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Metastable States and Population Dynamics in the Linkage Isomer Compound Sodium-nitro-prusside BERNARD DELLEY, JÜRG SCHEFER, Paul Scherrer Institut Switzerland, DOMINIK SCHANIEL, THEO WOIKE, U. Cologne — Two long-lived metastable states S1 and S2 can be produced in $Na_2[Fe(CN)_5NO]2H_2O$ by illumination with light in the spectral range 380-580 nm. Local minima in the ground state energy hypersurface as given by density functional theory are in agreement with the linkage isomerism model. We identify S2 with a side on bonded NO configuration and S1 with an inverted one. We have shown that that thermal properties, vibrational spectrum, optical properties and the Mossbauer spectrum are predicted in agreement with experiment. We find that the crystal model gives a significantly improved account of spectral differences between the ground and S1 state as compared to the free anion model. On the basis of the energy surfaces we estimate thermal depopulation rates and explore the dynamics of direct population of S1 induced by blue light.

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