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Supporting information for article:

Hirshfeld surface analysis to understand metal–ligand interactions in coordination polymers

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Table S1 Experimental crystal structures taken from CSD.

CSD	**CCDC**	**Reference**
ANAGOM	768736	Wang, C.-C., Song, Y.-X., Wang, Y.-L. Wang, P. (2011). *Chin. J. Inorg. Chem.* **27**, 361
BEBCOB	226101	Hu, M.-L., Xiao, H.-P.,Wang, S., Li, X.-H. (2003). *Acta Cryst.* C**59**, m454-m455
BEJZOG	1108224	Wołodkiewicz, W., Głowiak, T. (2003). *J. Coord. Chem.* **56**(7), 563-570
CUCAPI	1132177	Davey, G., Stephens, F. S. (1971). *Inorg. Phys. Theor.* 2577-2580
DIHLIQ	635865	Li, W., Li, M.-X., Shao, M., Zhu, S.-R. (2007). *Inorg, Chem. Comm.* **10**, 753-756
DUHHEV	1023878	Yang, L.-R., Liu, L., Lian, C., Liu, M.-H., Xu, Z.-H., Wang, L.-C., Guo, X., Long, Y.-S. (2015). *Dyes and Pigments.* **122**, 246-256
EXEKIC	823499	Hao, H.-J., Sun, D., Li, Y.-H., Liu, F.-J., Huang, R.-B., Zheng, L.-S. (2011). *Cryst. Growth Des.* **11**, 3564-3578
GOYWEY	988751	Penney, M. K., Giang, R., Klausmeyer, K. K. (2015). *Polyhedron*. **85**, 275-283.
HAYFEU	880042	Dharmalingam, S., Jeon, Y., Yoon, S. (2012). *Acta Cryst.* E**68**, m582-m583
IWOPOZ	239115	Gao, S., Huo, L.-H., Liu, J.-W., Chi, J.-L., Zhao, H. (2004). *Acta Cryst.* E**60**, m693-m695
JAFFII	1030630	Wu, H., Wang, C., Wang, F., Peng, H., Zhang, H., Bai, Y. (2015). *J. Chin. Chem. Soc.* **62**, 1028-1034
KAPJAP	1530888	Su, Y.-J., Wei, K.-X., Huang, B., Xu, W.-J., Zhang, W.-X., Zeng, M.-H., Chen, X.-M. (2017). *CrystEngComm*. **19**, 1725-1728
KEGKEN	602957	Brown, D. A., Fitzpatrick, N. J., Muller-Bunz, H., Ryan, A. T. (2006). *Inorg. Chem.* **45**, 4497.
KOQDOJ	145638	Kani, Y., Ohba, S., Nishida, Y. (2000). *Acta Cryst.* C**56**, e194
LOHMUS	950913	Popov, L. D. Levchenkov, S. I., Shcherbakov, I. N., Starikova, Z. A., Lukov, V. V., Kogan, V. A. (2014). *Coord Chem.* **40**, 281
LOLFEZ	993873	Banerjee, S., Rajakannu, P., Butcher, R. J., Murugavel, R. (2014). *CrystEngComm*. **16**, 8429-8441
MEVLII	162592	Shi, Q., Cao, R., Sun, D.-F., Hong, M.-C., Liang, Y.-C. (2001). *Polyhedron*. **20**, 3287-3293
MOVSIA	690731	Cao, X.-Y., Lin, Q.-P., Qin, Y.-Y., Zhang, J., Li, Z.-J., Cheng, J.-K., Yao, Y.-G. (2009). *Crystal Growth & Design*. **9**, n.1, 20-23

NIZTEW	649823	Martínez-Vargas, S., Hernández-Ortega, S., Toscano, R. A., Salazar-Mendoza, D., Valdés-Martínez, J. (2008). *CrystEngComm.* **10**, 86-94
NUKZUO	1224200	Hulme, C. E., Watkinson, M., Haynes, M., Pritchard, R. G., McAuliffe, C. A., Jaiboon, N., Beagley, B., Sousa, A., Bermejo, M. R., Fondo, M. (1997). *J. Chem. Soc., Dalton Trans.* 1805,1814
RIGSEG	654777	Lin, K.-H., Zhang, F.-F., Yu, Z.-Y., Min, S. (2007). *Acta Cryst.* E**63**, m1930
RULDUY	715857	Yan, S., Li, X., Zheng, X. (2009). *J. Mol. Struct.* **929**, 105-111
SORVOL	682181	Brown, K., Zolezzi, S., Aguirre, P., Venegas-Yazigi, D., Paredes-García, V., Baggio, R., Novak, M. A., Spodine, E. (2009). *Dalton Trans.* 1422-1427
TEXXUQ	602574	Effendy, Marchetti, F., Pettinari, C., Pettinari, R., Skelton, B. W., White, A. H. (2007). *Inorganica Chimica Acta*. **360**, 1451-1465
TEXYOL	602578	Effendy, Marchetti, F., Pettinari, C., Pettinari, R., Skelton, B. W., White, A. H. (2007). *Inorganica Chimica Acta*. **360**, 1451-1465
TEXZOM	602583	Effendy, Marchetti, F., Pettinari, C., Pettinari, R., Skelton, B. W., White, A. H. (2007). *Inorganica Chimica Acta*. **360**, 1451-1465
TEYBUV	602589	Effendy, Marchetti, F., Pettinari, C., Pettinari, R., Skelton, B. W., White, A. H. (2007). *Inorganica Chimica Acta*. **360**, 1451-1465
TICJOF	296080	Zhang, S., Wang, Z., Zhang, H., Cao, Y., Sun, Y., Chen, Y., Huang, C., Yu, X. (2007). *Inorg. Chim. Acta*. **360**, 2704-2710
UQUMEZ	825303	Wu, W.-P., Wang, J., Lu, L., He, X.-Y., Zou, L.-K. (2011). *Acta Cryst.* E**67**, m568
VUQLOJ	630068	Chen, P.-K., Qi, Y., Che, Y.-X., Zheng, J.-M. (2010). *CrystEngComm.* **12**, 720-724
WAJDOB	240377	Wen, Y.-H., Cheng, J.-K., Zhang, J., Li, Z.-J., Kang, Y., Yao, Y.-G. (2004). *Inorg. Chem. Comm.* **7**, 1120-1123
XOKQUK01	910187	Halaska, J., Cechova, D., Lawson, M. K., Ruzickova, Z., Jorik, V., Koman, M., Valko, M., Kozlevcar, B., Moncol, J. (2016). *Chem. Papers*, **70**, 101
XUPCUG	188085	Tao, J., Yin, X., Huang, R., Zheng, L. (2002). *Inorg. Chem. Comm.* **5**, 1000-1002
YORJUL	679712	Wu, W., Liu, J., Zeng F., Wu, Y. (2008). *Cryst. Res. Technol.* **43**(9), 991-994
YUHNIY	1306615	Hoang, N. N., Valach, F., Dunaj-Jurčo, M. (1995). *Acta Cryst.* C**51**, 1095-1097
ZAWREW	859609	Burrows, A. D., Mahon, M. F., Raithby, P. R., Warren, A. J., Teat, S. J., Warren, J. E. (2012). *CrystEngComm*. **14**, 3658-3666

Table S2 Selected geometric parameters (Å, °).

Cu1—O2	1.9168 (19)	C3—H3	0.93
Cu1—O3^{i}	1.9237 (19)	C4—C5	1.389 (4)
Cu1—N2	1.987 (2)	C4—C6	1.430 (4)
Cu1—N1	1.997 (2)	C5—C8	1.425 (4)
O1—C13	1.226 (4)	C6—C7	1.349 (5)
O2—C13	1.278 (4)	C6—H6	0.93
O3—C20	1.270 (4)	C7—C9	1.432 (5)
O4—C20	1.228 (4)	C7—H7	0.93
O5—N3	1.223 (3)	C8—C9	1.391 (4)
O6—N3	1.229 (3)	C9—C10	1.396 (5)
O7—H7A	0.855 (5)	C10—C11	1.362 (5)
O7—H7B	0.857 (5)	C10—H10	0.93
O8—H8A	0.860 (5)	C11—C12	1.391 (4)
O8—H8B	0.861 (5)	C11—H11	0.93
O9—H9A	0.861 (5)	C12—H12	0.93
O9—H9B	0.859 (5)	C13—C14	1.511 (4)
N1—C1	1.321 (4)	C14—C19	1.381 (4)
N1—C5	1.363 (4)	C14—C15	1.400 (4)
N2—C12	1.327 (4)	C15—C16	1.386 (4)
N2—C8	1.364 (4)	C15—C20	1.510 (4)
N3—C18	1.465 (4)	C16—C17	1.379 (4)
C1—C2	1.395 (4)	C16—H16	0.93
C1—H1	0.93	C17—C18	1.367 (4)
C2—C3	1.362 (5)	C17—H17	0.93
C2—H2	0.93	C18—C19	1.386 (4)
C3—C4	1.410 (5)	C19—H19	0.93
O2—Cu1—O3^{i}	91.58 (9)	C9—C7—H7	119
O2—Cu1—N2	169.02 (10)	N2—C8—C9	123.3 (3)
O3^{i}—Cu1—N2	94.40 (9)	N2—C8—C5	116.0 (2)
O2—Cu1—N1	94.69 (9)	C9—C8—C5	120.6 (3)
O3^{i}—Cu1—N1	161.86 (10)	C8—C9—C10	116.6 (3)

N2—Cu1—N1	82.38 (9)	C8—C9—C7	117.6 (3)
C13—O2—Cu1	115.85 (19)	C10—C9—C7	125.8 (3)
C20—O3—Cu1^{ii}	120.74 (18)	C11—C10—C9	120.2 (3)
H7A—O7—H7B	114 (2)	C11—C10—H10	119.9
H8A—O8—H8B	107 (2)	C9—C10—H10	119.9
H9A—O9—H9B	109 (2)	C10—C11—C12	119.8 (3)
C1—N1—C5	118.2 (2)	C10—C11—H11	120.1
C1—N1—Cu1	129.2 (2)	C12—C11—H11	120.1
C5—N1—Cu1	112.57 (19)	N2—C12—C11	121.9 (3)
C12—N2—C8	118.2 (3)	N2—C12—H12	119.1
C12—N2—Cu1	128.9 (2)	C11—C12—H12	119.1
C8—N2—Cu1	112.91 (18)	O1—C13—O2	125.9 (3)
O5—N3—O6	123.3 (3)	O1—C13—C14	119.6 (3)
O5—N3—C18	118.3 (2)	O2—C13—C14	114.4 (3)
O6—N3—C18	118.4 (3)	C19—C14—C15	119.9 (2)
N1—C1—C2	122.3 (3)	C19—C14—C13	117.7 (2)
N1—C1—H1	118.8	C15—C14—C13	122.1 (2)
C2—C1—H1	118.8	C16—C15—C14	119.2 (3)
C3—C2—C1	119.7 (3)	C16—C15—C20	116.4 (2)
C3—C2—H2	120.1	C14—C15—C20	124.4 (2)
C1—C2—H2	120.1	C17—C16—C15	121.4 (3)
C2—C3—C4	119.5 (3)	C17—C16—H16	119.3
C2—C3—H3	120.2	C15—C16—H16	119.3
C4—C3—H3	120.2	C18—C17—C16	118.1 (3)
C5—C4—C3	117.0 (3)	C18—C17—H17	121
C5—C4—C6	118.2 (3)	C16—C17—H17	121
C3—C4—C6	124.8 (3)	C17—C18—C19	122.7 (3)
N1—C5—C4	123.2 (3)	C17—C18—N3	119.0 (2)
N1—C5—C8	116.1 (2)	C19—C18—N3	118.3 (3)
C4—C5—C8	120.7 (3)	C14—C19—C18	118.7 (3)
C7—C6—C4	121.0 (3)	C14—C19—H19	120.6

C7—C6—H6	119.5	C18—C19—H19	120.6
C4—C6—H6	119.5	O4—C20—O3	125.8 (3)
C6—C7—C9	122.0 (3)	O4—C20—C15	118.7 (3)
C6—C7—H7	119	O3—C20—C15	115.3 (3)

Symmetry code(s): (i) *x*, *y*+1, *z*; (ii) *x*, *y*−1, *z*.

Table S3 Distances (Å) and angles (°) for H-bonds in compound **I**.

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
O7—H7A···O1	0.855 (10)	2.023 (10)	2.7239 (2)	138.7 (14)
O7—H7B···O9^{i}	0.856 (18)	1.96 (2)	2.7838 (2)	161 (1)
O8—H8A···O4^{ii}	0.86 (3)	1.95 (2)	2.7676 (2)	159 (1)
O8—H8B···O7	0.86 (3)	1.91 (3)	2.7706 (2)	177 (3)
O9—H9A···O7	0.86 (4)	1.96 (4)	2.7960 (2)	165 (4)
O9—H9B···O8^{i}	0.86 (3)	1.94 (3)	2.7788 (2)	165 (4)
C1—H1···O5^{iii}	0.93	2.42	3.2867 (2)	154
C3—H3···O4^{iv}	0.93	2.41	3.3380 (2)	175
C12—H12···O1^{ii}	0.93	2.56	3.4453 (2)	158

Symmetry code(s): (i) −*x*, *y*−1/2, −*z*+3/2; (ii) *x*, *y*+1, *z*; (iii) −*x*+1, *y*−1/2, −*z*+3/2; (iv) *x*, −*y*−3/2, *z*+1/2.

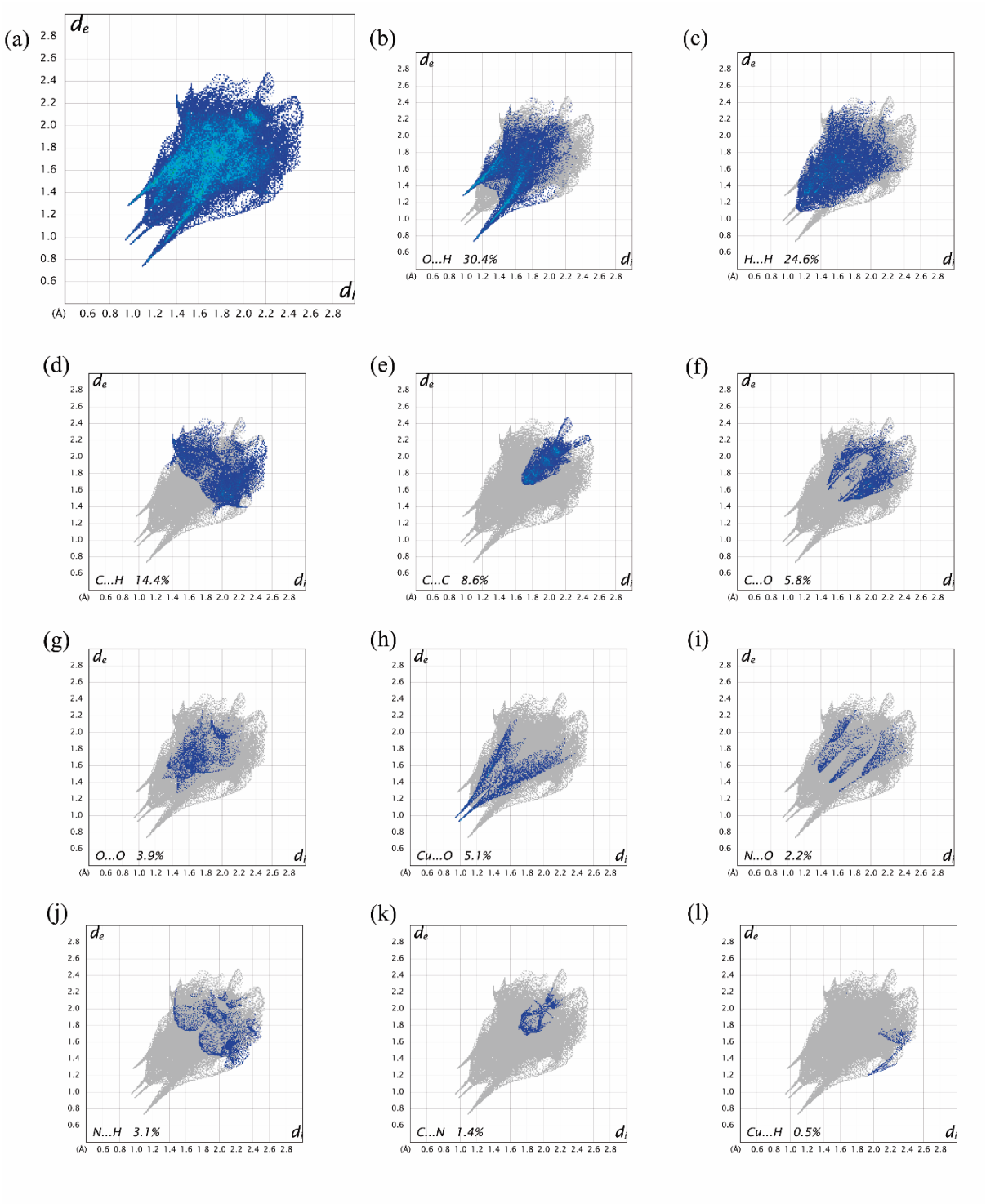

Figure S1 Fingerprint plots for (a) all contacts, (b) O···H 30.4%, (c) H···H 24.6%, (d) C···H 14.4%, (e) C···C 8.6%, (f) C···O 5.8%, (g) O···O 3.9%, (h) Cu···O 5.1%, (i) N···O 2.2%, (j) N···H 3.1%, (k) C···N 1.4%, and (l) Cu···H 0.5%.

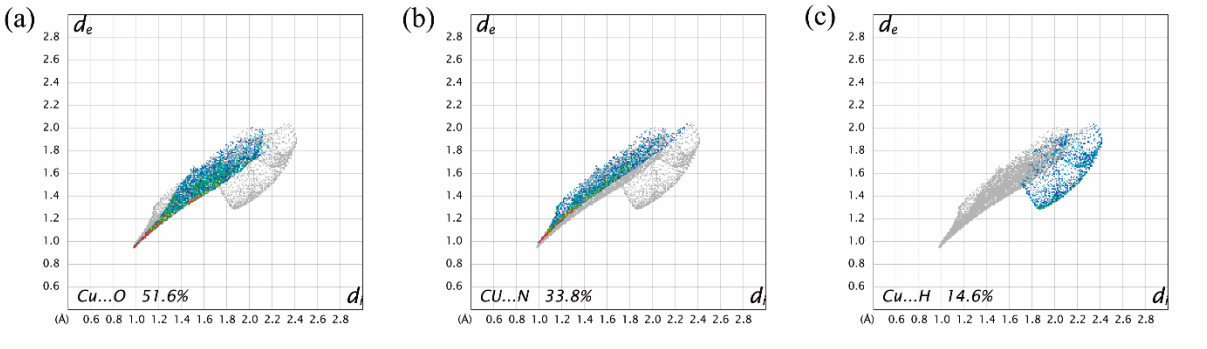

Figure S2 Fingerprint plots for the copper metal center highlighting the contacts (a) Cu···O, 51.6%, (b) Cu···N, 33.8%, and (c) Cu···H, 14.6%.

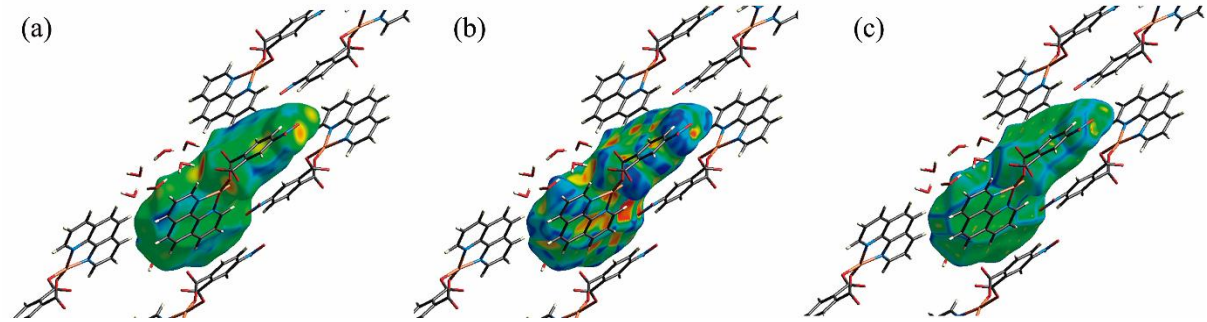

Figure S3 Hirshfeld Surface for compound **I** with the properties (a) d_e, (b) *Shape Index* (*S*) and (c) *Curvedness* (*C*) mapped on it.

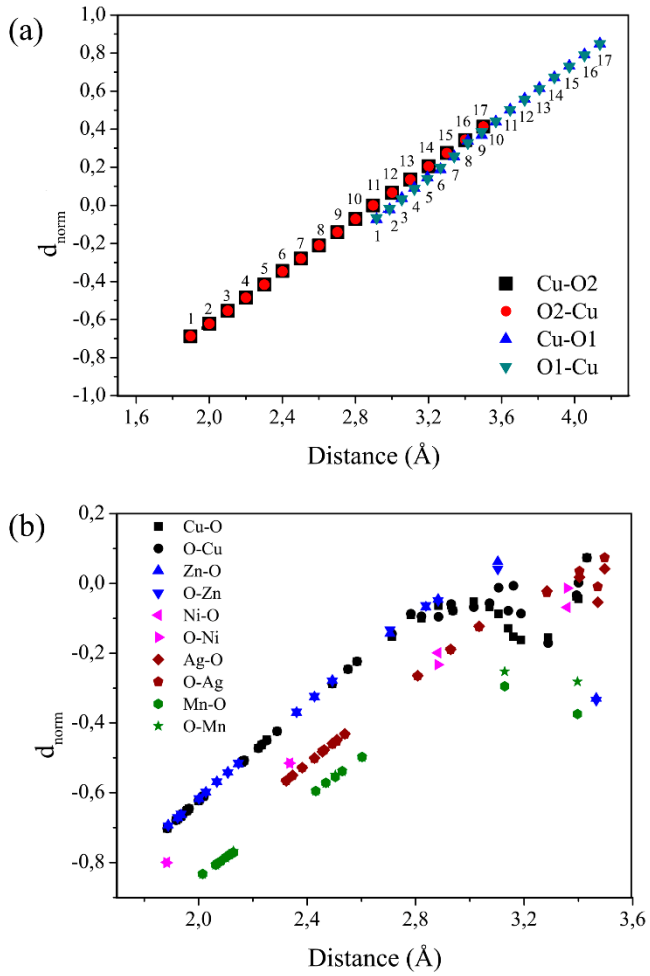

Figure S4 Graphics of distance (*d*) *vs.* d_{norm} for (a) simulated data, and (b) experimental data, showing the d_{norm} values taken from both the metal center surface and the carboxylate group surface.

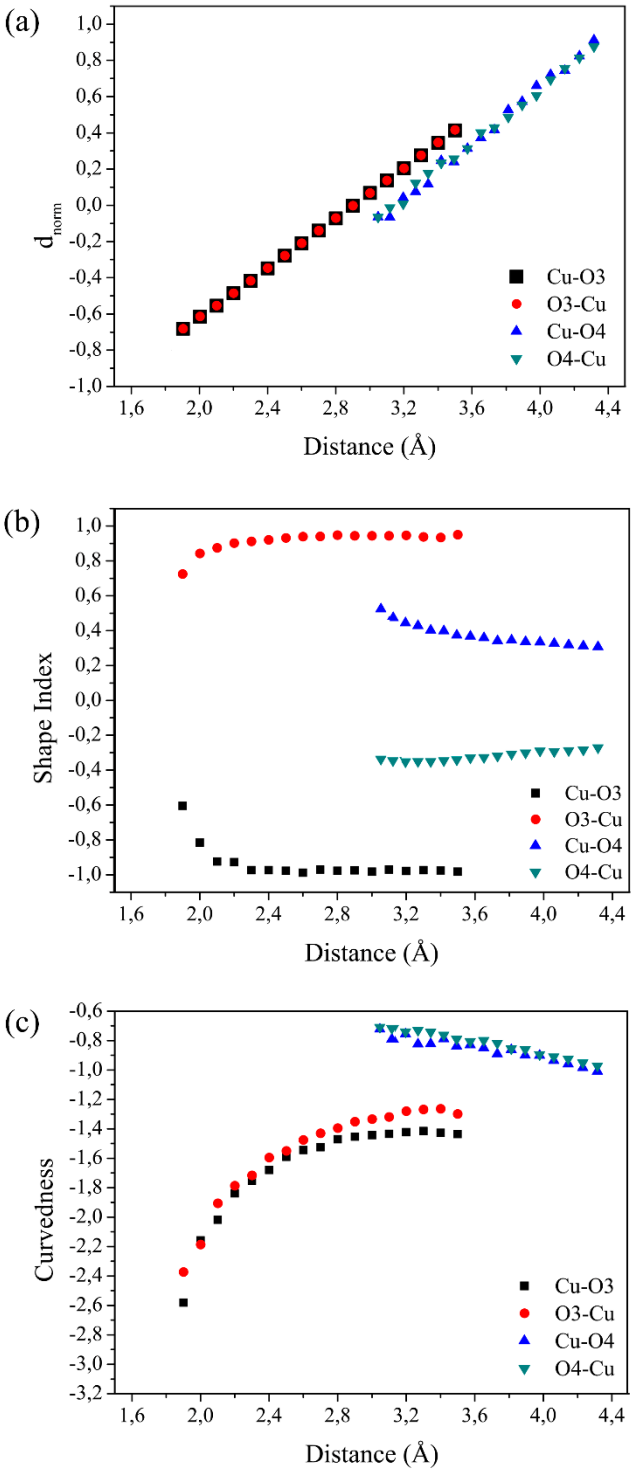

Figure S5 Graphics for the Cu-O3 and Cu-O4 distances vs (a) d_{norm}, (b) Shape Index (S), and (c) Curvedness (C).