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**Extension of the experimental electron density analysis to
metastable states: a case example of the spin crossover complex**



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SUPPORTING INFORMATION

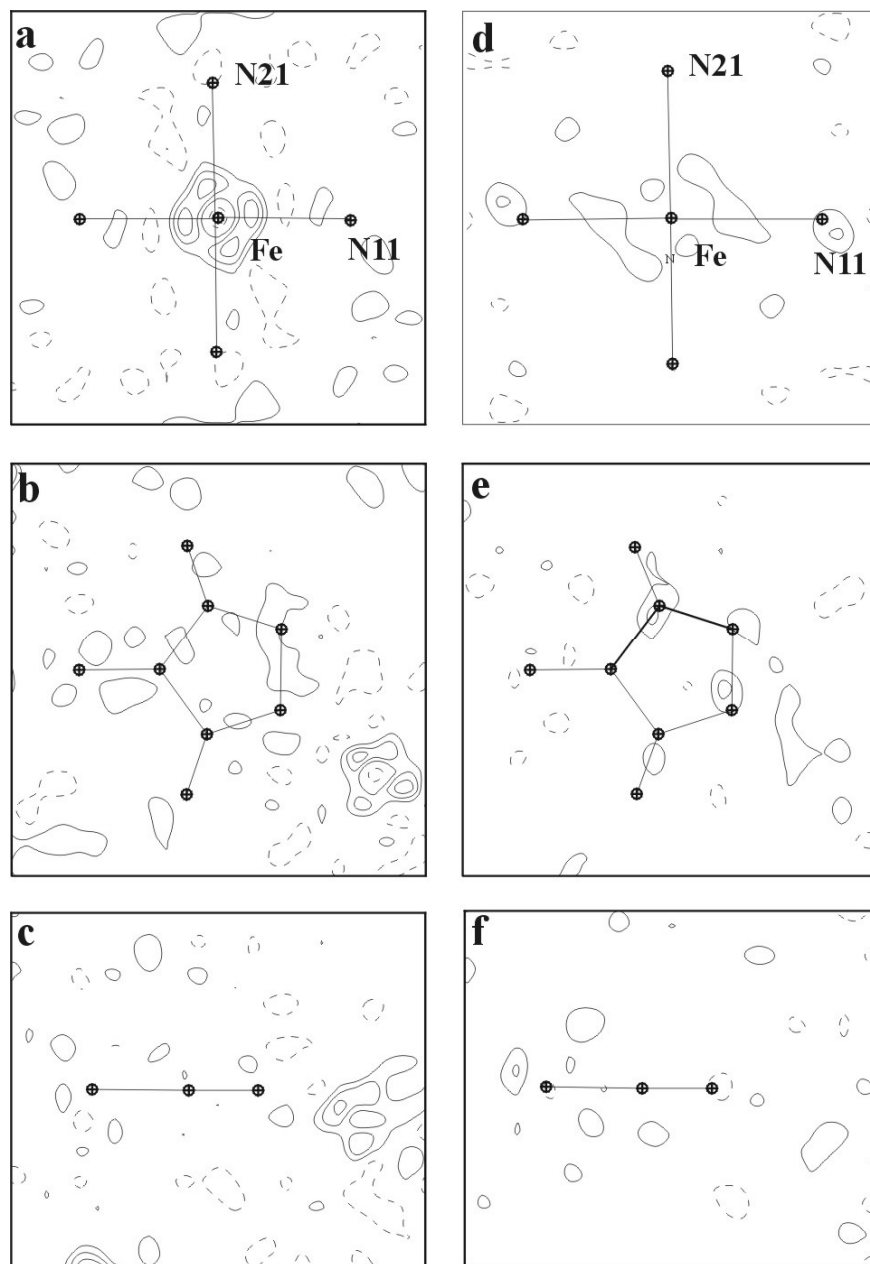


Figure 1. Residual electron density in the Fe-N11-N21, triazole ring and NCS plane for the HS (left) and LS (right) states. Contour levels : $0.1 \text{ e}\text{\AA}^{-3}$ positive solid lines and negative dashed.

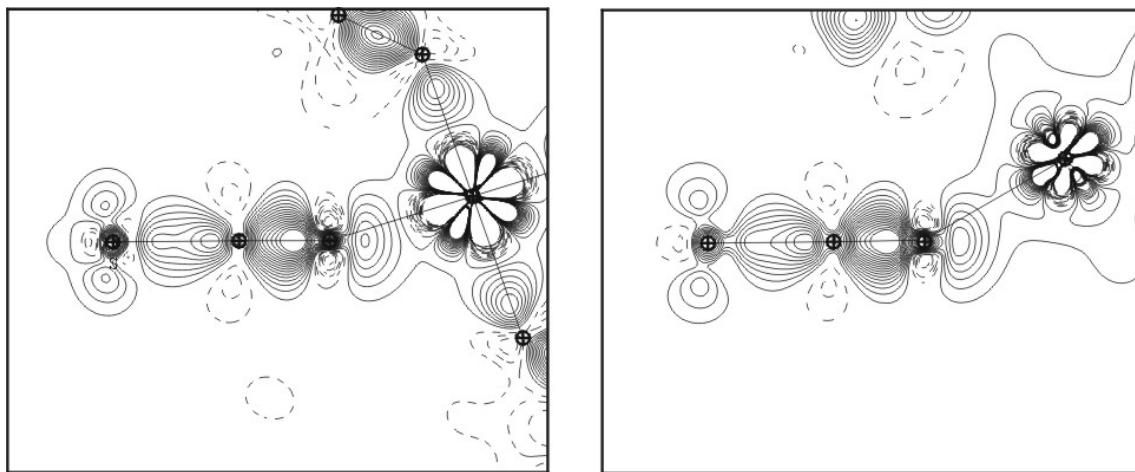


Figure 2. Static deformation density in the NCS plane for the LS (left) and HS (right) states. Contour levels : $0.05 \text{ e}\text{\AA}^{-3}$ positive solid lines and negative dashed.

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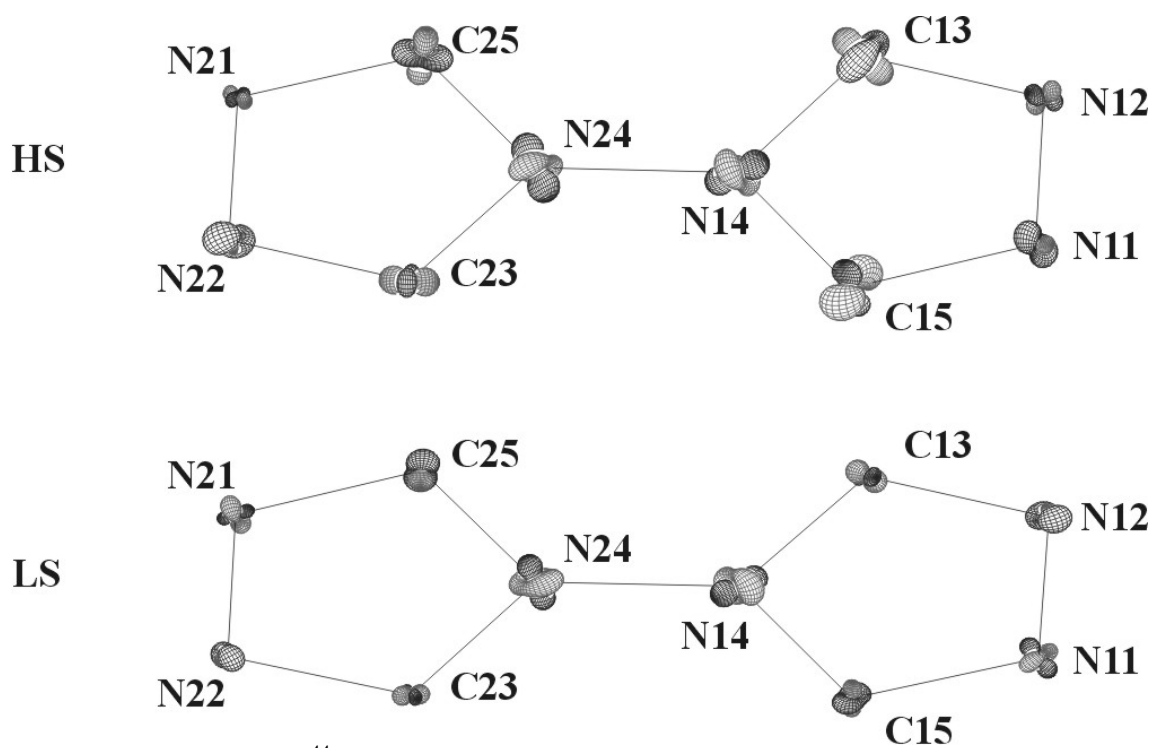


Figure 3. PEANUT plot⁴⁴ showing the RMS surfaces of the difference between the observed (refined) and rigid body (TLS model) atomic displacement parameters at the 100% probability level for the HS and LS states. Positive surface in grey, negative in black.