Supporting Information For:

Adabaticity of the Proton Coupled Electron Transfer Step in the Reduction of Superoxide Effected by Nickel Containing Superoxide Dismutase Metallopeptide-Based Mimics

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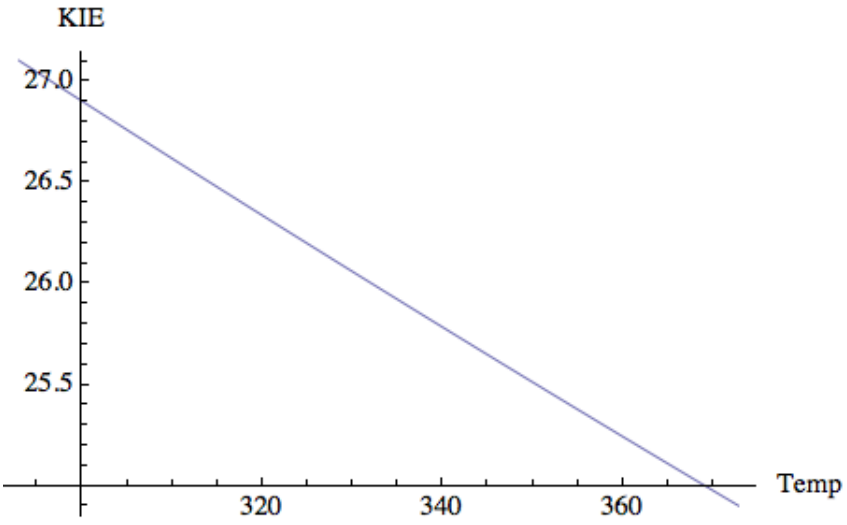

Figure 1: Temperature (K) KIE dependence using T^{ad} for $\mathbf{1}\cdots O_2^-$

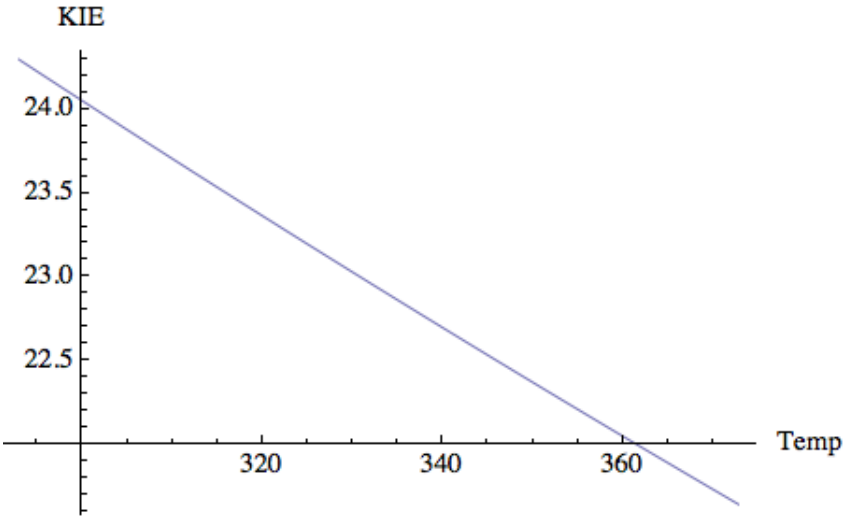

Figure 2: Temperature (K) KIE dependence using T^{sc} for $\mathbf{1}\cdots O_2^-$

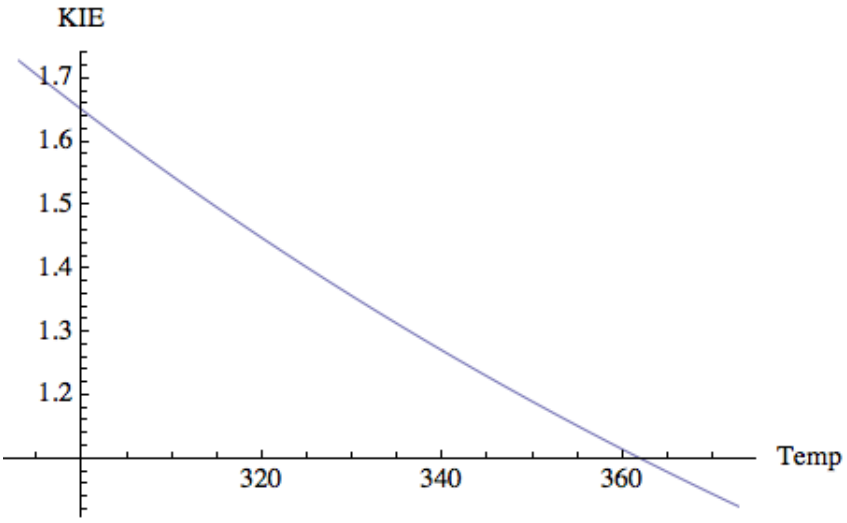

Figure 3: Temperature (K) KIE dependence using T^{na} for $\mathbf{1}\cdots O_2^-$

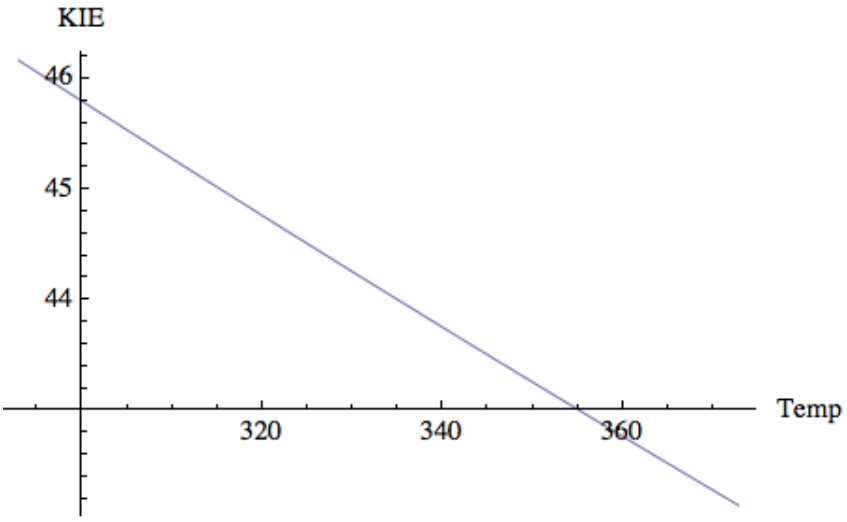

Figure 4: Temperature (K) KIE dependence using T^{ad} for $\mathbf{2}\cdots O_2^-$

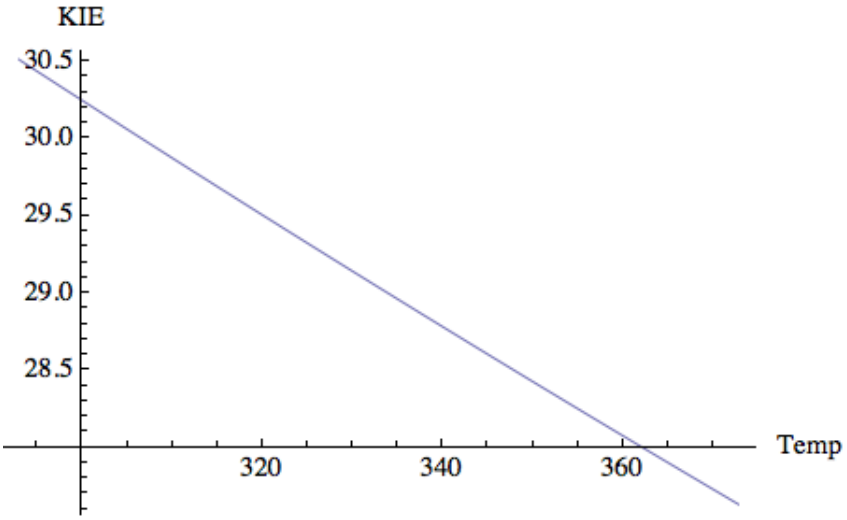

Figure 5: Temperature (K) KIE dependence using T^{sc} for $\mathbf{2}\cdots O_2^-$

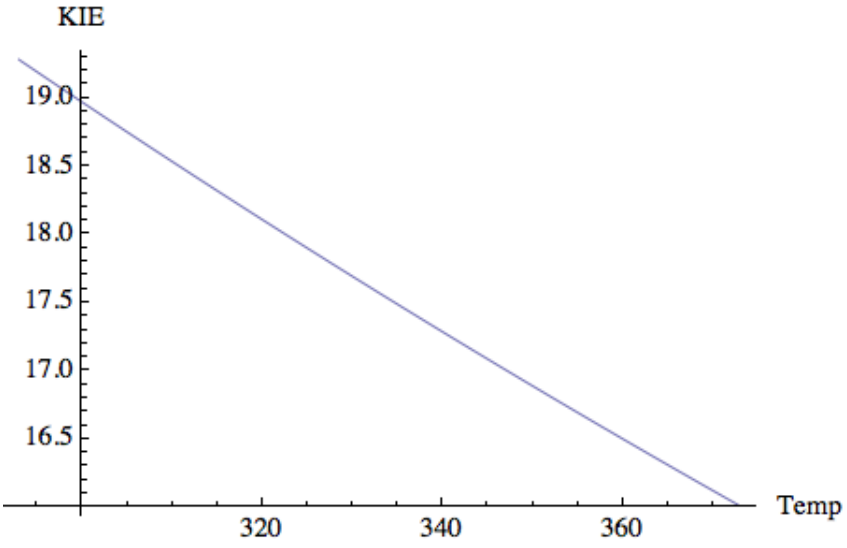

Figure 6: Temperature (K) KIE dependence using T^{na} for $\mathbf{2}\cdots O_2^-$

Table 1: Cartesian coordinations of the transition state structure of $\mathbf{1}\cdots O_2^-$.

Atom	x	y	z
Ni	0.00000	0.00000	0.00000
S	-1.93905	-0.76455	-0.77833
S	1.11017	-1.84777	-0.45222
N	1.53006	0.64120	0.88618
C	2.79267	-0.09550	0.82032
C	2.46437	-1.57802	0.79206
H	2.11069	-1.91116	1.77842
H	3.33312	-2.18748	0.49966
C	1.46572	1.80058	1.57778
C	0.05208	2.39434	1.52447
N	-0.68678	1.83481	0.36522
H	-0.42299	2.35872	-0.47732
H	-1.73768	1.95835	0.47494
C	-0.93691	-1.47687	-3.29469
C	-1.95077	-0.55880	-2.62971
H	-1.74811	0.49803	-2.85159
H	-1.00336	-1.38672	-4.39148
H	-2.97766	-0.78728	-2.95018
H	0.08655	-1.22595	-2.98134
H	-1.11167	-2.52640	-3.01524
H	-0.48785	2.10846	2.44012
H	0.11303	3.49336	1.49822
H	-3.01344	0.38794	-0.53426
H	3.33961	0.17631	-0.10290
H	3.42320	0.18029	1.68280
O	2.38574	2.34919	2.21818
O	-1.28750	-4.05525	-0.49082
H	-0.42878	-3.59787	-0.31796
H	-1.89353	-3.28863	-0.50180
O	-3.39429	2.34175	0.50379
O	-3.99617	1.46524	-0.31078

Table 2: Cartesian coordinations of the transition state structure of $\mathbf{2}\cdots O_2^-$.

Atom	x	y	z
Ni	0.18881	0.13182	-0.15367
S	-1.68483	-0.82162	-0.94329
S	1.33640	-1.67306	-0.72483
N	1.72939	0.77848	0.69026
C	3.02003	0.12735	0.49076
C	2.77453	-1.37283	0.41721
H	2.52379	-1.76452	1.41425
H	3.65288	-1.91570	0.03243
C	1.58265	1.75182	1.60966
C	0.12010	2.25776	1.68915
N	-0.61129	1.80880	0.46767
H	-0.45756	2.49617	-0.27741
H	-1.65250	1.72628	0.57945
C	-1.08366	-1.42047	-3.60901
C	-1.94308	-0.49521	-2.75699
H	-1.70398	0.55984	-2.95080
H	-1.30252	-1.27512	-4.68096
H	-3.01559	-0.64729	-2.95143
H	-0.01366	-1.22803	-3.43848
H	-1.27261	-2.47356	-3.35131
H	-3.03237	0.13429	-0.45697
H	3.46965	0.47058	-0.46094
H	3.70311	0.40206	1.31380
O	2.46789	2.25742	2.33847
O	-0.99228	-4.03587	-0.18602
H	-0.16832	-3.48471	-0.21421
H	-1.67270	-3.34164	-0.29463
O	-3.54284	1.86948	0.64965
O	-4.06689	0.87884	-0.07988
N	-1.38432	-1.59177	4.05131
C	-1.30549	-0.23922	4.36802
C	-0.86117	0.39959	3.22272
N	-0.67688	-0.53565	2.23044
C	-0.99373	-1.70871	2.74285
C	-0.59724	1.86717	2.99847
H	-1.57207	0.12172	5.35679
H	-0.88888	-2.64829	2.20335
C	-1.86055	-2.66066	4.91670
H	-1.86399	-2.30793	5.95559
H	-1.19493	-3.53233	4.84544
H	-2.88133	-2.96988	4.64568
H	0.18048	3.36082	1.70446
H	0.03188	2.25747	3.81582
H	-1.55203	2.42015	3.03991