Supporting information for article:

Electronic structure of two isostructural `paddle-wheel' complexes: a comparative study

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Appendix I.

Table SA1. Comparison of multipole refinement for (I) using non-averaged and merged data.

|                         | Non-merged (EXTI aniso) | merged (NO EXTI) | merged (EXTI isotropic) |
|-------------------------|-------------------------|------------------|-------------------------|
| R(F), R(F^2)            | 0.0186                  | 0.0118; 0.0281   | 0.0109; 0.0195          |
| Residual density        | +0.747/-0.357           | +0.383/-0.750    | +0.747/-0.357           |
| No. of diffractions     | 397256                  | 12311            | 12311                   |
| Charges                 |                         |                  |                         |
| Cu [-e]                 | 1.49                    | 2.03             | 1.59                    |
| O1 [-e]                 | -0.96                   | -0.98            | -0.98                   |
| O2 [-e]                 | -0.99                   | -1.00            | -1.02                   |
| O3 [-e]                 | -1.02                   | -0.97            | -1.02                   |
| O4 [-e]                 | -1.10                   | -1.02            | -1.05                   |
| O5 [-e]                 | -1.23                   | -1.13            | -1.22                   |
| Orbital                 |                         |                  |                         |
| Z2 [e; %]               | 2.015(4); 21.5 %        | 1.91; 21.7 %     | 2.01; 21.7 %            |
| XZ [e; %]               | 1.909(4); 20.4 %        | 1.78; 20.2 %     | 1.87; 20.2 %            |
| YZ [e; %]               | 2.086(4); 22.3 %        | 1.93; 21.9 %     | 2.03; 22.0 %            |
| X2-Y2 [e; %]            | 1.363(4); 14.6 %        | 1.28; 14.6 %     | 1.37; 14.8 %            |
| XY [e; %]               | 1.985(4); 22.1 %        | 1.90; 21.5 %     | 1.98; 21.4 %            |
| Σ [e]                  | 9.36                    | 8.81             | 9.26                    |
| AIM at BCP*             |                         |                  |                         |
| Cu-O1                   | 0.468(1); 12.462(1)     | 0.438(3); 12.091(5) | 0.468(3); 12.299(5) |
| Cu-O2                   | 0.448(1); 12.800(2)     | 0.445(3); 12.270(5) | 0.475(3); 12.473(5) |
| Cu-O3                   | 0.435(1); 11.363(1)     | 0.414(3); 10.949(5) | 0.441(3); 11.139(5) |
| Cu-O4                   | 0.410(1); 10.878(1)     | 0.339(3); 10.611(5) | 0.425(3); 10.760(5) |
| Cu-O5                   | 0.295(0); 7.026(1)      | 0.295(3); 6.930(3) | 0.295(3); 6.930(3) |
| Cu-Cu*                  | 0.057(0); 1.468(0)      | 0.052(0); 1.515(0) | 0.060(0); 1.683(0) |

# ρ_{BCP} [e/Å^3]; \nabla^2 \rho_{BCP} [e/Å^5]
Figures SA2. Residual densities in the plane defined by the atoms: \textit{atom1} – \textit{atom2} – \textit{atom3}.

| plane defined | Non-merged (EXTI aniso) | merged (NO EXTI) | merged (EXTI isotropic) |
|---------------|-------------------------|------------------|-------------------------|
| Cu-O1-O3      | ![Image](image1)         | ![Image](image2) | ![Image](image3)        |
| Cu-O2-O4      | ![Image](image4)         | ![Image](image5) | ![Image](image6)        |
Figures SA3. Error analysis for (I).

|                  | Non-merged (EXTI aniso) | merged (NO EXTI) | merged (EXTI isotropic) |
|------------------|-------------------------|------------------|-------------------------|
| Cu-O1-O5         | ![Image](image1.png)    | ![Image](image2.png)    | ![Image](image3.png)    |
| Normal probability distribution plot | ![Image](image4.png)    | ![Image](image5.png)    | ![Image](image6.png)    |
| c                | ![Image](image7.png)    | ![Image](image8.png)    | ![Image](image9.png)    |
Fractal analysis of the residual density

$F_{\text{obs}} - F_{\text{calc}}$ vs. $F_{\text{calc}}$

$F_{\text{obs}} - F_{\text{calc}}$ vs. $\sin(\theta)/\lambda$

Figures SA4 (see on the next pages). Static electron deformation densities of (I) in the plane defined by the atoms O(2)*, O(1), O(3). Contour spacing as in Fig. 2b. Symmetry code: * 1-x, 1-y, 1-z.
| 3.984 Å above the plane | 3.884 Å above the plane | 3.784 Å above the plane |
|------------------------|------------------------|------------------------|
| 3.684 Å above the plane | 3.584 Å above the plane | 3.484 Å above the plane |
| 3.384 Å above the plane | 3.284 Å above the plane | 3.184 Å above the plane |
| 3.084 Å above the plane | 2.984 Å above the plane | 2.884 Å above the plane |
|------------------------|------------------------|------------------------|
| 2.784 Å above the plane | 2.684 Å above the plane | 2.584 Å above the plane |
| 2.484 Å above the plane | 2.384 Å above the plane | 2.284 Å above the plane |
| 2.184 Å above the plane | 2.084 Å above the plane | 1.984 Å above the plane |
|-------------------------|-------------------------|-------------------------|
| 1.884 Å above the plane | 1.784 Å above the plane | 1.684 Å above the plane |
| 1.584 Å above the plane | 1.484 Å above the plane | 1.384 Å above the plane |
1.284 Å above the plane
1.184 Å above the plane
1.084 Å above the plane
0.984 Å above the plane
0.884 Å above the plane
0.784 Å above the plane
0.684 Å above the plane
0.584 Å above the plane
0.484 Å above the plane
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0.384 Å above the plane

In the plane O(2)*, O(1), O(3)

0.284 Å above the plane

0.184 Å above the plane

0.384 Å below the plane

0.484 Å below the plane

0.584 Å below the plane
| Depth below the plane |
|-----------------------|
| 1.584 Å               |
| 1.684 Å               |
| 1.784 Å               |
| 1.884 Å               |
| 1.984 Å               |
| 2.084 Å               |
| 2.184 Å               |
| 2.284 Å               |
| 2.384 Å               |
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2.484 Å below the plane
2.584 Å below the plane
2.684 Å below the plane

2.784 Å below the plane
2.884 Å below the plane
2.984 Å below the plane

3.084 Å below the plane
3.184 Å below the plane
3.284 Å below the plane