crystals

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Supplementary

Synthesis, Crystal Structure and Hirshfeld Topology Analysis of Polymeric Silver(I) Complex with *s*-Triazine-Type Ligand

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Table S1. Selected Interatomic distances [Å] for studied complex.

Ag1-N1	2.325(2)	Ag1-O11^{i}	2.565(2)
Ag1-O1	2.346(2)	Ag2-O6	2.672(3)
Ag1^{ii}-O1	2.685(2)	Ag2-O2	2.220(2)
Ag1-O8	2.699(1)	Ag2-N2	2.232(2)
Ag1-O9	2.699(2)	N1-C7	1.352(3)
N1-C9	1.371(3)	N2-C7	1.353(3)
N2-C8	1.366(3)	Cl1-O7	1.438(2)
Cl1-O8	1.445(2)	Cl1-O9	1.448(2)
Cl1-O10	1.451(2)	O3-Cl2	1.412(2)
N3-C9	1.339(3)	N3-C8	1.341(3)
Cl2-O5	1.439(2)	Cl2-O6	1.440(2)
Cl2-O4	1.443(2)	N5-C8	1.347(3)
N5-C18	1.464(3)	N5-C21	1.466(3)
N4-C9	1.345(3)	N4-C13	1.464(3)
N4-C10	1.470(3)	N6-C7	1.353(3)
N6-C14	1.464(3)	N6-C17	1.467(3)
C10-C11	1.521(3)	O11-C20	1.429(3)
O11-C19	1.436(3)	O11-Ag1	2.565(16)
C11-O12	1.441(3)	O12-C12	1.444(3)
C12-C13	1.513(3)	O13-C16	1.430(3)
O13-C15	1.441(3)	C14-C15	1.521(3)
C16-C17	1.515(3)	C18-C19	1.514(3)
C20-C21	1.515(3)		

(i) 1+x, y, z; (ii) -1+x, y, z.

Table S2. Selected Interatomic angles [°] for studied complex.

N1-Ag1-O1	163.26(7)	N1-Ag1-O11	104.52(6)
O1-Ag1-O11	86.15(6)	C7-N1-C9	113.76(18)
C7-N1-Ag1	117.55(13)	C9-N1-Ag1	103.47(13)
C7-N2-C8	113.79(18)	O2-Ag2-N2	156.41(7)
C8-N2-Ag2	115.30(14)	C7-N2-Ag2	118.27(13)
O8-Cl1-O9	109.13(10)	O7-Cl1-O10	109.52(11)
O8-Cl1-O10	109.46(11)	O9-Cl1-O10	109.39(10)
C9-N3-C8	114.23(18)	O3-Cl2-O5	109.94(14)
O3-Cl2-O6	110.38(16)	O5-Cl2-O6	107.04(14)
O3-Cl2-O4	110.71(12)	O5-Cl2-O4	109.79(12)
O6-Cl2-O4	108.90(14)	C8-N5-C18	122.13(18)
C8-N5-C21	123.14(19)	C18-N5-C21	114.57(18)
C9-N4-C13	122.68(18)	C9-N4-C10	123.17(18)
C13-N4-C10	113.47(17)	N3-C8-N5	118.24(19)
N3-C8-N2	124.7(2)	N5-C8-N2	117.08(19)
N3-C9-N4	119.36(19)	N3-C9-N1	124.18(19)
N4-C9-N1	116.45(19)	C7-N6-C14	121.69(18)
C7-N6-C17	122.38(18)	C14-N6-C17	112.73(17)
N1-C7-N2	124.22(19)	N1-C7-N6	117.59(19)
N2-C7-N6	118.15(19)	N4-C10-C11	110.00(18)
C20-O11-Ag1	117.77(13)	C20-O11-C19	109.17(17)
O12-C11-C10	111.38(19)	C19-O11-Ag1	131.06(13)
C11-O12-C12	109.06(17)	O12-C12-C13	110.64(18)
N6-C14-C15	109.28(19)	C16-O13-C15	109.99(17)
O13-C15-C14	111.58(19)	O11-C19-C18	110.82(18)
O13-C16-C17	110.39(18)	O11-C20-C21	111.63(19)
N6-C17-C16	108.99(18)	N5-C21-C20	109.27(19)
N5-C18-C19	109.06(19)	N4-C13-C12	109.36(18)

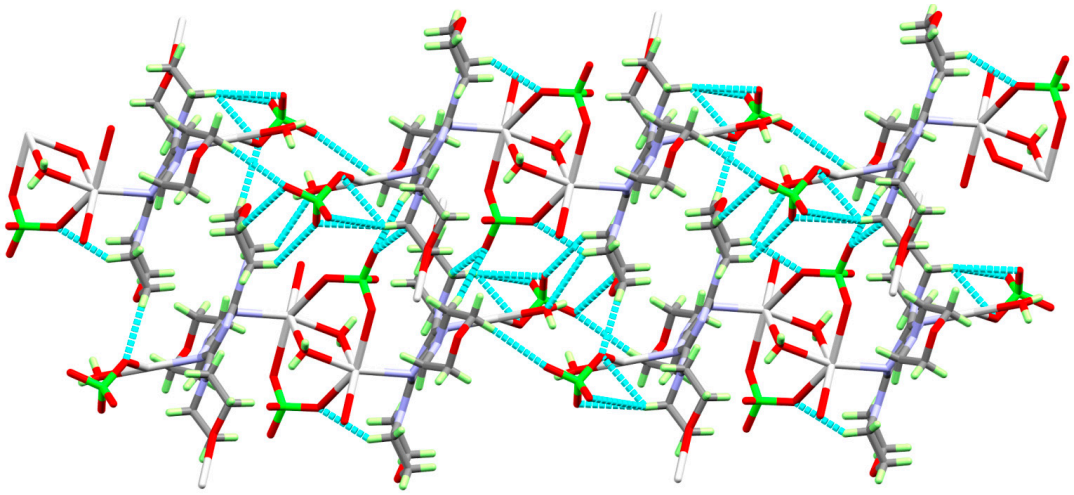

Figure S1 The hydrogen bonding network along the viewing b-direction in the studied silver(I) complex.

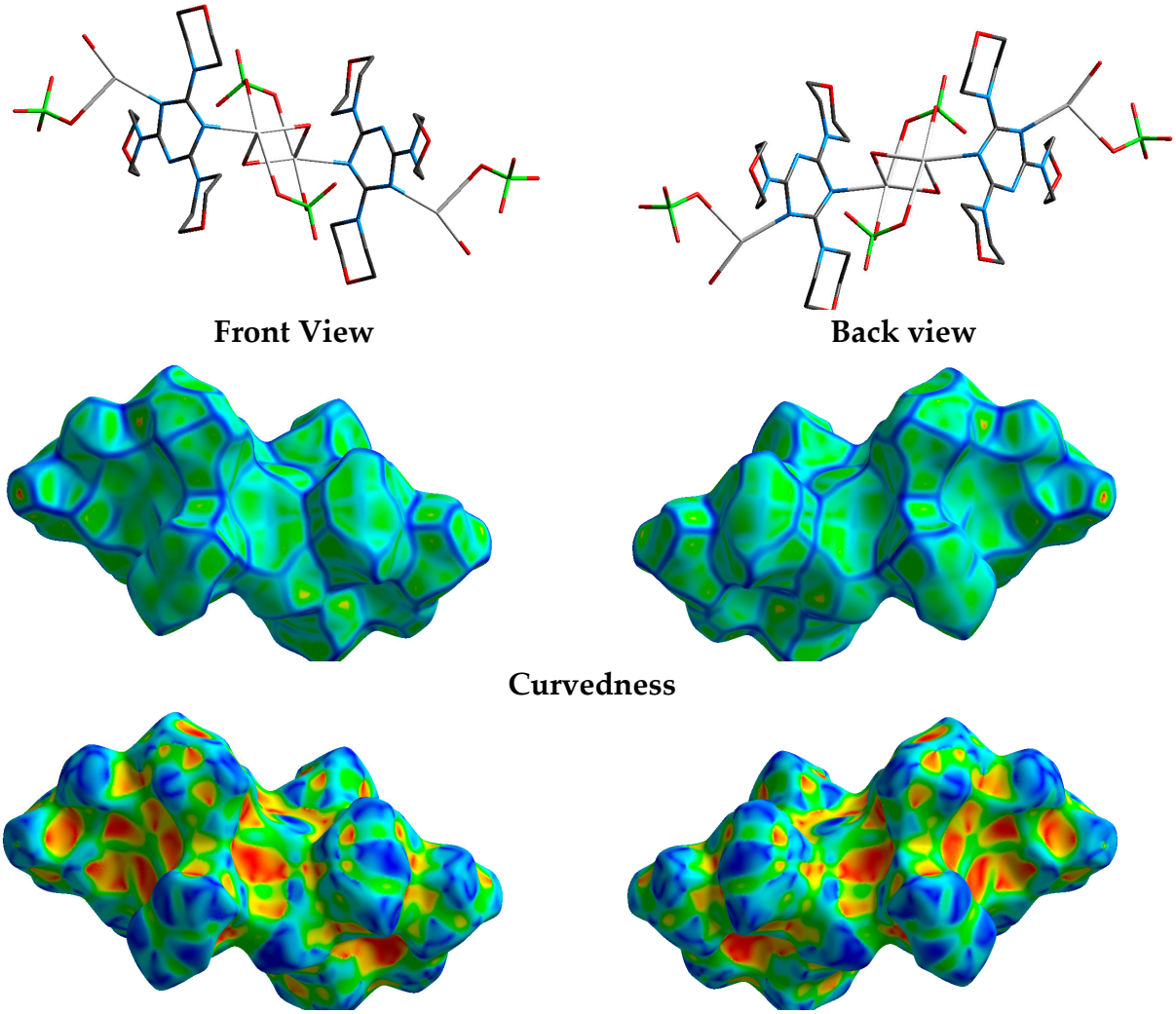

Figure S2. The shape index (SI) and curvedness Hirshfeld surfaces of the **$[Ag_2L(H_2O)_2(ClO_4)_2]_n$** complex.

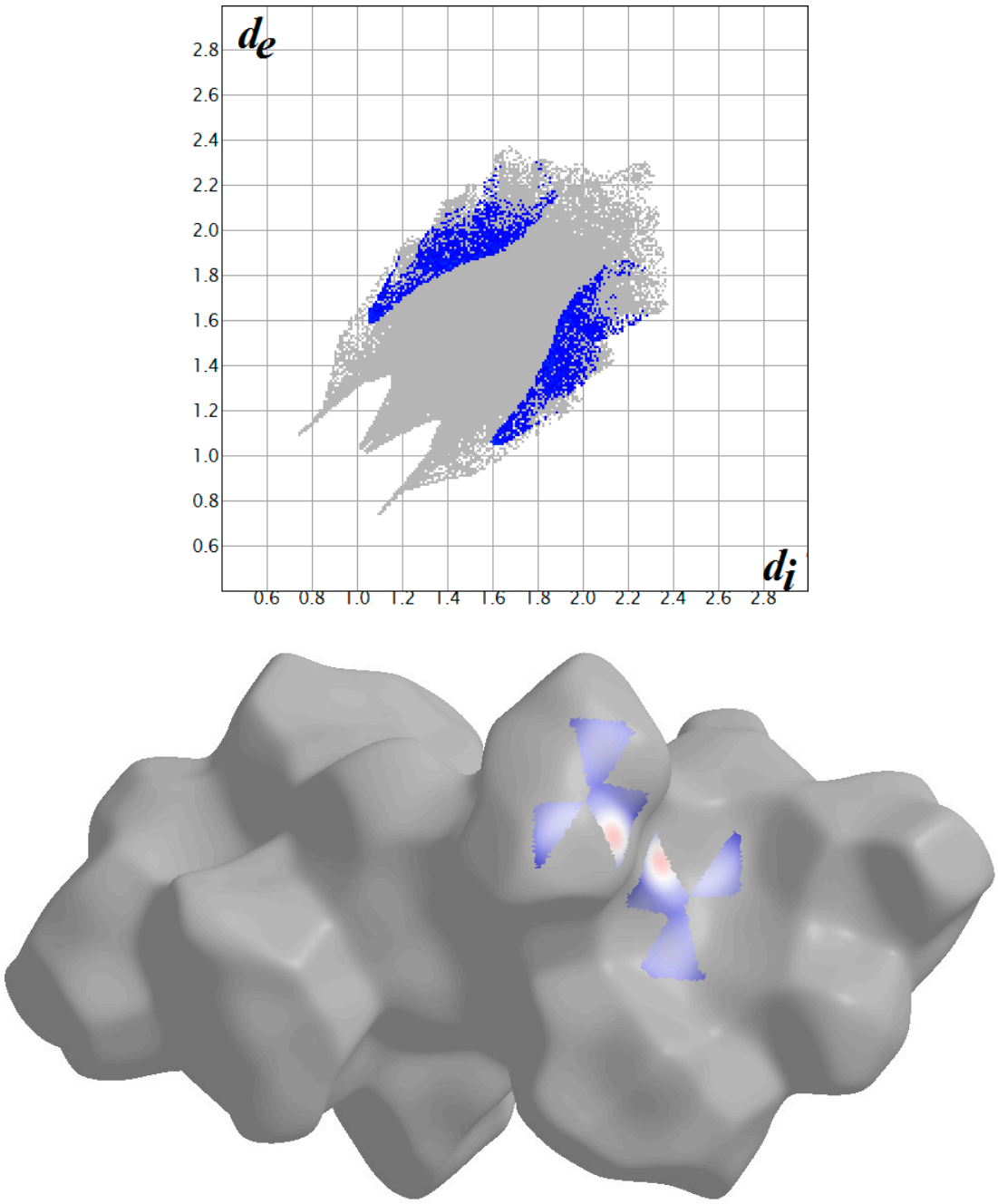

Figure S3. The decomposed fingerprint plot (upper) and d_{norm} map (lower) of the C…H interactions.

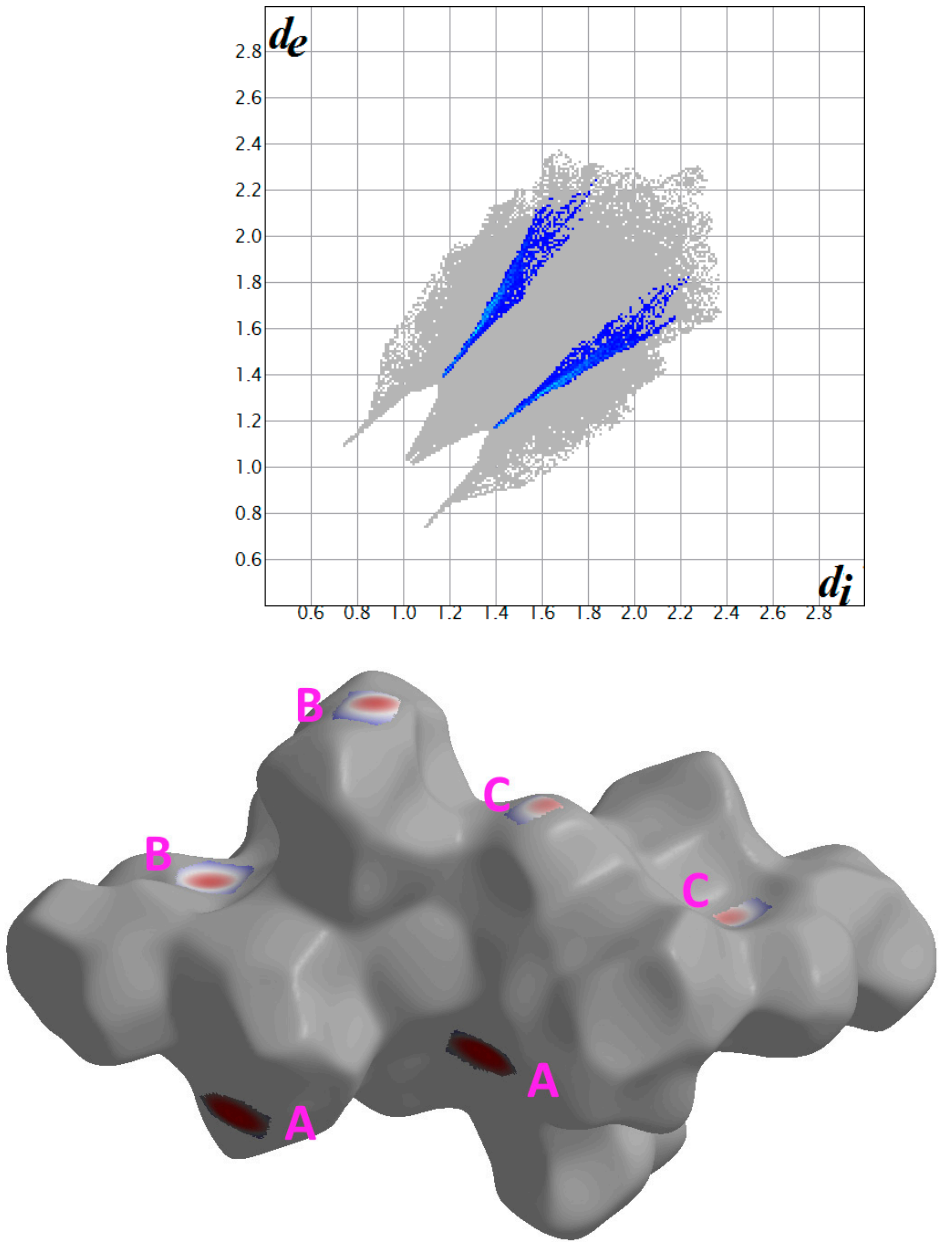

Figure S4. The decomposed FP plot (upper) and the d_{norm} map (lower) of the Ag...O interactions; A) Ag1…O11 (2.565 Å), B) Ag2….O12 (2.879 Å) and C) Ag2…O7 (2.996 Å). Note the significant difference of the red color intensity.

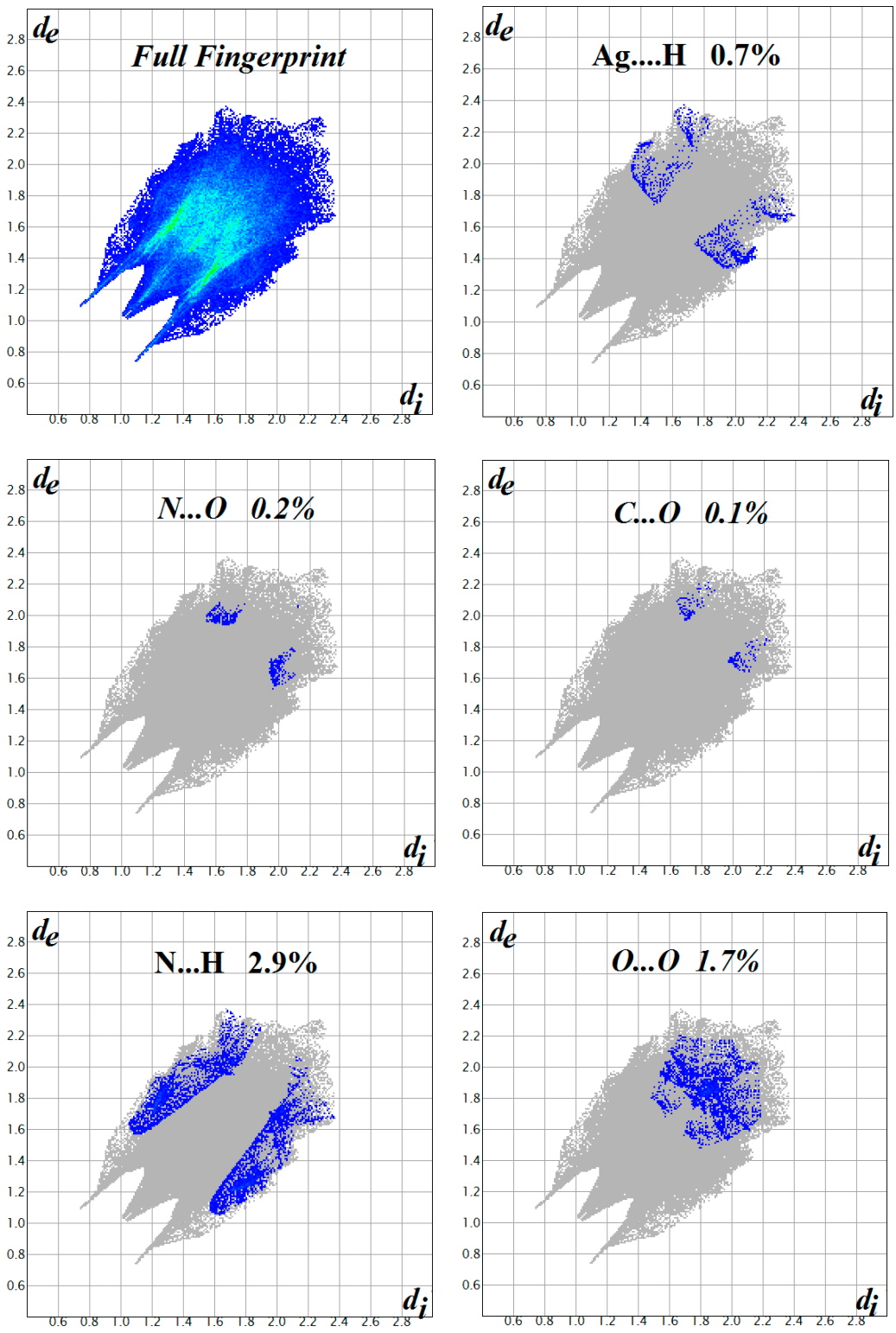

Figure S5. The decomposed fingerprint plot of the less important contacts observed in the crystal of the studied complex.

Table S3. The detailed intramolecular charge transfer interactions included in the Ag-N and Ag-O interactions using different DFT methods.

NBO$_i$	NBO$_i$	B97D	WB97XD	B3LYP	NBO$_i$	NBO$_i$	B97D	WB97XD	B3LYP
LP(1)N1	LP*(6)Ag1	7.13	3.64	5.31	LP(1)N2	LP*(6)Ag2	24.22	30.83	25.80
LP(1)N1	LP*(7)Ag1	3.67	12.10	6.63	LP(1)N2	LP*(7)Ag2	3.32	5.55	4.03
LP(1)N1	LP*(8)Ag1	0.77	1.27	0.93	LP(1)N2	LP*(8)Ag2	2.53	2.99	2.70
LP(1)N1	LP*(9)Ag1	1.72	1.56	1.76	LP(1)N2	LP*(9)Ag2	1.41	0.93	1.22
LP(1)O1	LP*(6)Ag1	0.22	0.00	0.13	LP(1)O2	LP*(6)Ag2	0.83	0.24	0.52
LP(1)O1	LP*(7)Ag1	2.60	4.15	3.18	LP(1)O2	LP*(7)Ag	0.57	0.56	0.56
LP(1)O1	LP*(9)Ag1	0.13	0.60	0.29	LP(1)O2	LP*(8)Ag2	3.46	3.41	3.49
LP(2)O1	LP*(6)Ag1	5.48	8.11	6.07	LP(1)O2	LP*(9)Ag2	0.14	0.73	0.30
LP(2)O1	LP*(7)Ag1	2.22	0.97	1.76	LP(2)O2	LP*(6)Ag2	22.20	27.62	23.39
LP(2)O1	LP*(9)Ag1	1.39	1.73	1.42	LP(2)O2	LP*(8)Ag2	4.57	7.31	5.44
					LP(2)O2	LP*(9)Ag2	0.45	0.31	0.38
LP(1)O1	LP*(6)Ag1^{ii}	1.92	1.13	1.53					
LP(1)O1	LP*(7)Ag1^{ii}	0.38	0.29	0.05					
LP(1)O1	LP*(9)Ag1^{ii}	2.96	2.97	2.90					
LP(2)O1	LP*(6)Ag1^{ii}	2.25	8.68	4.48					
LP(2)O1	LP*(7)Ag1^{ii}	7.37	5.79	7.30					
LP(2)O1	LP*(9)Ag1^{ii}	0.90	1.50	1.17					
LP(1)O8	LP*(6)Ag1	4.74	7.61	6.03	LP(1)O6	LP*(6)Ag2	3.29	5.30	4.07
LP(1)O8	LP*(7)Ag1	0.77	-	0.25	LP(1)O6	LP*(7)Ag2	7.63	8.78	8.15
LP(1)O8	LP*(8)Ag1	12.79	15.60	13.94	LP(1)O6	LP*(8)Ag2	1.95	3.33	2.50
LP(1)O8	LP*(9)Ag1	2.06	2.90	2.31	LP(2)O6	LP*(6)Ag2	0.13	0.16	0.18
LP(2)O8	LP*(6)Ag1	0.29	0.32	0.30	LP(2)O6	LP*(8)Ag2	0.20	0.41	0.27
LP(2)O8	LP*(7)Ag1	0.07	0.25	0.11	LP(2)O6	LP*(9)Ag2	0.79	0.89	0.82
LP(2)O8	LP*(8)Ag1	0.25	0.51	0.32	LP(3)O6	LP*(6)Ag2	7.57	7.99	7.14
LP(2)O8	LP*(9)Ag1	0.34	0.39	0.35	LP(3)O6	LP*(7)Ag2	2.62	2.98	2.69
LP(3)O8	LP*(6)Ag1	0.92	1.07	0.83	LP(3)O6	LP*(8)Ag2	0.29	0.44	0.33
LP(3)O8	LP*(7)Ag1	0.22	0.08	0.17					
LP(3)O8	LP*(8)Ag1	0.46	0.36	0.37					
LP(3)O8	LP*(9)Ag1	0.12	0.25	0.19					
LP(1)O9	LP*(6)Ag1	4.00	5.43	4.65					
LP(1)O9	LP*(7)Ag1	0.45	19.36	0.13					
LP(1)O9	LP*(8)Ag1	14.91	1.23	16.71					
LP(1)O9	LP*(9)Ag1	0.66	0.37	0.76					
LP(2)O9	LP*(6)Ag1	0.17	0.07	0.27					
LP(2)O9	LP*(8)Ag1	0.14	0.53	0.27					
LP(2)O9	LP*(9)Ag1	0.89	0.77	0.79					
LP(3)O9	LP*(6)Ag1	0.93	0.83	0.73					
LP(3)O9	LP*(7)Ag1	0.13	0.46	0.08					
LP(3)O9	LP*(8)Ag1	0.59	0.54	0.49					
LP(1)O11	LP*(6)Ag1	4.54	2.13	3.48					
LP(1)O11	LP*(7)Ag1	3.60	9.87	5.94					
LP(1)O11	LP*(8)Ag1	3.02	3.30	3.11					
LP(1)O11	LP*(9)Ag1	1.57	1.87	1.67					
LP(2)O11	LP*(6)Ag1	1.24	1.13	1.09					
LP(2)O11	LP*(7)Ag1	0.12	0.64	0.26					
LP(2)O11	LP*(8)Ag1	1.26	1.50	1.26					
LP(2)O11	LP*(9)Ag1	1.26	1.67	1.35					
LP(5)Ag1	LP*(7)Ag1	0.82	0.97	1.08					

Table S4. The AIM topological parameters calculated using different DFT methods.

	Ag-N/Ag-O (Å)	ρ (r) a.u.	G (r) a.u.	V (r) a.u.	H (r) a.u.	V(r)/G(r)	E_{int}(kcal/mol)
B97D							
Ag1-N1	2.325	0.0499	0.0713	-0.0761	-0.0048	1.07	23.87
Ag1-O1	2.346	0.0427	0.0611	-0.0626	-0.0016	1.03	19.66
Ag1-O8	2.699	0.0200	0.0224	-0.0240	-0.0016	1.07	7.53
Ag1^{ii}-O1	2.685	0.0207	0.0235	-0.0253	-0.0017	1.07	7.93
Ag1-O9	2.699	0.0203	0.0226	-0.0242	-0.0016	1.07	7.59
Ag1-O11	2.565	0.0270	0.0326	-0.0345	-0.0018	1.06	10.81
Ag2-N2	2.231	0.0585	0.0969	-0.1015	-0.0046	1.05	31.86
Ag2-O2	2.22	0.0519	0.0901	-0.0891	0.0009	0.99	27.97
Ag2-O6	2.672	0.0214	0.0250	-0.0262	-0.0012	1.05	8.22
Wb97XD							
Ag1-N1	2.325	0.0513	0.0720	-0.0773	-0.0054	1.07	24.26
Ag1-O1	2.346	0.0434	0.0616	-0.0635	-0.0018	1.03	19.91
Ag1-O8	2.699	0.0202	0.0226	-0.0244	-0.0018	1.08	7.64
Ag1^{ii}-O1	2.685	0.0208	0.0238	-0.0256	-0.0018	1.07	8.02
Ag1-O9	2.699	0.0205	0.0228	-0.0245	-0.0017	1.08	7.70
Ag1-O11	2.565	0.0274	0.0331	-0.0351	-0.0021	1.06	11.02
Ag2-N2	2.231	0.0607	0.0980	-0.1038	-0.0058	1.06	32.56
Ag2-O2	2.22	0.0531	0.0905	-0.0902	0.0003	1.00	28.30
Ag2-O6	2.672	0.0217	0.0253	-0.0266	-0.0013	1.05	8.33
B3LYP							
Ag1-N1	2.325	0.0509	0.0717	-0.0769	-0.0052	1.07	24.13
Ag1-O1	2.346	0.0432	0.0616	-0.0634	-0.0018	1.03	19.91
Ag1-O8	2.699	0.0202	0.0226	-0.0243	-0.0017	1.08	7.63
Ag1^{ii}-O1	2.685	0.0208	0.0238	-0.0256	-0.0017	1.07	8.02
Ag1-O9	2.699	0.0205	0.0228	-0.0245	-0.0017	1.07	7.68
Ag1-O11	2.565	0.0273	0.0330	-0.0350	-0.0020	1.06	10.97
Ag2-N2	2.231	0.0597	0.0976	-0.1029	-0.0053	1.05	32.30
Ag2-O2	2.22	0.0527	0.0906	-0.0902	0.0005	0.99	28.29
Ag2-O6	2.672	0.0216	0.0252	-0.0265	-0.0013	1.05	8.31

[a]ρ(r): Total electron density, [b]G(r): local electron kinetic energy density, [c]V(r): local electron potential energy density and [d]H(r): total energy density.

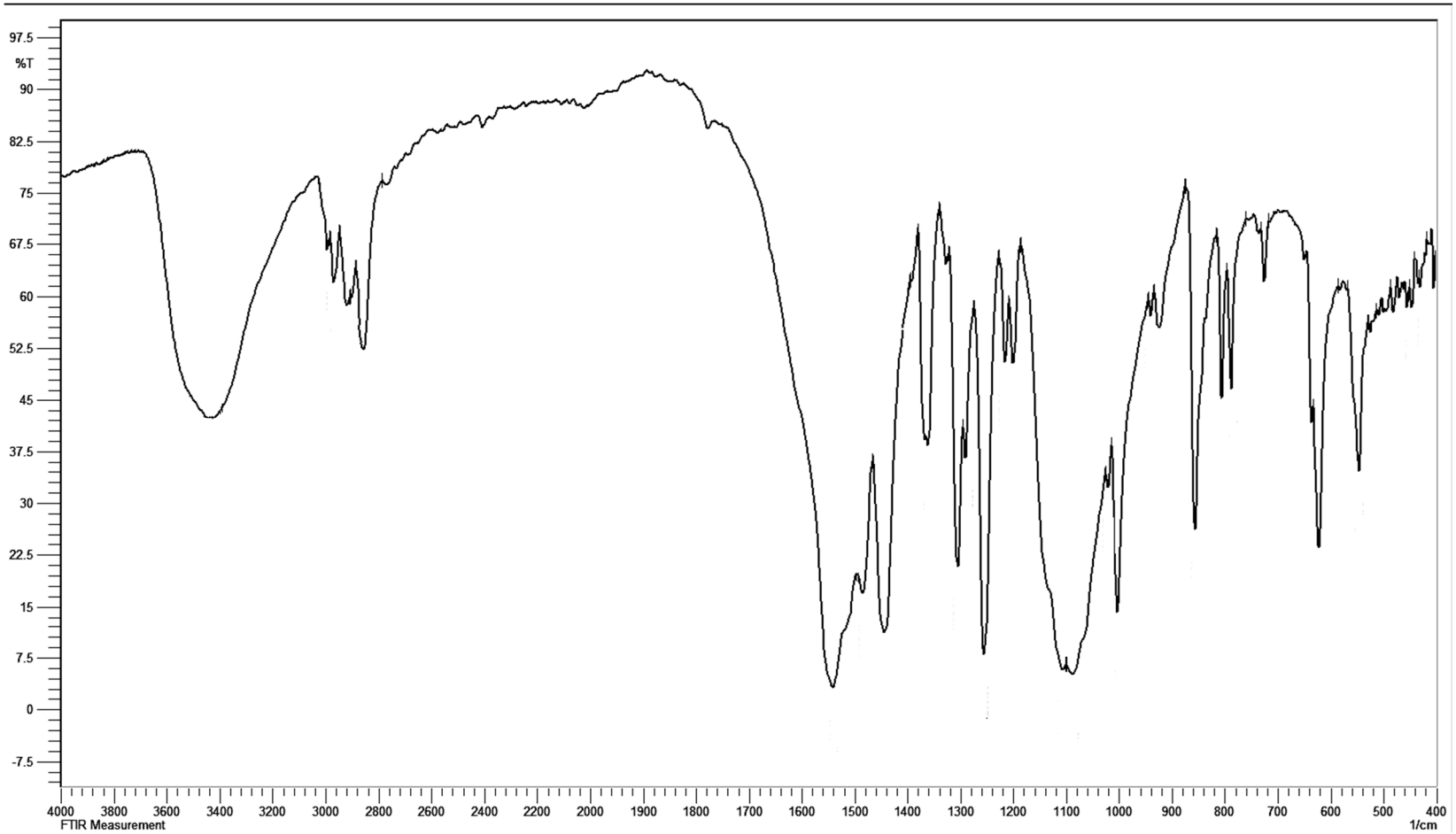

Figure S6. FTIR spectra of the studied complex.