Electronic Supplementary Information for Dalton Transactions


Urea Decomposition Facilitated by a Urease Model Complex: A Theoretical Investigation

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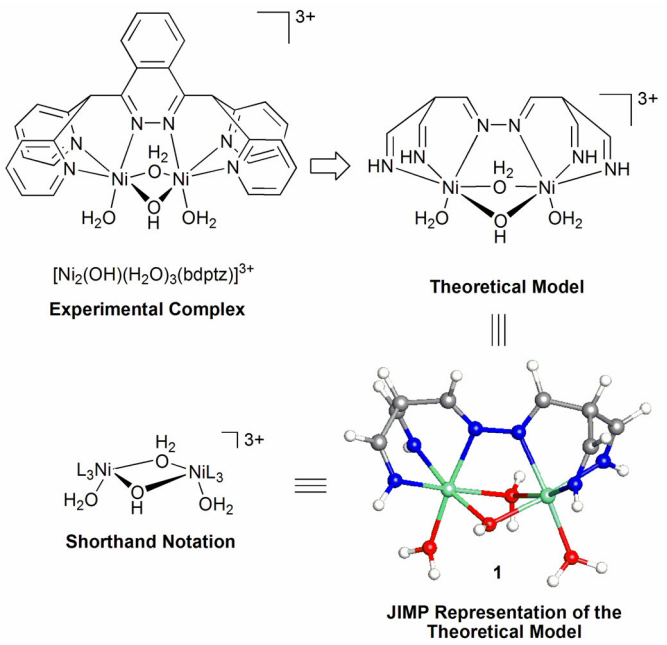
Colour versions of Scheme 2 and Figures 2-7 are presented below.




**Scheme 2** Outline of the theoretical model used to represent the dinickel cation $[Ni_2(bdptz)(\mu\text{-}OH)(\mu\text{-}H_2O)(H_2O)_2]^{3+}$ ($\mathbf{A}^{3+}$).

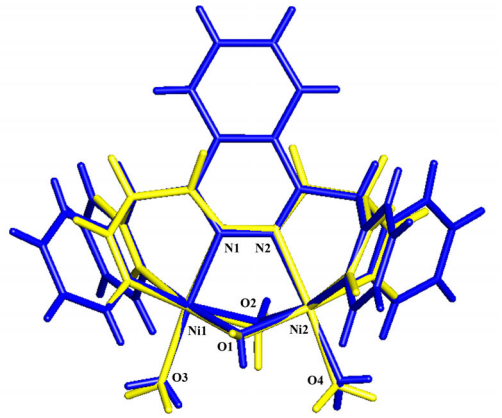



**Figure 2** Overlay of the calculated structure **1** (yellow), and the crystal structure of $[Ni_2(bdptz)(\mu\text{-}OH)(\mu\text{-}H_2O)(H_2O)_2]^{3+}$ ($\mathbf{A}^{3+}$) (blue).

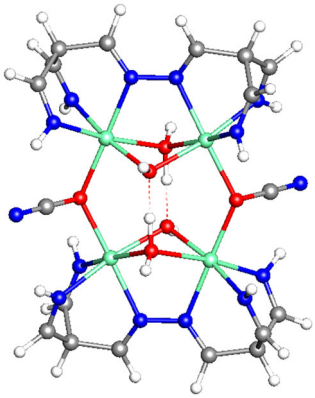


**Figure 3** JIMP representation of the calculated structure of the tetranickel complex **2**.

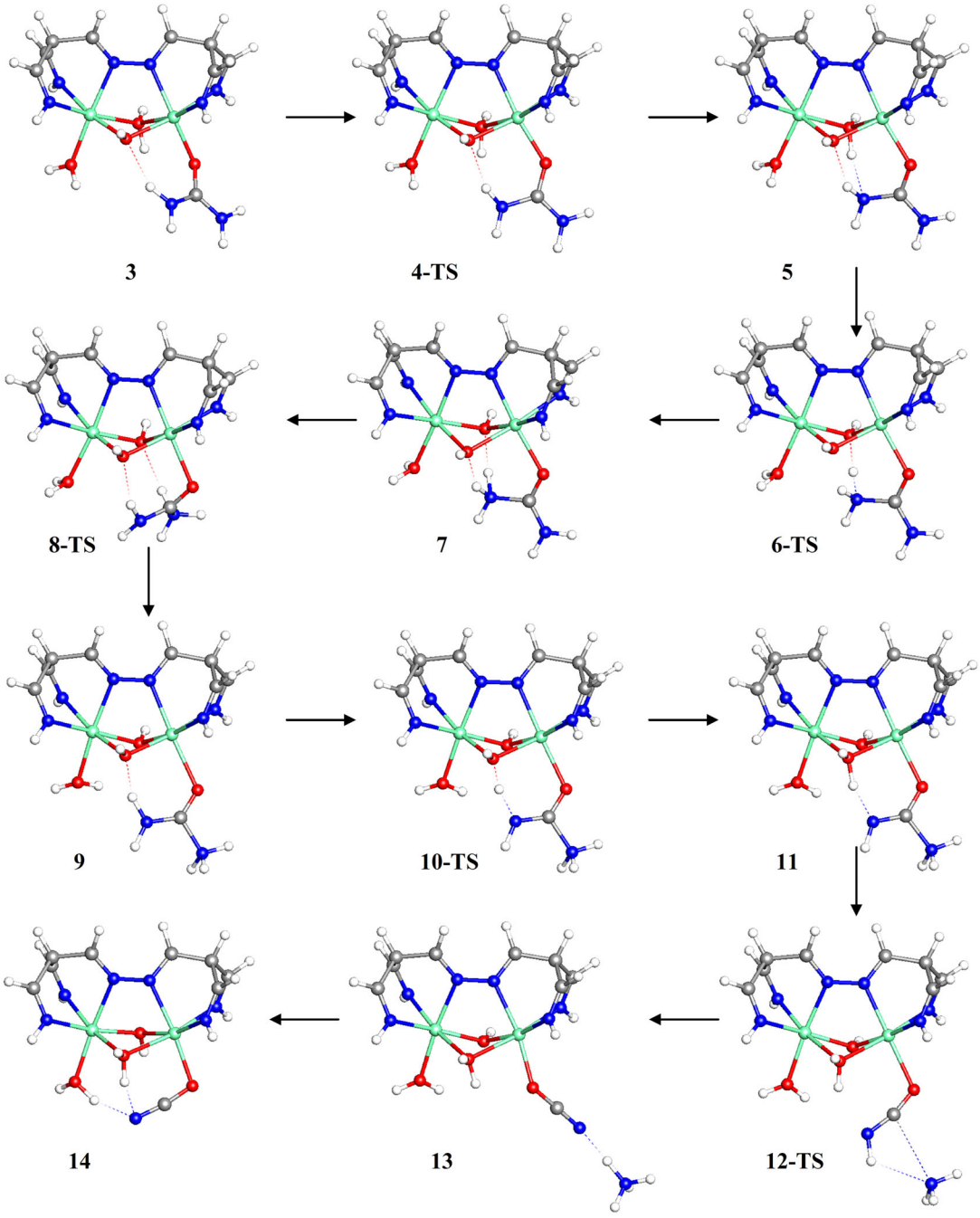



**Figure 4** JIMP representations of the intermediates and transition states in the calculated elimination pathway.

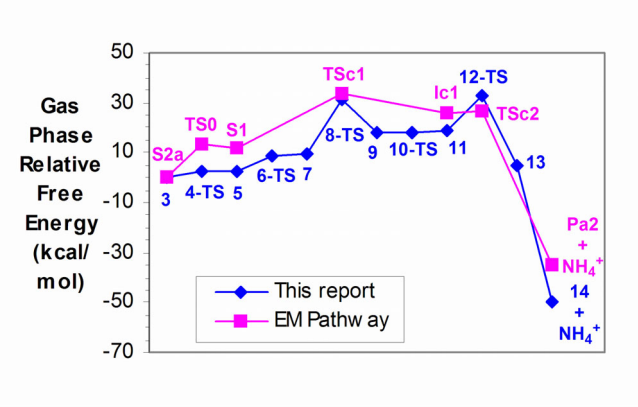
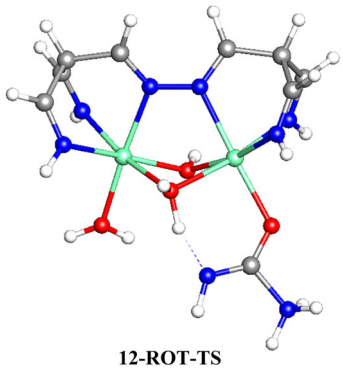
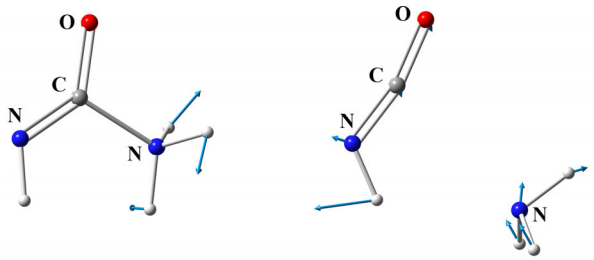



**Figure 5** A comparison of the gas-phase relative free energies of the transition states and intermediates in the elimination mechanisms proposed in this report (diamonds) and in reference 23 by EM (squares).



**12-ROT-TS**

**Figure 6** Transition state **12-ROT-TS**.




**12-ROT-TS**
Urea Closeup

**12-TS**
Urea Closeup

**Figure 7** GaussView 3.09 representation of the displacement vectors on the urea fragments in **12-ROT-TS** and **12-TS**.