

Table 5S**Bond Lengths of H₂BT and its complexes**

No.	Ligand H ₂ BT		Co-complex		Cu-complex		Ni-complex	
	Bond name	Bond length (Å°)	Bond name	Bond length (Å°)	Bond name	Bond length (Å°)	Bond name	Bond length (Å°)
1	C(20)-O(25)	1.382	O(31)-H(49)	0.978	O(28)-H(44)	0.977	O(29)-C(30)	1.291
2	C(20)-C(21)	1.404	O(31)-H(48)	0.977	O(28)-H(43)	0.977	O(28)-H(46)	0.977
3	C(19)-C(20)	1.422	O(28)-C(29)	1.296	O(27)-H(42)	0.975	O(28)-H(45)	0.977
4	C(18)-H(34)	1.088	O(27)-C(29)	1.286	O(27)-H(41)	0.976	O(27)-C(30)	1.290
5	C(18)-C(19)	1.465	Co(26)-O(31)	2.201	O(28)-Cu(26)	2.083	O(29)-Ni(26)	2.092
6	N(16)-C(18)	1.303	Co(26)-O(28)	2.024	O(27)-Cu(26)	2.300	O(28)-Ni(26)	2.135
7	N(15)-H(33)	1.016	Co(26)-O(27)	2.072	O(25)-Cu(26)	2.071	O(27)-Ni(26)	2.122
8	N(15)-N(16)	1.391	O(25)-Co(26)	2.122	O(24)-Cu(26)	5.090	O(25)-Ni(26)	2.005
9	C(14)-O(17)	1.247	O(24)-Co(26)	2.011	O(23)-H(40)	0.977	O(23)-H(44)	0.977
10	C(14)-N(15)	1.380	C(18)-O(23)	1.381	C(18)-O(23)	1.376	C(16)-H(39)	1.094

11	C(12)-H(32)	1.096	N(15)-Co(26)	2.044	C(16)-H(35)	1.093	C(16)-C(17)	1.452
12	C(12)-H(31)	1.102	N(15)-C(16)	1.319	N(15)-Cu(26)	1.970	N(15)-Ni(26)	2.054
13	C(12)-C(14)	1.530	N(14)-N(15)	1.396	N(15)-C(16)	1.316	N(15)-C(16)	1.316
14	C(11)-O(13)	1.225	C(13)-O(24)	1.307	N(14)-N(15)	1.398	N(14)-N(15)	1.412
15	C(11)-C(12)	1.555	C(13)-N(14)	1.341	C(13)-O(25)	1.295	C(13)-O(25)	1.299
16	N(10)-H(30)	1.029	C(11)-O(25)	1.256	C(13)-N(14)	1.339	C(13)-N(14)	1.331
17	N(10)-C(11)	1.394	N(10)-C(11)	1.378	N(10)-C(11)	1.389	C(11)-O(24)	1.240
18	C(8)-N(10)	1.392	C(8)-N(10)	1.401	N(9)-Cu(26)	4.984	N(10)-H(36)	1.032
19	C(8)-N(9)	1.303	C(8)-N(9)	1.306	C(8)-N(10)	1.315	N(10)-C(11)	1.384
20	C(8)-S(7)	1.795	C(5)-N(9)	1.389	C(8)-N(9)	1.353	C(8)-N(10)	1.387