



STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 77 (2021)

Supporting information for article:

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using CuK α and MoK α X-ray Diffraction Data**

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List of content:

- **Tables S1-S6** Statistical parameters for IAM, TAAM, HAR and BODD refinements of **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.
- **Tables S7-S9** Similarity index (S) and mean similarity index (\bar{S}) calculated for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.
- **Tables S10-S13** Results of lattice energy calculations.
- **Figure S1** ORTEP view of the molecular structures obtained with the neutron experiment.
- **Figures S2-S4** F_o^2 vs F_c^2 plots for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.
- **Figures S5-S7** Normal probability plots for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.
- **Figures S8-S13** Comparison of bonds for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.
- **Figures S14-S27** Comparison of angles for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.
- **Figure S28** Overlay of selected geometries of **2Cu**, **2Mo** and **2Neu** used for lattice energy calculations.
- **Figure S29** Comparison of selected bonds and angles for **2Cu**.
- **Figures S30-S32** Difference between ADPs of neutron and analysed model for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.
- **Figures S33-S35** Residual density maps for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.

- **Figures S36-S38** Fractal plots for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.
- **Figures S39-S41** Deformation density maps for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**.

Table S1 Statistical parameters for IAM, TAAM and BODD refinements of **1Mo** and **1Cu**.

	IAM Mo	IAM Cu	TAAM Mo Shade	TAAM Mo iso	TAAM Cu Shade	TAAM Cu iso	BODD Mo	BODD Cu
R[F ² > 2σ(F ²)]	0.028	0.034	0.015	0.018	0.014	0.020	0.023	0.027
wR(F ²)	0.095	0.086	0.050	0.057	0.033	0.063	0.080	0.068
# of reflections	10114	1767	9849	9849	1767	1767	10114	1767
# of fit parameters	128	128	160	171	160	171	131	131
Goodness of fit	1.05	1.10	1.58	1.77	0.81	2.23	0.90	0.87
Δρ _{max}	0.70	0.27	0.33	0.33	0.25	0.11	0.40	0.25
Δρ _{min}	-0.31	-0.28	-0.21	-0.33	-0.28	-0.17	-0.34	-0.28

Table S2 Statistical parameters for HAR refinements of **1Mo** and **1Cu**.

	HAR Mo aniso	HAR Mo Shade	HAR Mo iso	HAR Cu aniso	HAR Cu Shade	HAR Cu iso
R[F ² > 2σ(F ²)]	0.015	0.015	0.017	0.013	0.013	0.016
wR(F ²)	0.024	0.025	0.012	0.017	0.018	0.022
# of reflections	9828	9826	9828	1767	1767	1767
# of fit parameters	226	160	160	226	160	160
chi ²	2.35	2.39	2.94	1.47	1.59	2.47
Goodness of fit	1.53	1.55	1.72	1.21	1.26	1.57
Δρ _{max}	0.20	0.22	0.22	0.08	0.08	0.09
Δρ _{min}	-0.15	-0.15	-0.16	-0.11	-0.11	-0.14

Table S3 Statistical parameters for IAM, TAAM and BODD refinements of **2Mo** and **2Cu**.

	IAM Mo	IAM Cu	TAAM Mo Shade	TAAM Mo iso	TAAM Cu Shade	TAAM Cu iso	BODD Mo	BODD Cu
R[F ² > 2σ(F ²)]	0.024	0.028	0.018	0.023	0.014	0.017	0.022	0.024
wR(F ²)	0.064	0.077	0.035	0.038	0.043	0.046	0.055	0.067
# of reflections	9942	1383	9779	9779	796	796	9942	1383
# of fit parameters	99	99	127	139	127	139	102	102
Goodness of fit	0.99	1.09	0.82	0.89	1.73	1.55	0.84	0.96
Δρ _{max}	0.30	0.32	0.24	0.32	0.12	0.12	0.23	0.21
Δρ _{min}	-0.25	-0.21	-0.32	-0.46	-0.11	-0.11	-0.22	-0.20

Table S4 Statistical parameters for HAR refinements of **2Mo** and **2Cu**.

	HAR Mo aniso	HAR Mo Shade	HAR Mo iso	HAR Cu aniso	HAR Cu Shade	HAR Cu iso
R[F ² > 2σ(F ²)]	0.021	0.021	0.022	0.011	0.012	0.013
wR(F ²)	0.015	0.015	0.017	0.017	0.020	0.021
# of reflections	9776	9776	9776	796	796	796
# of fit parameters	199	127	127	199	127	127
chi ²	0.50	0.52	0.62	2.05	2.50	2.76
Goodness of fit	0.71	0.72	0.79	1.43	1.58	1.66
Δρ _{max}	0.16	0.15	0.15	0.05	0.05	0.05
Δρ _{min}	-0.19	-0.19	-0.19	-0.05	-0.04	-0.06

Table S5 Statistical parameters for IAM, TAAM and BODD refinements of **3Mo** and **3Cu**.

	IAM Mo	IAM Cu	TAAM Mo Shade	TAAM Mo iso	TAAM Cu Shade	TAAM Cu iso	BODD Mo	BODD Cu
R[F ² > 2σ(F ²)]	0.044	0.034	0.051	0.031	0.025	0.022	0.045	0.028
wR(F ²)	0.129	0.104	0.074	0.07	0.078	0.065	0.129	0.088

# of reflections	3266	627	3113	3113	627	627	5044	627
# of fit parameters	62	62	55	60	55	60	65	65
Goodness of fit	1.07	1.10	1.56	1.51	2.54	2.13	1.01	0.96
$\Delta\rho_{\max}$	0.78	0.31	0.49	0.44	0.20	0.17	0.22	0.15
$\Delta\rho_{\min}$	-0.29	-0.28	-0.42	-0.29	-0.34	-0.16	-0.22	-0.28

Table S6 Statistical parameters for HAR refinements of **3Mo** and **3Cu**.

	HAR Mo	HAR Mo	HAR Mo	HAR Cu	HAR Cu	HAR Cu
	aniso	Shade	iso	aniso	Shade	iso
R[F ² > 2 σ (F ²)]	0.038	0.039	0.039	0.019	0.19	0.023
wR(F ²)	0.031	0.032	0.032	0.029	0.027	0.035
# of reflections	3113	3113	3113	627	627	627
# of fit parameters	88	66	66	88	66	66
chi ²	1.86	1.91	1.91	3.82	3.14	5.21
Goodness of fit	1.36	1.38	1.38	1.96	1.77	2.28
$\Delta\rho_{\max}$	0.16	0.17	0.17	0.07	0.07	0.09
$\Delta\rho_{\min}$	-0.17	-0.17	-0.17	-0.08	-0.08	-0.09

Table S7 Similarity index (S) and mean similarity index (\bar{S}) calculated for **1Mo** and **1Cu**.

	HAR Mo	HAR Mo	HAR Cu	HAR Cu	TAAM Mo	TAAM Cu
	aniso	Shade	aniso	Shade	aniso	aniso
mean overlap (\bar{S})	1.43	0.70	2.13	0.96	0.72	1.14
H9A	0.95	0.48	1.96	0.61	0.49	0.62
H9B	0.87	1.41	0.74	1.91	1.48	2.09
H1N	3.62	1.24	8.57	1.52	1.26	1.89
H8	0.40	0.38	0.51	0.65	0.45	0.84
H10A	0.85	0.82	1.84	1.14	0.84	1.14
H10C	2.00	1.00	0.38	1.07	0.97	1.22

H10B	0.22	0.88	1.11	1.17	0.89	1.27
H2	2.22	0.51	1.66	0.77	0.51	0.98
H3	2.43	0.33	2.75	0.39	0.33	0.64
H7	1.66	0.43	2.41	0.84	0.48	1.17
H4	0.51	0.27	1.48	0.44	0.25	0.64

Table S8 Similarity index (S) and mean similarity index (\bar{S}) calculated for **2Mo** and **2Cu**.

	HAR Mo aniso	HAR Mo Shade	HAR Cu aniso	HAR Cu Shade	TAAM Mo aniso	TAAM Cu aniso
mean overlap (\bar{S})	2.16	0.78	10.19/17.67	1.19	0.79	1.34
H1A	3.47	1.77	n/a	2.15	1.73	2.17
H5A	0.98	0.91	1.51	1.19	0.93	1.51
H5B	2.46	0.86	7.20	1.32	0.91	1.69
H11	1.17	0.65	35.20	0.82	0.70	1.18
H12	1.28	0.99	4.46	1.13	1.06	1.36
H13	2.83	0.43	15.25	0.77	0.50	1.07
H14	0.6	0.3	3.14	0.36	0.28	0.45
H15	4.7	0.78	4.01	1.46	0.78	1.63
H1B	2.52	1.64	3.48	2.06	1.57	1.96
H2	2.21	0.2	20.90	1.36	0.23	0.89
H3	1.53	0.26	6.28	0.68	0.27	1.01
H4	2.14	0.53	10.64	0.95	0.58	1.13

Table S9 Similarity index (S) and mean similarity index (\bar{S}) calculated for **3Mo** and **3Cu**.

	HAR Mo aniso	HAR Mo Shade	HAR Cu aniso	HAR Cu Shade	TAAM Mo aniso	TAAM Cu aniso
mean overlap (\bar{S})	4.14	0.47	5.80	0.74	0.73	1.18

H4	3.19	0.43	9.29	0.89	1.11	1.11
H5	0.33	0.70	3.76	1.77	1.80	3.89
H3	3.31	0.51	1.69	0.52	0.30	0.46
H2	1.32	0.17	8.24	0.06	0.17	0.10
H1	12.54	0.55	6.01	0.46	0.25	0.34

Table S10 Lattice energy calculation results for **1Neu**, **2Neu**, **3Neu**, **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**. Results are shown in kJ/mol. Calculations were performed using CRYSTAL17 at the DFT/B3LYP level of theory and applying the DFT-D3(ATM) dispersion correction, using cc-pVDZ basis set. Calculations for neutron datasets were performed with and without geometry optimization.

	1Neu	2Neu	3Neu			
Neutron	-260.19	-309.16	-193.26			
Neutron (optimized)	-260.34	-313.42	-193.92			
	1Mo	1Cu	2Mo	2Cu	3Mo	3Cu
IAM	-257.29	-258.66	-301.06	-301.42	-193.67	-192.68
HAR ani	-257.59	-259.58	-299.77	-290.55	-192.22	-190.86
HAR iso	-257.80	-260.21	-298.08	-289.49	-191.55	-190.62
HAR Shade	-257.60	-260.12	-299.25	-293.31	-191.55	-190.79
TAAM Shade	-258.95	-260.07	-301.75	-301.92	-190.98	-194.03
TAAM iso	-259.01	-260.19	-302.05	-302.06	-190.98	-193.50
BODD	-257.34	-259.69	-300.95	-301.32	-194.27	-193.70

Table S11 Differences between lattice energy calculation results for CuK α and MoK α data of **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**. Results are shown in kJ/mol. Calculations were performed using CRYSTAL17 at the DFT/B3LYP level of theory and applying the DFT-D3(ATM) dispersion correction, using cc-pVDZ basis set.

	Δ IAM	Δ BODD	Δ HAR _{SHADE}	Δ TAAM _{SHADE}	Δ HAR _{iso}	Δ TAAM _{iso}	Δ HAR _{ani}
1Cu-1Mo	-1.37	-2.36	-2.53	-1.12	-2.42	-1.19	-1.99
2Cu-2Mo	-0.36	-0.37	5.94	-0.17	8.59	-0.01	9.22
3Cu-3Mo	0.99	0.57	0.76	-3.06	0.92	-2.52	1.36

Table S12 Differences between lattice energy calculation results for model and optimized neutron data of **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**. Results are shown in kJ/mol. Calculations were performed using CRYSTAL17 at the DFT/B3LYP level of theory and applying the DFT-D3(ATM) dispersion correction, using cc-pVDZ basis set.

	1Mo	1Cu	2Mo	2Cu	3Mo	3Cu
IAM	3.05	1.69	12.35	12.00	0.25	1.24
HAR ani	2.75	0.76	13.65	22.87	1.70	3.07
HAR iso	2.54	0.13	15.34	23.93	2.38	3.30
HAR Shade	2.74	0.22	14.16	20.11	2.37	3.13
TAAM Shade	1.39	0.27	11.67	11.50	2.94	-0.11
TAAM iso	1.33	0.15	11.37	11.36	2.94	0.43
BODD	3.00	0.65	12.46	12.10	-0.35	0.22

Table S13 Differences between lattice energy calculation results for model and neutron data (without geometry optimization) of **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**. Results are shown in kJ/mol. Calculations were performed using CRYSTAL17 at the DFT/B3LYP level of theory and applying the DFT-D3(ATM) dispersion correction, using cc-pVDZ basis set.

	1Mo	1Cu	2Mo	2Cu	3Mo	3Cu
IAM	2.90	1.53	8.10	7.74	-0.42	0.57
HAR ani	2.59	0.61	9.39	18.61	1.04	2.40
HAR iso	2.39	-0.03	11.08	19.68	1.71	2.63

HAR Shade	2.59	0.06	9.91	15.85	1.71	2.46
TAAM Shade	1.24	0.12	7.41	7.24	2.28	-0.78
TAAM iso	1.18	-0.01	7.11	7.10	2.28	-0.24
BODD	2.85	0.49	8.21	7.84	-1.02	-0.45

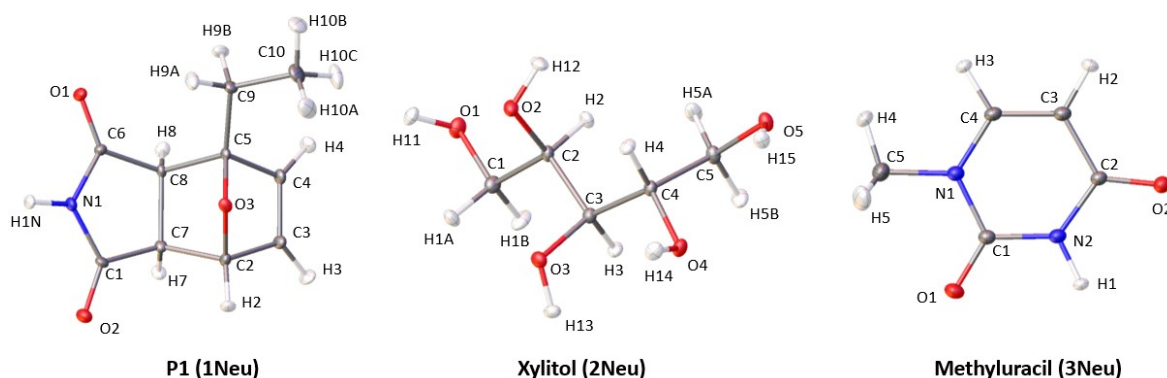
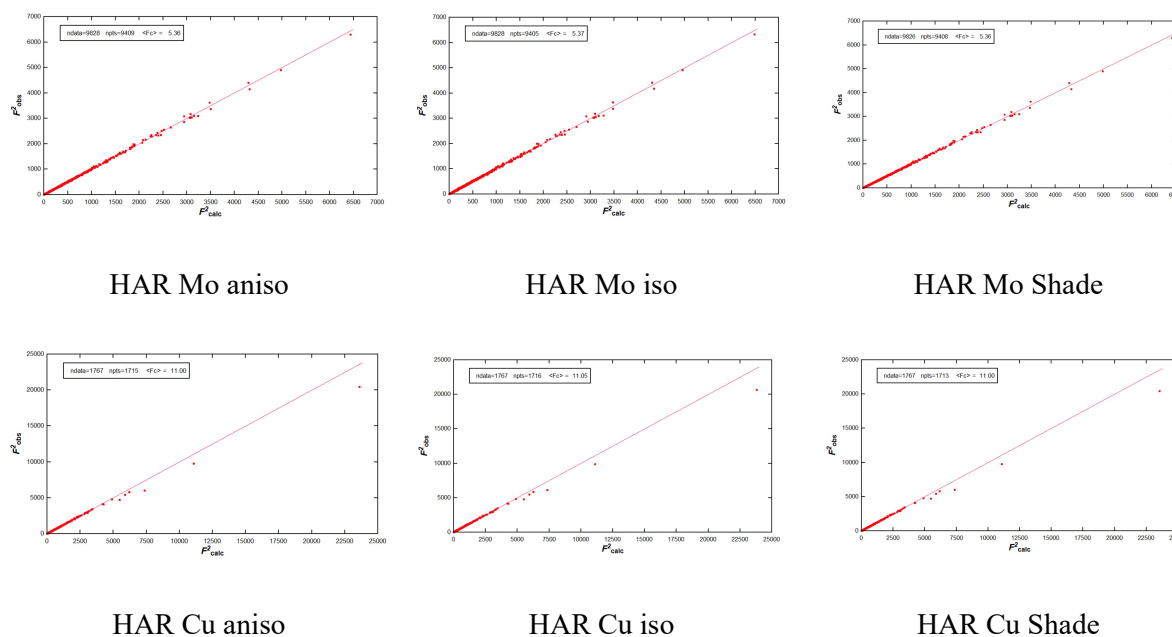
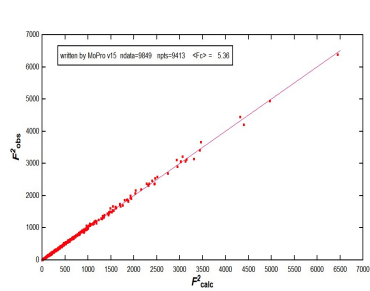
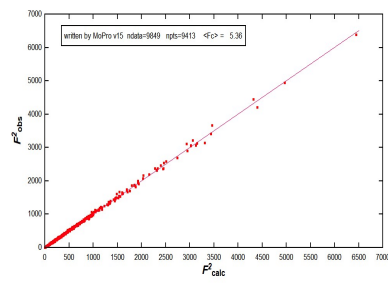


Figure S1 An ORTEP view of the molecular structure obtained with the neutron experiment. Atomic displacement ellipsoids are drawn at the 50% probability level. Data for compounds **2Neu** (Madsen *et al.*, 2003) and **3Neu** (McMullan & Craven, 1989) were available in the CSD.

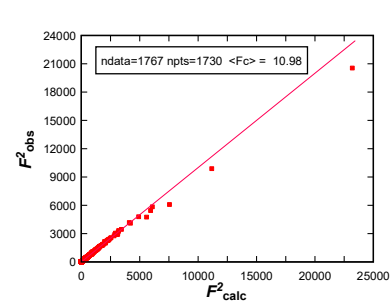




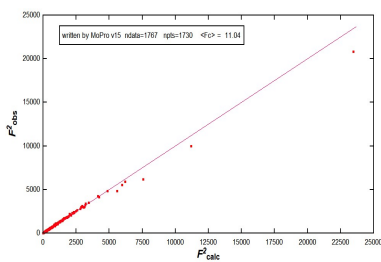
TAAM Mo Shade



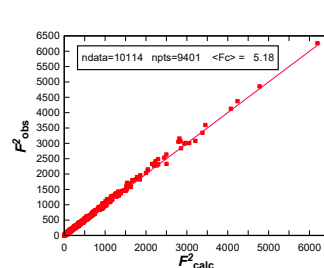
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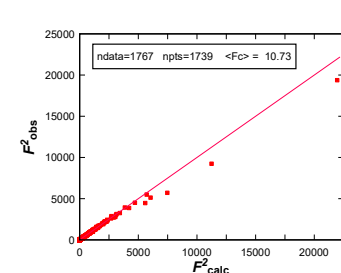
TAAM Cu Shade



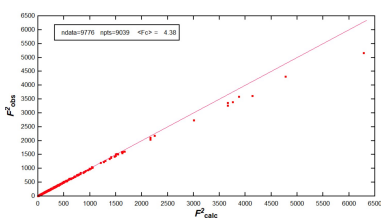
TAAM Cu iso



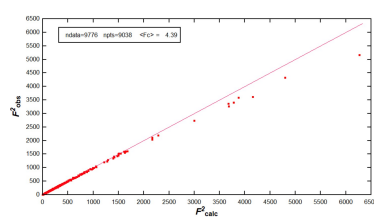
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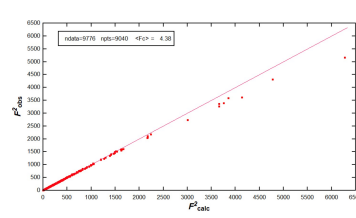
BODD Cu

Figure S2 F_o^2 vs F_c^2 plots for **1Mo** and **1Cu**.

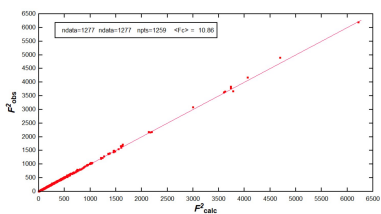
HAR Mo aniso



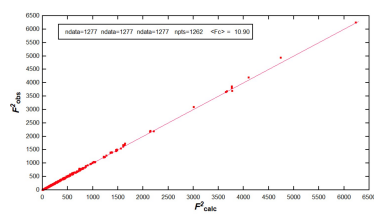
HAR Mo iso



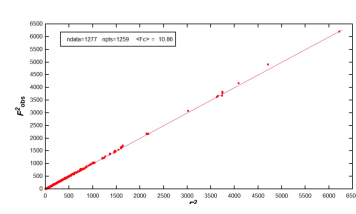
HAR Mo Shade



HAR Cu aniso



HAR Cu iso



HAR Cu Shade

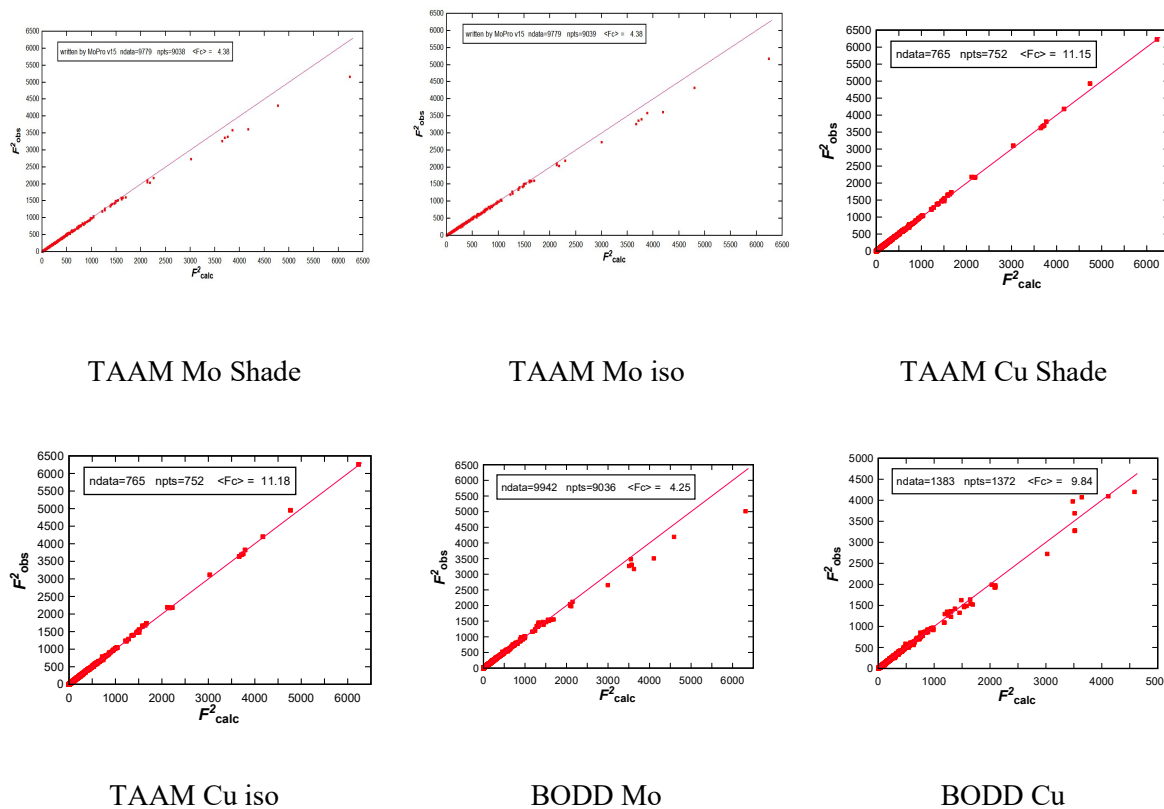
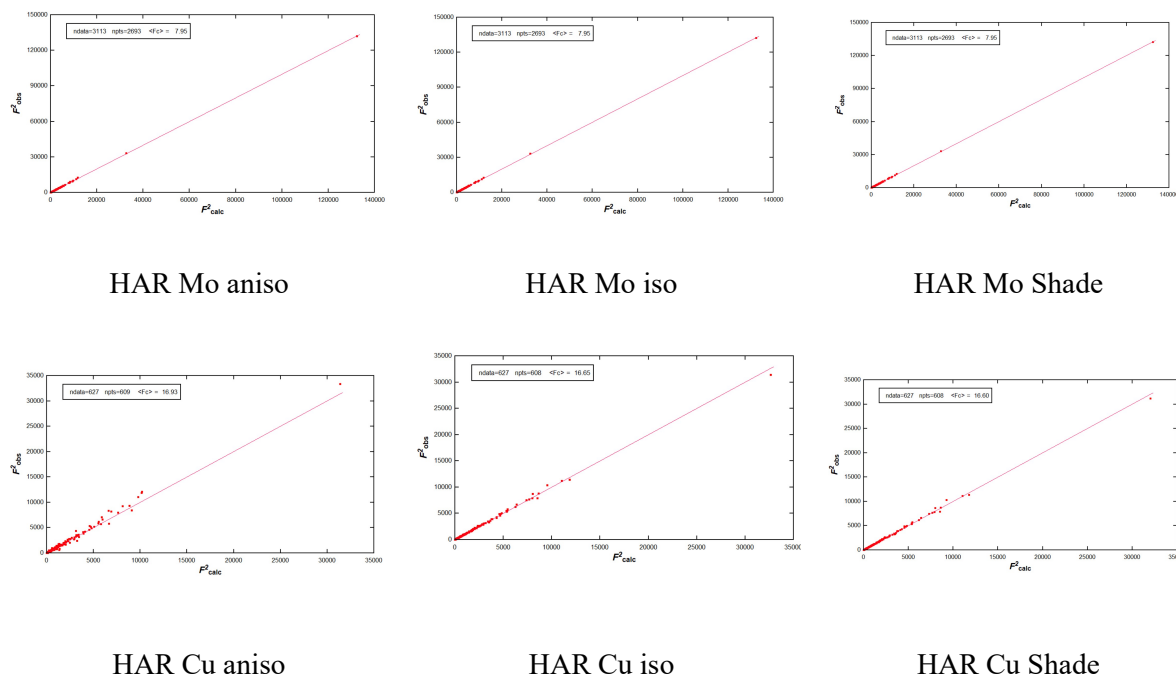


Figure S3 F_o^2 vs F_c^2 plots for 2Mo and 2Cu.



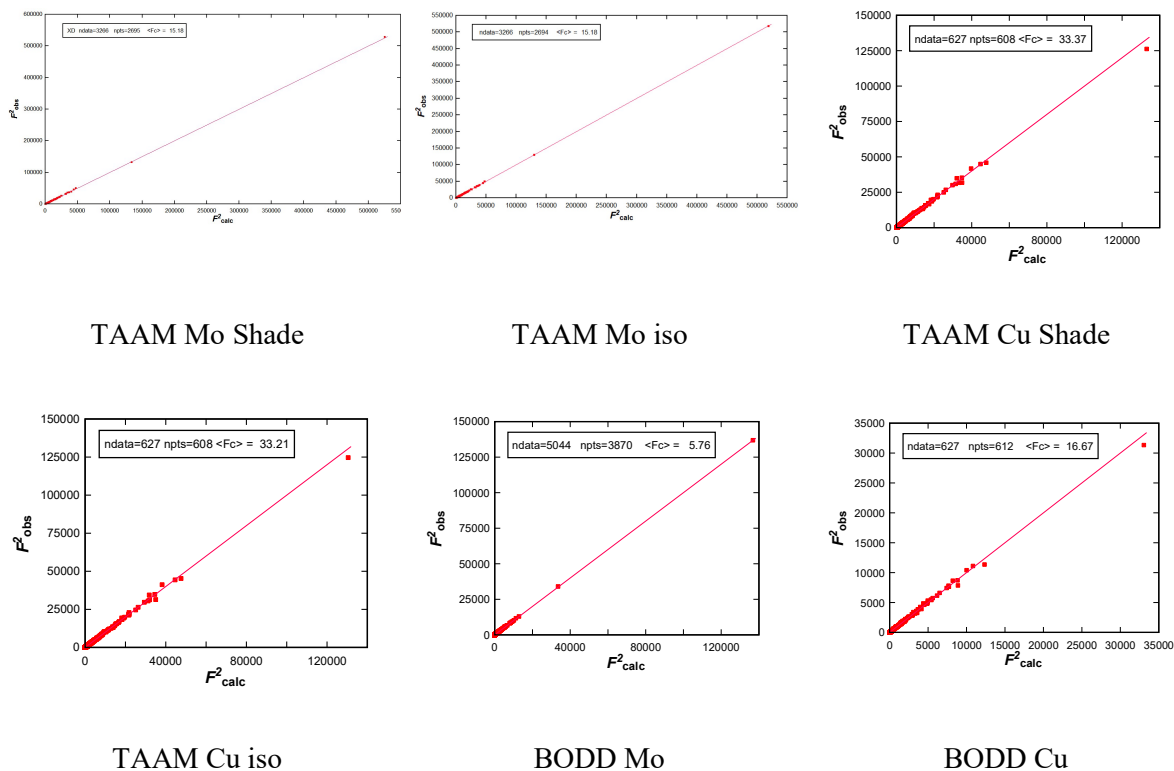
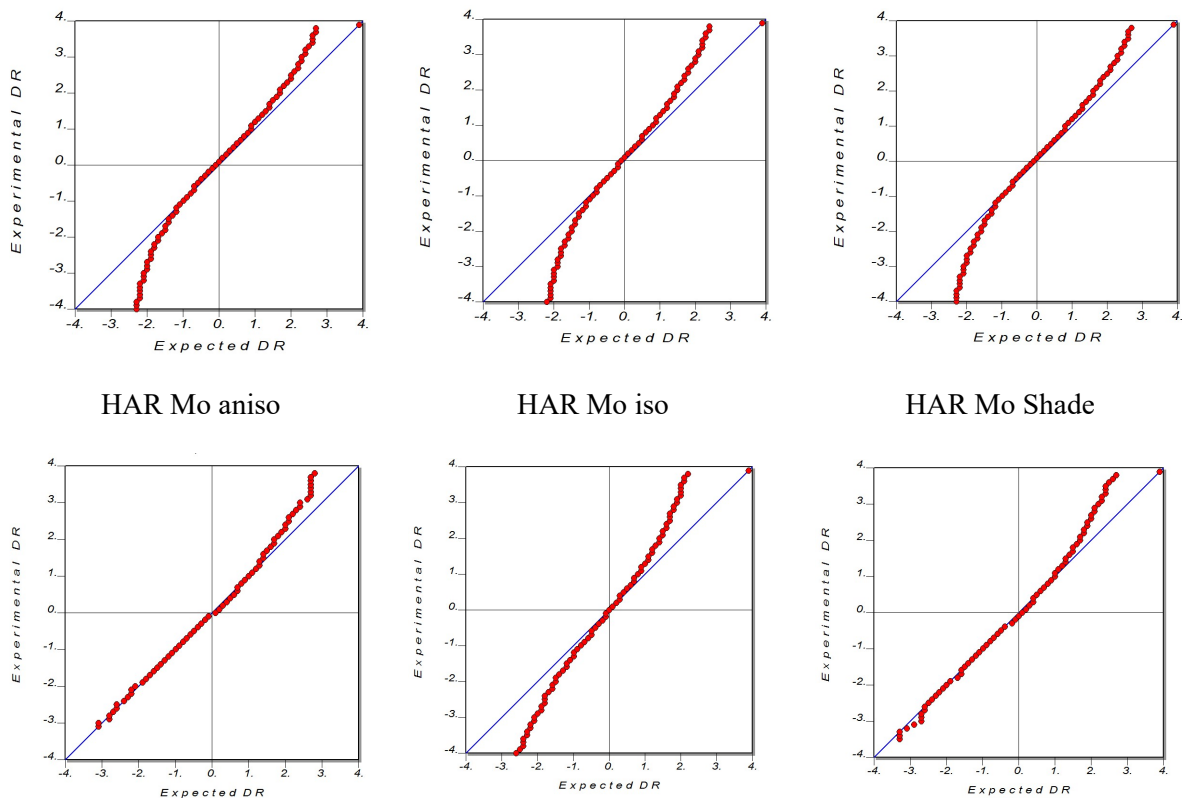


Figure S4 F_o^2 vs F_c^2 plots for 3Mo and 3Cu.



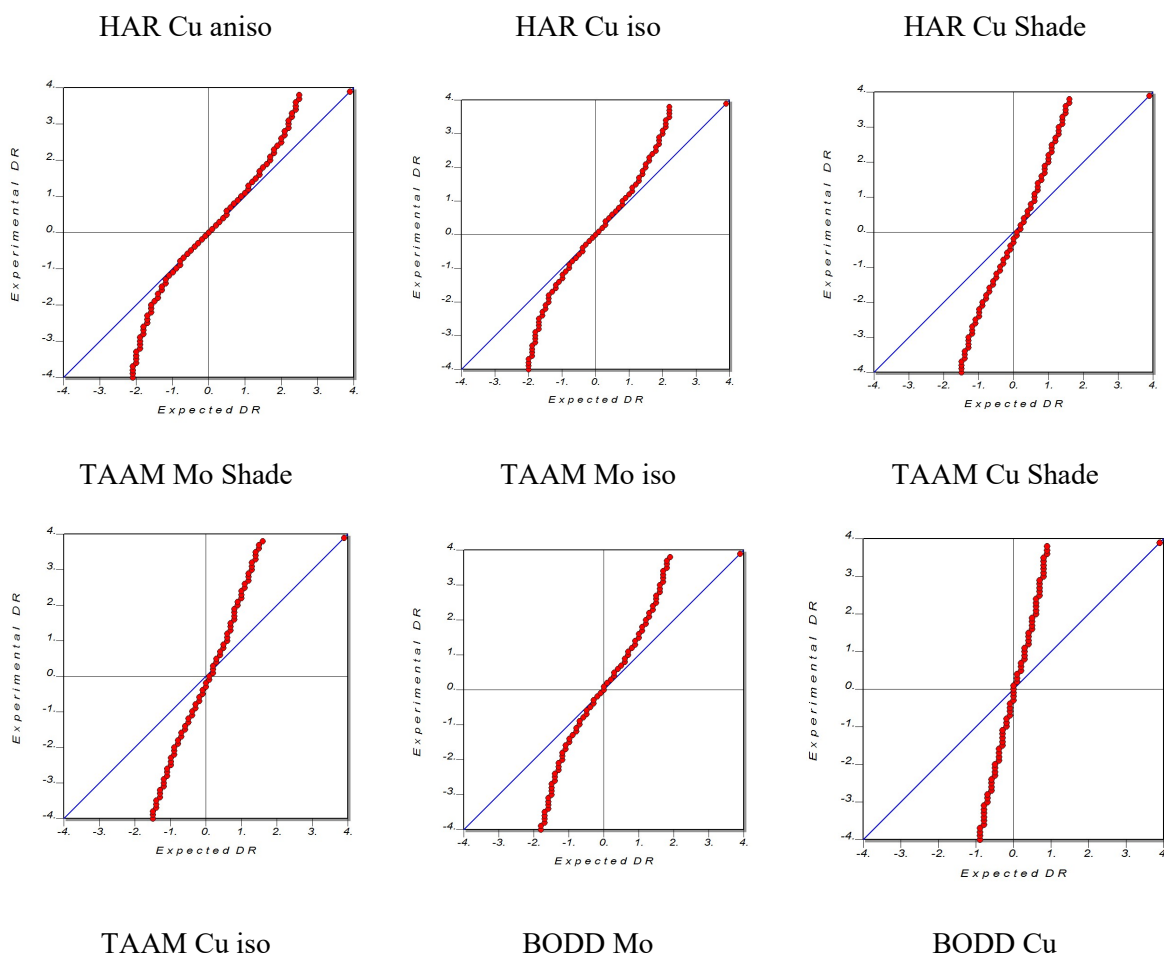
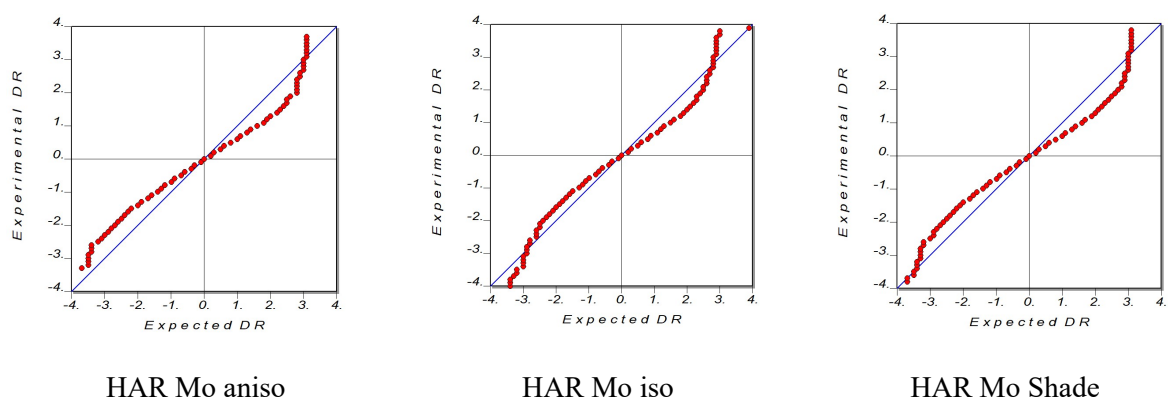


Figure S5 Normal probability plots for **1Mo** and **1Cu**.



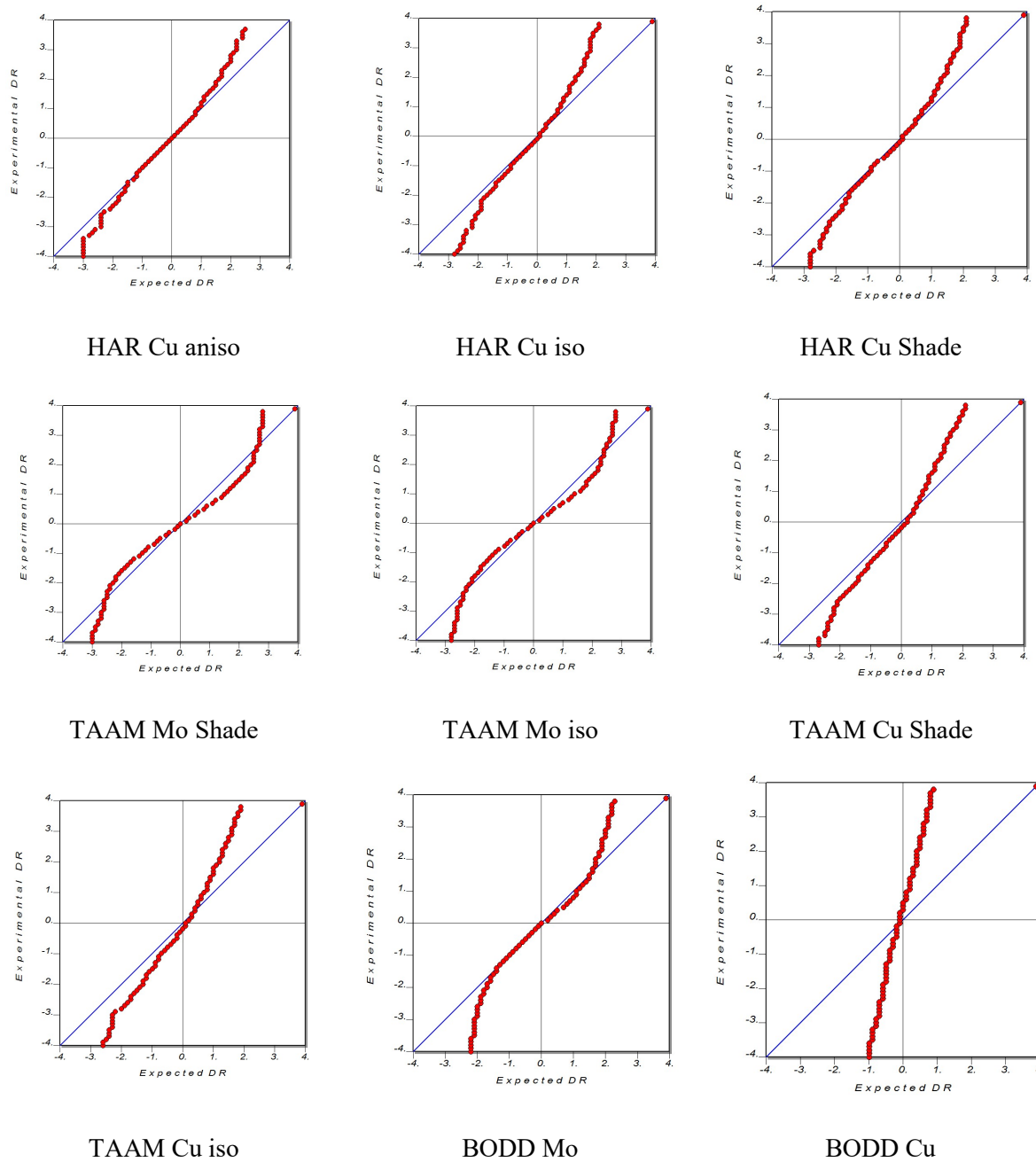


Figure S6 Normal probability plots for **2Mo** and **2Cu**.

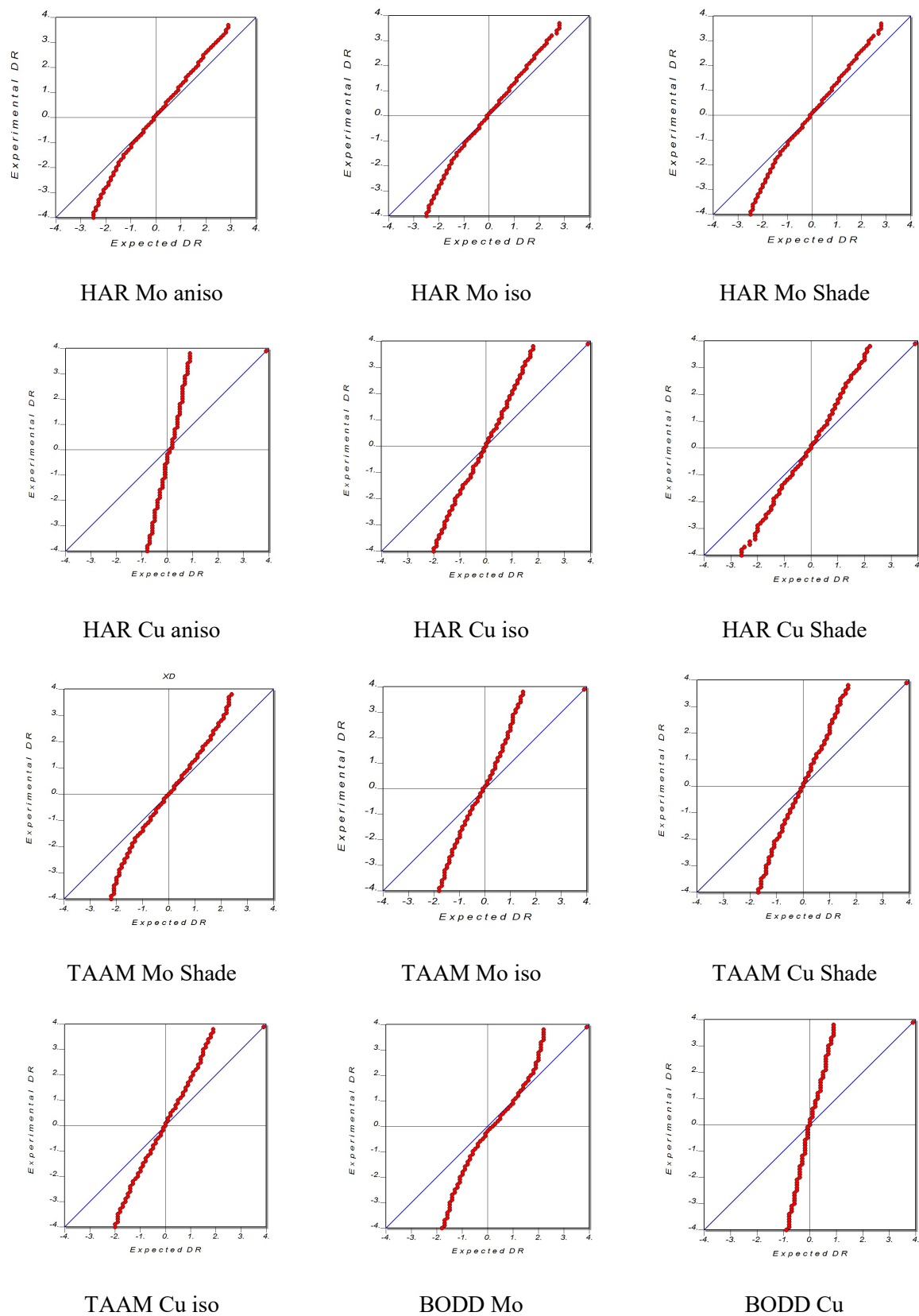


Figure S7 Normal probability plots for **3Mo** and **3Cu**.

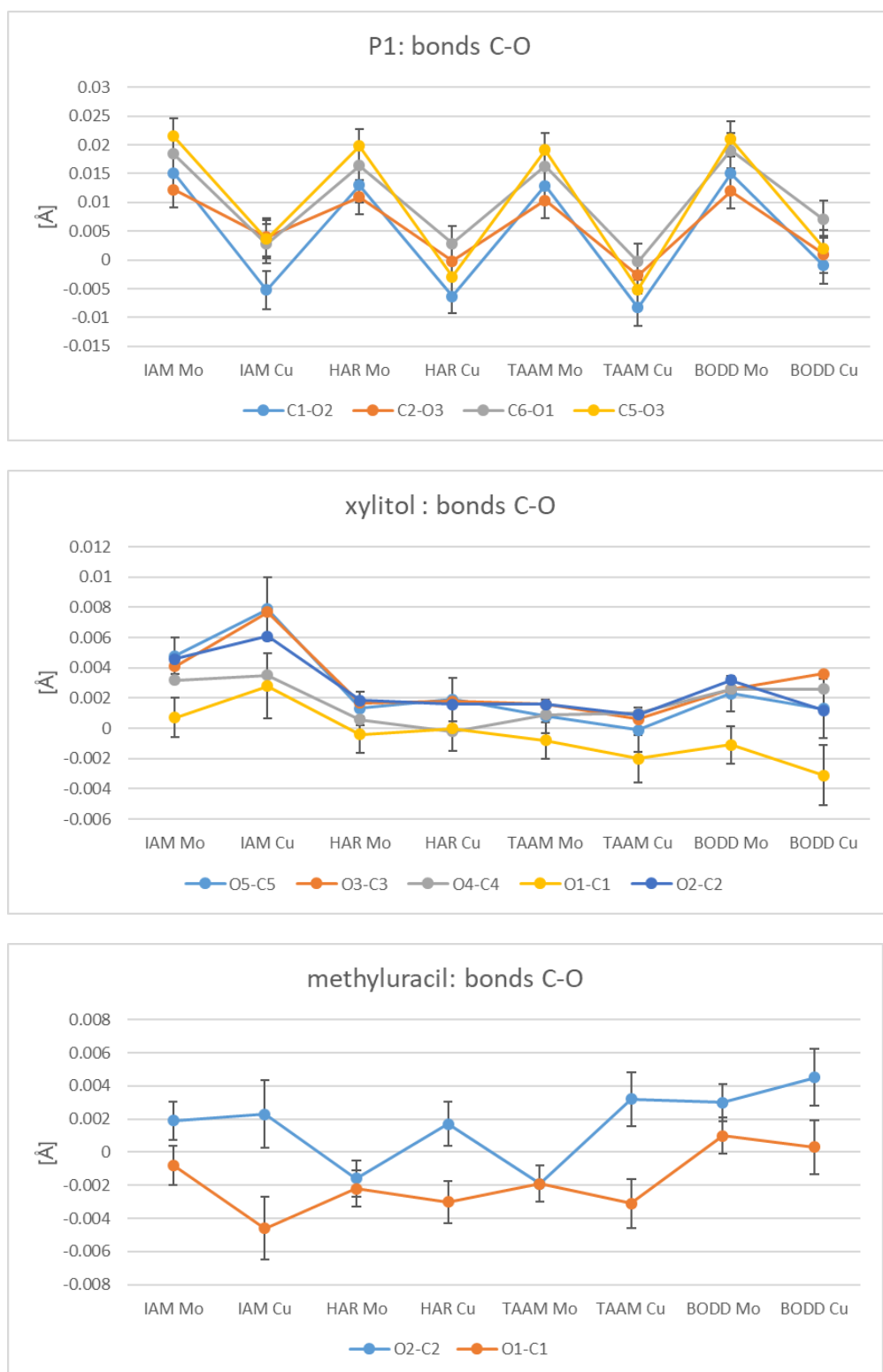


Figure S8 Comparison of C-O bonds for 1Mo, 1Cu, 2Mo, 2Cu, 3Mo and 3Cu. Values on plot represent difference between values obtained with analysed model and neutron data in angstroms.

Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

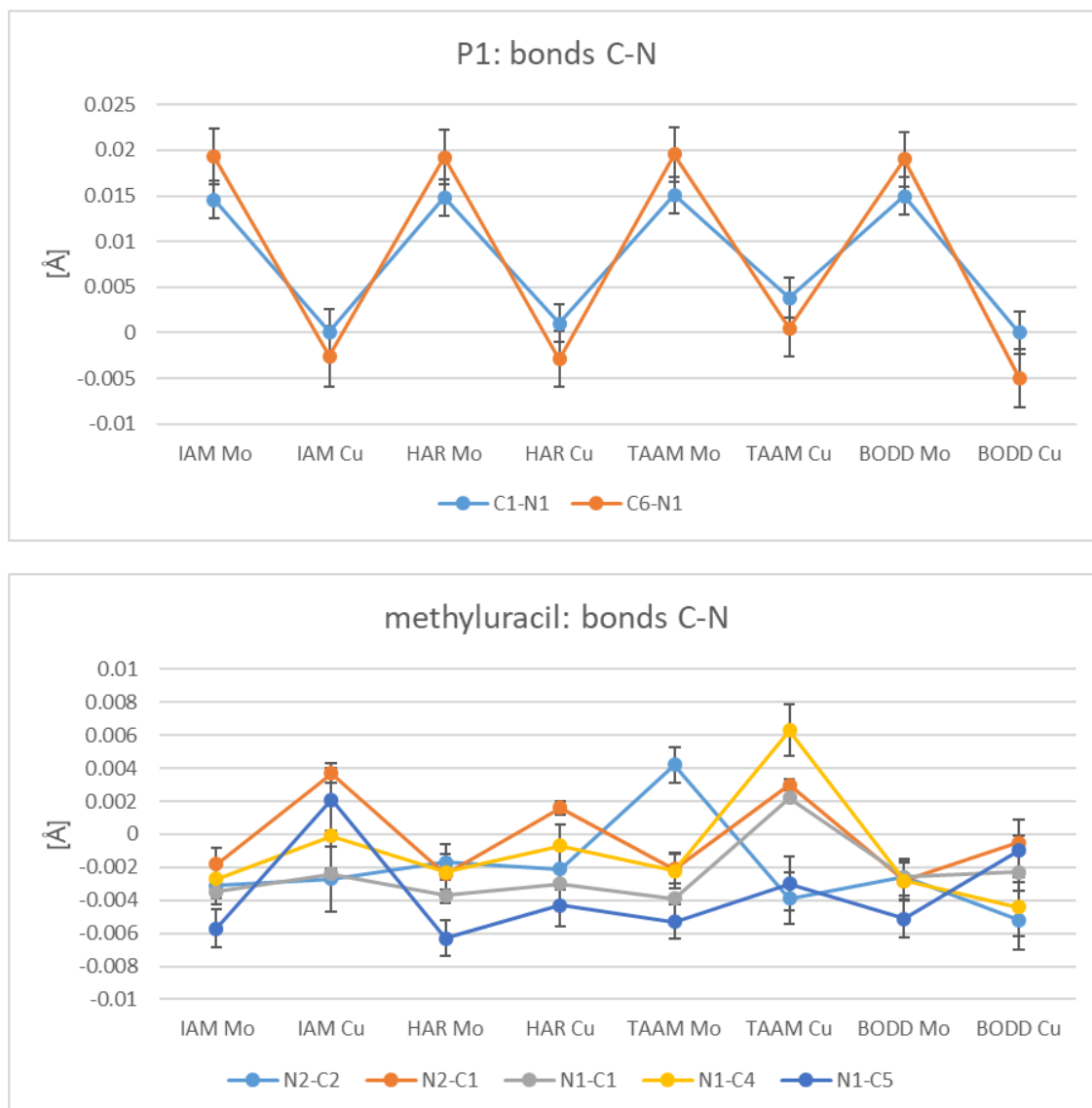


Figure S9 Comparison of C-N bonds for **1Mo**, **1Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data in angstroms. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

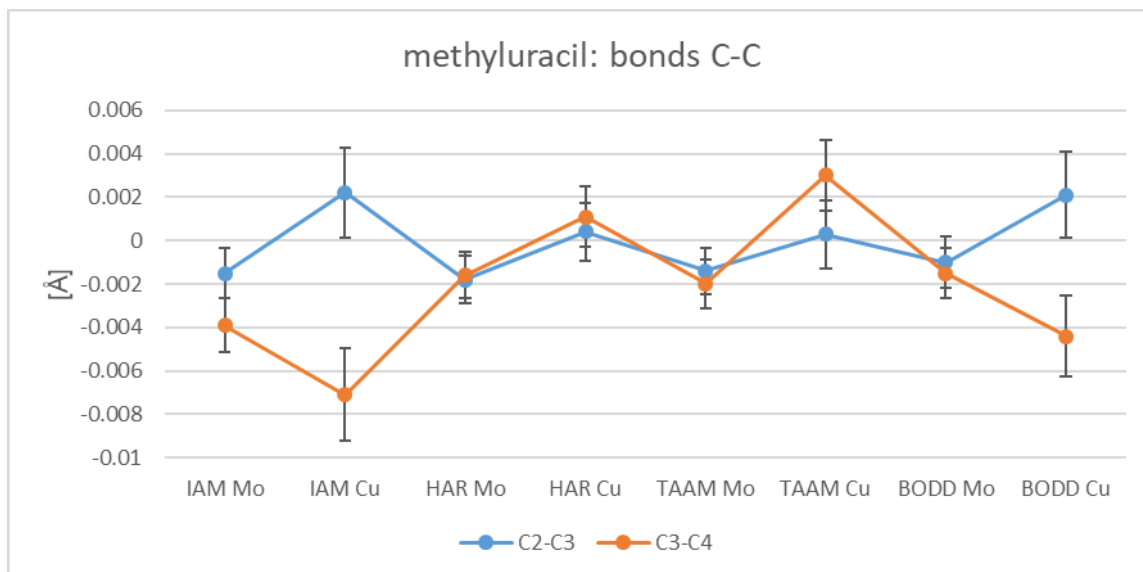
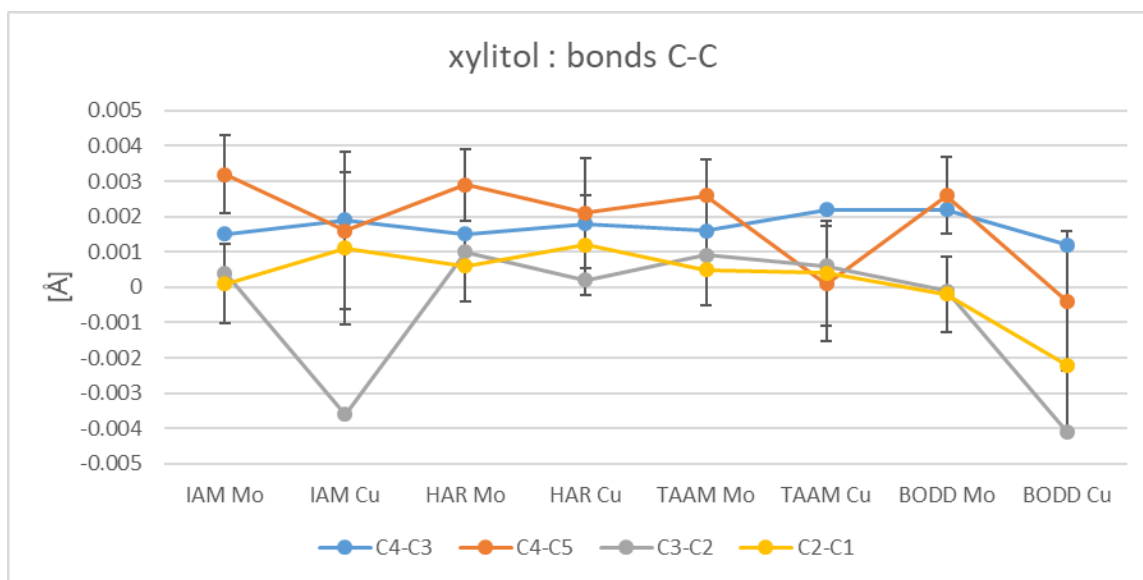
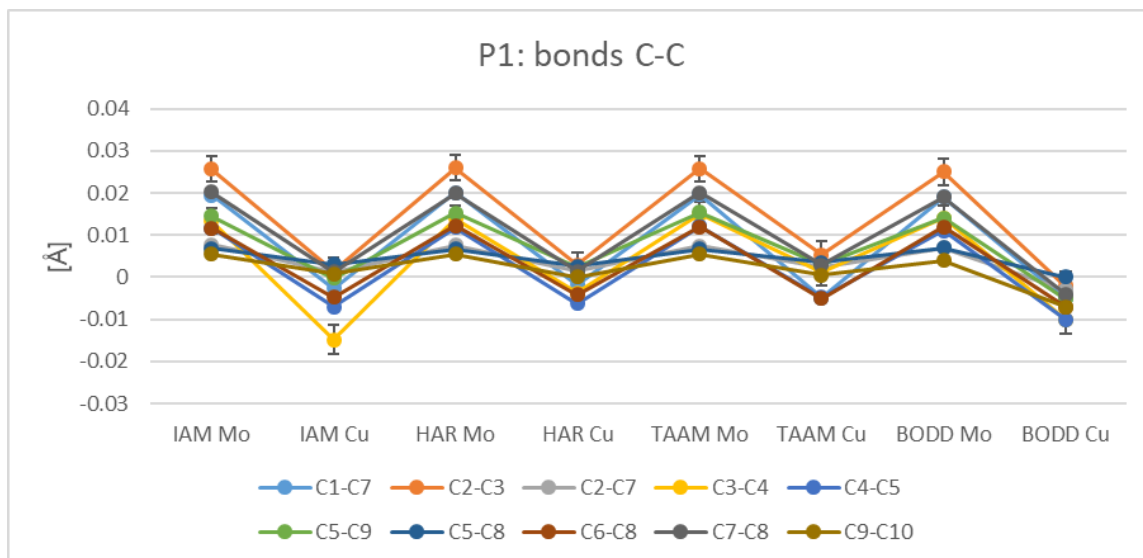
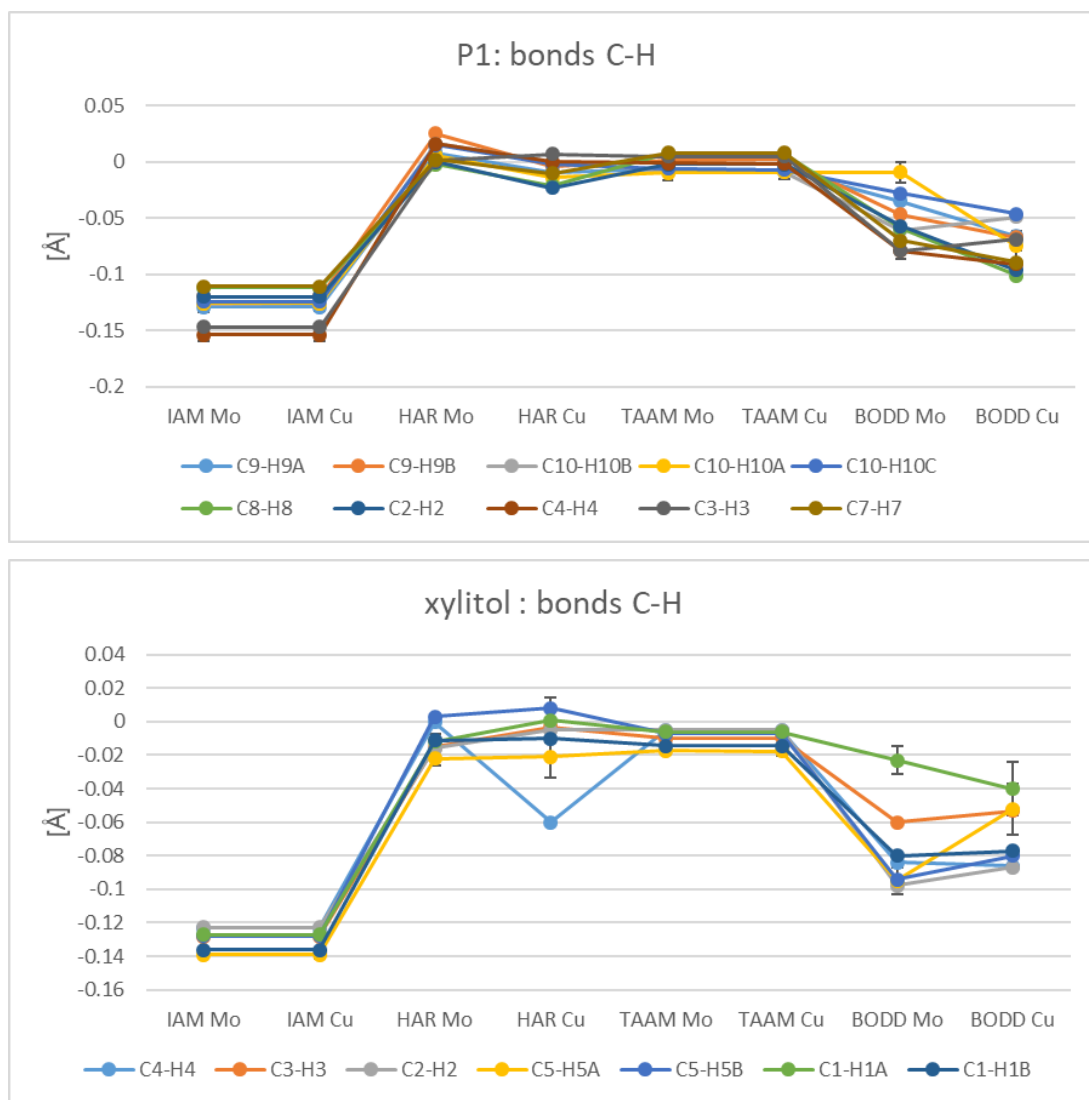


Figure S10 Comparison of C-C bonds for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data in angstroms. Lines on plot have no physical meaning, however help in visual analysis. For clarity, estimated standard deviations of P1 (**1Mo** and **1Cu**) were shown only for C2-C3 and C3-C4 bonds.



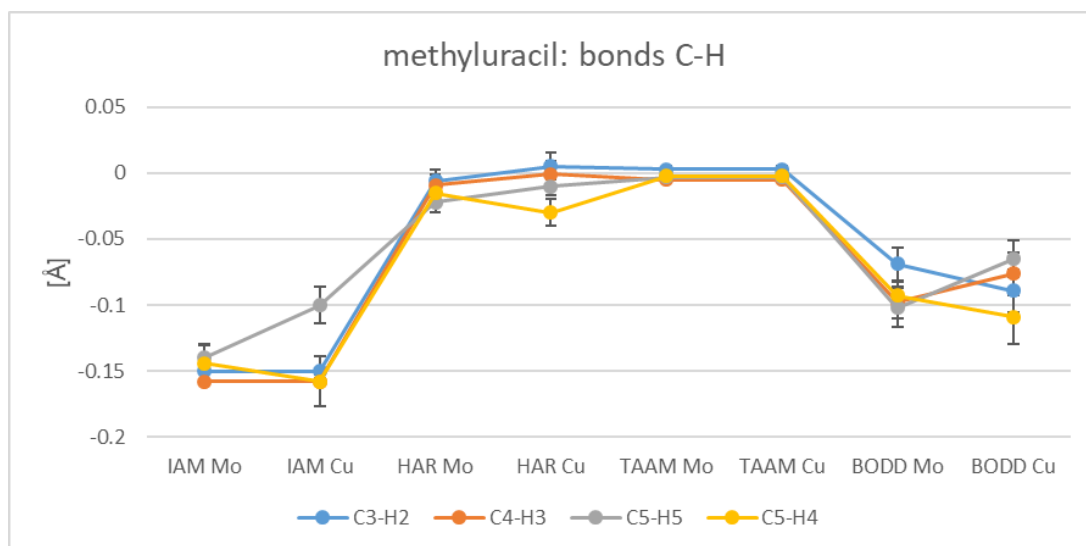
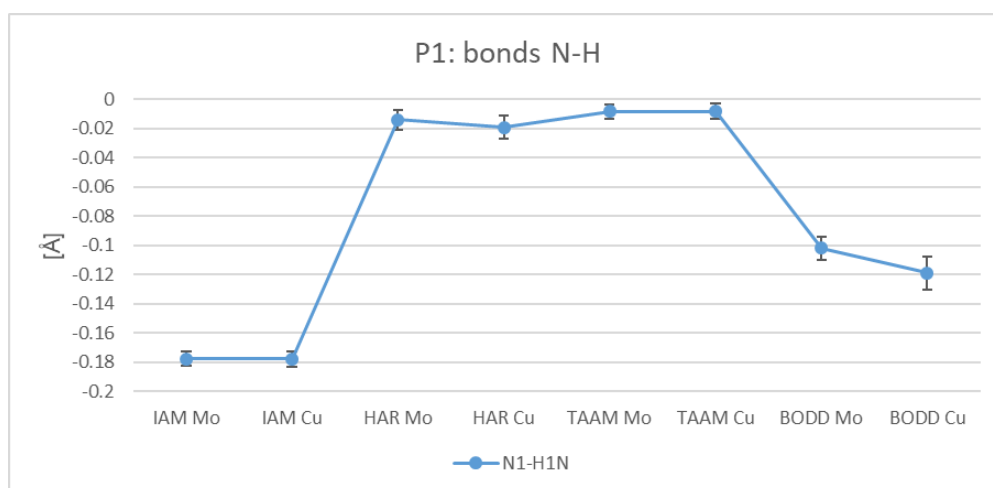


Figure S11 Comparison of C-H bonds for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data in angstroms. Lines on plot have no physical meaning, however help in visual analysis. For clarity, estimated standard deviations of P1 (**1Mo** and **1Cu**) were shown only for C10-H10A and C4-H4 bonds, whereas estimated standard deviations of xylitol (**2Mo** and **2Cu**) were shown only for C1-H1A and C5-H5A bonds.



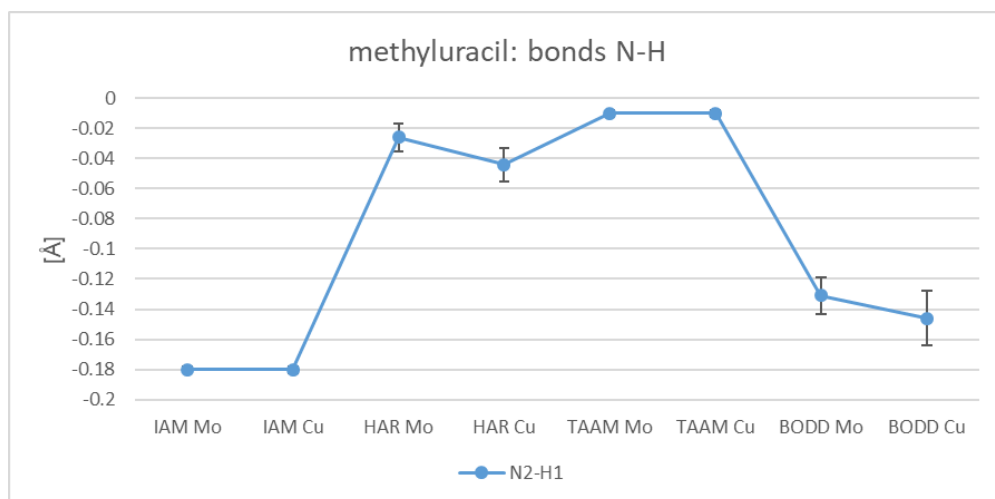


Figure S12 Comparison of N-H bonds for **1Mo**, **1Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data in angstroms. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

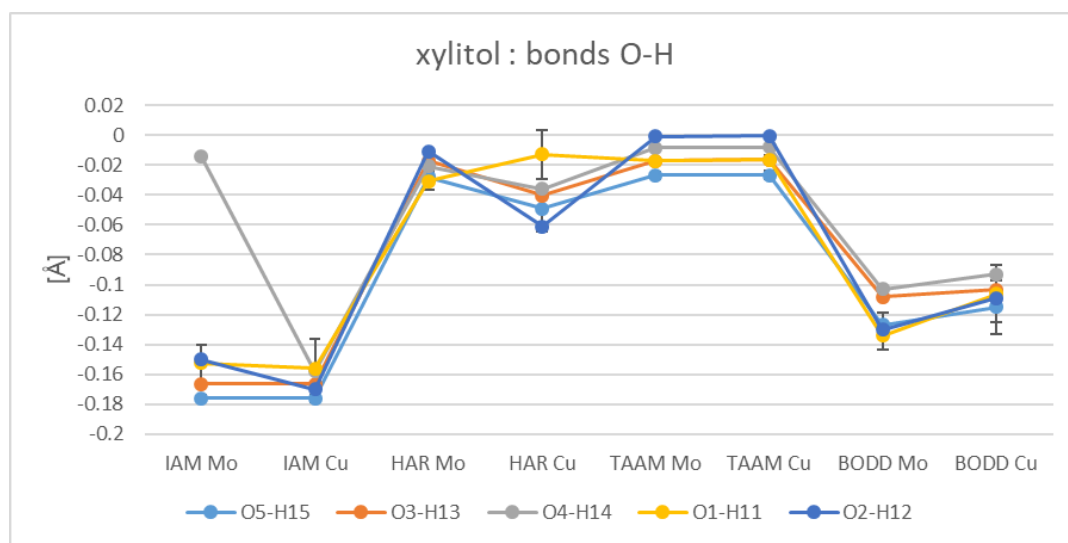


Figure S13 Comparison of O-H bonds for **2Mo** and **2Cu**. Values on plot represent difference between values obtained with analysed model and neutron data in angstroms. Lines on plot have no physical meaning, however help in visual analysis. For clarity, estimated standard deviations were shown only for O1-H11 and O5-H15 bonds.

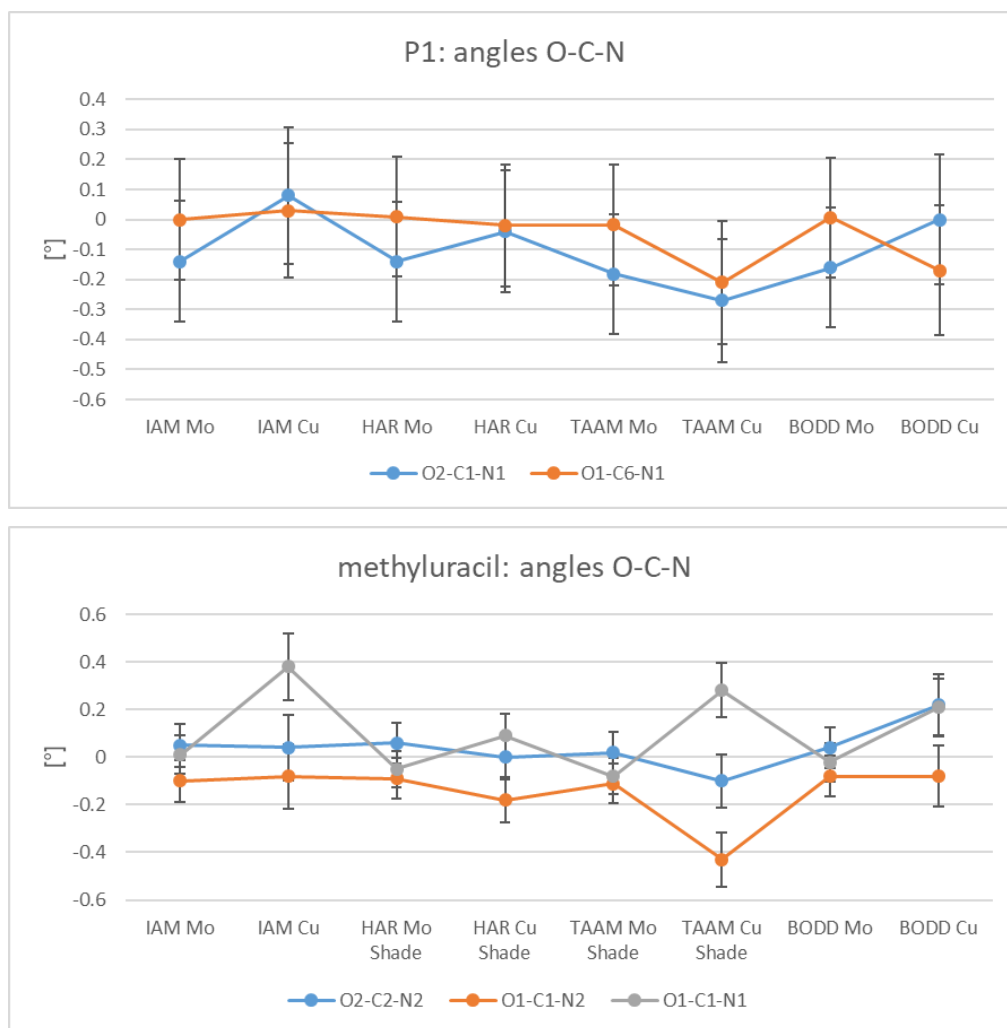


Figure S14 Comparison of O-C-N angles for **1Mo**, **1Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

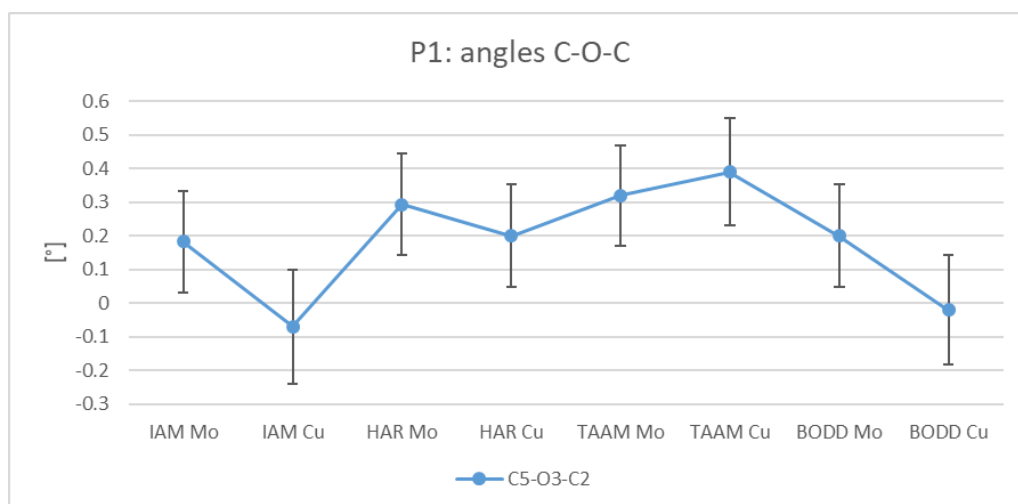


Figure S15 Comparison of C-O-C angles for **1Mo** and **1Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

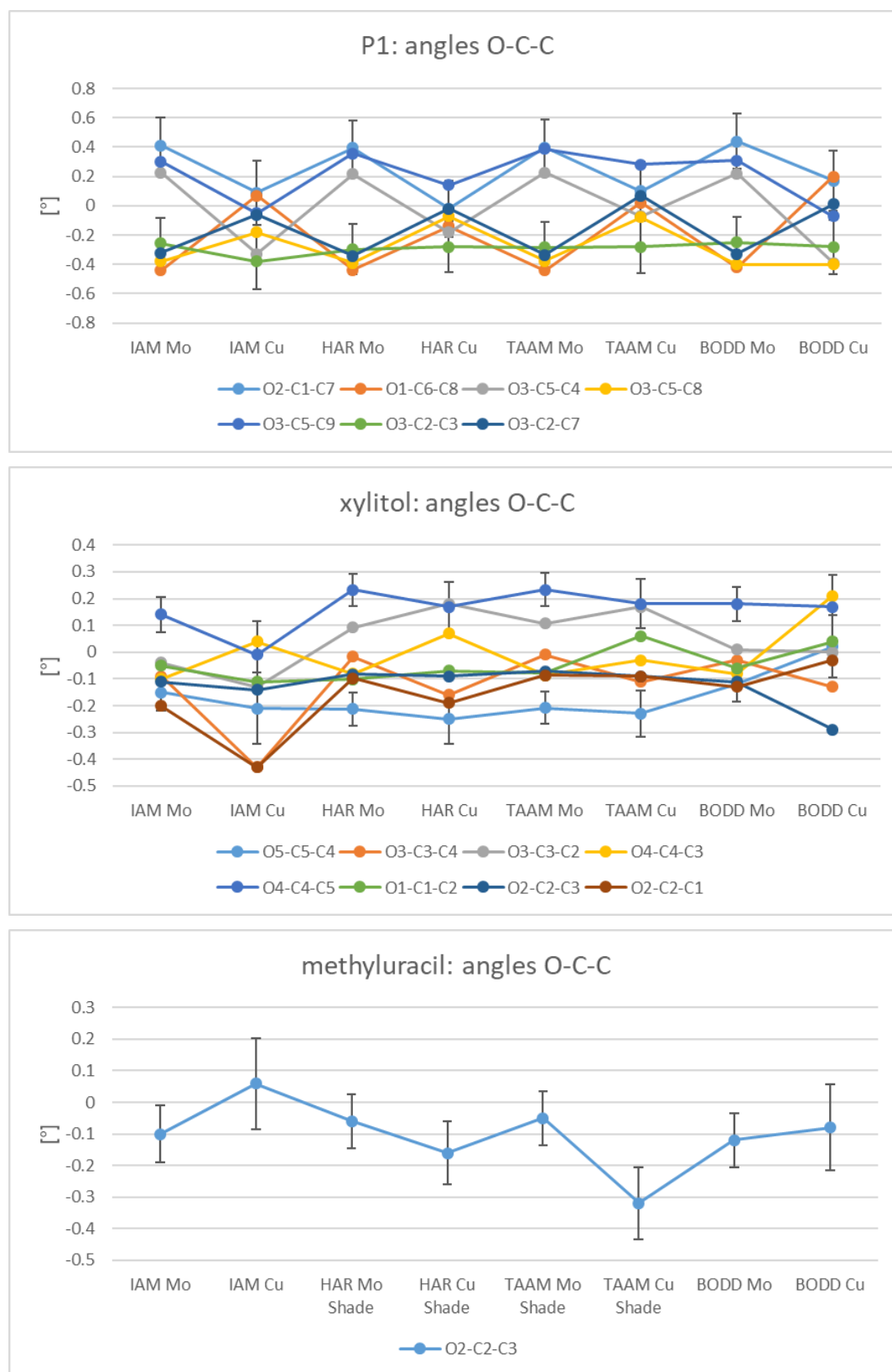


Figure S16 Comparison of O-C-C angles for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For clarity, estimated standard deviations of **1Mo** and **1Cu** were shown only for O3-C2-C3 and O2-C1-C7 angles.

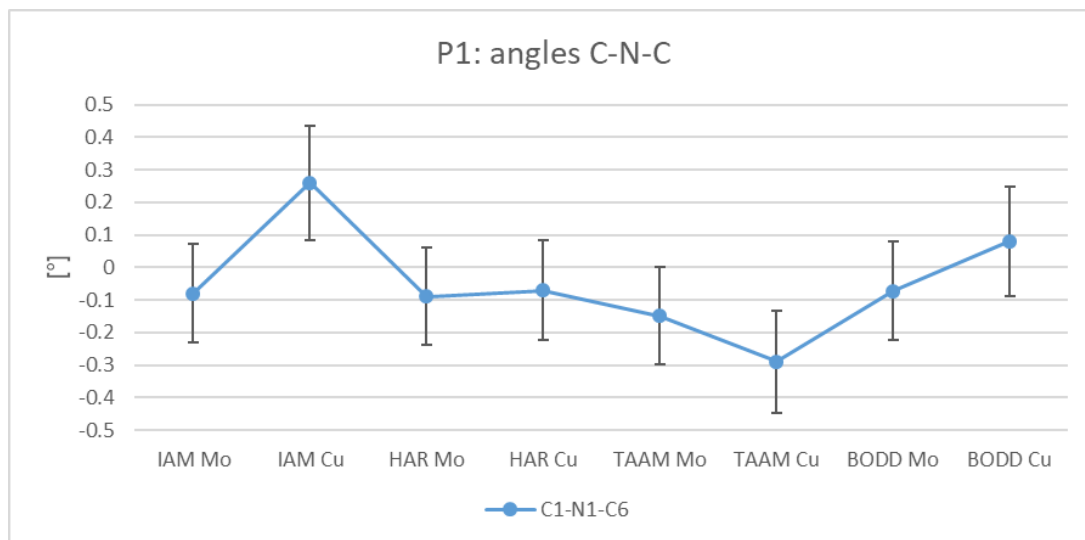


Figure S17 Comparison of C-N-C angles for **1Mo**, **1Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

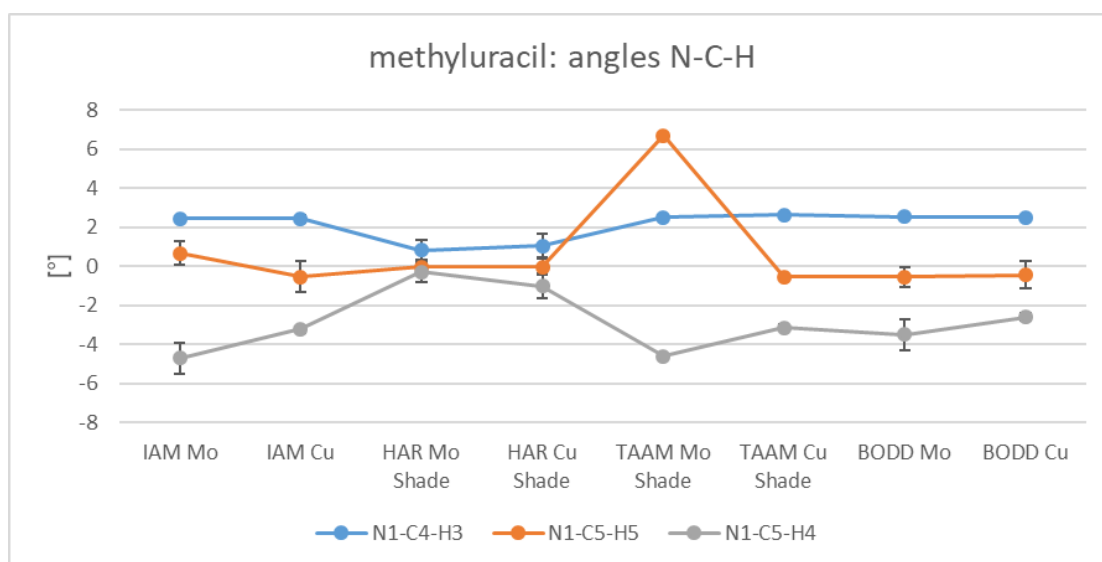


Figure S18 Comparison of N-C-H angles for **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

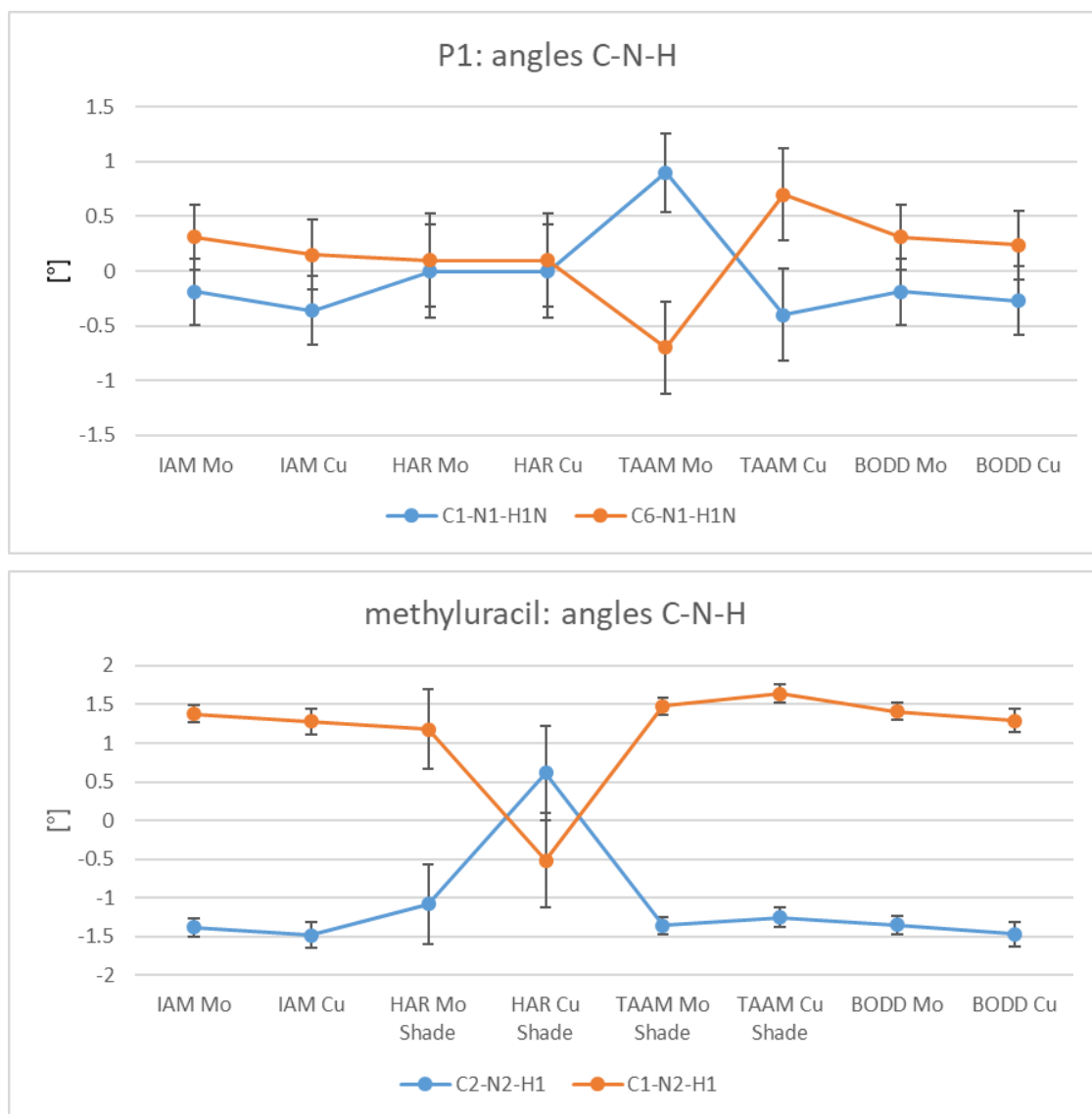


Figure S19 Comparison of C-N-H angles for **1Mo**, **1Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

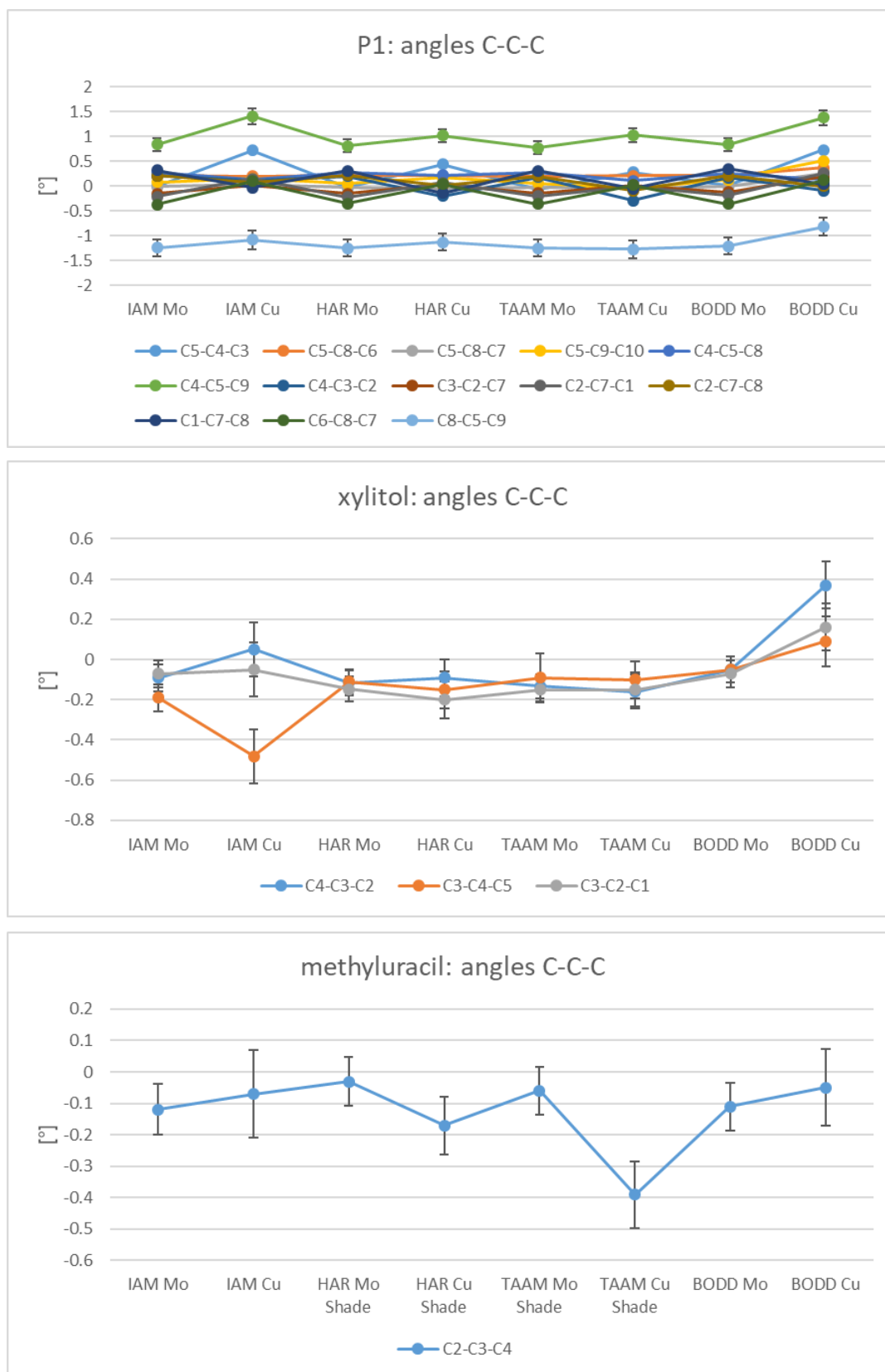


Figure S20 Comparison of C-C-C angles for 1Mo, 1Cu, 2Mo, 2Cu, 3Mo and 3Cu. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot

have no physical meaning, however help in visual analysis. For clarity, estimated standard deviations of P1 (**1Mo** and **1Cu**) were shown only for C4-C5-C9 and C8-C5-C9 angles.

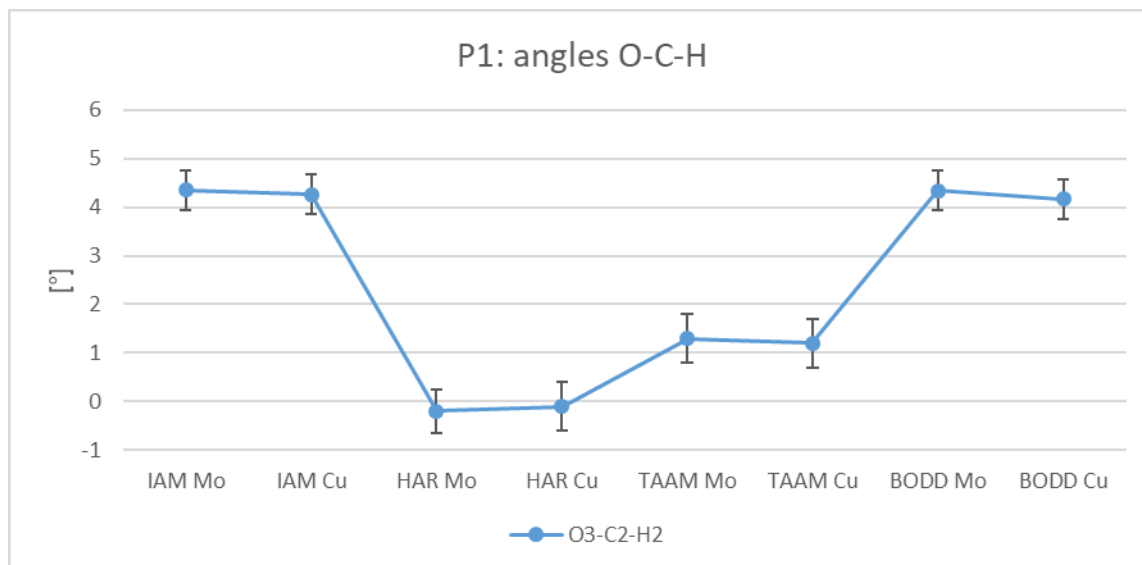


Figure S21 Comparison of O-C-H angles for **1Mo**, **1Cu**, **2Mo** and **2Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For clarity, estimated standard deviations of **2Mo** and **2Cu** were shown only for O5-C5-H5B and O1-C1-H1B angles.

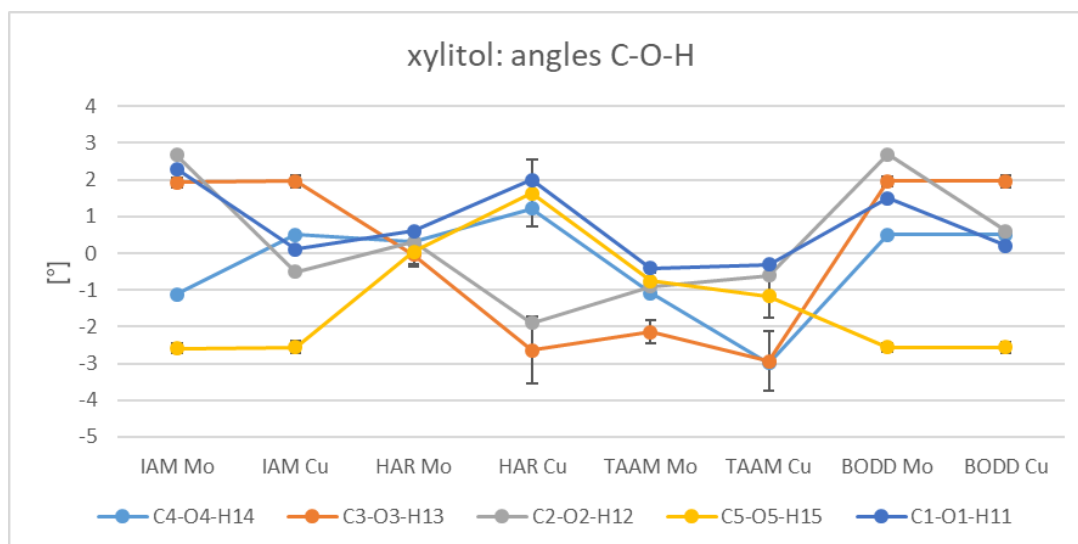
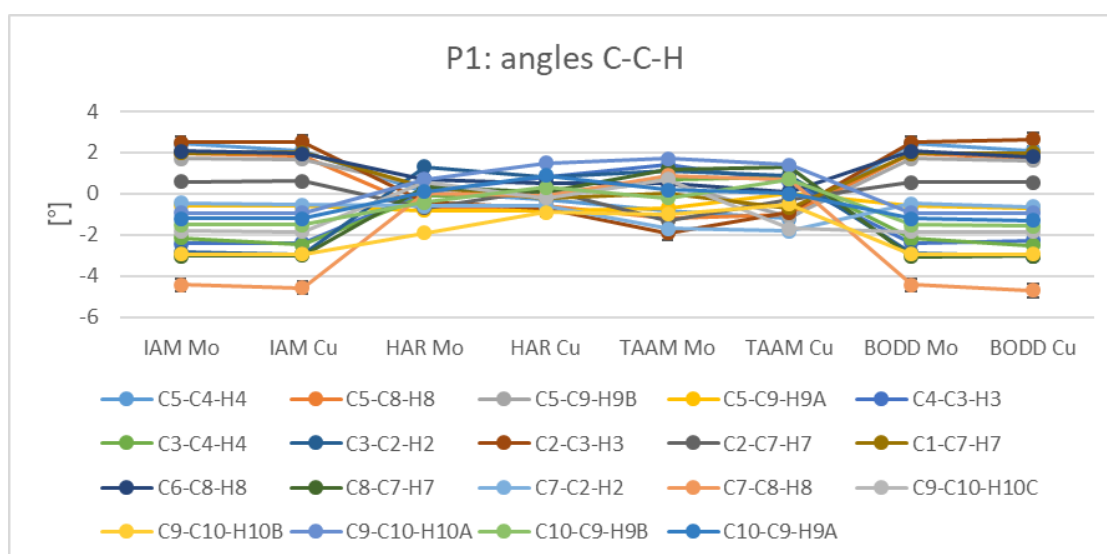


Figure S22 Comparison of C-O-H angles for **2Mo** and **2Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For clarity, estimated standard deviations were shown only for C3-O3-H12 and C5-O5-H15 angles.



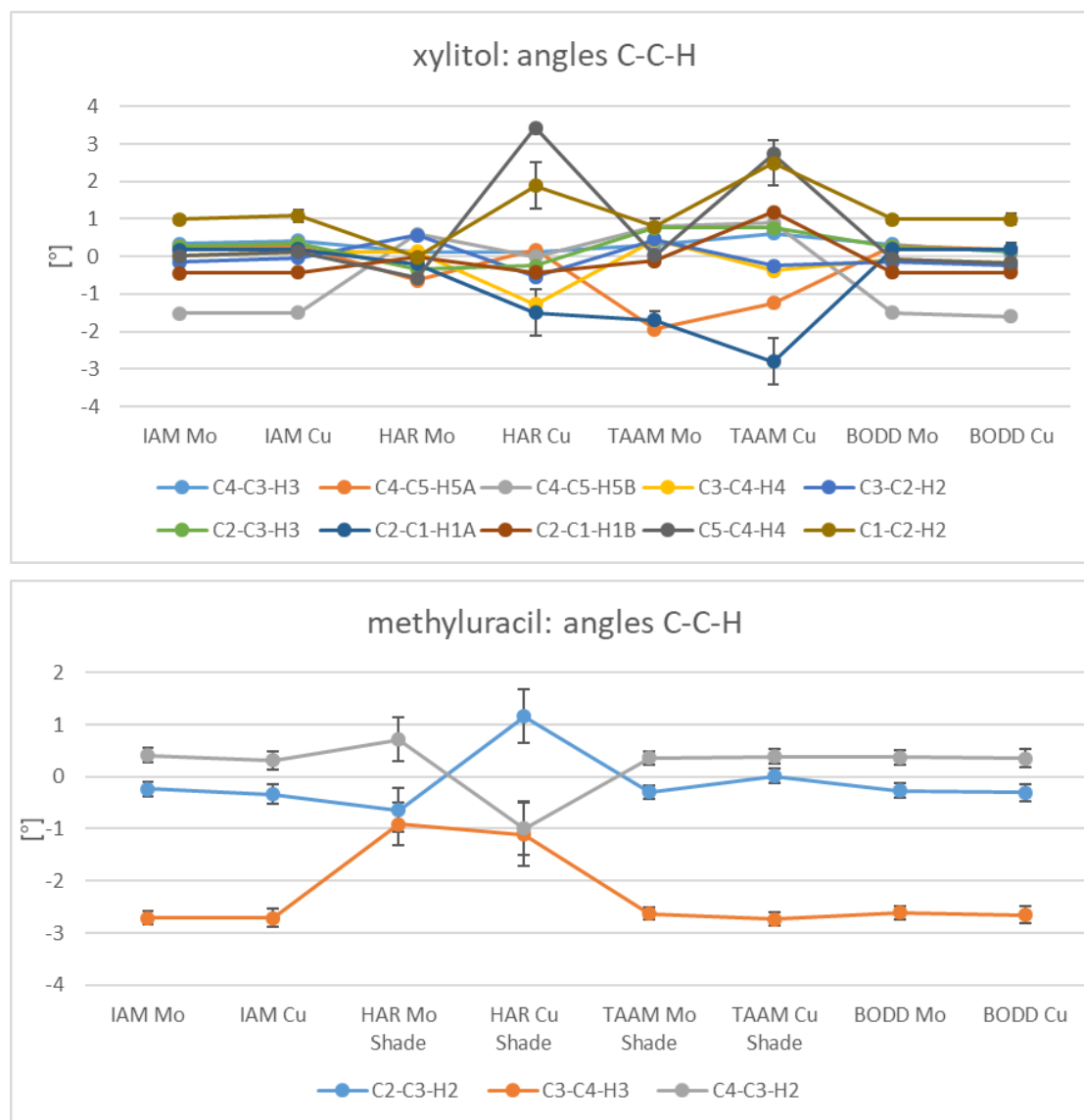


Figure S23 Comparison of C-C-H angles for **1Mo**, **1Cu**, **2Mo**, **2Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For clarity, estimated standard deviations of **1Mo** and **1Cu** were shown only for C2-C3-H3 and C7-C8-H8 angles, whereas estimated standard deviations of **2Mo** and **2Cu** were shown only for C1-C2-H2 and C2-C1-H1A angles.

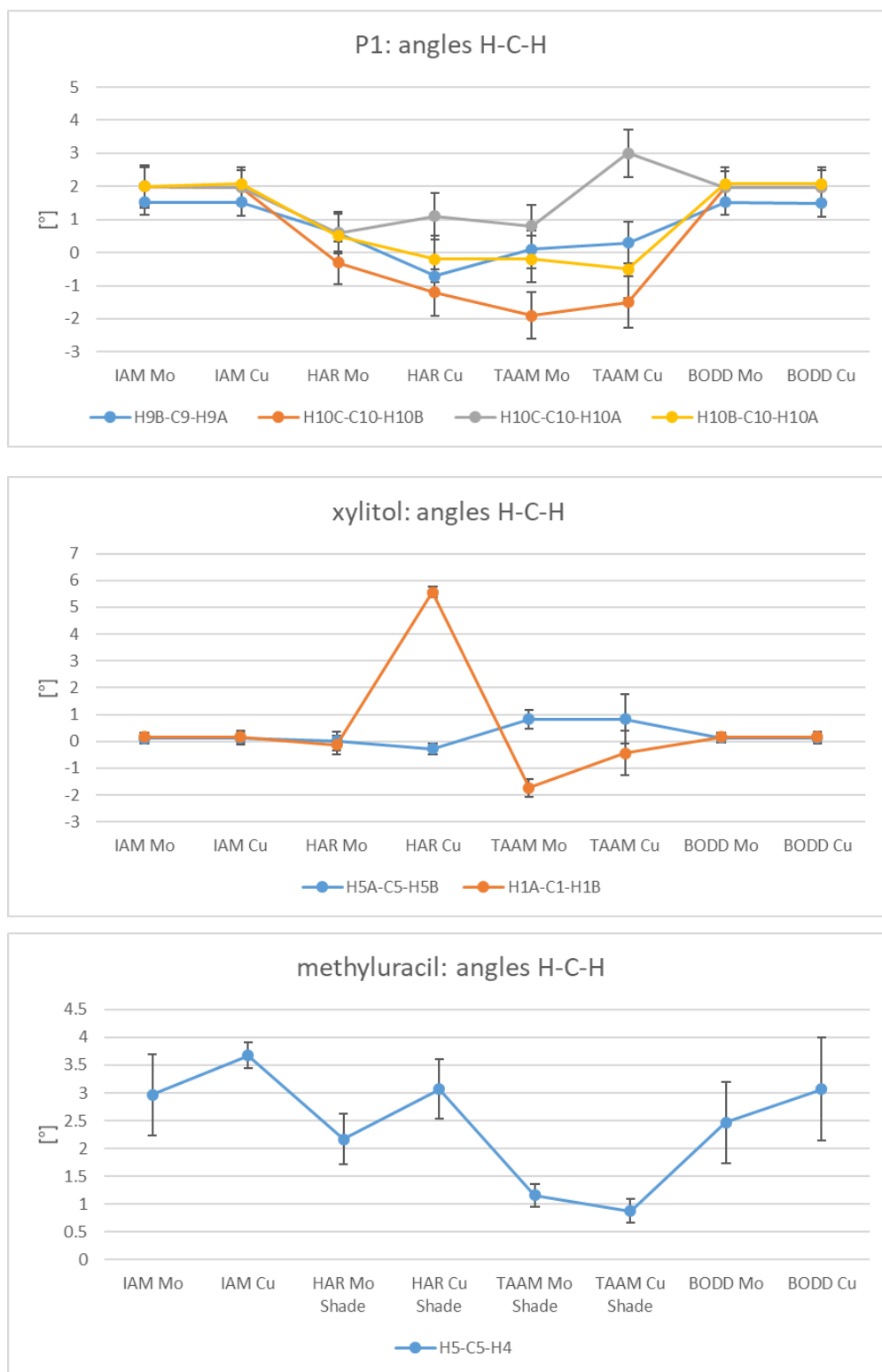


Figure S24 Comparison of H-C-H angles for 1Mo, 1Cu, 2Mo, 2Cu, 3Mo and 3Cu. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

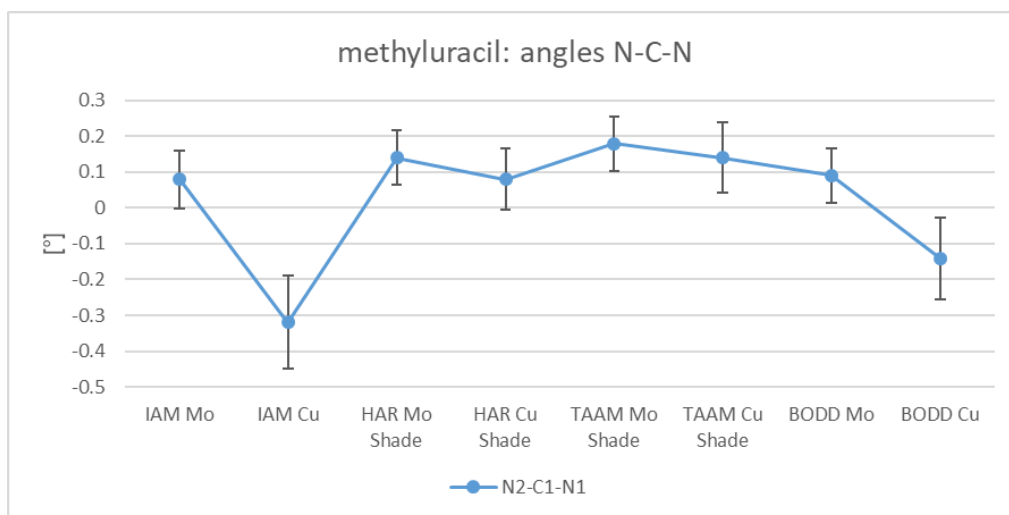


Figure S25 Comparison of N-C-N angles for **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

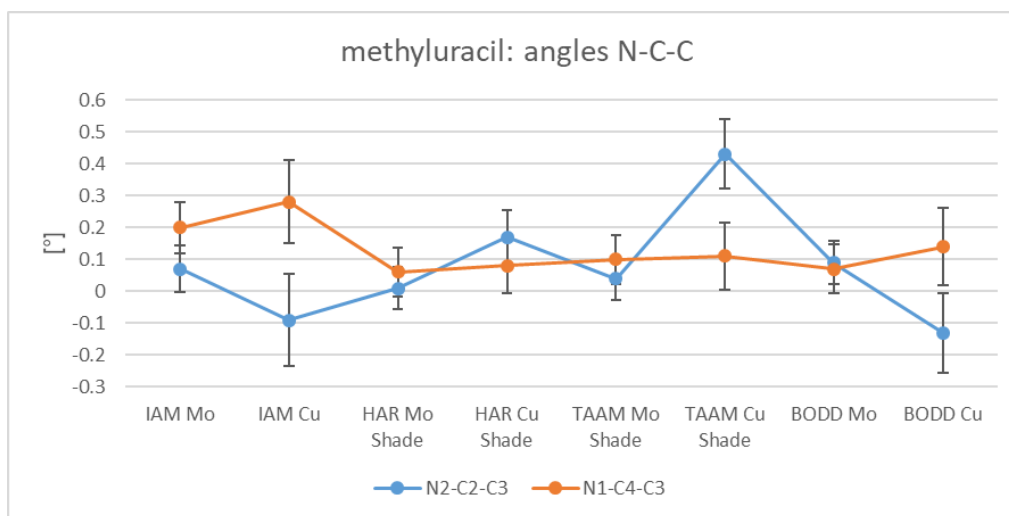
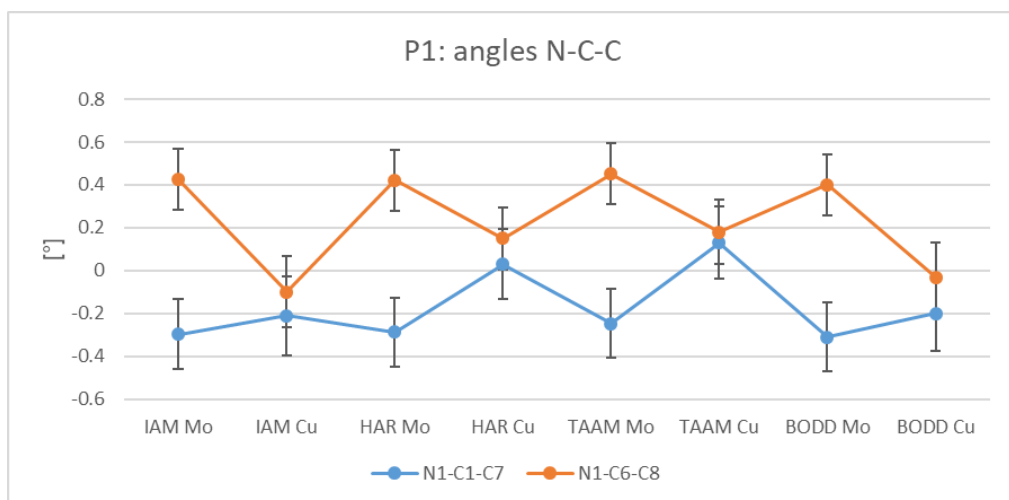


Figure S26 Comparison of N-C-C angles for **1Mo**, **1Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.

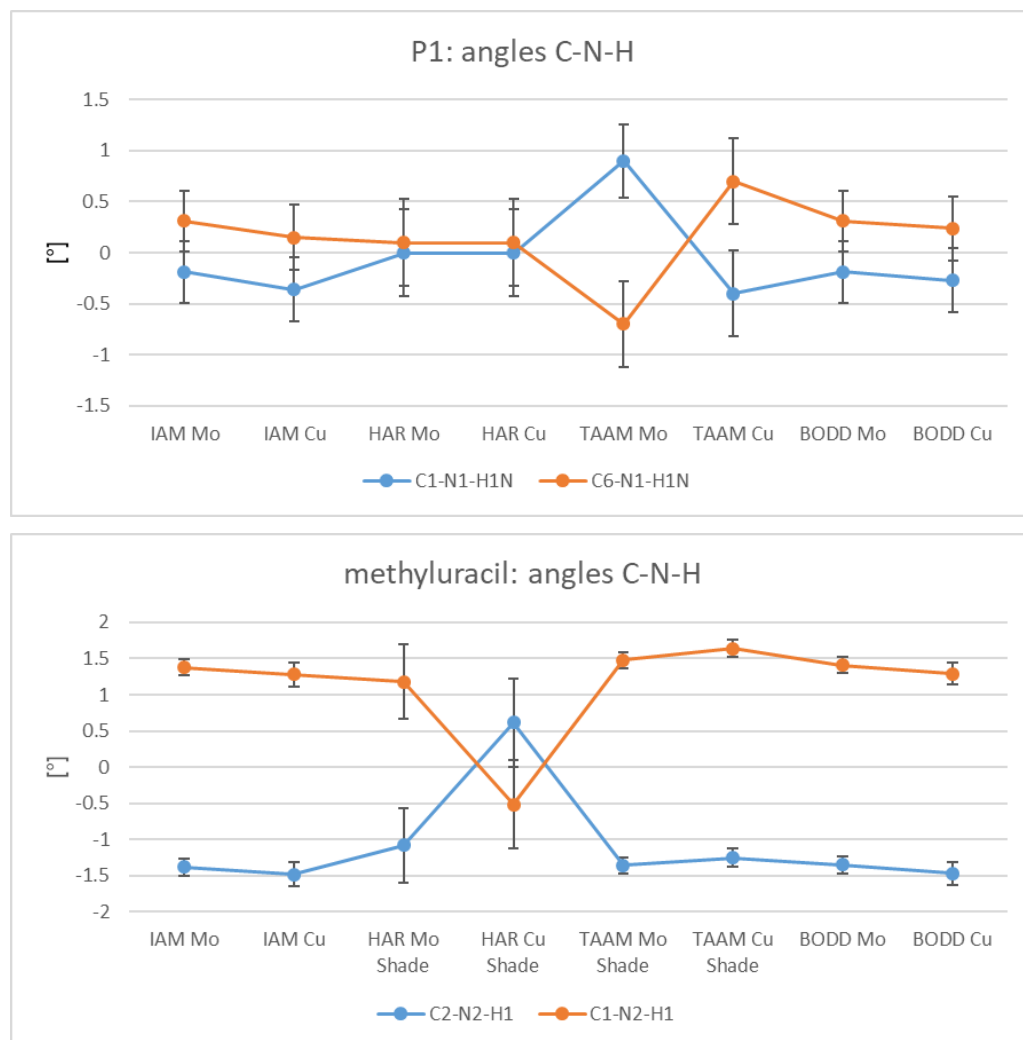
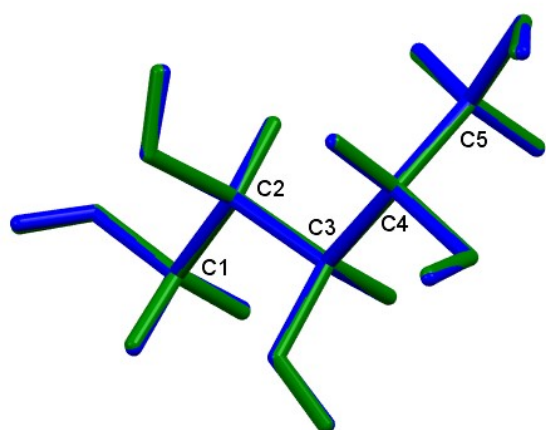
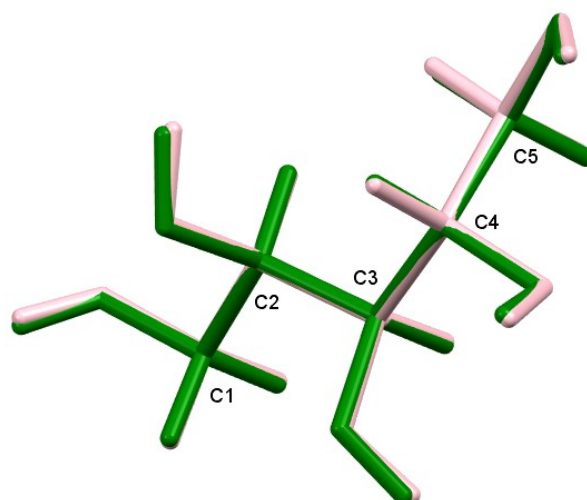
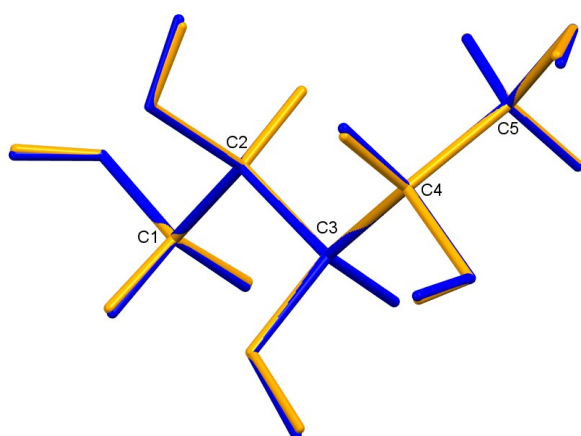


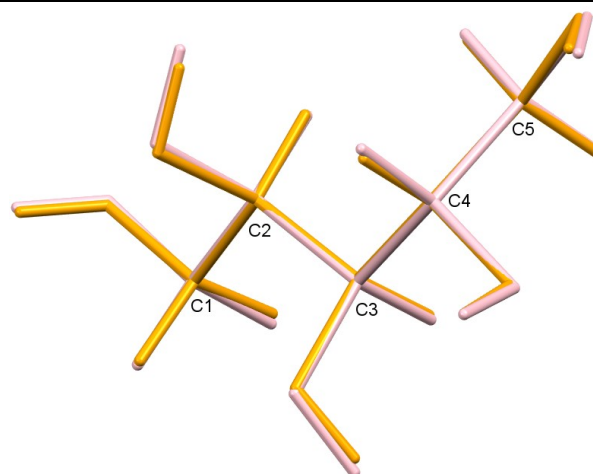
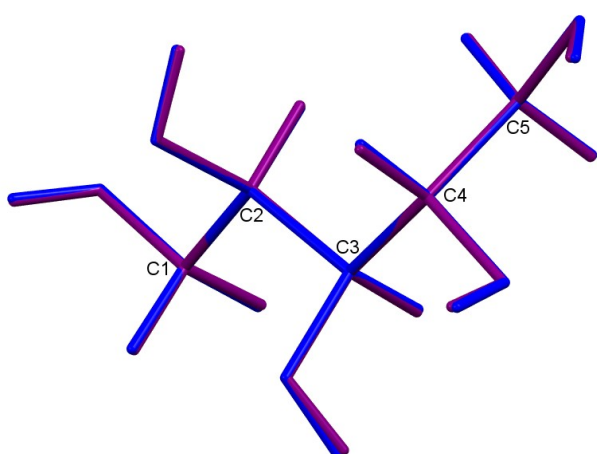
Figure S27 Comparison of C-N-H angles for **1Mo**, **1Cu**, **3Mo** and **3Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.



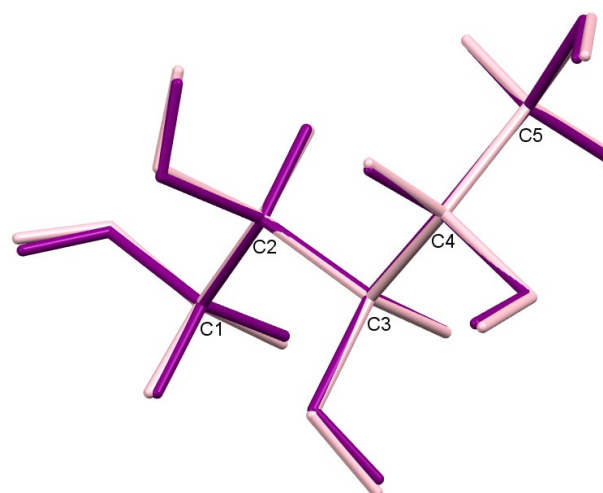
Neu (blue) /IAM Cu (green)

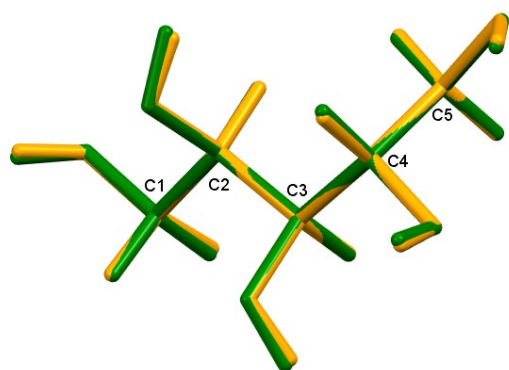
Neu_{opt} (pink)/IAM Cu (green)

Neu (blue) /HAR Cu SHADE (orange)

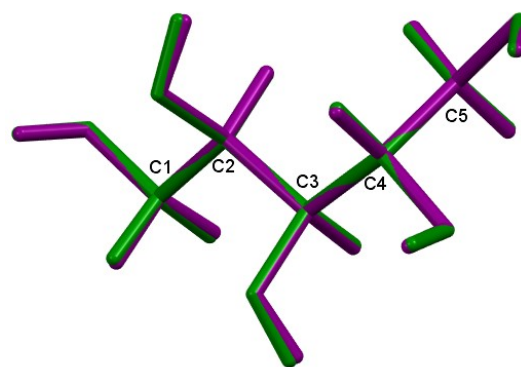
Neu_{opt} (pink)/HAR Cu SHADE (orange)

Neu(blue)/TAAM Cu SHADE (purple)

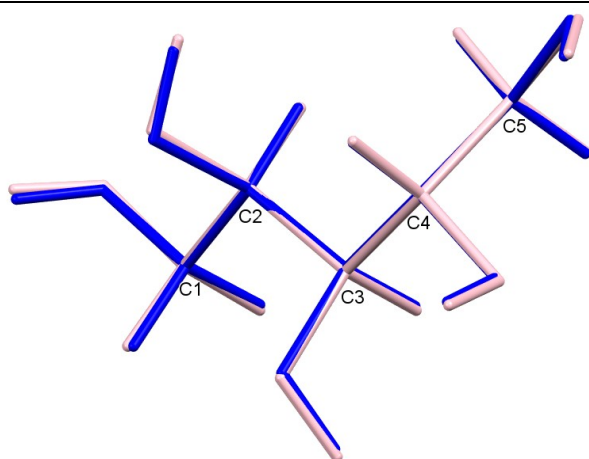
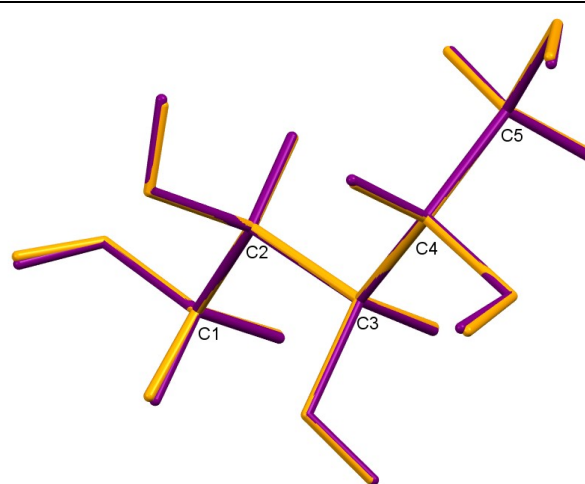
Neu_{opt} (pink)/TAAM Cu SHADE (purple)



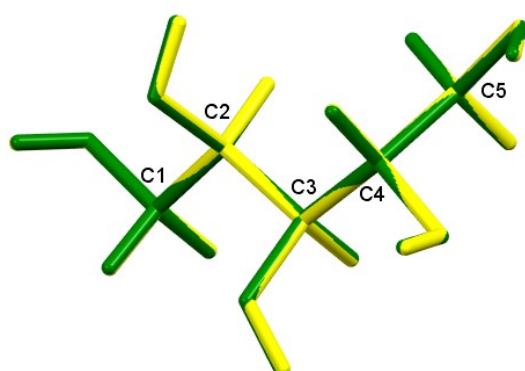
IAM Cu (green)/ HAR Cu SHADE (orange)



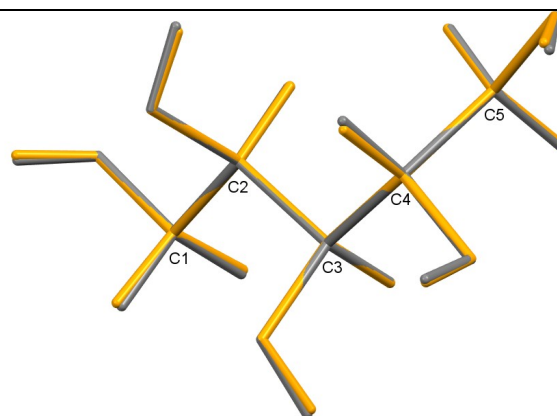
IAM Cu (green)/ TAAM Cu SHADE (purple)

Neu_{opt} (pink)/Neu (blue)

TAAM Cu SHADE (purple) /HAR Cu SHADE (orange)



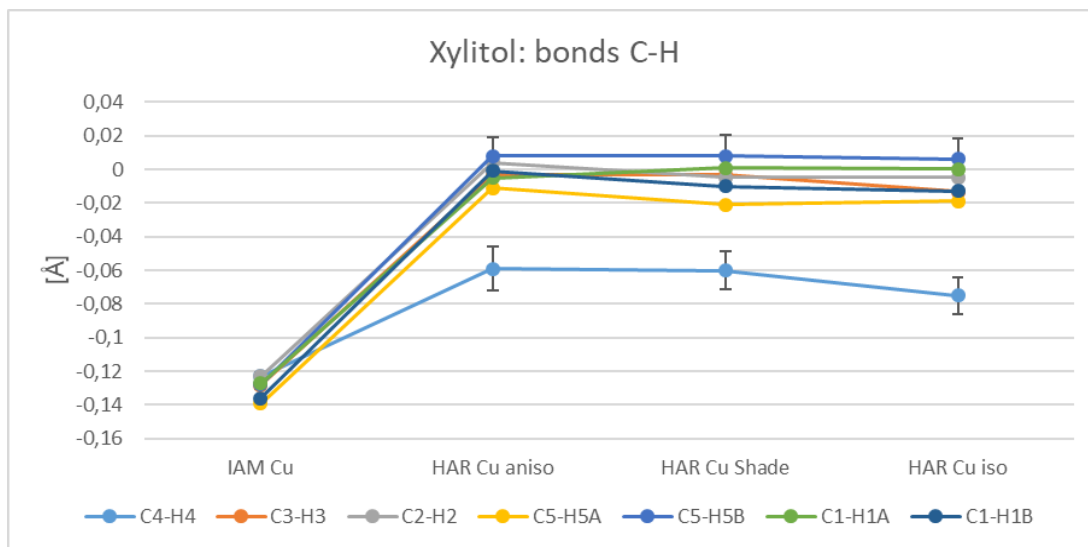
IAM Cu (green)/IAM Mo (yellow)



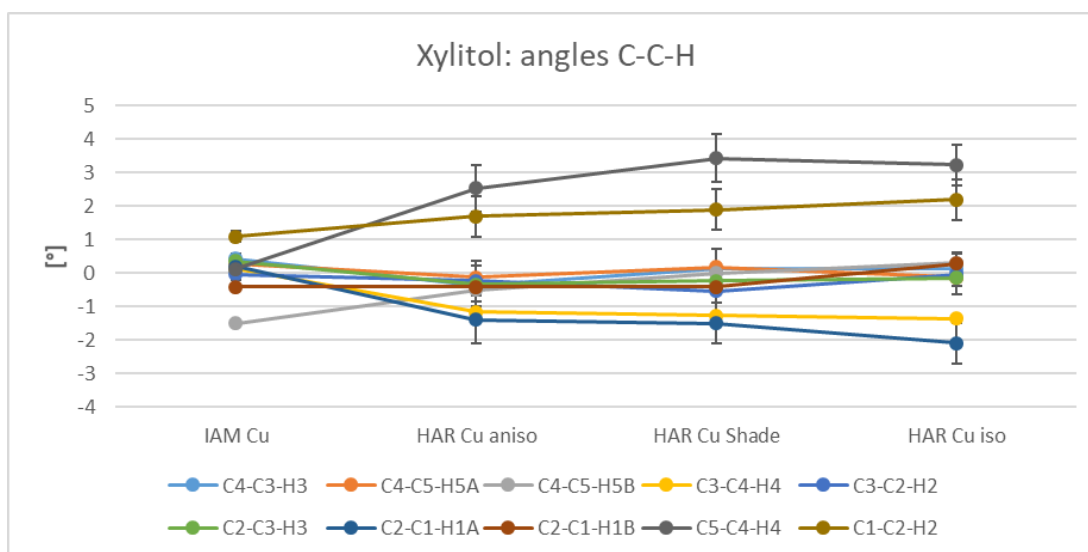
HAR Cu SHADE (orange) / HAR Mo SHADE (grey)

Figure S28 Overlay of selected geometries of **2Cu**, **2Mo** and **2Neu** used for lattice energy calculations.

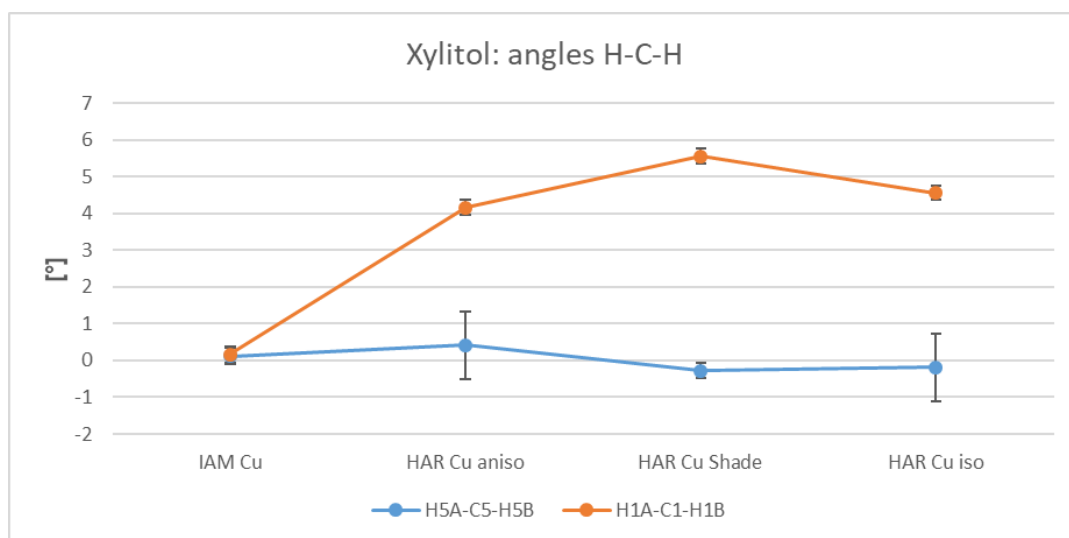
a)



b)



c)



d)

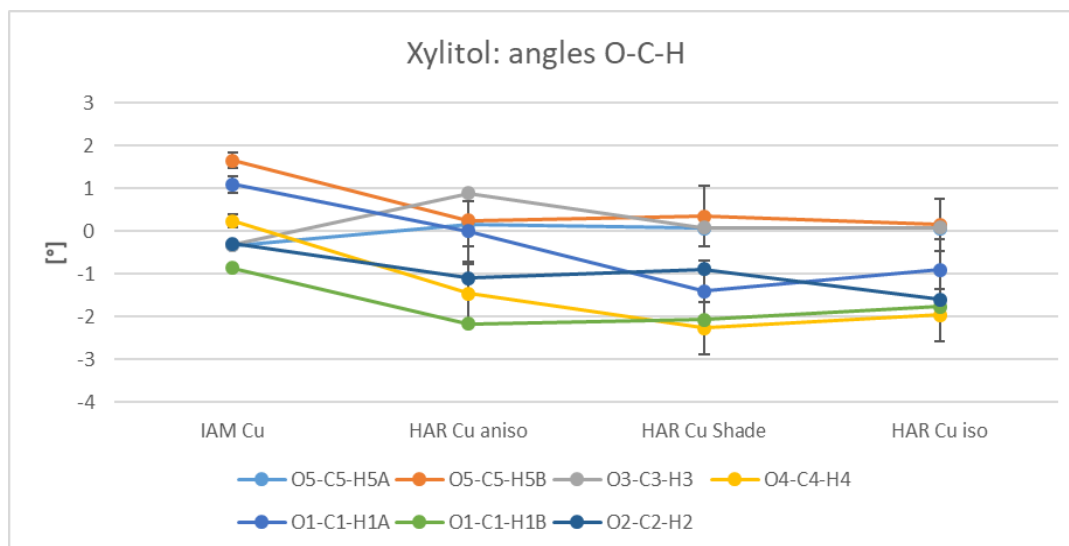
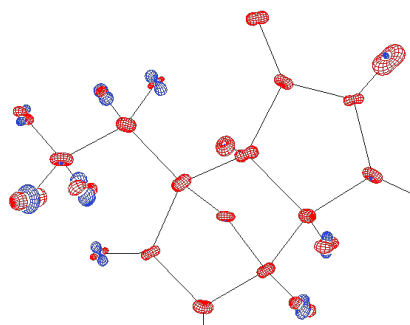
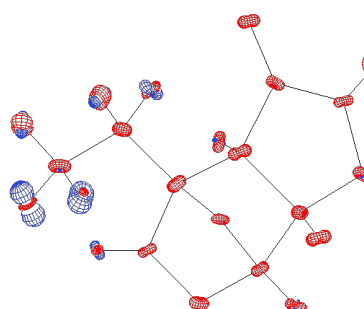


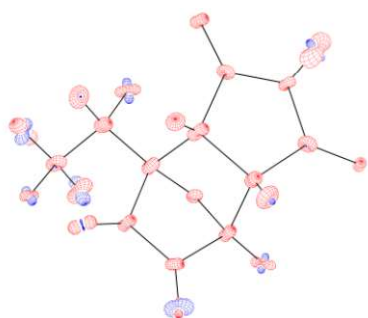
Figure S29 Comparison of a) C-H bonds, b) C-C-H angles, c) H-C-H angles and d) O-C-H angles for **2Cu**. Values on plot represent difference between values obtained with analysed model and neutron data. Lines on plot have no physical meaning, however help in visual analysis. For each plot estimated standard deviations were added.



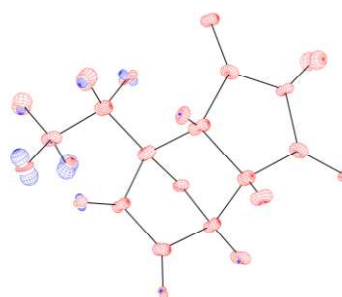
HAR Mo aniso



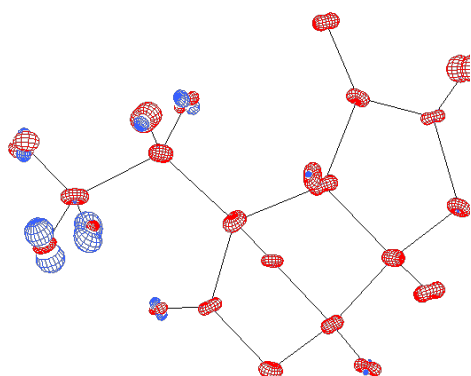
HAR Mo Shade



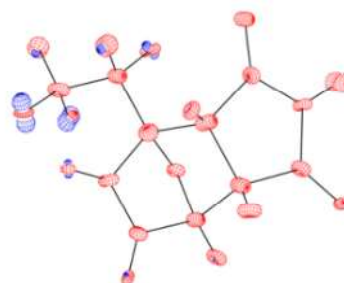
HAR Cu aniso



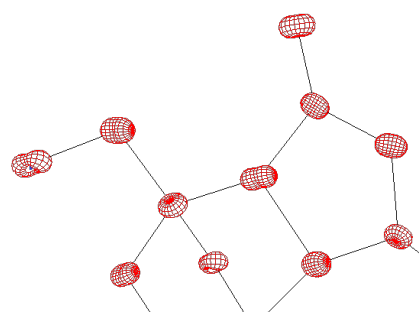
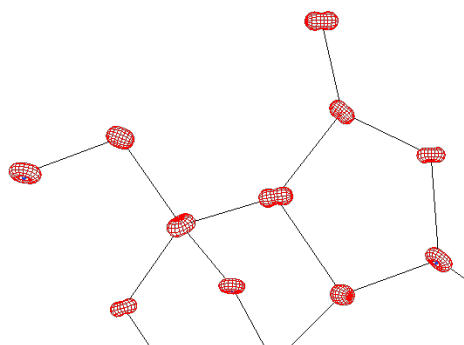
HAR Cu Shade



TAAM Mo Shade



TAAM Cu Shade



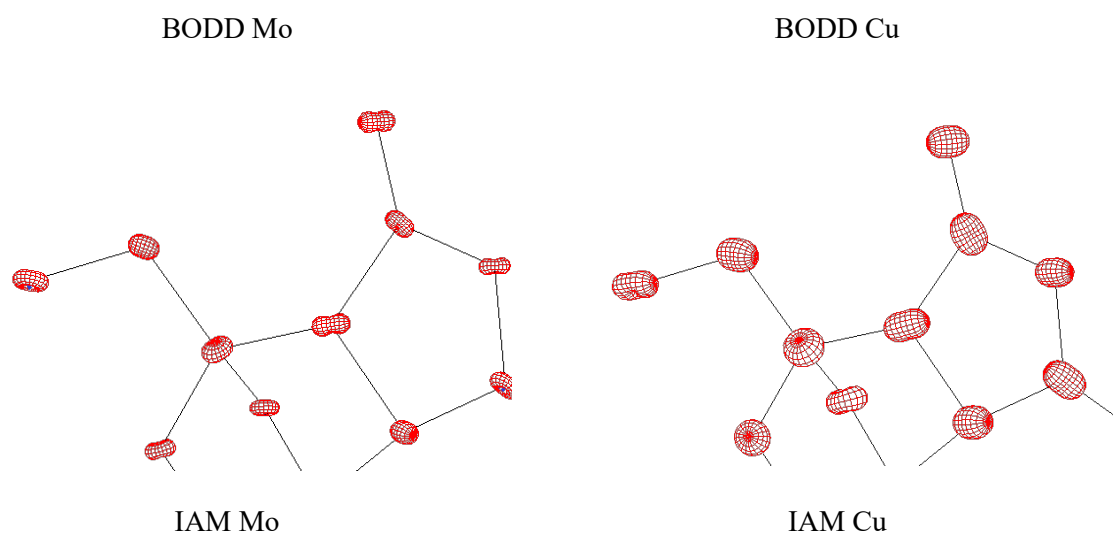
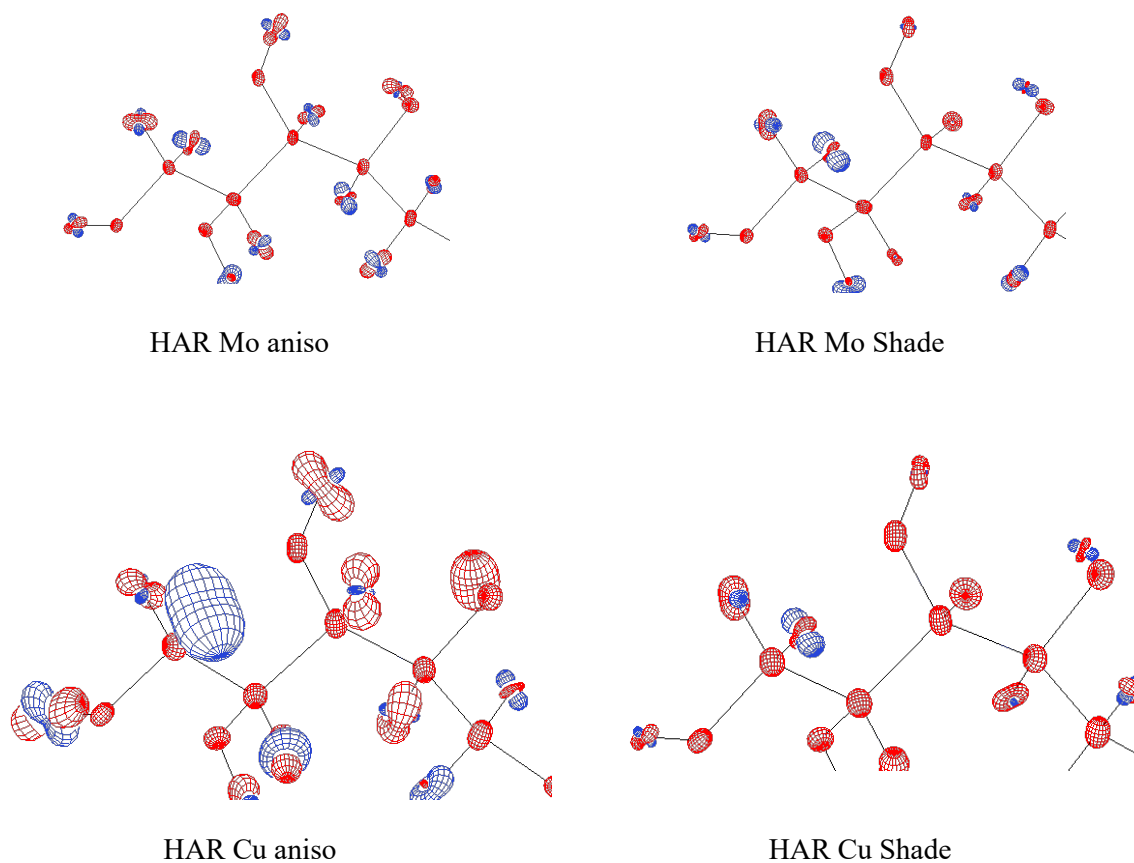


Figure S30 Difference between ADPs of neutron and analysed model for **1Cu** and **1Mo**. Two-step overlay algorithm and 2.0 scale were applied using PEANUT software.



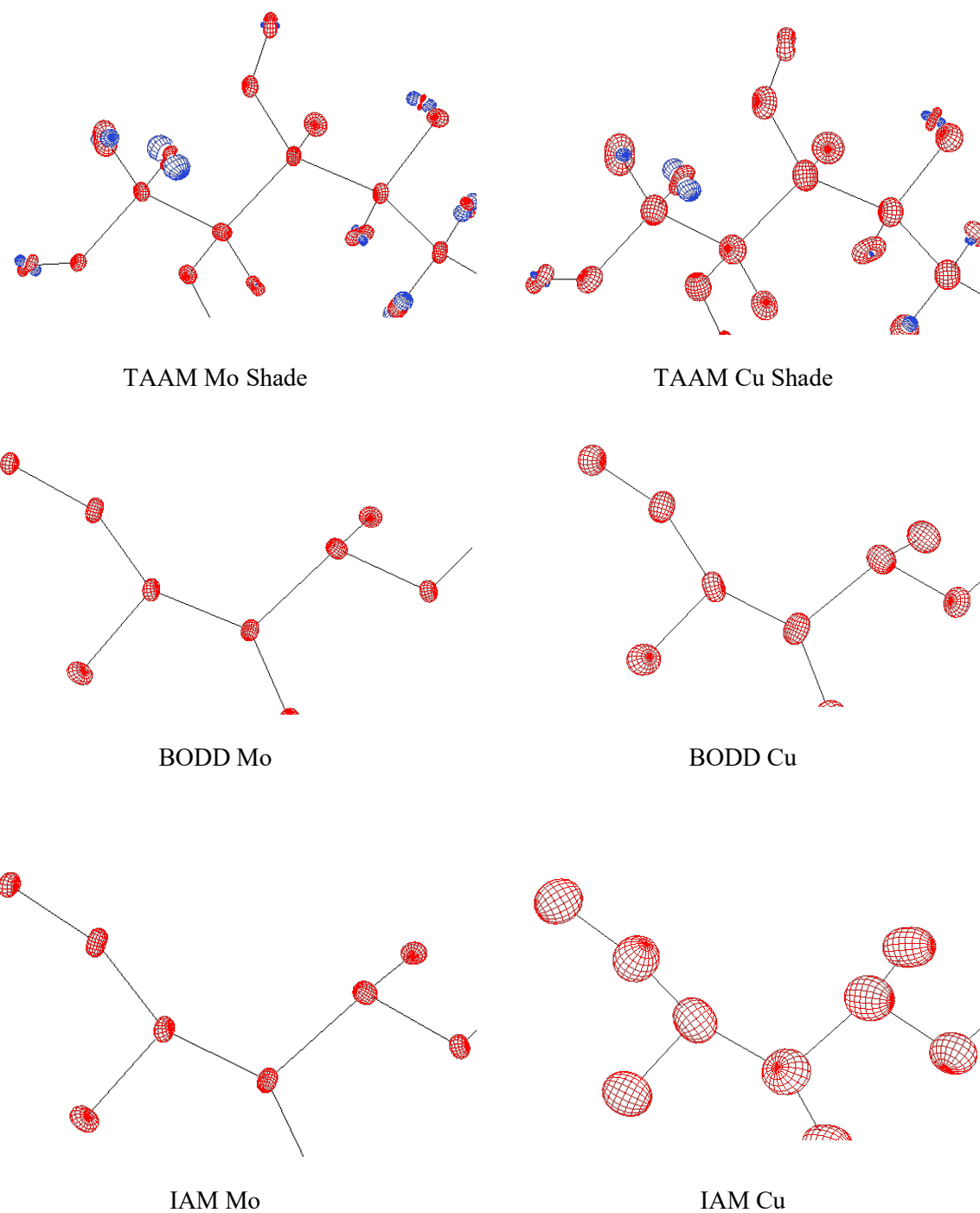
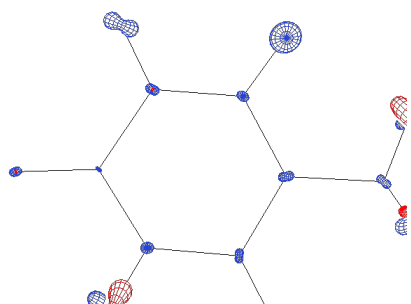
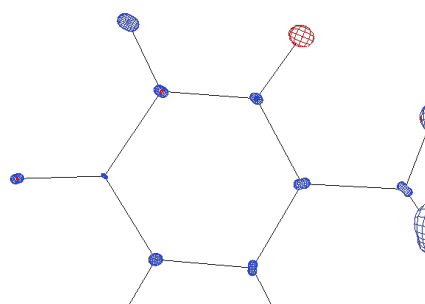


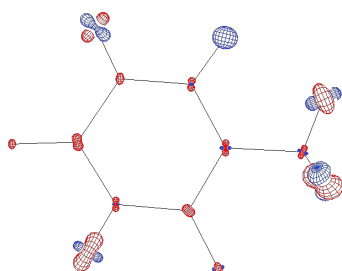
Figure S31 Difference between ADPs of neutron and analysed model for **2Cu** and **2Mo**. Two-step overlay algorithm and 2.0 scale were applied using PEANUT software.



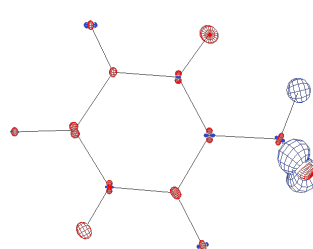
HAR Mo aniso



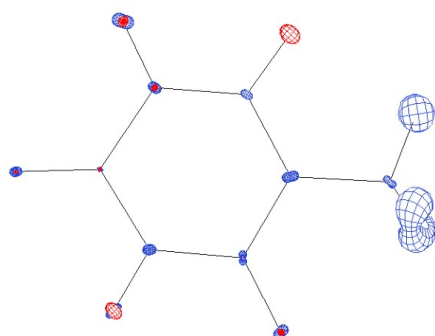
HAR Mo Shade



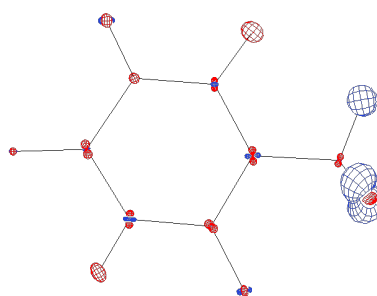
HAR Cu aniso



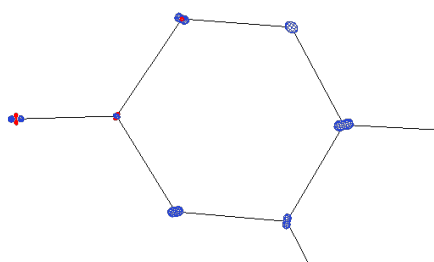
HAR Cu Shade



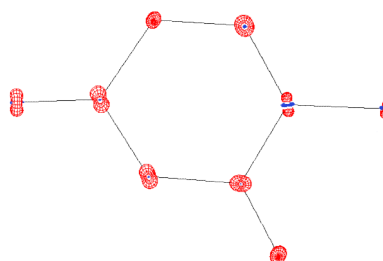
TAAM Mo Shade



TAAM Cu Shade



BODD Mo



BODD Cu

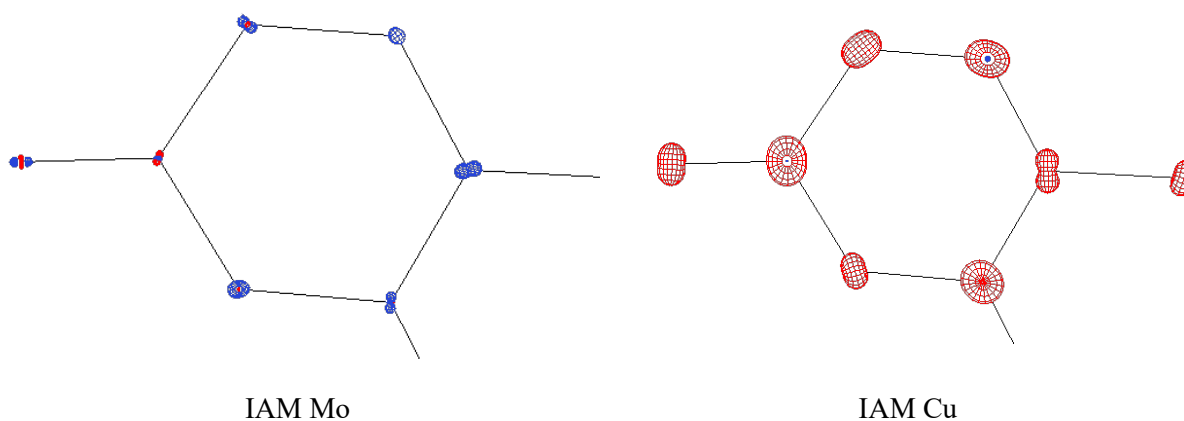
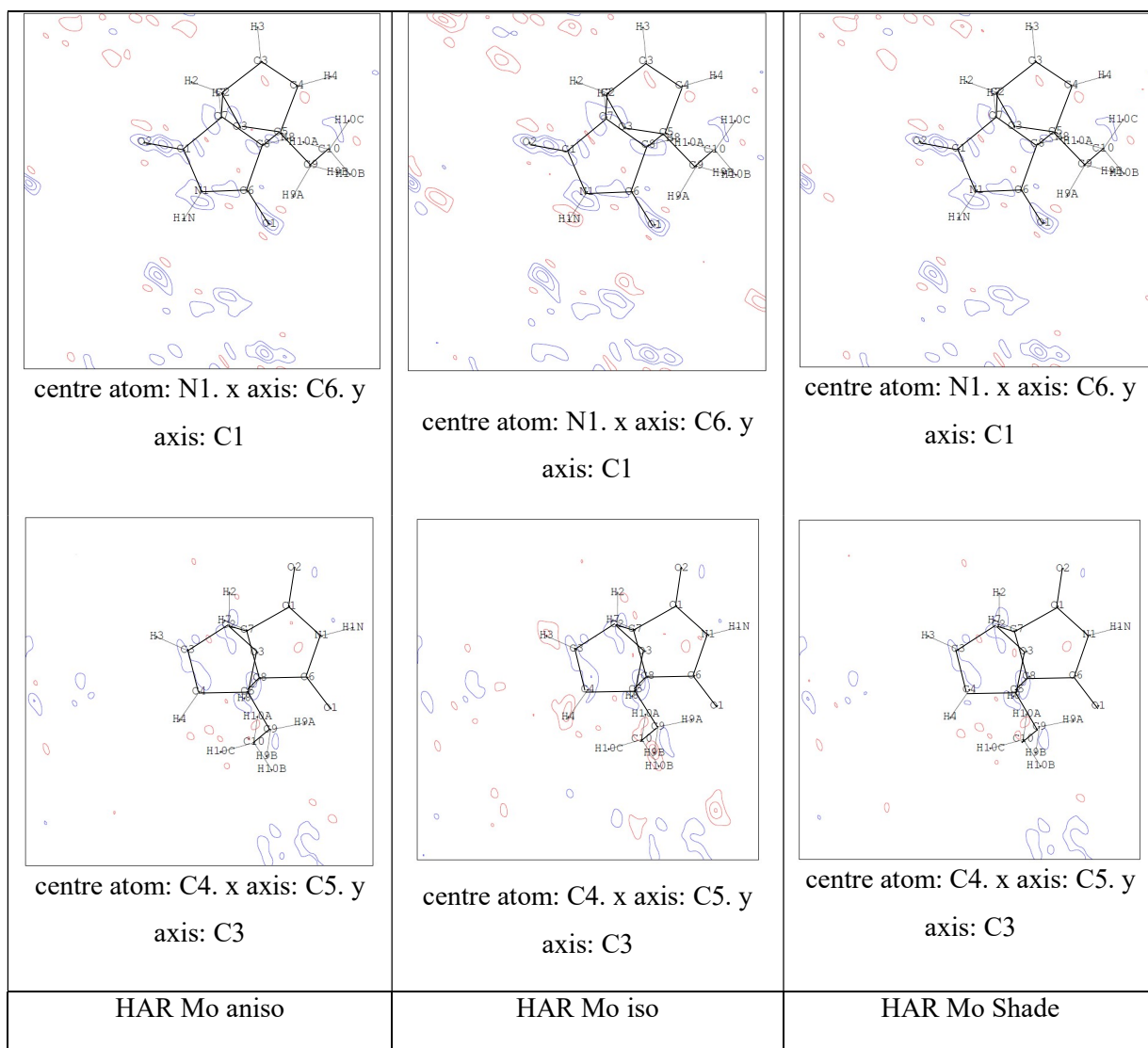
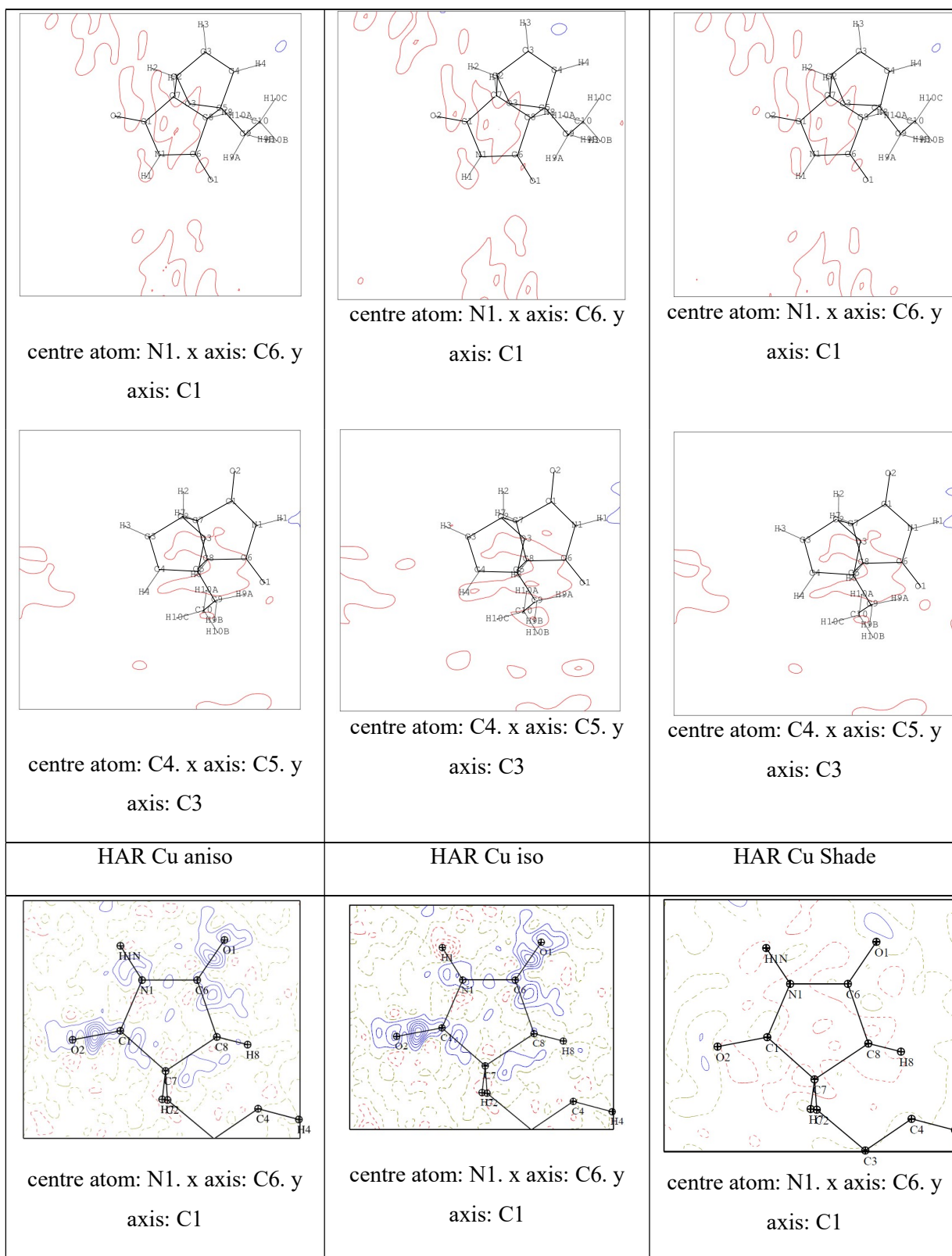
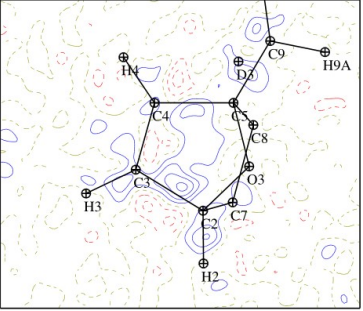
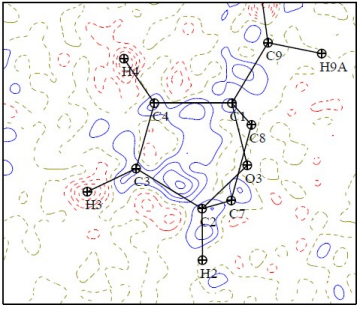
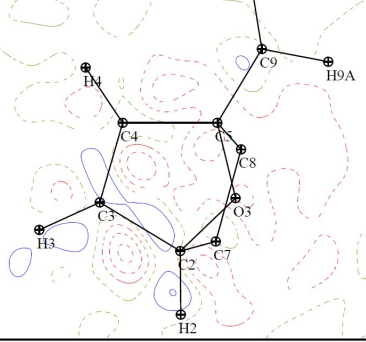
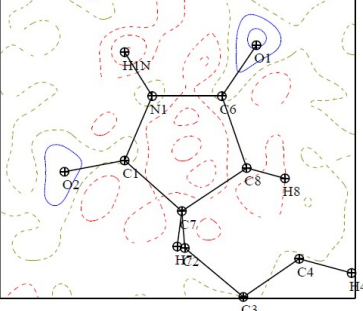
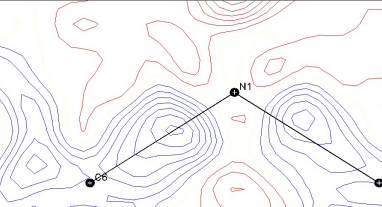
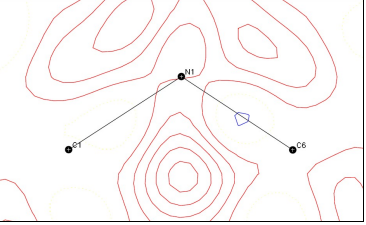
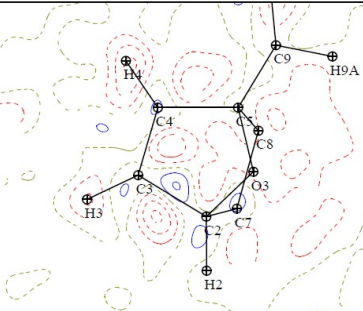
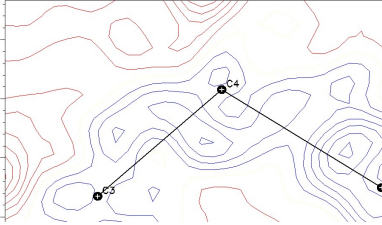
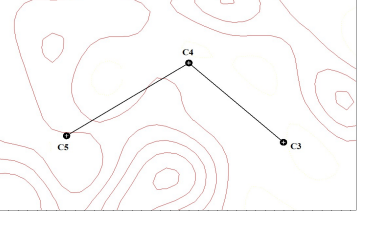
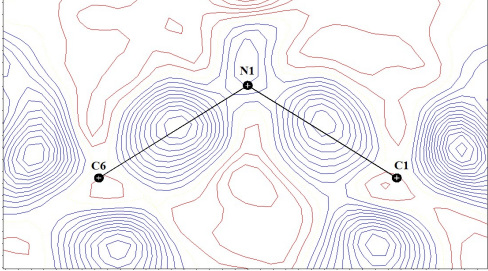
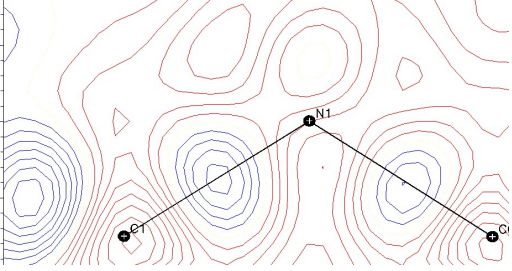


Figure S32 Difference between ADPs of neutron and analysed model for **3Cu** and **3Mo**. Two-step overlay algorithm and 2.0 scale were applied using PEANUT software.





 <p>centre atom: C4. x axis: C5. y axis: C3</p>	 <p>centre atom: C4. x axis: C5. y axis: C3</p>	 <p>centre atom: C4. x axis: C5. y axis: C3</p>
TAAM Mo Shade	TAAM Mo iso	TAAM Cu Shade
 <p>centre atom: N1. x axis: C6. y axis: C1</p>	 <p>centre atom: N1. x axis: C6. y axis: C1</p>	 <p>centre atom: N1. x axis: C6. y axis: C1</p>
 <p>centre atom: C4. x axis: C5. y axis: C3</p>	 <p>centre atom: C4. x axis: C5. y axis: C3</p>	 <p>centre atom: C4. x axis: C5. y axis: C3</p>
TAAM Cu iso	BODD Mo	BODD Cu
		

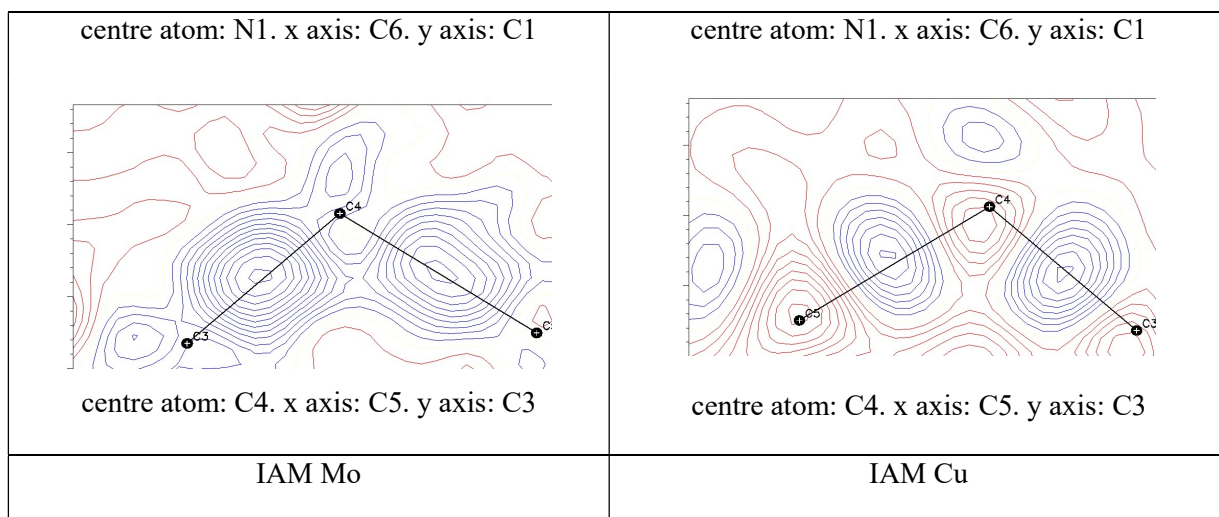
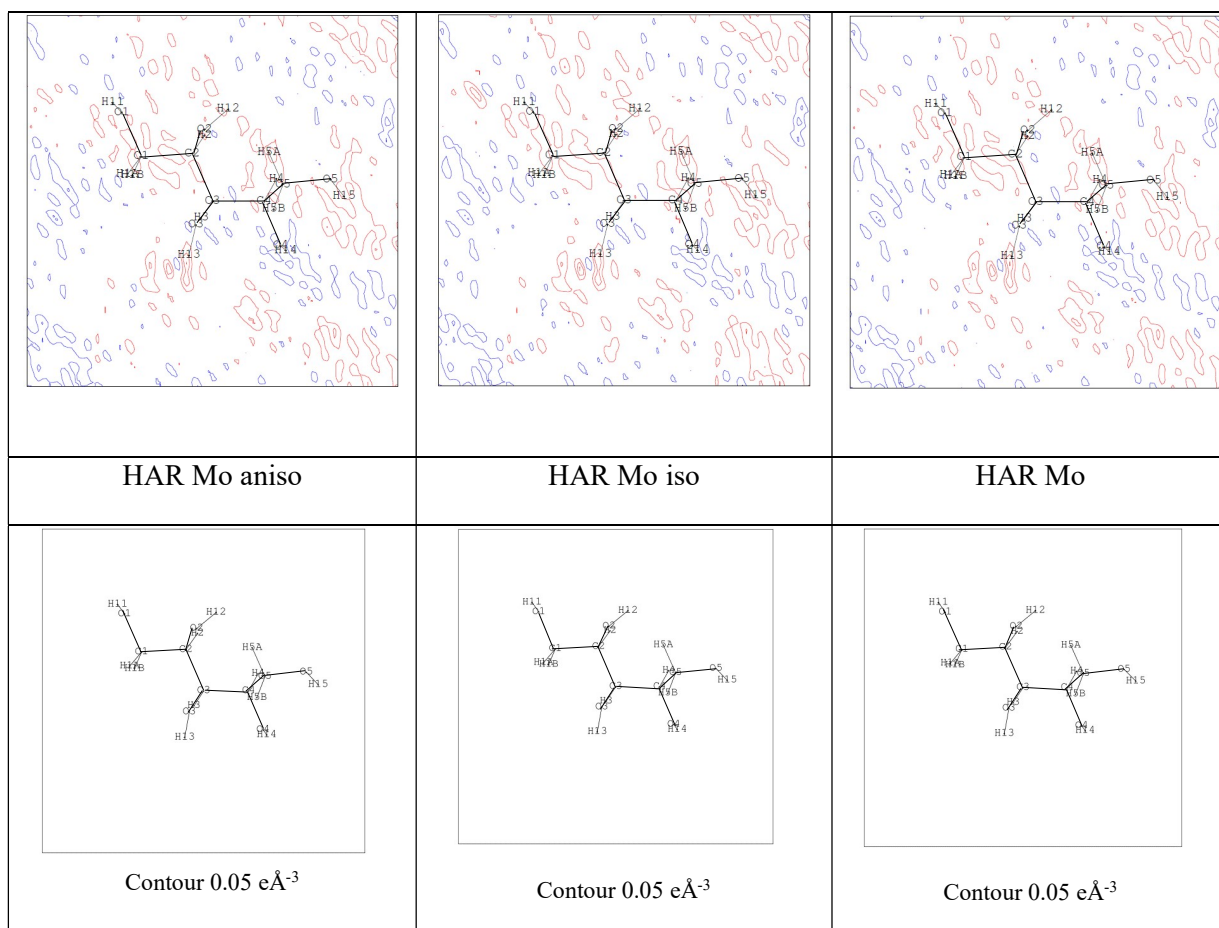


Figure S33 Residual density maps of **1Cu** and **1Mo**. All maps are presented with contours levels with intervals $\pm 0.05 \text{ e}\text{\AA}^{-3}$. Blue lines represent positive values and red lines the negative ones. Maps were prepared for centre atom: N1, x axis: C6 and y axis: C1 or centre atom: C4, x axis: C5 and y axis: C3. Details are given below the maps.



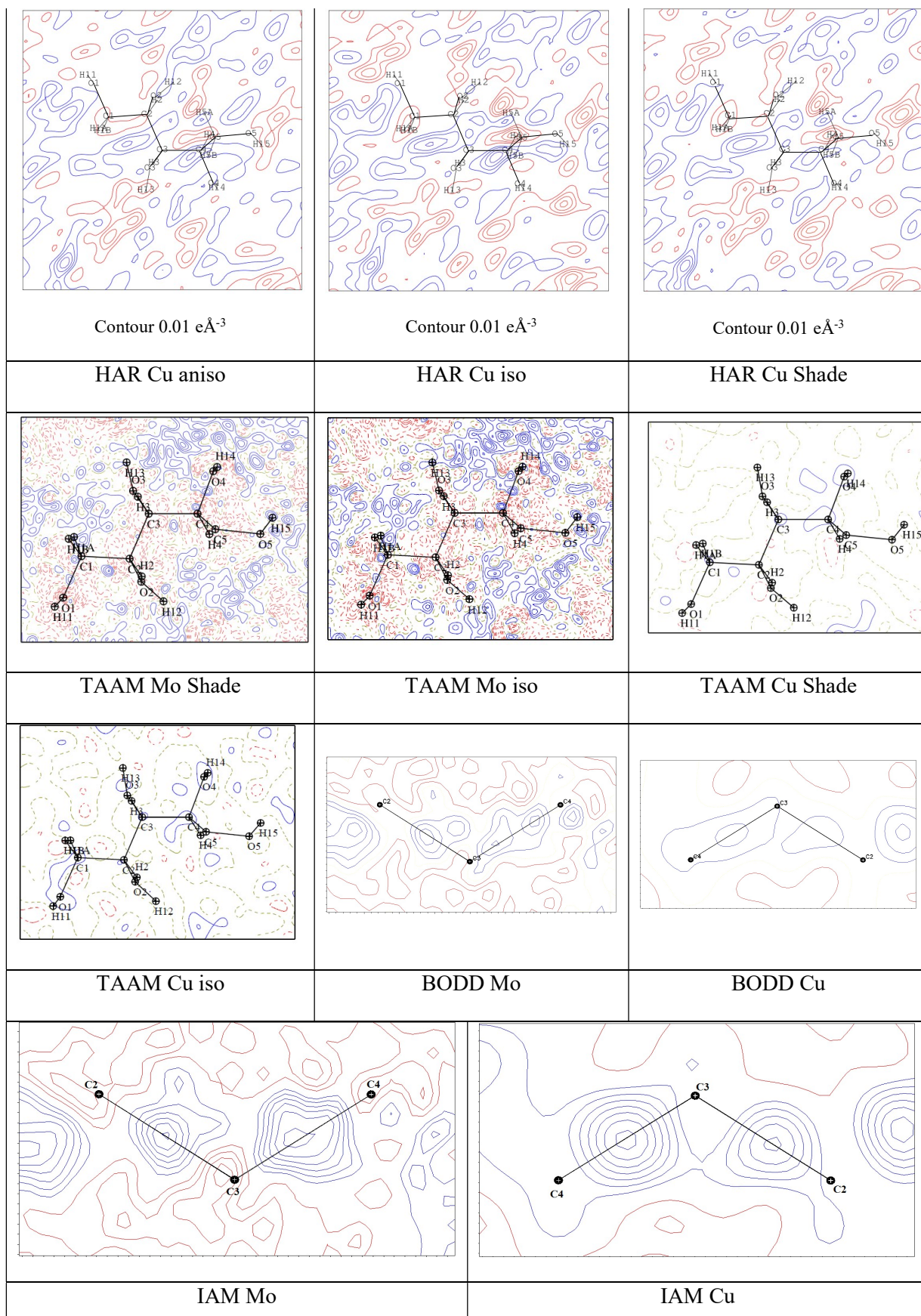
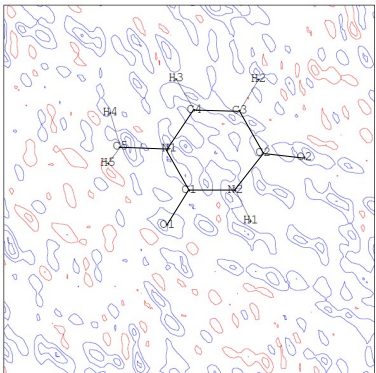
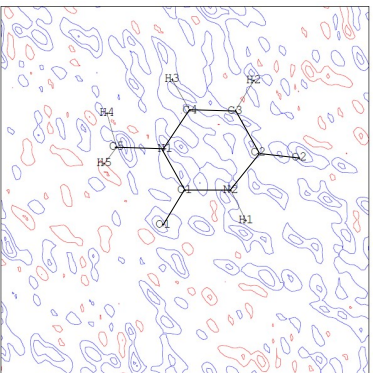
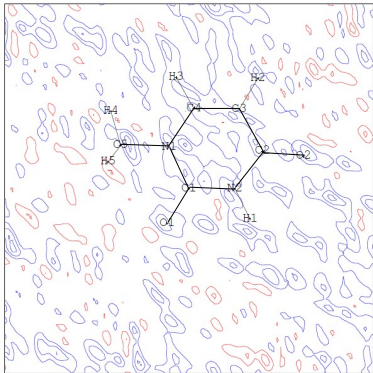
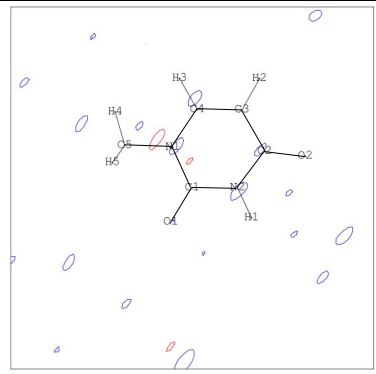
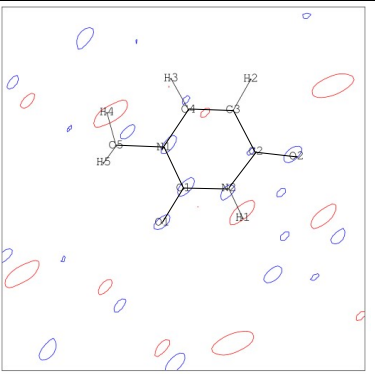
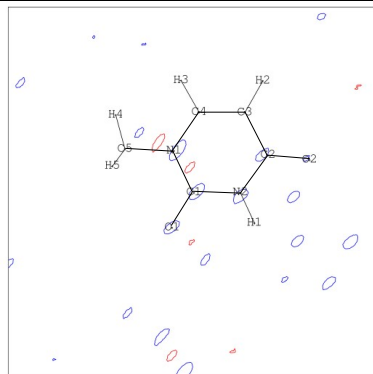
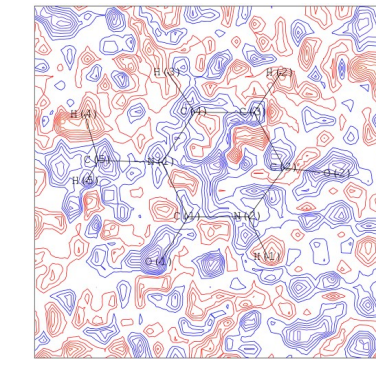
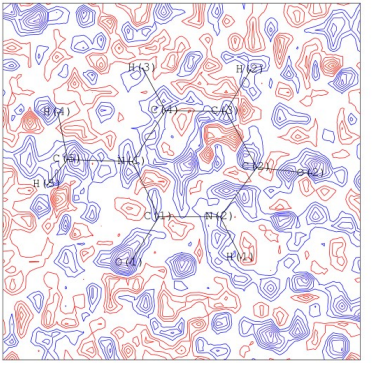
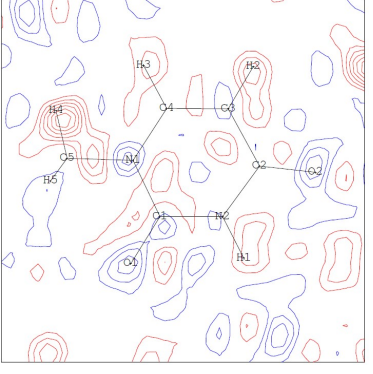


Figure S34 Residual density maps of 2Cu and 2Mo. All maps are presented for centre atom: C3, x axis: C4 and y axis: C2 with contours levels with intervals ± 0.05 eÅ⁻³. Blue lines represent positive

values and red lines the negative ones. Additionally for HAR Cu refinements maps with contour levels with intervals $\pm 0.01 \text{ e}\text{\AA}^{-3}$ are available. These maps are additionally captioned below.

		
HAR Mo aniso	HAR Mo iso	HAR Mo Shade
		
HAR Cu aniso	HAR Cu iso	HAR Cu Shade
		
TAAM Mo Shade	TAAM Mo iso	TAAM Cu Shade

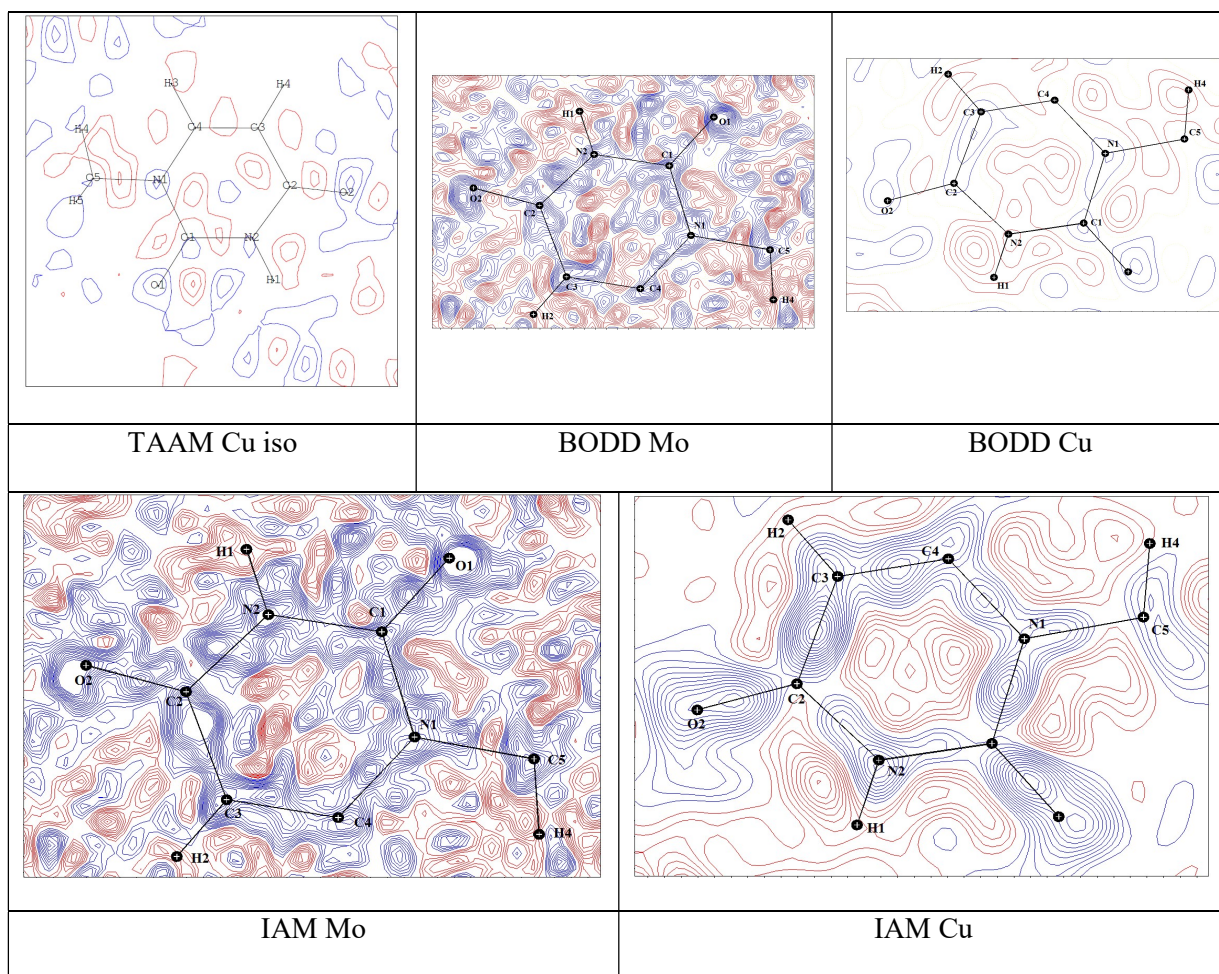
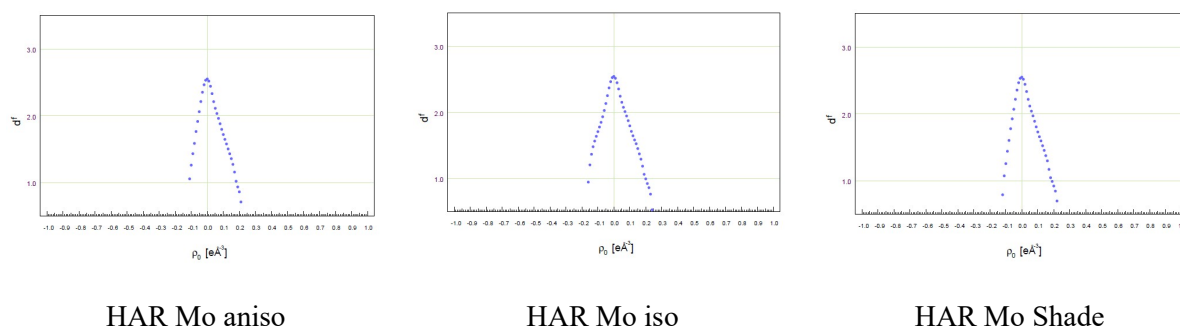


Figure S35 Residual density maps of **3Cu** and **3Mo**. All maps are presented for centre atom: C1, x axis: N2 and y axis: C4 with contours levels with intervals $\pm 0.05 \text{ e}\text{\AA}^{-3}$. Blue lines represent positive values and red lines the negative ones.



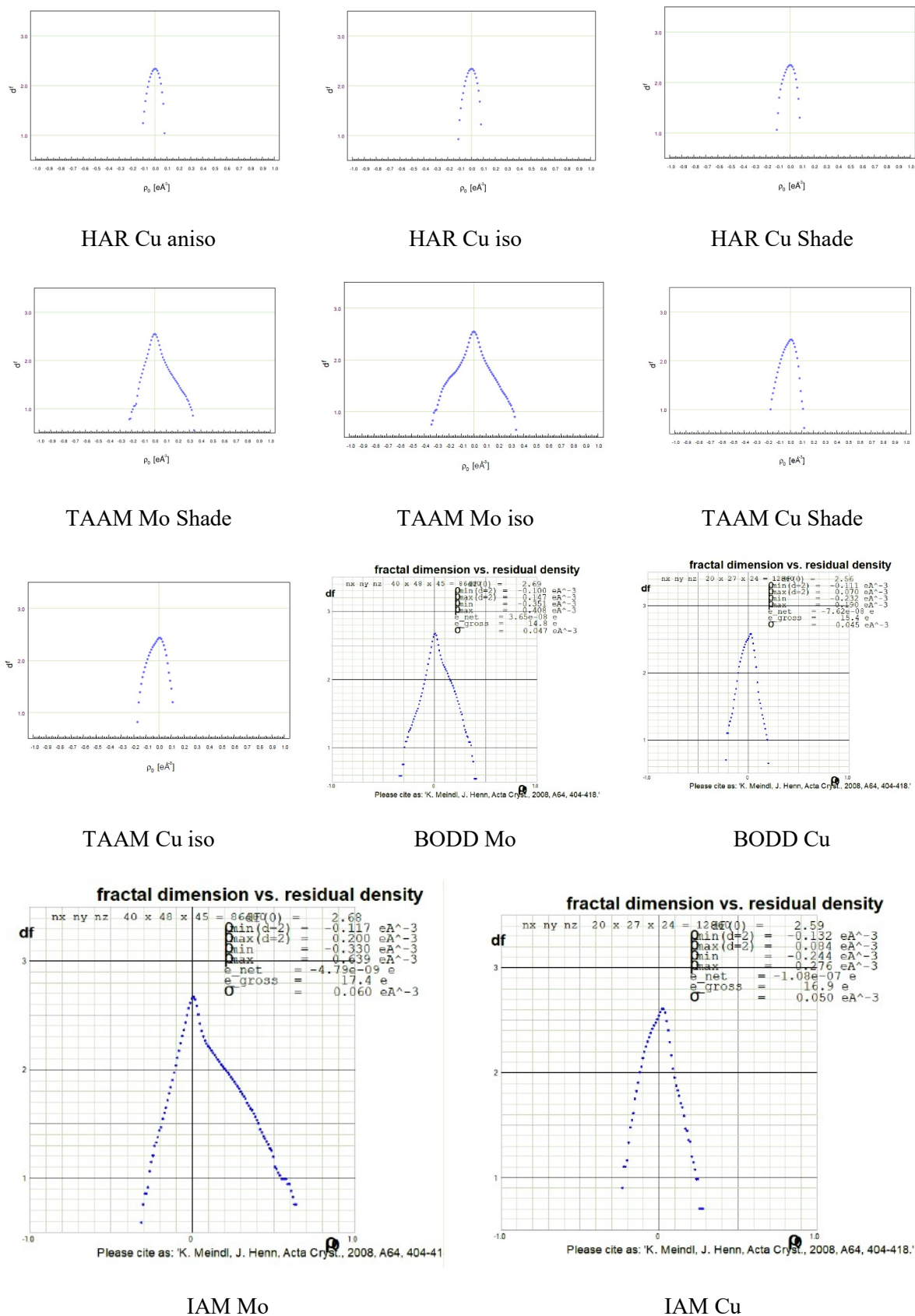
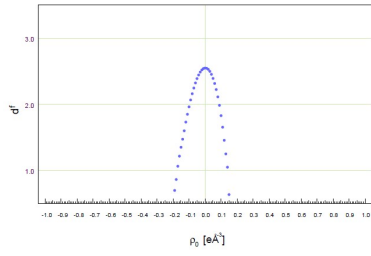
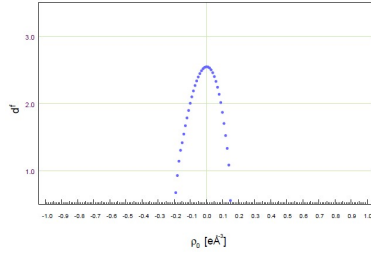


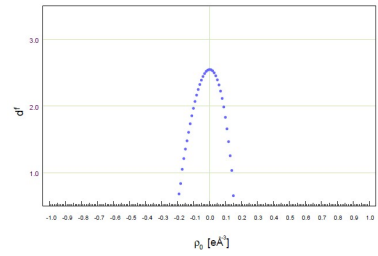
Figure S36 Fractal plots for 1Cu and 1Mo.



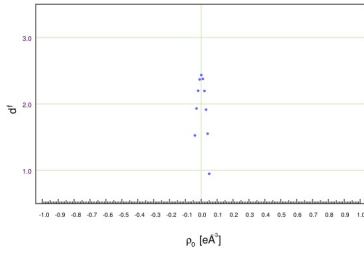
HAR Mo aniso



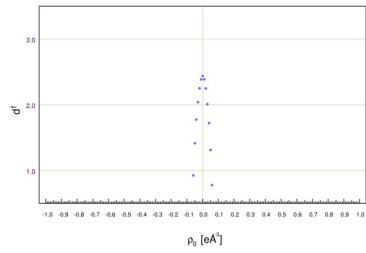
HAR Mo iso



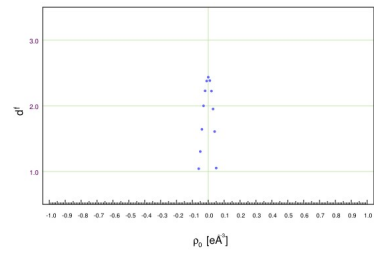
HAR Mo Shade



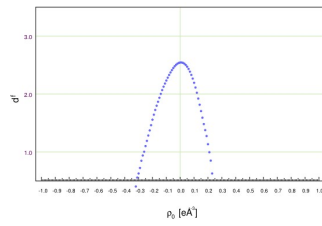
HAR Cu aniso



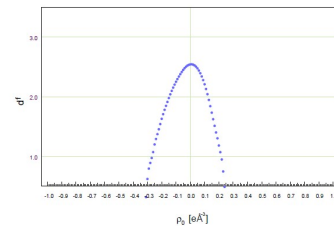
HAR Cu iso



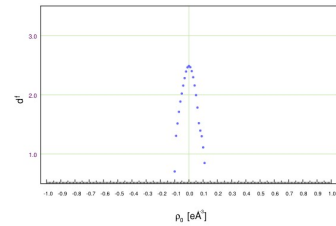
HAR Cu Shade



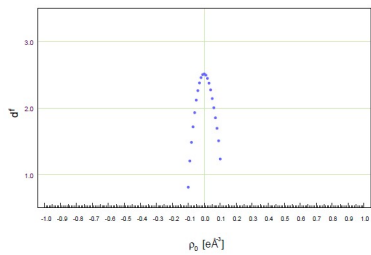
TAAM Mo Shade



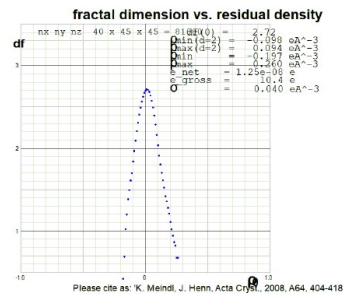
TAAM Mo iso



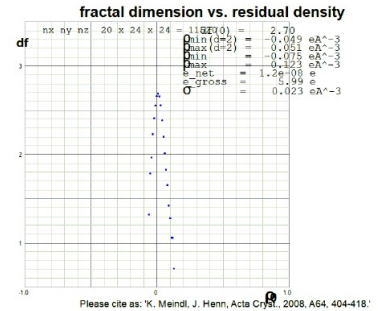
TAAM Cu Shade



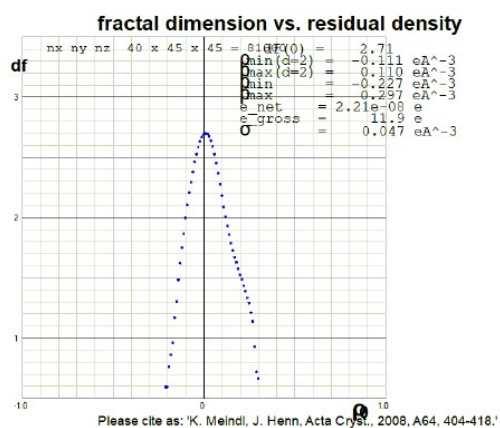
TAAM Cu iso



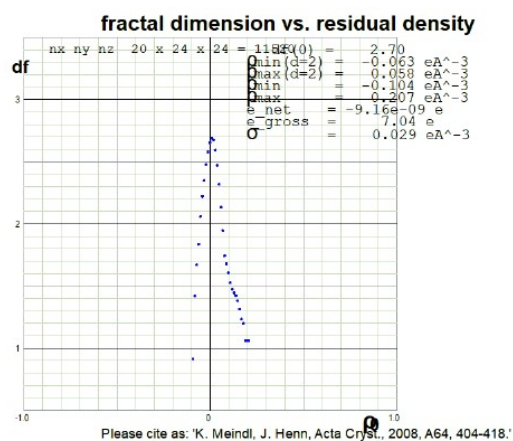
BODD Mo



BODD Cu

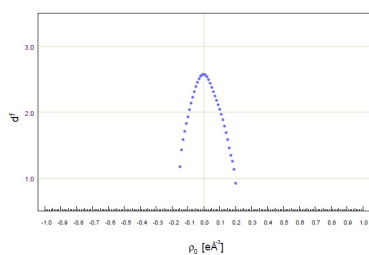


IAM Mo

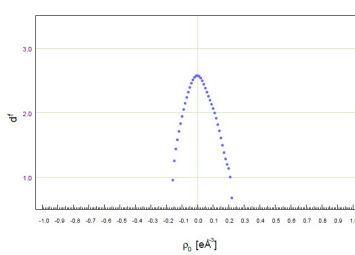


IAM Cu

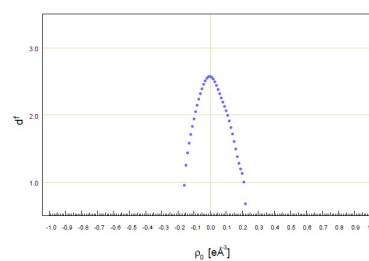
Figure S37 Fractal plots for 2Cu and 2Mo.



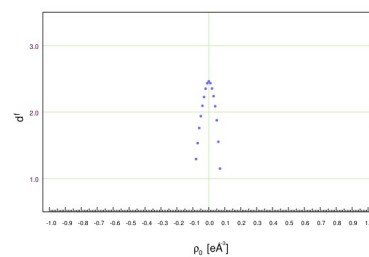
HAR Mo aniso



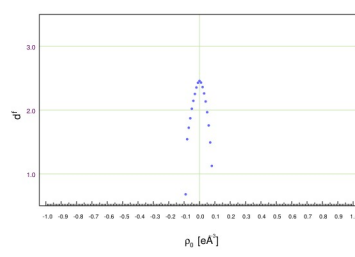
HAR Mo iso



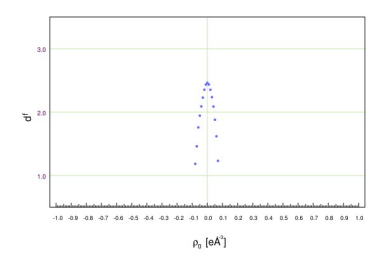
HAR Mo Shade



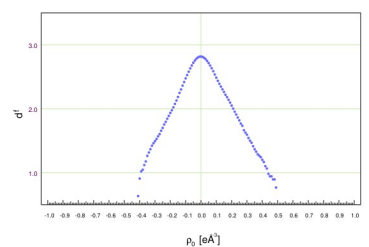
HAR Cu aniso



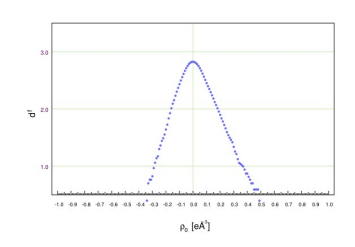
HAR Cu iso



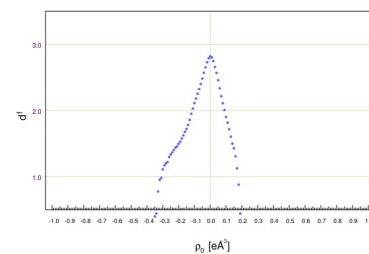
HAR Cu Shade



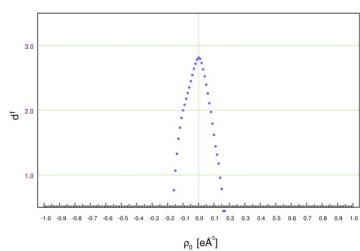
TAAM Mo Shade



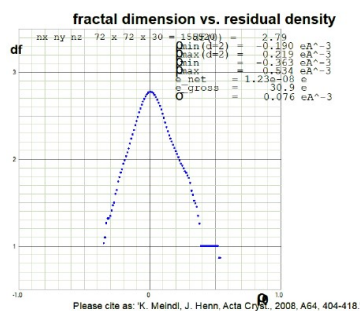
TAAM Mo iso



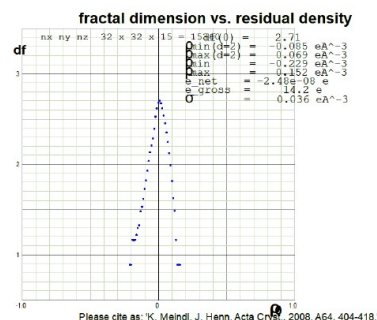
TAAM Cu Shade



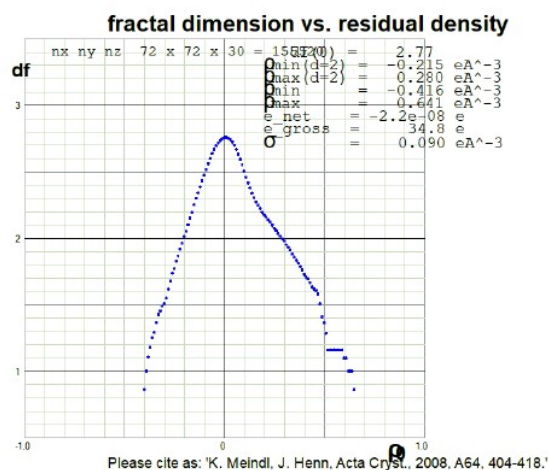
TAAM Cu iso



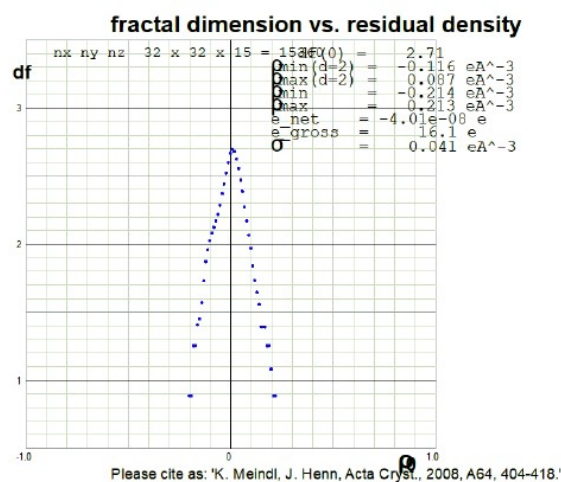
BODD Mo



BODD Cu

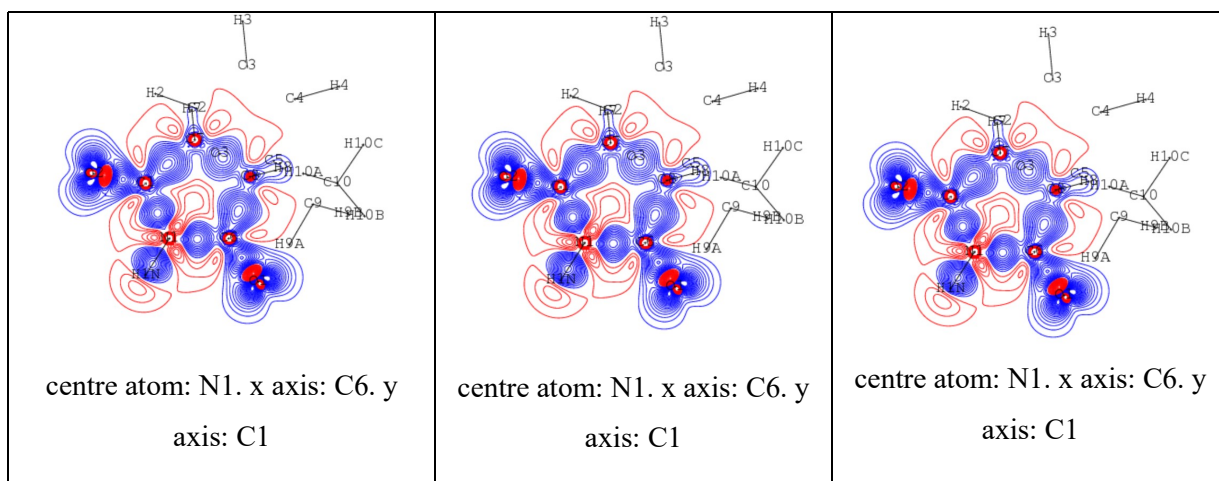


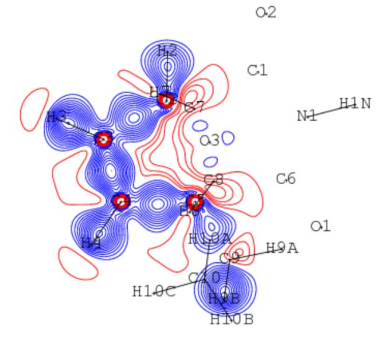
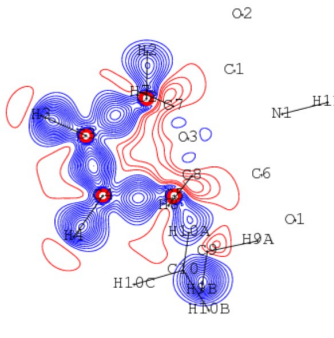
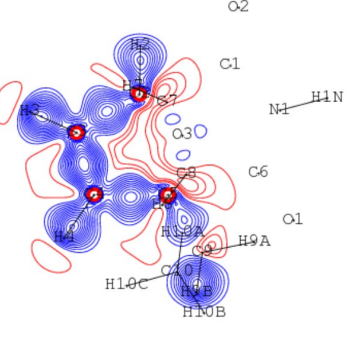
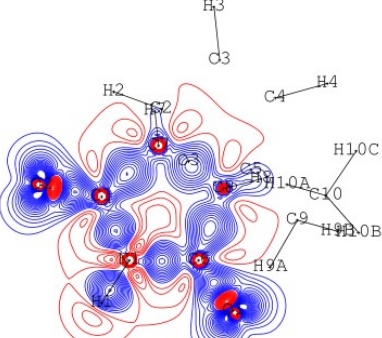
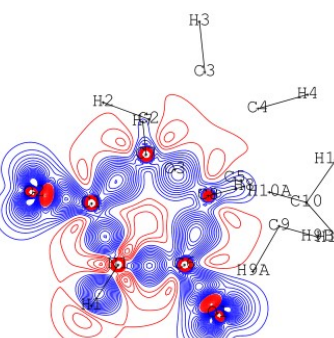
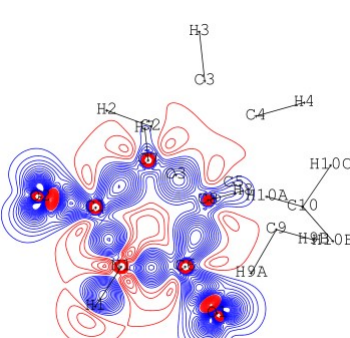
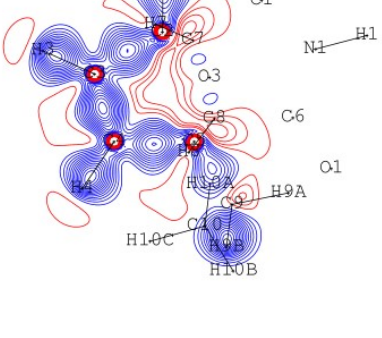
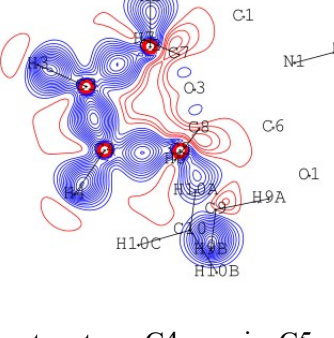
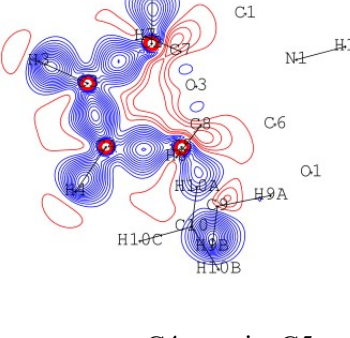
IAM Mo

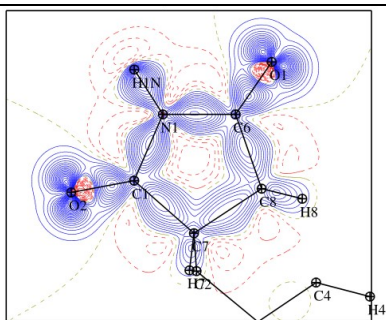


IAM Cu

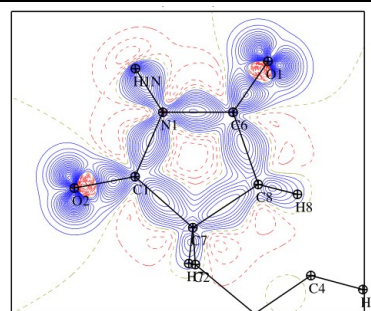
Figure S38 Fractal plots for 3Cu and 3Mo.



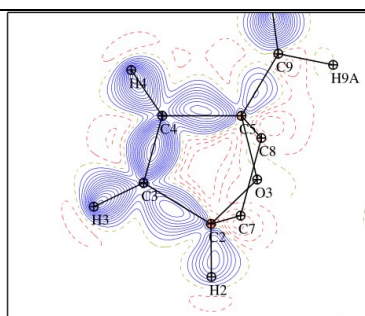
 <p>centre atom: C4. x axis: C5. y axis: C3</p>	 <p>centre atom: C4. x axis: C5. y axis: C3</p>	 <p>centre atom: C4. x axis: C5. y axis: C3</p>
HAR Mo aniso	HAR Mo iso	HAR Mo Shade
 <p>centre atom: N1. x axis: C6. y axis: C1</p>	 <p>centre atom: N1. x axis: C6. y axis: C1</p>	 <p>centre atom: N1. x axis: C6. y axis: C1</p>
HAR Cu aniso	HAR Cu iso	HAR Cu Shade
 <p>centre atom: C4. x axis: C5. y axis: C3</p>	 <p>centre atom: C4. x axis: C5. y axis: C3</p>	 <p>centre atom: C4. x axis: C5. y axis: C3</p>
HAR Cu aniso	HAR Cu iso	HAR Cu Shade



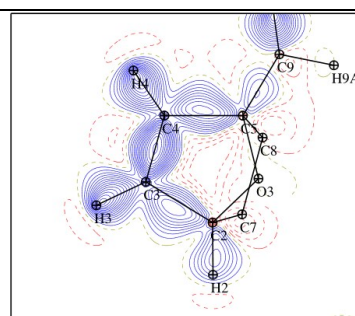
centre atom: N1. x axis: C6. y axis: C1



centre atom: N1. x axis: C6. y axis: C1



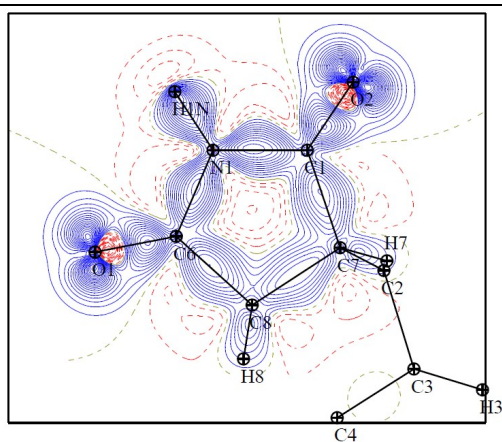
centre atom: C4. x axis: C5. y axis: C3



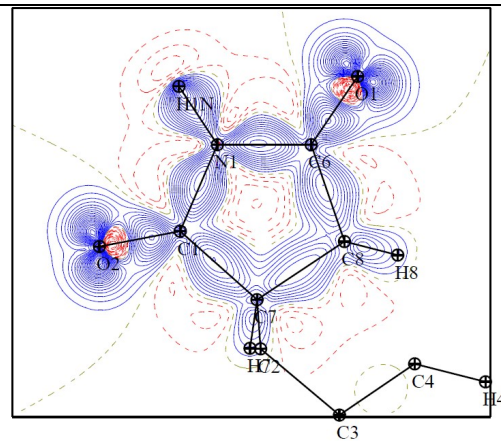
centre atom: C4. x axis: C5. y axis: C3

TAAM Mo Shade

TAAM Mo iso



centre atom: N1. x axis: C6. y axis: C1



centre atom: N1. x axis: C6. y axis: C1

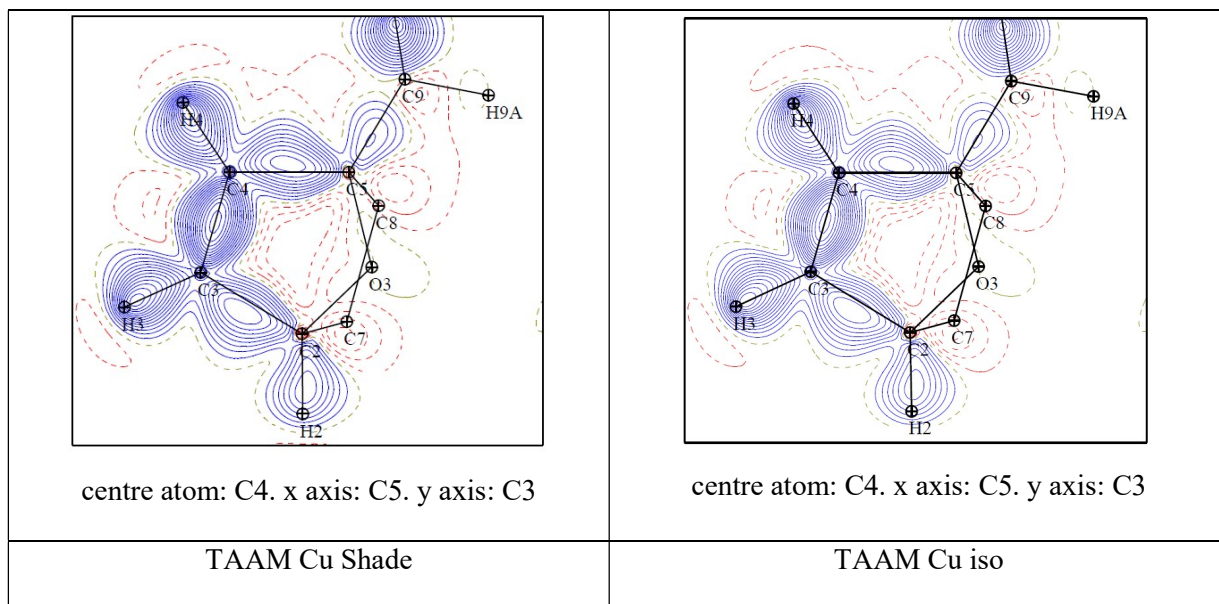
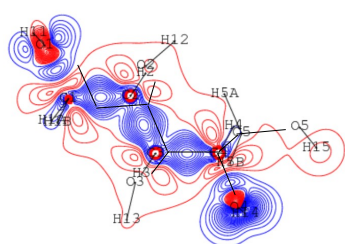
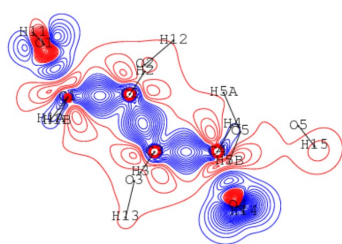


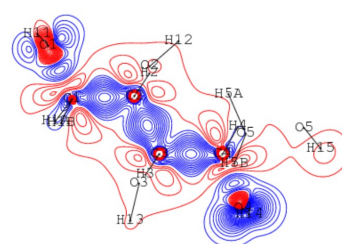
Figure S39 Deformation density maps of **1Cu** and **1Mo**. All maps are presented with contour levels with intervals $\pm 0.05 \text{ e}\text{\AA}^{-3}$. Blue lines represent positive values and red lines the negative ones. Maps were prepared for centre atom: N1, x axis: C6 and y axis: C1 or centre atom: C4, x axis: C5 and y axis: C3. Details are given below the maps.



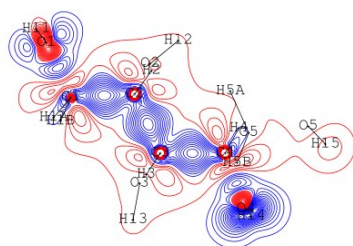
HAR Mo aniso



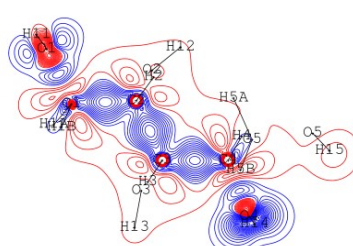
HAR Mo iso



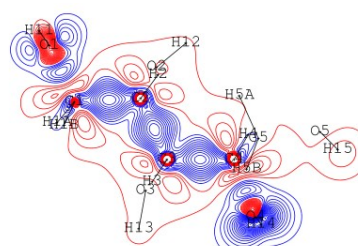
HAR Mo Shade



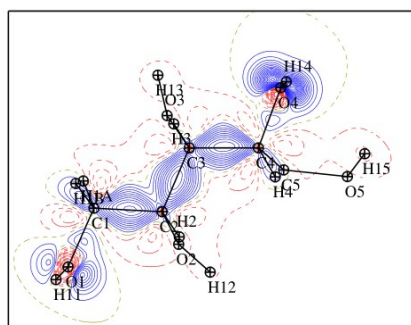
HAR Cu aniso



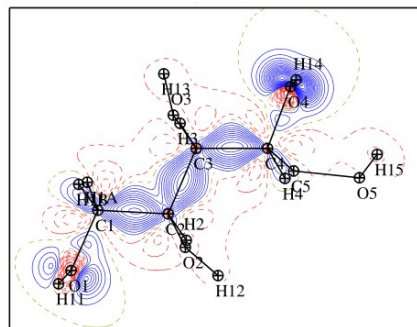
HAR Cu iso



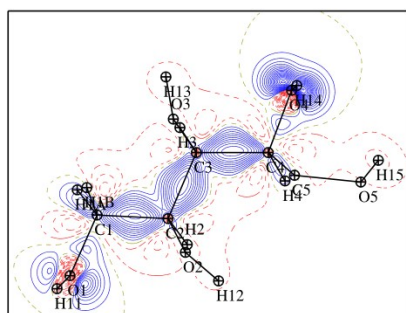
HAR Cu Shade



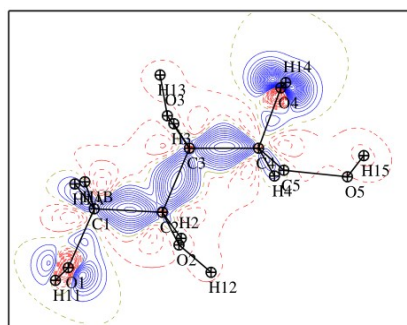
TAAM Mo Shade



TAAM Mo iso

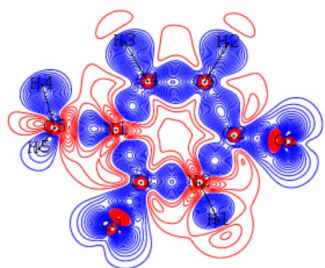


TAAM Cu Shade

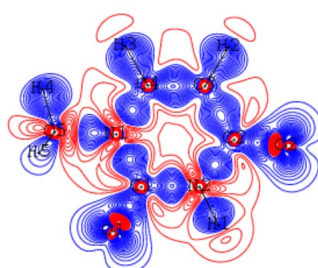


TAAM Cu iso

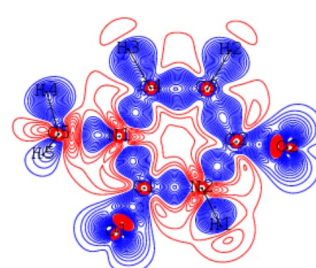
Figure S40 Deformation density maps of **2Cu** and **2Mo**. All maps are presented for centre atom: C3. x axis: C4 and y axis: C2 with contours levels with intervals $\pm 0.05 \text{ e}\text{\AA}^{-3}$. Blue lines represent positive values and red lines the negative ones.



HAR Mo aniso



HAR Mo iso



HAR Mo Shade

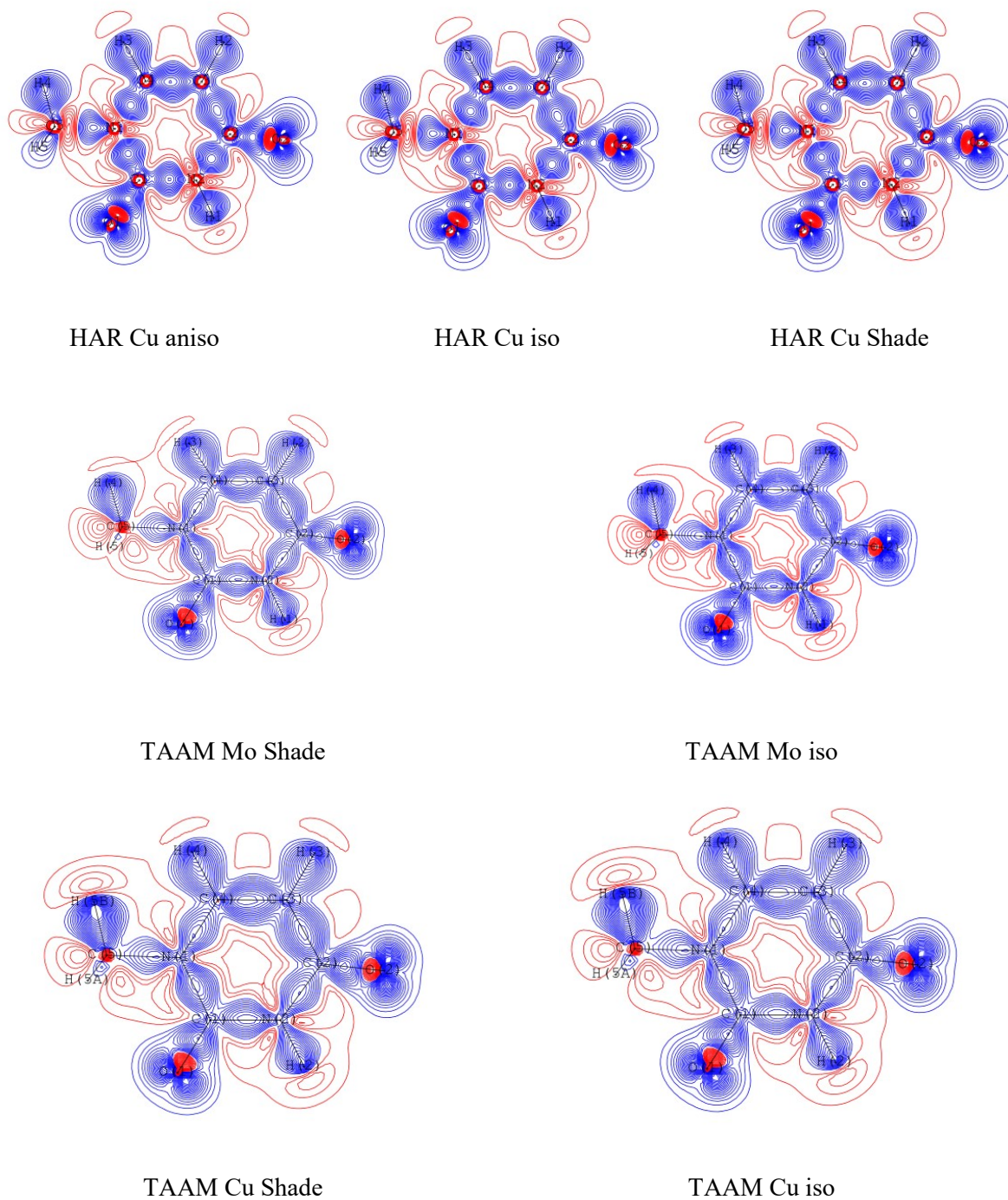


Figure S41 Deformation density maps of **3Cu** and **3Mo**. All maps are presented for centre atom: C1. x axis: N2 and y axis: C4 with contours levels with intervals $\pm 0.05 \text{ e}\text{\AA}^{-3}$. Blue lines represent positive values and red lines the negative ones.