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Red Emissive Diarylboron Diketonate Crystals: Aggregation-induced Color Change and Amplified Spontaneous Emission

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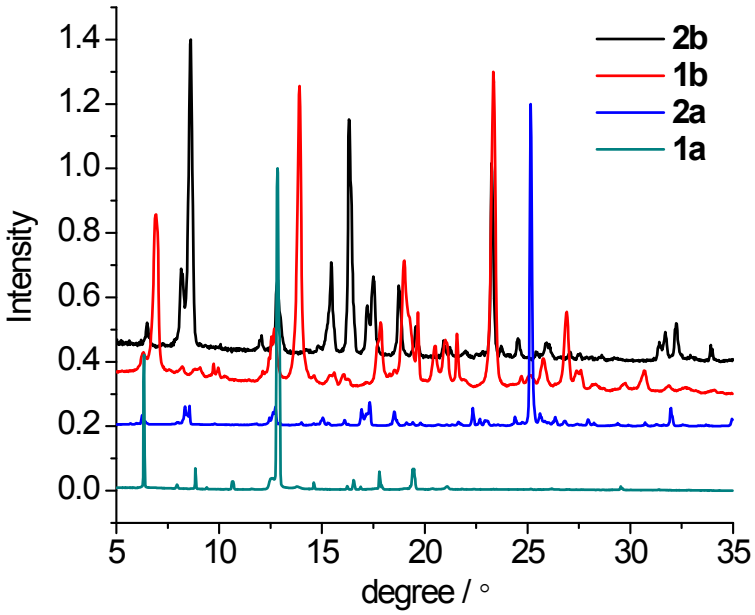

Fig. S1 PXRD patterns of different crystals.

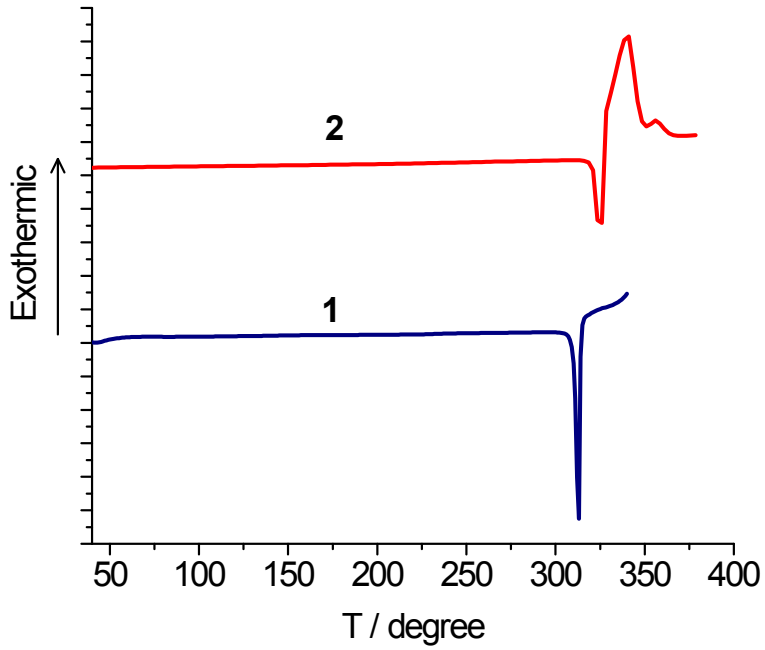

Fig. S2 The first heating curves of boron compounds **1** and **2** at a heating rate of 10 °C/min.

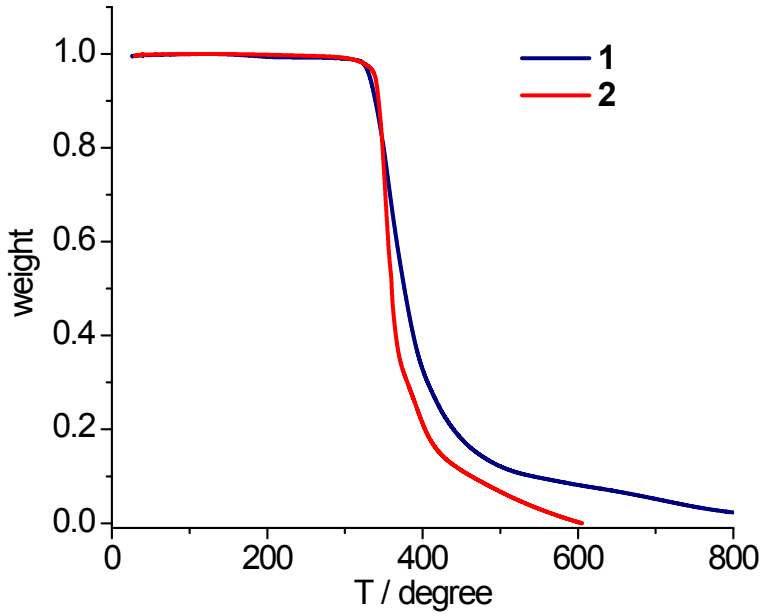

Fig. S3 TGA curves of **1** and **2** at a heating rate of 10 °C/min.

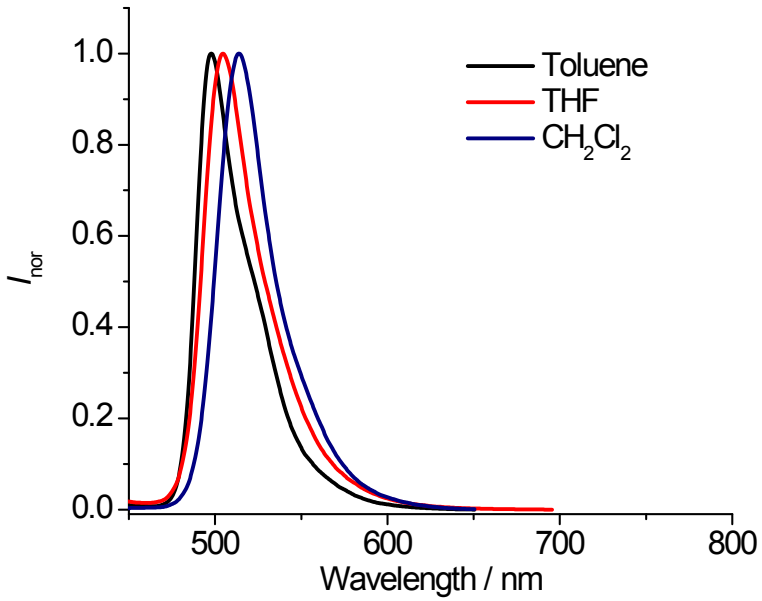

Fig. S4 Solvent-dependent emission spectra of boron compound **1**.

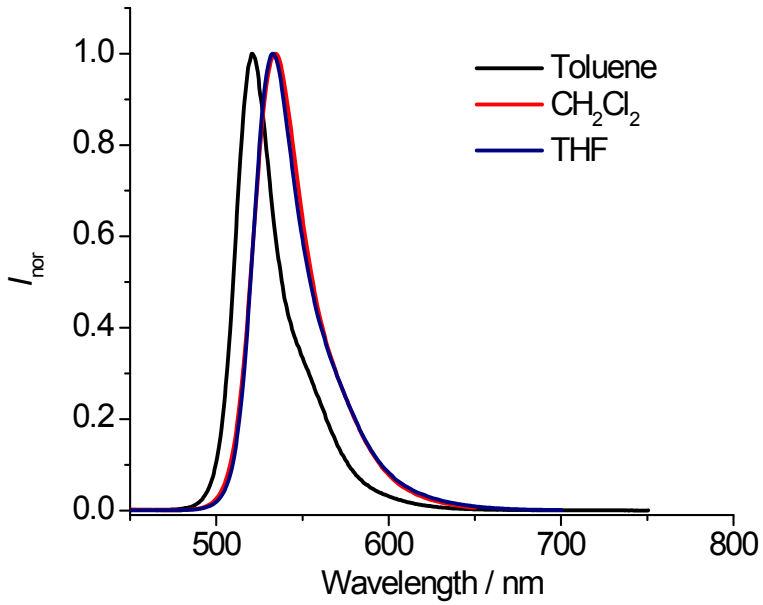

Fig. S5 Solvent-dependent emission spectra of boron compound **2**.

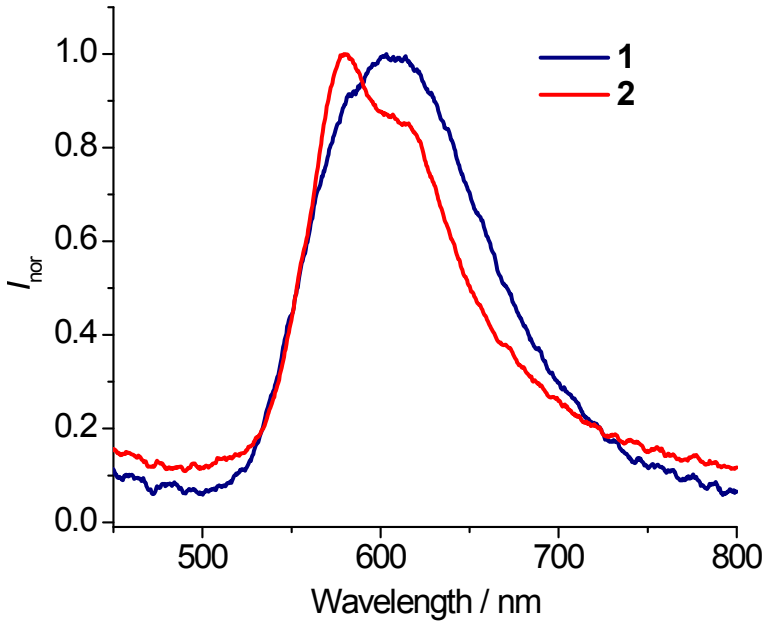

Fig. S6 PL spectra of thin films prepared by thermally vacuum sublimation approach.

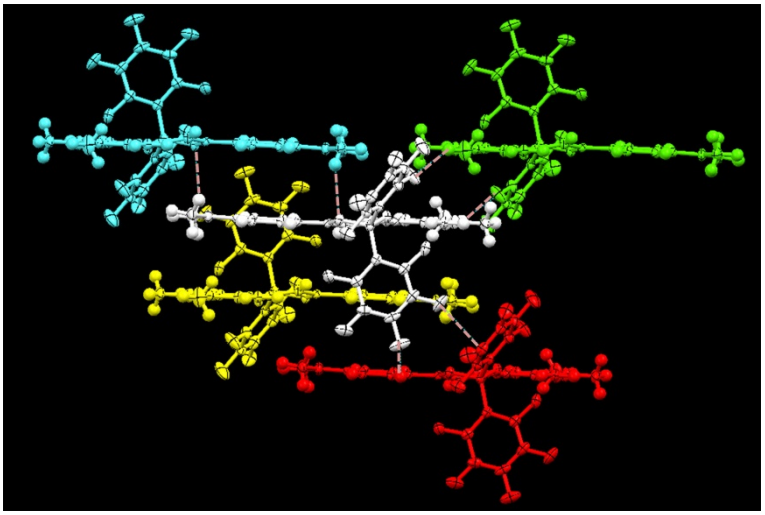

Fig. S7 Intermolecular interactions in crystal **2**: one molecule (white color) contact with four molecules through π ‒ π (yellow color), C–H···O (blue color), and C–H···F (red color) interactions.

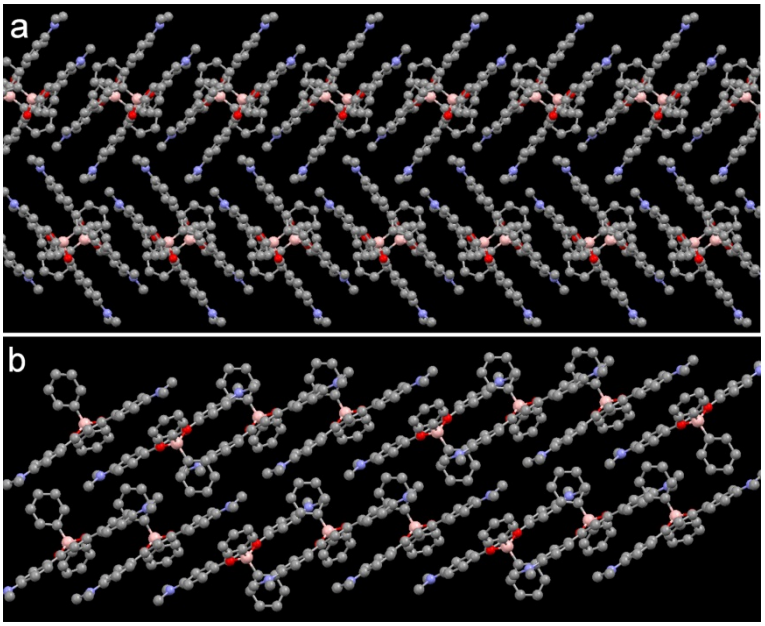

Fig. S8 Comparison of crystal packing structure between polymorphs **1a** (a) and **1b** (b).

Table S1 Selected bond lengths [Å] and angles [°] for **1a**, **1b** and **2a**.

Crystal 1a

B(1)-O(1)	1.516(4)	B(1)-O(2)	1.517(4)
B(1)-C(26)	1.603(4)	B(1)-C(20)	1.608(5)
O(1)-B(1)-O(2)	107.3(2)	O(1)-B(1)-C(26)	109.0(2)
O(2)-B(1)-C(26)	107.2(2)	O(1)-B(1)-C(20)	109.0(3)
O(2)-B(1)-C(20)	108.6(2)	C(26)-B(1)-C(20)	115.6(3)
C(7)-O(1)-B(1)	117.5(2)	C(9)-O(2)-B(1)	117.9(2)
C(21)-C(20)-B(1)	122.4(3)	C(25)-C(20)-B(1)	121.7(3)

Crystal 1b

B(1)-O(1)	1.508(9)	B(2)-O(4)	1.500(9)
B(1)-O(2)	1.514(9)	B(2)-O(3)	1.523(8)
B(1)-C(26)	1.574(10)	B(2)-C(51)	1.564(11)
B(1)-C(20)	1.617(11)	B(2)-C(57)	1.610(11)
B(3)-O(6)	1.504(9)	B(3)-C(88)	1.596(12)
B(3)-O(5)	1.533(9)	B(3)-C(82)	1.589(11)
O(1)-B(1)-O(2)	108.0(5)	O(4)-B(2)-O(3)	107.5(5)
O(1)-B(1)-C(26)	107.9(7)	O(4)-B(2)-C(51)	107.4(7)
O(2)-B(1)-C(26)	107.6(6)	O(3)-B(2)-C(51)	108.0(6)
O(1)-B(1)-C(20)	110.0(6)	O(4)-B(2)-C(57)	108.6(6)
O(2)-B(1)-C(20)	108.9(7)	O(3)-B(2)-C(57)	108.9(6)
C(26)-B(1)-C(20)	114.3(6)	C(51)-B(2)-C(57)	116.2(6)
C(25)-C(20)-B(1)	120.5(8)	C(52)-C(51)-B(2)	121.7(8)
C(21)-C(20)-B(1)	121.7(7)	C(56)-C(51)-B(2)	124.1(7)
O(6)-B(3)-O(5)	107.5(5)	C(88)-B(3)-C(82)	115.8(6)
O(6)-B(3)-C(88)	109.2(7)	C(69)-O(5)-B(3)	121.3(6)
O(5)-B(3)-C(88)	108.8(7)	C(71)-O(6)-B(3)	120.6(6)
O(6)-B(3)-C(82)	107.8(7)	C(83)-C(82)-B(3)	120.6(5)
O(5)-B(3)-C(82)	107.4(7)	C(87)-C(82)-B(3)	119.3(5)

Crystal 2a

B(1)-O(1)	1.495(3)	B(1)-O(2)	1.495(3)
B(1)-C(26)	1.630(4)	B(1)-C(20)	1.634(4)
O(1)-B(1)-O(2)	108.8(2)	O(1)-B(1)-C(26)	105.8(2)
O(2)-B(1)-C(26)	110.5(2)	O(1)-B(1)-C(20)	112.0(2)
O(2)-B(1)-C(20)	106.9(2)	C(26)-B(1)-C(20)	112.8(2)
C(7)-O(1)-B(1)	120.0(2)	C(9)-O(2)-B(1)	117.7(2)
C(25)-C(20)-B(1)	118.6(2)	C(21)-C(20)-B(1)	127.8(2)

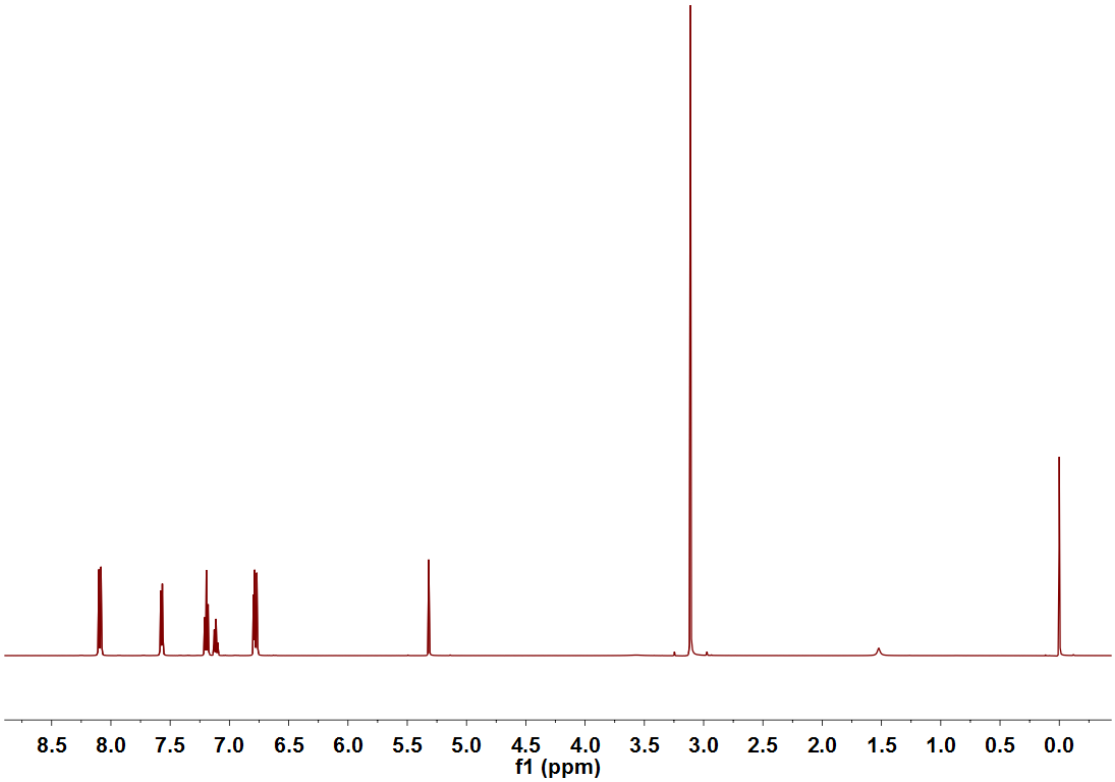

Fig. S9 ^{1}H NMR spectra of **1** recorded in CD_2Cl_2 (500 MHz).

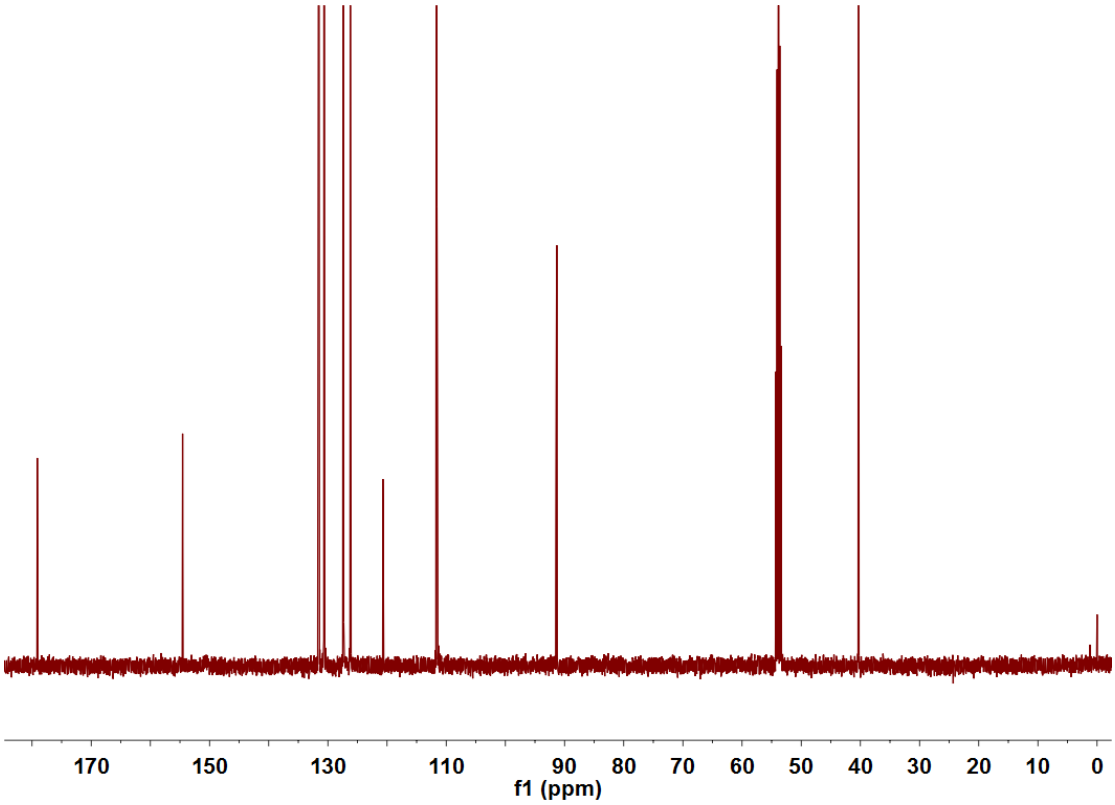

Fig. S10 ^{13}C NMR spectra of **1** recorded in CD_2Cl_2 (125 MHz).

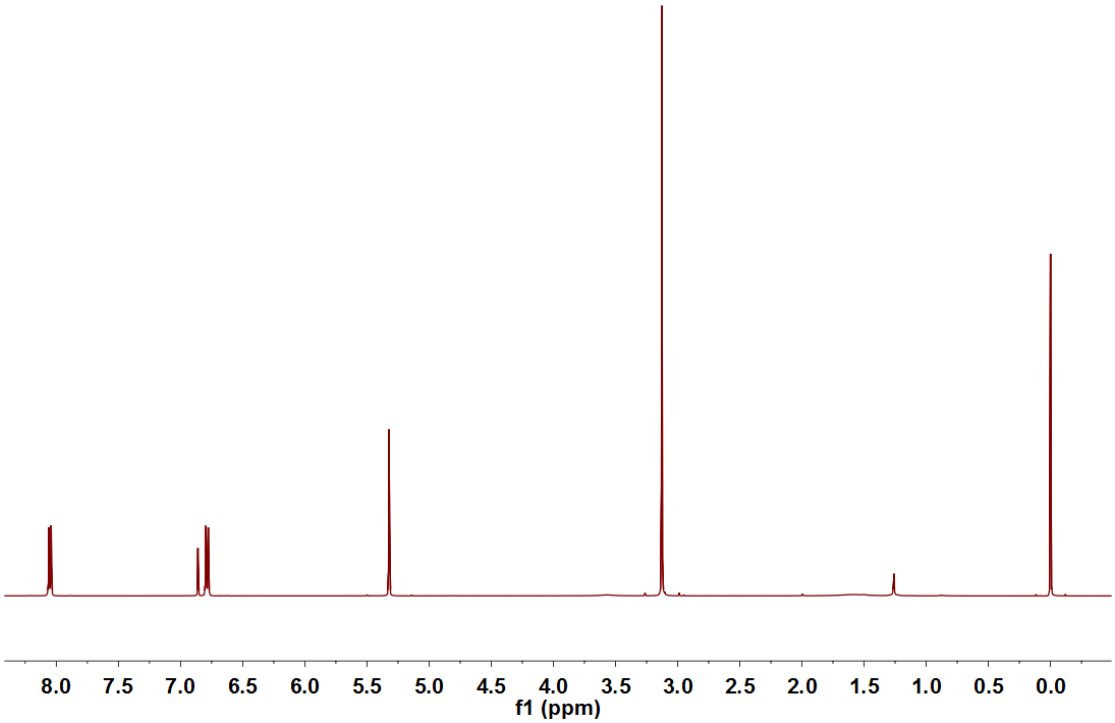

Fig. S11 ^{1}H NMR spectra of **2** recorded in CD_2Cl_2 (500 MHz).

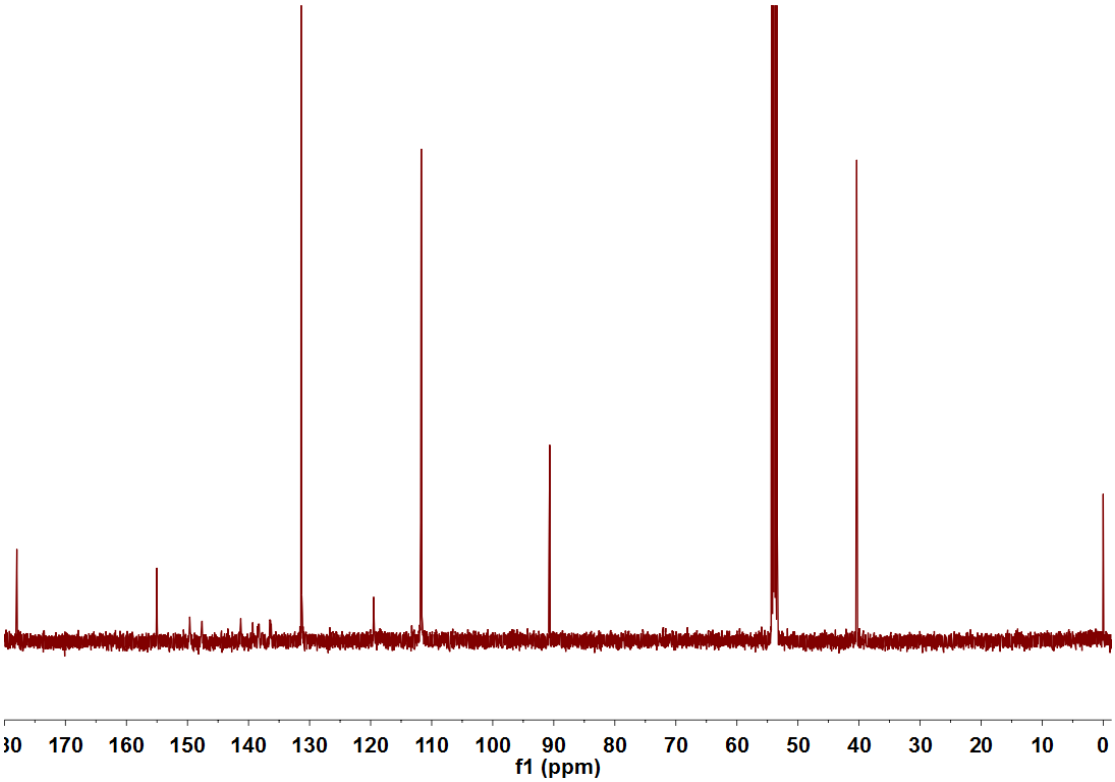

Fig. S12 ^{13}C NMR spectra of **2** recorded in CD_2Cl_2 (125 MHz).