

Synthesis, crystal structure, aggregation-induced emission (AIE) and electroluminescence properties of a novel emitting material based on pyrrolo[3,2-b]pyrrole

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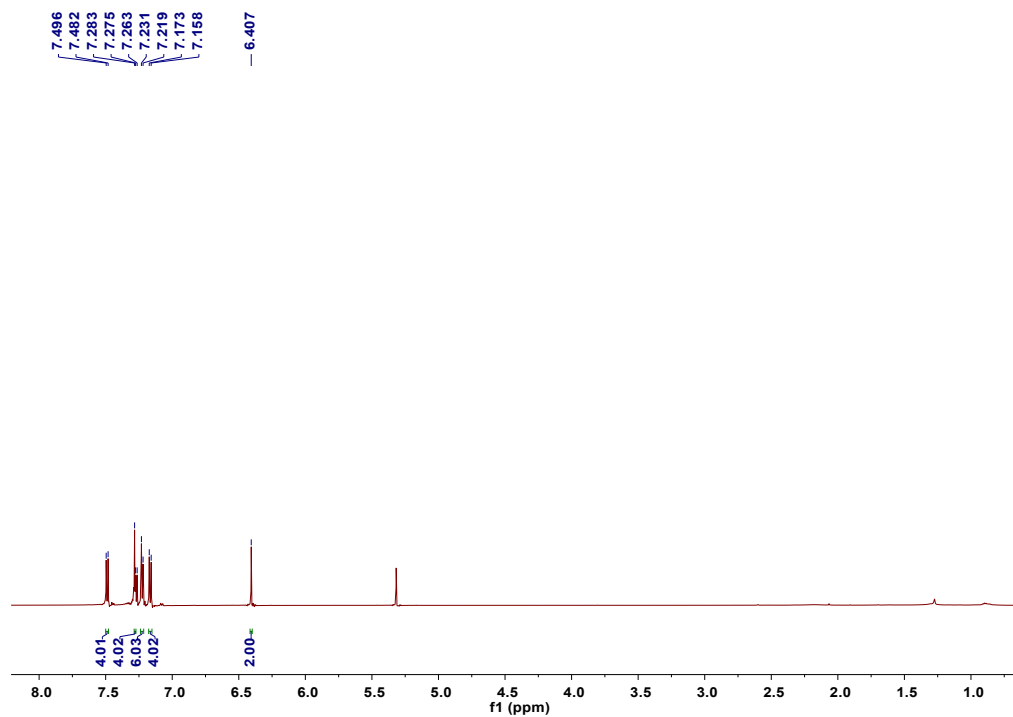
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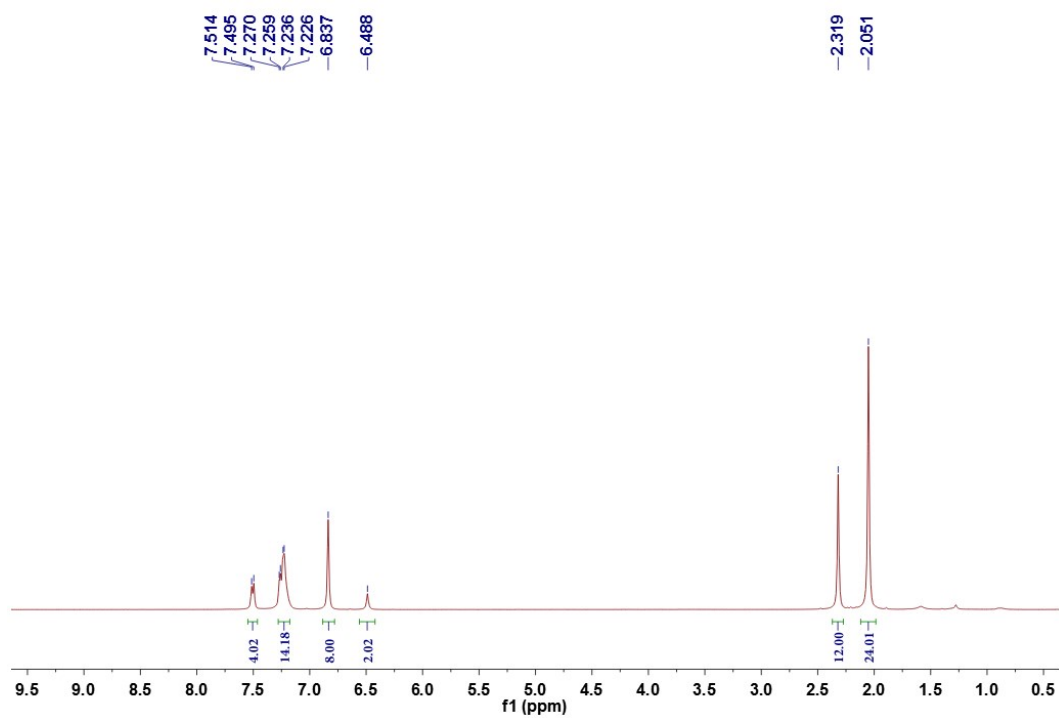
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Hongbo Wang[#] and Jinnan Huo[#] have equal contribution

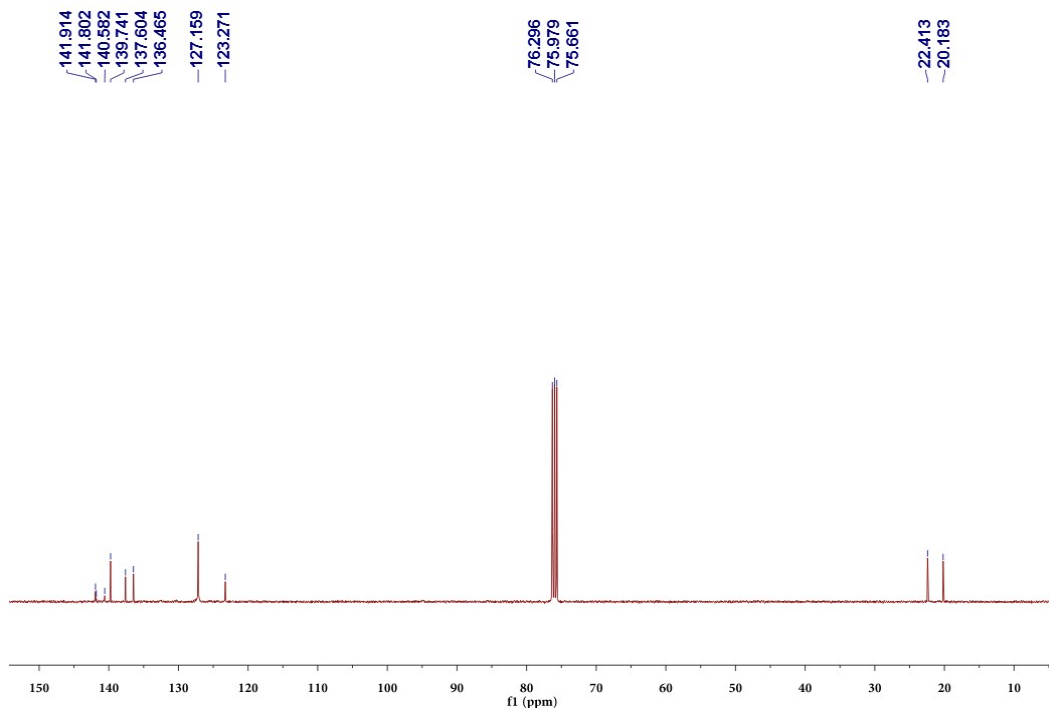
Electronic Supplementary Information (ESI)



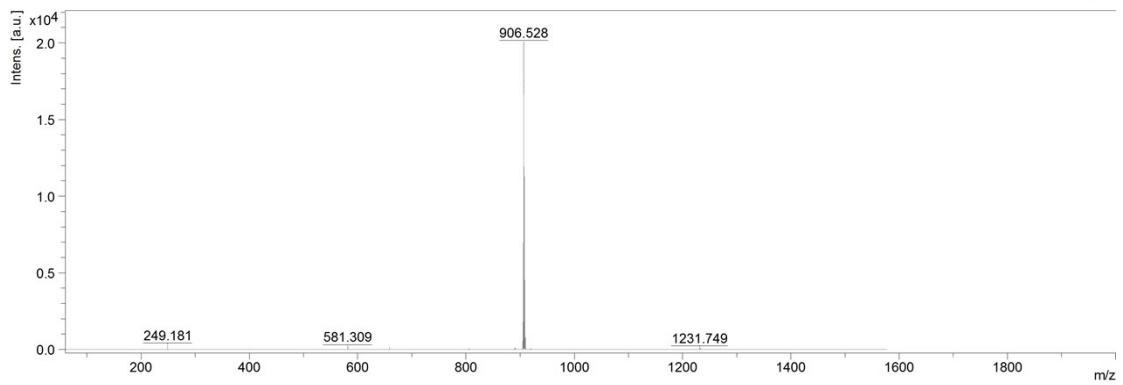
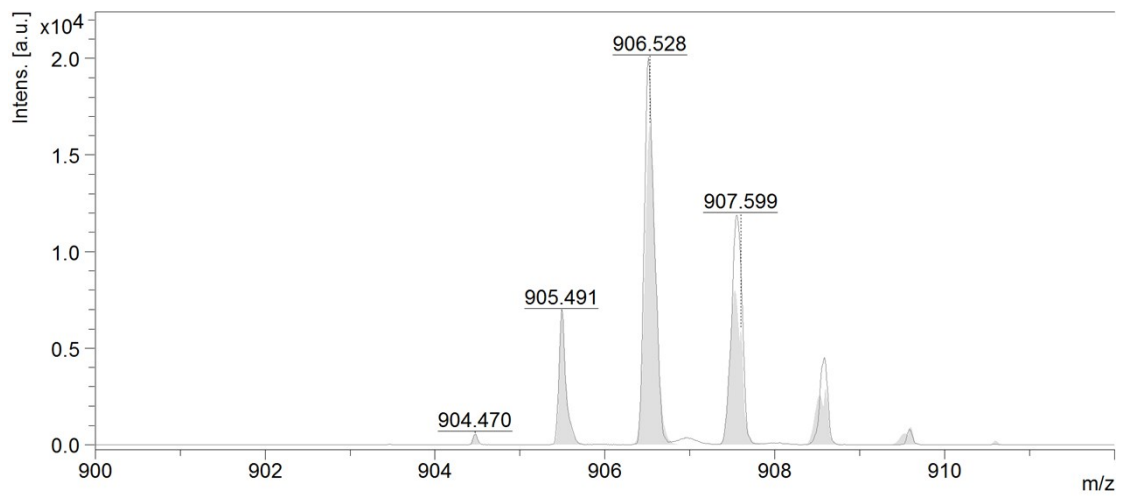
¹H NMR of compound 1



¹H NMR of DMBPDPP



^{13}C NMR of DMBPDPP



Mass spectra of DMBPDPP

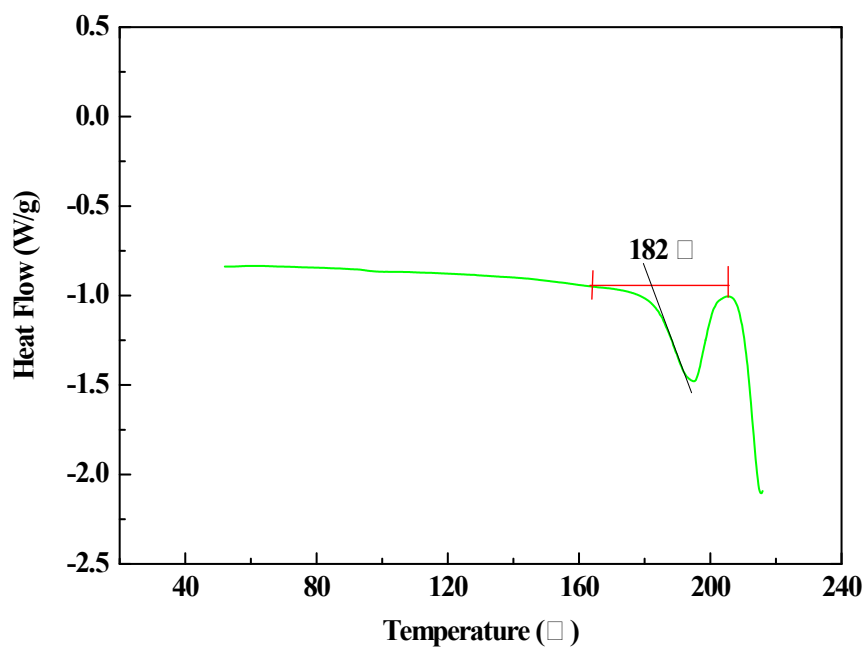
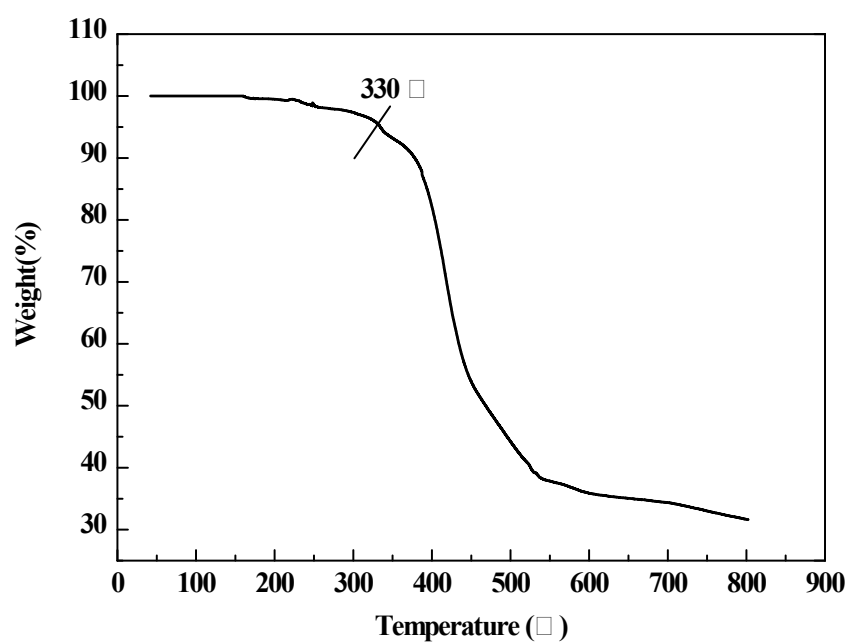


Fig. S1 TGA and DSC curves of DMBPDPP

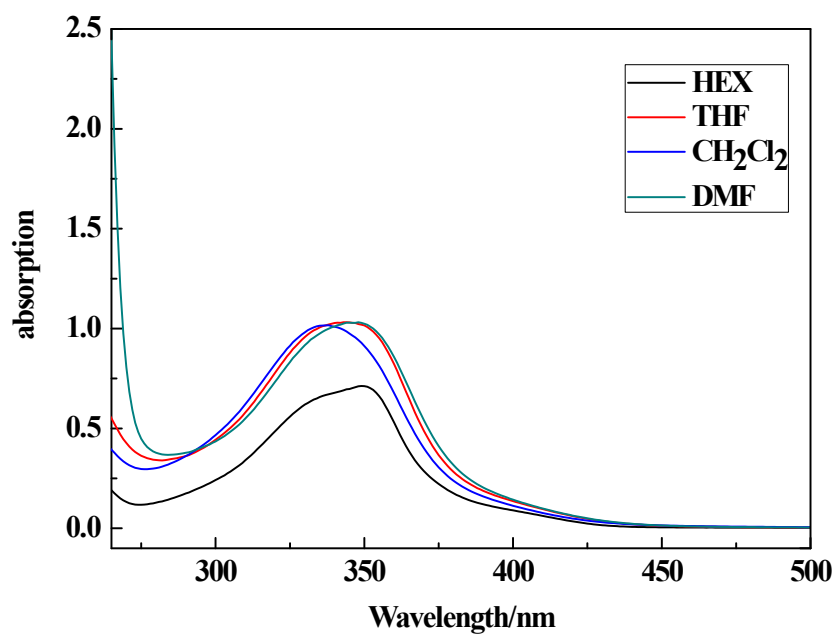


Fig. S2 UV-vis absorption spectra of DMBPDPP in different polar solvents (10^{-5} mol/L)

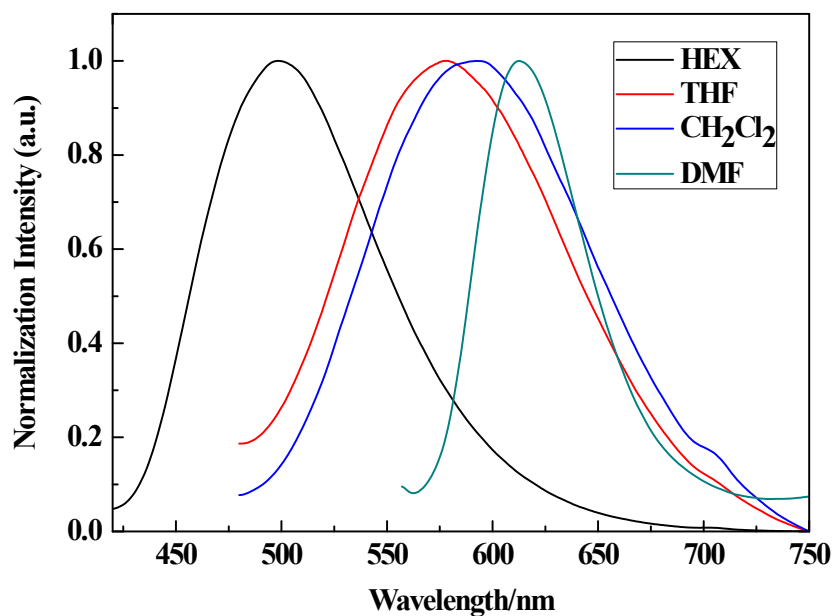


Fig. S3 Fluorescence emission spectra of DMBPDPP in different polar solvents (10^{-5} mol/L)

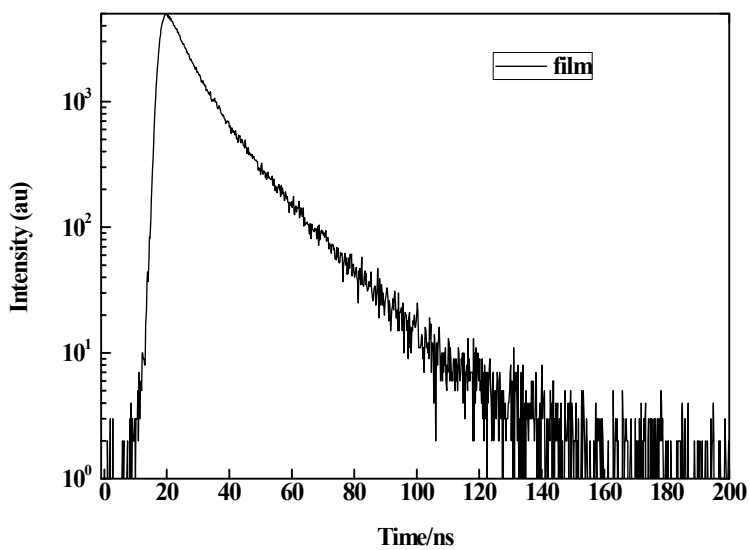


Fig. S4 Transient decay curves of DMBPDPP solid film at 300K

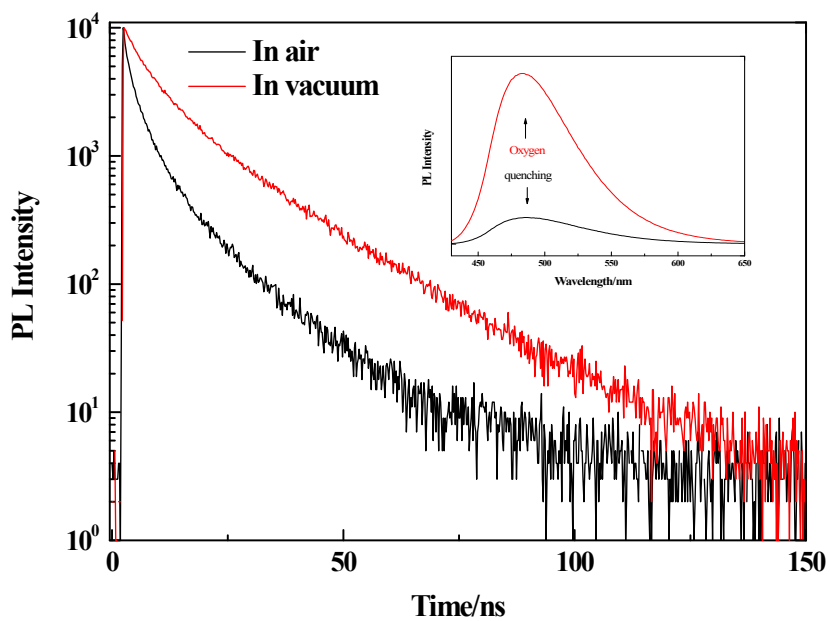


Fig.S5 Transient PL decay curves of DMBPDPP solid film in air/vacuum. Inset depicts PL spectra of DMBPDPP solid film in air/vacuum.

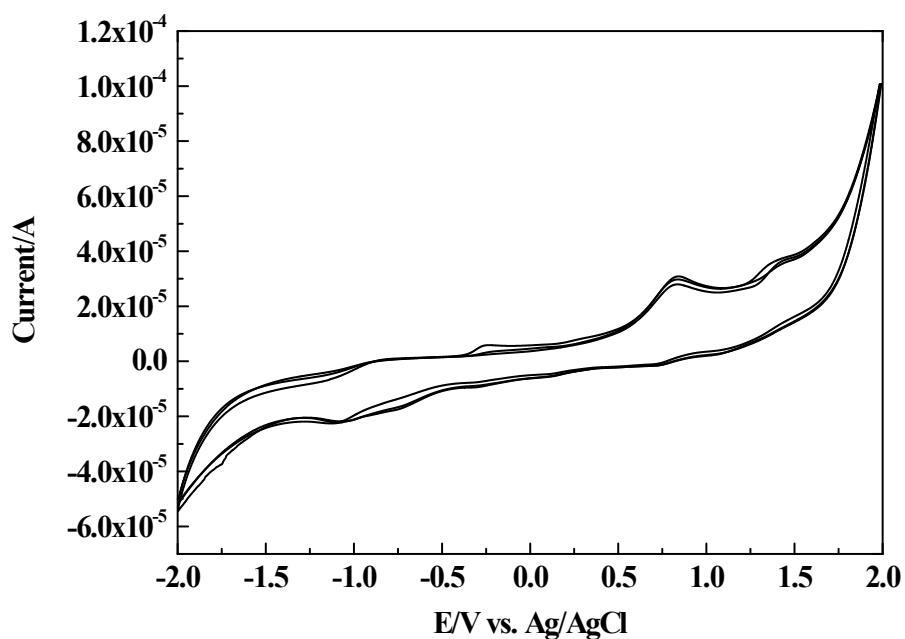


Fig. S6 The cyclic voltammogram curves of DMBPDPP in THF solvent (10^{-3} mol/L)

Table S1 Bond Distances of DMBPDPP (\AA)

Natation-1	Atom(I)	Atom(J)	Bond Distance	Natation	Atom(I)	Atom(J)	Bond Distance
1	N1	C22	1.416(3)	2	N1	C25	1.387(4)
3	N1	C28	1.406(3)	4	N2	C26	1.376(4)
5	N2	C36	1.402(4)	6	N2	C43	1.431(3)
7	C1	B1	1.576(5)	8	C10	B1	1.580(4)
9	C19	B1	1.551(4)	10	C19	C20	1.396(4)
11	C19	C24	1.391(4)	12	C43	C44	1.375(4)
13	C43	C48	1.392(4)	14	C45	C46	1.378(4)
15	C46	C47	1.404(4)	16	C46	B2	1.590(4)
17	C49	C50	1.405(5)	18	C49	C54	1.433(4)
19	C49	B2	1.571(5)	20	C58	C59	1.413(5)
21	C58	C63	1.421(5)	22	C58	B2	1.561(5)

Table S2 Torsion Angles of DMBPDPP

Torsion Angles	a	Torsion Angles	a
C25-N1 -C22 -C21	131.6(3)	C25-N1-C22-C23	-46.0(4)
C28-N1-C22-C21	-36.9(4)	C22-N1-C28-C27	169.9(3)
C22-N1-C28-C29	-17.9(5)	C43-N2-C26-C25	-167.5(3)
C43-N2-C36-C35	165.7(3)	C43-N2-C36-C37	-19.4(5)
C26-N2-C43-C44	-53.0(4)	C26-N2-C43-C48	124.8(3)
C36-N2-C43-C44	143.3(3)	C36-N2-C43-C48	-39.0(4)
N1-C28-C29-C30	-36.8(4)	N1-C28-C29-C34	147.4(3)
C27-C28-C29-C30	134.0(3)	C27-C28-C29-C34	-41.9(5)
N2-C36-C37-C38	152.0(3)	N2-C36-C37-C42	-30.0(5)
C35-C36-C37-C38	-34.0(5)	C10-B1-C1-C2	-116.9(4)
C10-B1-C1-C6	68.4(4)	C19-B1-C1-C2	60.3(4)
C19-B1-C1-C6	-114.4(3)	C1-B1-C10-C11	51.8(4)
C1-B1-C10-C15	-130.9(3)	C19-B1-C10-C11	-125.4(3)
C19-B1-C10-C15	51.9(4)	C46-B2-C49-C50	49.9(4)