1)-C(14)	1.7231(18)	C(25)-C(80)	1.660(6)	C(14)-S(1)-C(15)	92.34(9)	C(18)-C(15)-S(1)	120.88(14)
	S(1)-C(15)	1.7275(19)	C(25)-C(80')	1.663(6)	C(4)-N(1)-C(1)	104.93(14)	C(17)-C(16)-C(6)	120.03(16)
	N(1)-C(4)	1.319(2)	C(26)-C(28)	1.389(3)	C(4)-N(2)-C(3)	106.38(14)	C(16)-C(17)-C(8)	121.61(16)
	N(1)-C(1)	1.373(2)	C(29)-C(32)	1.361(4)	C(4)-N(2)-C(6)	126.50(15)	C(23)-C(18)-C(30)	118.1(2)
	N(2)-C(4)	1.378(2)	C(30)-C(35)	1.375(3)	C(3)-N(2)-C(6)	126.99(14)	C(23)-C(18)-C(15)	122.27(19)
	N(2)-C(3)	1.389(2)	C(32)-C(35)	1.366(4)	N(1)-C(1)-C(3)	111.38(15)	C(30)-C(18)-C(15)	119.60(19)
	N(2)-C(6)	1.438(2)			N(1)-C(1)-C(2)	127.05(15)	C(14)-C(19)-C(9)	113.08(17)
	C(1)-C(3)	1.377(2)			C(3)-C(1)-C(2)	121.56(16)	C(27)-C(20)-C(11)	121.6(2)
	C(1)-C(2)	1.431(2)			C(10)-C(2)-C(11)	120.47(17)	C(26)-C(21)-C(5)	121.0(2)
	C(2)-C(10)	1.400(2)			C(10)-C(2)-C(1)	121.86(17)	C(10)-C(22)-C(27)	119.08(19)
	C(2)-C(11)	1.412(3)			C(11)-C(2)-C(1)	117.66(16)	C(18)-C(23)-C(29)	120.7(2)
	C(3)-C(5)	1.437(3)			C(1)-C(3)-N(2)	105.05(15)	C(28)-C(24)-C(7)	122.2(2)
	C(4)-C(14)	1.456(3)			C(1)-C(3)-C(5)	123.16(16)	C(81)-C(25)-C(82')	129.5(5)
	C(5)-C(21)	1.409(3)			N(2)-C(3)-C(5)	131.66(16)	C(81)-C(25)-C(82)	111.1(8)
	C(5)-C(7)	1.425(3)			N(1)-C(4)-N(2)	112.26(16)	C(82')-C(25)-C(82)	43.4(4)
	C(6)-C(12)	1.374(2)			N(1)-C(4)-C(14)	122.46(16)	C(81)-C(25)-C(81')	40.6(6)
	C(6)-C(16)	1.375(2)			N(2)-C(4)-C(14)	125.22(15)	C(82')-C(25)-C(81')	122.0(4)
	C(7)-C(24)	1.406(3)			C(21)-C(5)-C(7)	119.11(18)	C(82)-C(25)-C(81')	138.6(6)
	C(7)-C(11)	1.462(3)			C(21)-C(5)-C(3)	124.77(18)	C(81)-C(25)-C(8)	114.8(4)
	C(8)-C(13)	1.390(2)			C(7)-C(5)-C(3)	116.08(16)	C(82')-C(25)-C(8)	115.1(2)
	C(8)-C(17)	1.390(2)			C(12)-C(6)-C(16)	119.82(15)	C(82)-C(25)-C(8)	109.1(5)
	C(8)-C(25)	1.528(3)			C(12)-C(6)-N(2)	119.67(14)	C(81')-C(25)-C(8)	111.0(4)
	C(9)-C(15)	1.362(3)			C(16)-C(6)-N(2)	120.51(15)	C(81)-C(25)-C(80)	61.9(6)
	C(9)-C(19)	1.397(3)			C(24)-C(7)-C(5)	117.53(18)	C(82')-C(25)-C(80)	97.0(4)
	C(10)-C(22)	1.370(3)			C(24)-C(7)-C(11)	121.46(18)	C(82)-C(25)-C(80)	56.4(5)
	C(11)-C(20)	1.410(3)			C(5)-C(7)-C(11)	120.96(17)	C(81')-C(25)-C(80)	102.1(4)
	C(12)-C(13)	1.372(2)			C(13)-C(8)-C(17)	116.81(16)	C(8)-C(25)-C(80)	106.2(2)
	C(14)-C(19)	1.368(2)			C(13)-C(8)-C(25)	121.73(16)	C(81)-C(25)-C(80')	107.6(6)
	C(15)-C(18)	1.466(3)			C(17)-C(8)-C(25)	121.45(16)	C(82')-C(25)-C(80')	67.3(4)
	C(16)-C(17)	1.373(2)			C(15)-C(9)-C(19)	114.09(17)	C(82)-C(25)-C(80')	110.5(5)
	C(18)-C(23)	1.379(3)			C(22)-C(10)-C(2)	120.86(19)	C(81')-C(25)-C(80')	69.4(4)
	C(18)-C(30)	1.388(3)			C(20)-C(11)-C(2)	116.78(17)	C(8)-C(25)-C(80')	103.4(2)
	C(20)-C(27)	1.362(3)			C(20)-C(11)-C(7)	122.69(18)	C(80)-C(25)-C(80')	150.3(3)
	C(21)-C(26)	1.368(3)			C(2)-C(11)-C(7)	120.52(16)	C(21)-C(26)-C(28)	120.2(2)
	C(22)-C(27)	1.386(3)			C(13)-C(12)-C(6)	119.66(16)	C(20)-C(27)-C(22)	121.21(19)
	C(23)-C(29)	1.384(3)			C(12)-C(13)-C(8)	122.05(16)	C(24)-C(28)-C(26)	119.9(2)
	C(24)-C(28)	1.367(3)			C(19)-C(14)-C(4)	133.14(17)	C(32)-C(29)-C(23)	120.5(3)
	C(25)-C(81)	1.403(9)			C(19)-C(14)-S(1)	110.47(14)	C(35)-C(30)-C(18)	120.4(2)
	C(25)-C(82')	1.436(4)			C(4)-C(14)-S(1)	116.38(12)	C(29)-C(32)-C(35)	119.4(3)
	C(25)-C(82)	1.446(11)			C(9)-C(15)-C(18)	128.99(18)	C(32)-C(35)-C(30)	120.9(3)

	C(25)-C(81')	1.487(7)			C(9)-C(15)-S(1)	110.00(15)		
Compounds	Bond lengths (Å)				Bond angles (°)			
Py-TPI	S(1)-C(17)	1.7253(15)	C(26)-C(27)	1.382(2)	C(17)-S(1)-C(18)	92.50(7)	C(15)-C(14)-C(12)	119.24(13)
	S(1)-C(18)	1.7272(15)	C(28)-C(39)	1.363(2)	C(7)-N(1)-C(10)	106.10(11)	C(15)-C(14)-C(17)	118.75(13)
	N(1)-C(7)	1.3796(18)	C(29)-C(32)	1.394(2)	C(7)-N(1)-C(4)	124.69(11)	C(12)-C(14)-C(17)	121.98(13)
	N(1)-C(10)	1.3920(17)	C(29)-C(38)	1.431(2)	C(10)-N(1)-C(4)	127.36(11)	C(22)-C(15)-C(14)	121.83(14)
	N(1)-C(4)	1.4410(17)	C(30)-C(36)	1.348(2)	C(7)-N(2)-C(3)	104.80(12)	C(37)-C(16)-C(2)	121.11(14)
	N(2)-C(7)	1.3192(18)	C(32)-C(42)	1.375(3)	C(19)-C(1)-C(8)	120.50(13)	C(31)-C(17)-C(14)	131.49(14)
	N(2)-C(3)	1.3750(18)	C(35)-C(42)	1.380(3)	C(19)-C(1)-C(3)	122.06(14)	C(31)-C(17)-S(1)	110.22(11)
	C(1)-C(19)	1.401(2)	C(37)-C(39)	1.390(2)	C(8)-C(1)-C(3)	117.43(13)	C(14)-C(17)-S(1)	118.23(11)
	C(1)-C(8)	1.413(2)	C(38)-C(41)	1.334(2)	C(16)-C(2)-C(11)	119.24(13)	C(25)-C(18)-C(7)	123.92(13)
	C(1)-C(3)	1.4344(19)	C(40)-C(45)	1.527(2)	C(16)-C(2)-C(10)	124.61(13)	C(25)-C(18)-S(1)	110.22(11)
	C(2)-C(16)	1.403(2)	C(40)-C(43)	1.527(2)	C(11)-C(2)-C(10)	116.04(12)	C(7)-C(18)-S(1)	125.85(11)
	C(2)-C(11)	1.4260(19)	C(40)-C(44)	1.538(3)	C(10)-C(3)-N(2)	111.50(12)	C(21)-C(19)-C(1)	120.49(15)
	C(2)-C(10)	1.4371(19)			C(10)-C(3)-C(1)	121.76(13)	C(34)-C(20)-C(4)	119.19(13)
	C(3)-C(10)	1.3716(19)			N(2)-C(3)-C(1)	126.72(13)	C(19)-C(21)-C(33)	119.93(15)
	C(4)-C(26)	1.378(2)			C(26)-C(4)-C(20)	120.38(13)	C(15)-C(22)-C(6)	120.86(14)
	C(4)-C(20)	1.386(2)			C(26)-C(4)-N(1)	121.13(12)	C(33)-C(23)-C(8)	121.66(15)
	C(5)-C(6)	1.422(2)			C(20)-C(4)-N(1)	118.47(12)	C(35)-C(24)-C(13)	119.14(15)
	C(5)-C(12)	1.427(2)			C(6)-C(5)-C(12)	120.25(13)	C(35)-C(24)-C(36)	122.86(15)
	C(5)-C(13)	1.427(2)			C(6)-C(5)-C(13)	119.45(13)	C(13)-C(24)-C(36)	118.00(13)
	C(6)-C(22)	1.389(2)			C(12)-C(5)-C(13)	120.29(13)	C(18)-C(25)-C(31)	113.25(14)
	C(6)-C(41)	1.437(2)			C(22)-C(6)-C(5)	118.80(13)	C(4)-C(26)-C(27)	119.68(13)
	C(7)-C(18)	1.456(2)			C(22)-C(6)-C(41)	122.32(14)	C(26)-C(27)-C(9)	121.48(13)
	C(8)-C(23)	1.413(2)			C(5)-C(6)-C(41)	118.87(14)	C(39)-C(28)-C(11)	122.07(15)
	C(8)-C(11)	1.462(2)			N(2)-C(7)-N(1)	112.35(12)	C(32)-C(29)-C(13)	118.65(16)
	C(9)-C(34)	1.393(2)			N(2)-C(7)-C(18)	122.04(13)	C(32)-C(29)-C(38)	122.55(16)
	C(9)-C(27)	1.394(2)			N(1)-C(7)-C(18)	125.61(12)	C(13)-C(29)-C(38)	118.79(14)
	C(9)-C(40)	1.531(2)			C(23)-C(8)-C(1)	117.02(13)	C(36)-C(30)-C(12)	121.83(14)
	C(11)-C(28)	1.403(2)			C(23)-C(8)-C(11)	122.65(14)	C(17)-C(31)-C(25)	113.79(14)
	C(12)-C(14)	1.411(2)			C(1)-C(8)-C(11)	120.33(12)	C(42)-C(32)-C(29)	121.04(17)
	C(12)-C(30)	1.435(2)			C(34)-C(9)-C(27)	117.34(13)	C(23)-C(33)-C(21)	120.39(14)
	C(13)-C(24)	1.416(2)			C(34)-C(9)-C(40)	119.70(13)	C(20)-C(34)-C(9)	121.92(13)
	C(13)-C(29)	1.421(2)			C(27)-C(9)-C(40)	122.95(13)	C(42)-C(35)-C(24)	120.35(17)
	C(14)-C(15)	1.394(2)			C(3)-C(10)-N(1)	105.23(12)	C(30)-C(36)-C(24)	121.92(15)
	C(14)-C(17)	1.478(2)			C(3)-C(10)-C(2)	122.91(13)	C(16)-C(37)-C(39)	119.90(15)
	C(15)-C(22)	1.379(2)			N(1)-C(10)-C(2)	131.62(12)	C(41)-C(38)-C(29)	121.67(15)
	C(16)-C(37)	1.368(2)			C(28)-C(11)-C(2)	117.46(13)	C(28)-C(39)-C(37)	120.21(15)
	C(17)-C(31)	1.359(2)			C(28)-C(11)-C(8)	121.50(13)	C(45)-C(40)-C(43)	108.66(16)
	C(18)-C(25)	1.365(2)			C(2)-C(11)-C(8)	121.03(13)	C(45)-C(40)-C(9)	109.26(14)
	C(19)-C(21)	1.369(2)			C(14)-C(12)-C(5)	118.96(13)	C(43)-C(40)-C(9)	112.64(13)
	C(20)-C(34)	1.380(2)			C(14)-C(12)-C(30)	123.37(13)	C(45)-C(40)-C(44)	109.69(16)
	C(21)-C(33)	1.392(2)			C(5)-C(12)-C(30)	117.60(13)	C(43)-C(40)-C(44)	107.90(15)
	C(23)-C(33)	1.368(2)			C(24)-C(13)-C(29)	119.83(14)	C(9)-C(40)-C(44)	108.66(14)
	C(24)-C(35)	1.398(2)			C(24)-C(13)-C(5)	120.34(13)	C(38)-C(41)-C(6)	121.35(16)
	C(24)-C(36)	1.432(2)			C(29)-C(13)-C(5)	119.82(14)	C(32)-C(42)-C(35)	120.98(16)
	C(25)-C(31)	1.407(2)			C(17)-S(1)-C(18)	92.50(7)	C(15)-C(14)-C(12)	119.24(13)