

Models and Methods for Computing Reduction Potentials, pK_a s and Binding Constants: The Aquacobalamin System

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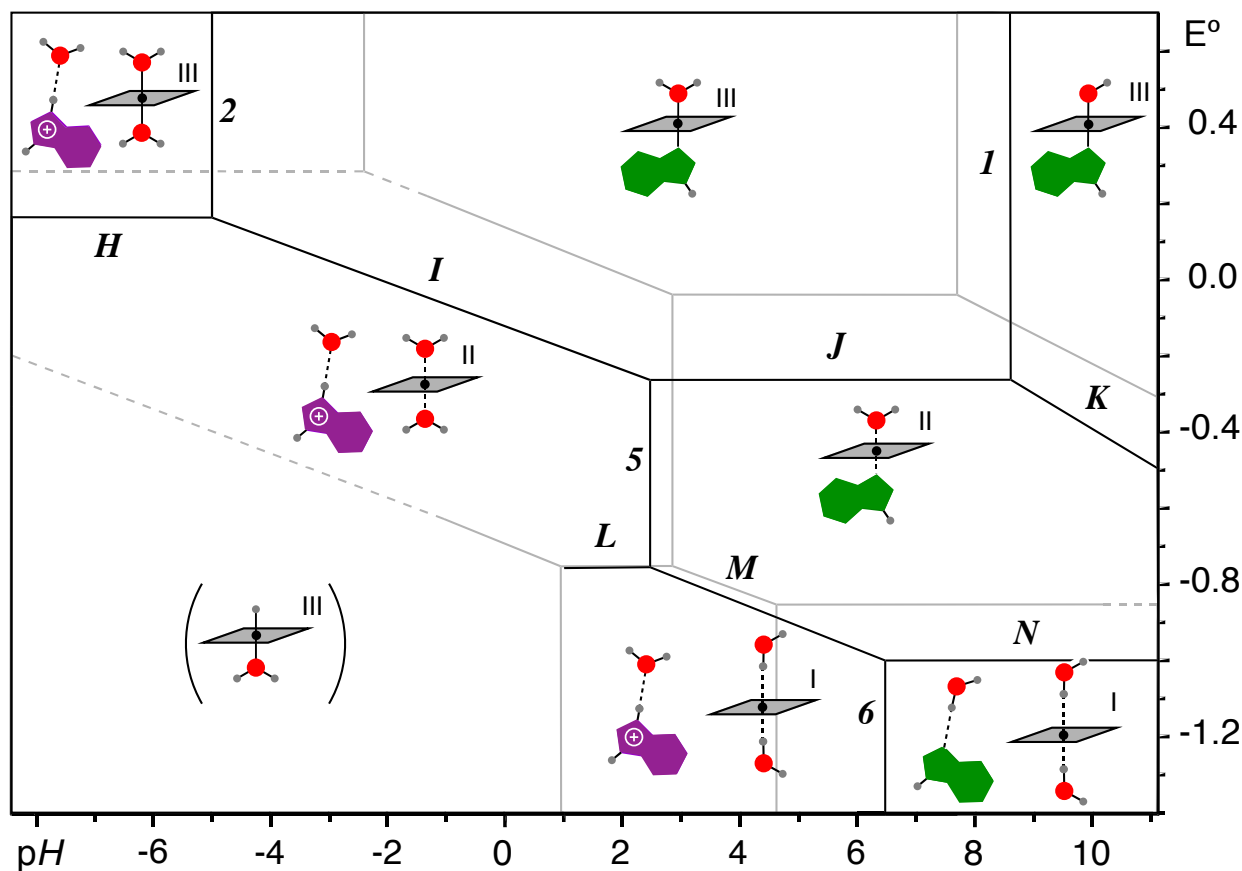


Figure 2. Experimental (gray) and computed (black) Pourbaix diagram for aquacobalamin. Upper-case letters refer to model reduction reactions and numbers refer to pK_a s. Hydridocob(III)alamin was not included in the computed Pourbaix diagram.