

**Table S3.** The DFT bond angle data of the investigated compounds.

	<b>4c</b>		<b>6c</b>		<b>11c</b>
C(29)-C(30)-C(20)	121.3	C(27)-C(28)-C(18)	121.2	C(30)-C(31)-C(26)	120.3
C(30)-C(29)-C(28)	119.6	C(28)-C(27)-C(26)	119.3	C(31)-C(30)-C(29)	119.6
Cl(31)-C(28)-C(29)	119.6	Cl(29)-C(26)-C(27)	119.5	Cl(32)-C(29)-C(30)	119.4
Cl(31)-C(28)-C(27)	119.7	Cl(29)-C(26)-C(25)	119.7	Cl(32)-C(29)-C(28)	119.6
C(29)-C(28)-C(27)	120.7	C(27)-C(26)-C(25)	120.7	C(30)-C(29)-C(28)	121.0
C(28)-C(27)-C(26)	119.1	C(26)-C(25)-C(24)	119.4	C(29)-C(28)-C(27)	119.0
C(27)-C(26)-C(20)	121.8	C(25)-C(24)-C(18)	121.2	C(28)-C(27)-C(26)	120.9
C(24)-N(25)-C(8)	116.5	C(22)-N(23)-C(8)	116.5	C(31)-C(26)-C(27)	119.1
N(25)-C(24)-C(23)	122.8	N(23)-C(22)-C(21)	122.8	C(31)-C(26)-N(25)	125.2
C(24)-C(23)-N(22)	120.9	C(22)-C(21)-N(20)	120.9	C(27)-C(26)-N(25)	115.7
C(23)-N(22)-C(21)	116.9	C(21)-N(20)-C(19)	116.9	C(26)-N(25)-N(24)	114.0
N(22)-C(21)-C(8)	122.2	N(20)-C(19)-C(8)	122.3	N(25)-N(24)-C(15)	116.5
C(30)-C(20)-C(26)	117.5	C(28)-C(18)-C(24)	118.2	C(22)-N(23)-C(8)	116.5
C(30)-C(20)-C(19)	124.9	C(28)-C(18)-C(16)	121.9	N(23)-C(22)-C(21)	122.8
C(26)-C(20)-C(19)	117.6	C(24)-C(18)-C(16)	119.9	C(22)-C(21)-N(20)	120.9
C(20)-C(19)-C(15)	132.3	C(16)-N(17)-C(13)	111.4	C(21)-N(20)-C(19)	116.9
C(16)-N(17)-C(13)	112.1	C(18)-C(16)-N(17)	118.8	N(20)-C(19)-C(8)	122.2
O(18)-C(16)-N(17)	124.6	C(18)-C(16)-C(15)	126.2	C(16)-N(17)-C(13)	111.8
O(18)-C(16)-C(15)	122.8	N(17)-C(16)-C(15)	115.0	C(18)-C(16)-N(17)	119.0
N(17)-C(16)-C(15)	112.6	C(16)-C(15)-S(14)	110.7	C(18)-C(16)-C(15)	125.8
C(19)-C(15)-C(16)	120.6	C(15)-S(14)-C(13)	88.1	N(17)-C(16)-C(15)	115.2
C(19)-C(15)-S(14)	129.9	N(17)-C(13)-S(14)	114.8	N(24)-C(15)-C(16)	134.6
C(16)-C(15)-S(14)	109.4	N(17)-C(13)-N(12)	126.2	N(24)-C(15)-S(14)	115.9
C(15)-S(14)-C(13)	87.8	S(14)-C(13)-N(12)	118.9	C(16)-C(15)-S(14)	109.5
N(17)-C(13)-S(14)	118.0	H(38)-N(12)-C(13)	112.0	C(15)-S(14)-C(13)	88.0
N(17)-C(13)-N(12)	125.8	H(38)-N(12)-N(10)	107.8	N(17)-C(13)-S(14)	115.5
S(14)-C(13)-N(12)	116.1	C(13)-N(12)-N(10)	120.0	N(17)-C(13)-N(12)	124.6
H(40)-N(12)-C(13)	115.0	N(12)-N(10)-C(9)	117.0	S(14)-C(13)-N(12)	119.9
H(40)-N(12)-N(10)	110.2	C(11)-C(9)-N(10)	124.9	H(41)-N(12)-C(13)	113.1
C(13)-N(12)-N(10)	123.5	C(11)-C(9)-C(5)	119.2	H(41)-N(12)-N(10)	108.7
N(12)-N(10)-C(9)	117.6	N(10)-C(9)-C(5)	115.9	C(13)-N(12)-N(10)	121.2
C(11)-C(9)-N(10)	125.1	N(23)-C(8)-C(19)	120.6	N(12)-N(10)-C(9)	117.2
C(11)-C(9)-C(5)	119.2	N(23)-C(8)-N(7)	121.2	C(11)-C(9)-N(10)	125.0
N(10)-C(9)-C(5)	115.6	C(19)-C(8)-N(7)	118.2	C(11)-C(9)-C(5)	119.2
N(25)-C(8)-C(21)	120.7	H(34)-N(7)-C(8)	114.0	N(10)-C(9)-C(5)	115.8
N(25)-C(8)-N(7)	121.2	H(34)-N(7)-C(2)	114.1	N(23)-C(8)-C(19)	120.7
C(21)-C(8)-N(7)	118.1	C(8)-N(7)-C(2)	132.0	N(23)-C(8)-N(7)	121.2
H(36)-N(7)-C(8)	113.9	C(5)-C(6)-C(1)	122.3	C(19)-C(8)-N(7)	118.2
H(36)-N(7)-C(2)	114.1	C(9)-C(5)-C(6)	121.6	H(37)-N(7)-C(8)	114.0
C(8)-N(7)-C(2)	132.0	C(9)-C(5)-C(4)	121.0	H(37)-N(7)-C(2)	114.0
C(5)-C(6)-C(1)	122.3	C(6)-C(5)-C(4)	117.4	C(8)-N(7)-C(2)	132.0
C(9)-C(5)-C(6)	121.6	C(5)-C(4)-C(3)	121.0	C(5)-C(6)-C(1)	122.3

C(9)-C(5)-C(4)	121.0	C(4)-C(3)-C(2)	121.1	C(9)-C(5)-C(6)	121.6
C(6)-C(5)-C(4)	117.4	N(7)-C(2)-C(3)	116.8	C(9)-C(5)-C(4)	121.0
C(5)-C(4)-C(3)	121.0	N(7)-C(2)-C(1)	124.7	C(6)-C(5)-C(4)	117.4
C(4)-C(3)-C(2)	121.1	C(3)-C(2)-C(1)	118.5	C(5)-C(4)-C(3)	121.0
N(7)-C(2)-C(3)	116.7	C(6)-C(1)-C(2)	119.7	C(4)-C(3)-C(2)	121.1
N(7)-C(2)-C(1)	124.7			N(7)-C(2)-C(3)	116.7
C(3)-C(2)-C(1)	118.5			N(7)-C(2)-C(1)	124.7
C(6)-C(1)-C(2)	119.7			C(3)-C(2)-C(1)	118.5
				C(6)-C(1)-C(2)	119.7