

**Table S2.** The DFT bond length data of the investigated compounds.

	<b>4c</b>		<b>6c</b>		<b>11c</b>
C(29)-C(30)	1.39	C(27)-C(28)	1.40	C(30)-C(31)	1.39
C(28)-Cl(31)	1.75	C(26)-Cl(29)	1.76	C(29)-Cl(32)	1.76
C(28)-C(29)	1.40	C(26)-C(27)	1.398	C(29)-C(30)	1.40
C(27)-C(28)	1.40	C(25)-C(26)	1.396	C(28)-C(29)	1.40
C(26)-C(27)	1.39	C(24)-C(25)	1.396	C(27)-C(28)	1.396
C(24)-N(25)	1.34	C(22)-N(23)	1.343	C(26)-C(31)	1.41
C(23)-C(24)	1.39	C(21)-C(22)	1.391	C(26)-C(27)	1.405
N(22)-C(23)	1.35	N(20)-C(21)	1.349	N(25)-C(26)	1.415
C(21)-N(22)	1.32	C(19)-N(20)	1.323	N(24)-N(25)	1.278
C(20)-C(30)	1.41	C(18)-C(28)	1.407	C(22)-N(23)	1.343
C(20)-C(26)	1.41	C(18)-C(24)	1.407	C(21)-C(22)	1.391
C(19)-C(20)	1.46	C(16)-C(18)	1.477	N(20)-C(21)	1.349
C(16)-O(18)	1.22	C(16)-N(17)	1.392	C(19)-N(20)	1.323
C(16)-N(17)	1.40	C(15)-C(16)	1.37	C(16)-C(18)	1.5
C(15)-C(19)	1.35	S(14)-C(15)	1.743	C(16)-N(17)	1.369
C(15)-C(16)	1.52	C(13)-N(17)	1.3	C(15)-N(24)	1.37
S(14)-C(15)	1.77	C(13)-S(14)	1.773	C(15)-C(16)	1.395
C(13)-N(17)	1.30	N(12)-H(38)	1.015	S(14)-C(15)	1.775
C(13)-S(14)	1.808	N(12)-C(13)	1.391	C(13)-N(17)	1.317
N(12)-H(40)	1.015	N(10)-N(12)	1.417	C(13)-S(14)	1.754
N(12)-C(13)	1.359	C(9)-C(11)	1.509	N(12)-H(41)	1.015
N(10)-N(12)	1.411	C(9)-N(10)	1.295	N(12)-C(13)	1.38
C(9)-C(11)	1.507	C(8)-N(23)	1.338	N(10)-N(12)	1.415
C(9)-N(10)	1.298	C(8)-C(19)	1.424	C(9)-C(11)	1.508
C(8)-N(25)	1.337	N(7)-H(34)	1.012	C(9)-N(10)	1.296
C(8)-C(21)	1.423	N(7)-C(8)	1.384	C(8)-N(23)	1.338
N(7)-H(36)	1.012	C(5)-C(9)	1.486	C(8)-C(19)	1.423
N(7)-C(8)	1.385	C(5)-C(6)	1.404	N(7)-H(37)	1.012
C(5)-C(9)	1.484	C(4)-C(5)	1.411	N(7)-C(8)	1.384
C(5)-C(6)	1.405	C(3)-C(4)	1.386	C(5)-C(9)	1.485
C(4)-C(5)	1.411	C(2)-N(7)	1.404	C(5)-C(6)	1.404
C(3)-C(4)	1.385	C(2)-C(3)	1.414	C(4)-C(5)	1.411
C(2)-N(7)	1.402	C(1)-C(6)	1.397	C(3)-C(4)	1.385
C(2)-C(3)	1.414	C(1)-C(2)	1.405	C(2)-N(7)	1.403
C(1)-C(6)	1.396			C(2)-C(3)	1.414
C(1)-C(2)	1.406			C(1)-C(6)	1.397
				C(1)-C(2)	1.405