

Table 6S

Bond angles of H₂BT and its complexes

No.	Ligand H ₂ BT		Co-complex		Cu-complex		Ni-complex	
	Bond angle name	Bond angle (°)	Bond angle name	Bond angle(°)	Bond angle name	Bond angle (°)	Bond angle name	Bond angle(°)
1	C(24)-C(19)-C(18)	122.634	H(49)-O(31)-Co(26)	100.890	H(44)-O(28)-Cu(26)	110.668	C(30)-O(29)-Ni(26)	89.877
2	C(20)-C(19)-C(18)	119.425	H(48)-O(31)-Co(26)	106.664	H(43)-O(28)-Cu(26)	111.941	H(46)-O(28)-H(45)	104.094
3	H(34)-C(18)-C(19)	117.400	C(29)-O(28)-Co(26)	90.074	H(42)-O(27)-Cu(26)	111.502	H(46)-O(28)-Ni(26)	111.954
4	H(34)-C(18)-N(16)	122.635	C(29)-O(27)-Co(26)	88.241	H(41)-O(27)-Cu(26)	115.191	H(45)-O(28)-Ni(26)	111.855
5	C(19)-C(18)-N(16)	119.962	O(31)-Co(26)-O(28)	89.525	O(28)-Cu(26)-O(27)	89.336	C(30)-O(27)-Ni(26)	88.544
6	C(18)-N(16)-N(15)	118.178	O(31)-Co(26)-O(27)	85.756	O(28)-Cu(26)-O(25)	109.881	O(29)-Ni(26)-O(28)	94.598
7	H(33)-N(15)-N(16)	110.926	O(31)-Co(26)-O(25)	84.488	O(28)-Cu(26)-O(24)	123.397	O(29)-Ni(26)-O(27)	63.399
8	H(33)-N(15)-C(14)	116.658	O(31)-Co(26)-O(24)	86.337	O(28)-Cu(26)-N(15)	150.638	O(29)-Ni(26)-O(25)	96.071
9	N(16)-N(15)-C(14)	130.118	O(31)-Co(26)-N(15)	165.748	O(28)-Cu(26)-N(9)	152.254	O(29)-Ni(26)-O(24)	100.296
10	O(17)-C(14)-N(15)	123.868	O(28)-Co(26)-O(27)	64.923	O(27)-Cu(26)-O(25)	105.436	O(29)-Ni(26)-N(15)	165.428
11	O(17)-C(14)-C(12)	121.893	O(28)-Co(26)-O(25)	165.614	O(27)-Cu(26)-O(24)	82.985	O(28)-Ni(26)-O(27)	97.520
12	N(15)-C(14)-C(12)	114.229	O(28)-Co(26)-O(24)	108.174	O(27)-Cu(26)-N(15)	113.799	O(28)-Ni(26)-O(25)	99.305
13	H(32)-C(12)-H(31)	107.166	O(28)-Co(26)-N(15)	96.262	O(27)-Cu(26)-N(9)	69.454	O(28)-Ni(26)-O(24)	128.433
14	H(32)-C(12)-C(14)	113.457	O(27)-Co(26)-O(25)	101.507	O(25)-Cu(26)-O(24)	26.043	O(28)-Ni(26)-N(15)	99.975
15	H(32)-C(12)-C(11)	105.954	O(27)-Co(26)-O(24)	169.530	O(25)-Cu(26)-N(15)	82.224	O(27)-Ni(26)-O(25)	154.427
16	H(31)-C(12)-C(14)	106.191	O(27)-Co(26)-N(15)	108.494	O(25)-Cu(26)-N(9)	61.871	O(27)-Ni(26)-O(24)	133.249
17	H(31)-C(12)-C(11)	106.252	O(25)-Co(26)-O(24)	84.537	O(24)-Cu(26)-N(15)	79.176	O(27)-Ni(26)-N(15)	114.234
18	C(14)-C(12)-C(11)	117.212	O(25)-Co(26)-N(15)	92.624	O(24)-Cu(26)-N(9)	39.119	O(25)-Ni(26)-O(24)	30.505

19	O(13)-C(11)- C(12)	120.358	O(24)-Co(26)- N(15)	79.490	N(15)-Cu(26)-N(9)	57.093	O(25)-Ni(26)- N(15)	81.577
20	O(13)-C(11)- N(10)	126.370	Co(26)-O(25)- C(11)	128.625	Cu(26)-O(25)- C(13)	105.867	O(24)-Ni(26)- N(15)	70.464
21	C(12)-C(11)- N(10)	113.212	Co(26)-O(24)- C(13)	96.580	Cu(26)-O(24)- C(11)	71.041	Ni(26)-O(25)- C(13)	109.230
22	H(30)-N(10)- C(11)	113.904	Co(26)-N(15)- C(16)	137.810	Cu(26)-N(15)- C(16)	133.646	Ni(26)-O(24)- C(11)	40.599
23	H(30)-N(10)- C(8)	118.087	Co(26)-N(15)- N(14)	104.818	Cu(26)-N(15)- N(14)	112.707	Ni(26)-N(15)- C(16)	137.639
24	C(11)-N(10)- C(8)	127.996	C(16)-N(15)- N(14)	116.890	Cu(26)-N(9)-C(8)	114.897	Ni(26)-N(15)- N(14)	110.256
25	C(8)-N(9)-C(5)	110.186	N(15)-N(14)- C(13)	109.458	Cu(26)-N(9)-C(5)	123.460	C(16)-N(15)- N(14)	111.343