Supporting materials:

^{17}O ESEEM evidence for exchange of the axial oxo ligand in the molybdenum center of the high pH form of sulfite oxidase

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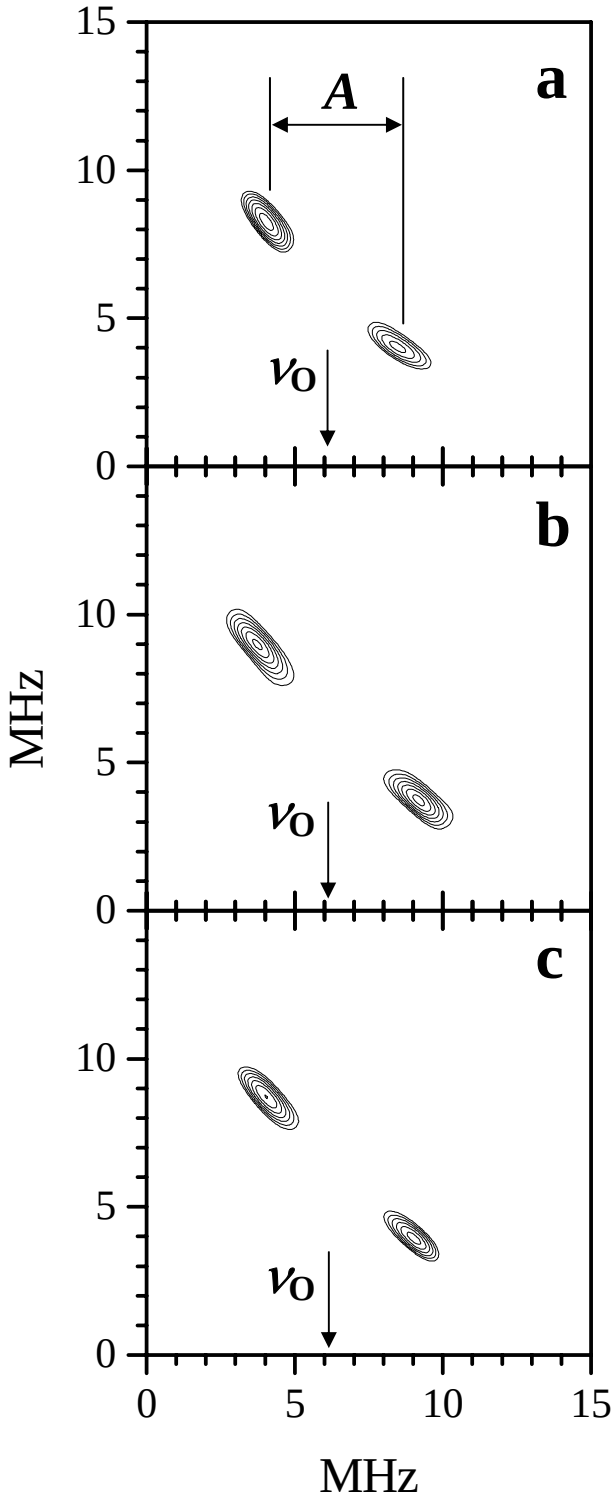

Figure S1. (++) quadrants of the ^{17}O HYSCORE spectra of *hpH* SO in $H_2{}^{17}O$ obtained at turning points of the EPR spectrum. The magnetic fields corresponding to panels (a), (b) and (c) are, respectively, 1052 mT (g_Z), 1063.2 mT (g_Y) and 1068.4 mT (g_X). Other experimental conditions: mw frequency, 29.252 GHz; mw pulses, 4×15 ns; time interval τ between the first and second mw pulses, 200 ns; measurement temperature, 20 K. The value of the ^{17}O Zeeman frequency, ν_O, is indicated by an arrow in each panel. Panel (a) also shows how the *hfi* constant is measured.

Scheme S1: Proposed process for the exchange of axial (ax) and equatorial (eq) oxygen groups with ^{17}O enriched water in metal (M) compounds with a *cis*-MO(OH) structure (adapted from ref 24). The species in the boxes predominate at equilibrium.