Supplementary Material (ESI) for Faraday Discussions

Implications for the Mechanism of Sulfite Oxidizing Enzymes from Pulsed EPR Spectroscopy and DFT Calculations for "Difficult" Nuclei

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Supplementary Data

Optimized XYZ atom coordinates of the sulfate-bound Mo(V) computational model:

C	2.258992	-3.485989	1.207005
C	0.793709	-3.884065	1.384943
S	-0.368040	-2.504367	1.851116
S	-3.054947	0.077112	2.542035
O	-2.240590	-0.193256	3.779660
O	-4.047345	-0.995895	2.184897
O	-3.593511	1.480602	2.444255
C	-0.684819	0.549445	-4.364000
C	0.356239	0.079850	-5.380252
C	-0.459525	-0.120743	-3.026998
S	-1.294122	0.552940	-1.615208
C	0.303466	-1.233953	-2.943837
S	0.576351	-2.081178	-1.402327
C	0.959718	-1.850314	-4.154041
O	0.465079	-1.346605	-5.414157
Mo	-0.303897	-0.580378	0.362920
O	-1.909521	0.054966	1.241059
O	0.999043	0.420416	0.876039
H	2.370168	-2.755387	0.395664
H	2.880425	-4.369075	0.961801
H	2.653848	-3.031862	2.129670
H	0.686577	-4.618508	2.200008
H	0.421683	-4.352411	0.459878
H	-0.616687	1.646777	-4.253702
H	-1.703805	0.334389	-4.738186
H	0.086371	0.383605	-6.405710
H	1.344105	0.525271	-5.134038
H	0.779189	-2.937615	-4.178989
H	2.062758	-1.700209	-4.115261

Optimized XYZ atom coordinates of the sulfite-bound Mo(V) computational model:

C	2.236654	-3.317426	1.253743
C	0.789887	-3.786536	1.406904
S	-0.437037	-2.454628	1.839344
S	-3.120279	-0.423676	2.742918
O	-4.504943	-0.676336	2.156376
O	-3.039920	0.898041	3.501829
C	-0.566212	0.579400	-4.474622
C	0.459451	0.026733	-5.463799
C	-0.421581	-0.090734	-3.125861
S	-1.241840	0.661068	-1.744810
C	0.254073	-1.258338	-3.017955
S	0.447924	-2.111147	-1.466425
C	0.885452	-1.932720	-4.210073
O	0.462481	-1.403576	-5.487929
Mo	-0.395382	-0.535307	0.290539
O	-2.019019	0.004139	1.042527
O	0.877301	0.492768	0.853818
H	2.318503	-2.583330	0.441276
H	2.905622	-4.168390	1.018740
H	2.593299	-2.841731	2.181257
H	0.704171	-4.527108	2.219607
H	0.457743	-4.270235	0.474745
H	-0.420542	1.670280	-4.371170
H	-1.589717	0.436940	-4.872045
H	0.237059	0.343104	-6.497466
H	1.472095	0.399368	-5.196590
H	0.619964	-3.002804	-4.232181
H	1.996294	-1.870998	-4.148114