Supporting Information

Blended Hydrogen Atom Abstraction and Proton-Coupled Electron Transfer Mechanisms of Closed-Shell Molecules

*Chunsen Li, David Danovich and Sason Shaik**

Institute of Chemistry and the Lise-Meitner-Minerva Center for Computational Quantum Chemistry, The Hebrew University of Jerusalem, 91904 Jerusalem, Israel

Email S.S.: sason@yfaat.ch.huji.ac.il

Table S1. B3LYP with different basis sets calculated *BDE*, *D* and *RE* in kcal mol^{-1}. In the case of $(CH_3)_2COH$•, CCSD(T) with correlation consistent basis sets was employed as well.

Y-H (bond)	Basis set	BDE[a]	D[a]	RE[a]
Cl_2CrO_2H• (O-H)	Def2-TZVP//LACVP	75.3	92.2	16.9
	def2-TZVP//LACVP**	75.9	90.4	14.5
	6-311++G**	76.9	94.2	17.3
	def2-TZVP//6-311++G**	76.0	93.8	17.8
MnO_4H^-• (O-H)	def2-TZVP//LACVP**	75.7	94.1	18.3
	6-311++G** opt	77.2	95.8	18.6
	def2-TZVP//6-311++G**	75.9	95.3	19.4
CH_4 (C-H)	6-311++G** opt	101.4	108.5	7.1
	Def2-TZVP//6-311++G**	101.3	108.5	7.2
C_6H_{12} axial (C-H)	6-311++G**//6-31G	93.4	101.0	7.6
	6-311++G** opt	93.5	100.5	7.0
	Def2-TZVP//6-311++G**	93.3	100.4	7.1
C_6H_{12} equatorial (C-H)	6-311++G** opt	93.6	100.8	7.2
	Def2-TZVP//6-311++G**	93.3	100.8	7.5
C_6H_8 (C-H)	6-311++G** opt	69.5	89.9	20.4
DHA (C-H)	6-311++G** opt	72.8	88.2	15.4
	Def2-TZVP//6-311++G**	72.1	88.1	16.0
$(CH_3)_2COH$• (O-H)	6-311++G** opt	23.3	52.3	29.0
	Def2-TZVP opt	22.7	52.0	29.3
	CCSD(T)/6-311++G**// B3LYP/6-311++G**	20.3	46.4	26.1
	CCSD(T)/Def2-TZVP// B3LYP/6-311++G**	18.7	46.1	27.4
	CCSD(T)/aug-cc-pVTZ// B3LYP/6-311++G**	22.2	49.1	26.9
	CCSD(T)/aug-cc-pVQZ// B3LYP/6-311++G**	22.4	50.1	27.7
$PhC(CH_3)_2$• (C-H)	6-311++G** opt	46.0	77.4	31.4
$PhCH_3$ (C-H)	6-311++G** opt	85.3	97.8	12.5
	6-311+G*//6-31G	85.0	97.3	12.3
	6-311++G**//6-31G	85.3	97.8	12.5
	Def2-TZVP//6-31G	85.1	97.9	12.8

[a] With ZPE correction. Note that corresponding values in ref. 21e were computed using LACV3P++**

Table S2. B3LYP with different basis sets calculated ΔE_{ST} (in kcal mol^{-1}).

Molecue	Basis set	ΔE_{ST}
Cl_2CrO_2	6-311++G**	45.2
	LACV3P+*//LACVP*	40.1

	def2-TZVP//LACVP*	45.0
	def2-TZVP	45.4
MnO_4^-	6-311++G**	34.8
	def2-TZVP//LACVP	33.0
	def2-TZVP	35.5
$KMnO_4$	6-311++G**	34.7
$(CH_3)_2C=O$	6-311++G**	139.9[a] (89.0)[b]
α-MS	6-311++G**	82.9

[a] π to π* excitation. [b] lone pair of O atom to π* of C=O excitation.

Table S3. B3LYP calculated barriers $\Delta E^{\ddagger}$ (kcal mol^{-1}) for Identity Reactions.

reactions	Basis set	$\Delta E^{\ddagger a}$
CH_3•/CH_4	6-311++G**	14.6
	Def2-TZVP//6-311++G**	15.0
C_6H_{11}•/C_6H_{12} ax.	6-311++G**	15.6
	Def2-TZVP//6-311++G**	16.2
C_6H_{11}•/C_6H_{12} eq.	6-311++G**	15.0
	Def2-TZVP//6-311++G**	15.5
DHA_{yl}•/DHA	6-311++G**	17.2
	Def2-TZVP//6-311++G**	17.8
allyl•/propene	6-311++G**	19.4
	Def2-TZVP//6-311++G**	19.8
C_6H_7•/C_6H_8 [b]	6-311++G**	20.6
	Def2-TZVP//6-311++G**	21.2
CrO_2Cl_2/CrO_2Cl_2H•	6-311++G**	11.5
	Def2-TZVP//6-311++G**	11.6
	LACV3P++**//LACVP**	11.0
$KMnO_4$/$KMnO_4H$• [c]	6-311++G**	11.6
	Def2-TZVP//6-311++G**	12.2
	LACV3P++**//LACVP**	11.9
MnO_4^-/MnO_4H• [d]	6-311++G**	15.0
$(CH_3)_2CO$/$(CH_3)_2COH$•	6-311++G**	10.3
	Def2-TZVP//6-311++G**	10.3
$Ph(CH_3)C{=}CH_2$/$Ph(CH_3)_2C$•	6-311++G**	23.2
	Def2-TZVP//6-311++G**	23.5

[a] Including ZPE correction. [b] C_6H_8 is 1,4-cyclohexadiene. [c] Note that the corresponding value in ref. 21e was computed using LACV3P++**. [d] RC is calculated by fixing H-O distance of MnO3OH---OMnO3.

Table S4. B3LYP/6-311++G** calculated open-shell singlet (OSS), triplet (T), closed-shell singlet (CSS) barriers $\Delta E^{\ddagger}$ and singlet reaction driving force $\Delta E_{RC->IH}$ (kcal mol^{-1}) for Nonidentity H-Abstraction reactions.

reactions	$\Delta E^{\ddagger}$(OS)[a]	$\Delta E_{RC->IH}$[a]	$\Delta E^{\ddagger}$(CS)sp[a,b]	$\Delta E^{\ddagger}$(CS)opt[a,c]	$\Delta E^{\ddagger}$(T)sp[a,b]
MnO_4^- + CH_4	27.3	23.4	31.4	30.9	37.8
$KMnO_4$ + CH_4	26.3	18.2			
MnO_4^- + C_6H_{12}	23.3	16.4	27.3	30.0	32.4
$KMnO_4$ + C_6H_{12}	19.6	9.6			
MnO_4^- + DHA	14.6	-5.2	15.1	15.6	28.4
$KMnO_4$ + DHA	15.3	-2.8			
MnO_4^- + $PhCH_3$	20.0	7.0	21.6	23.3	31.7
$KMnO_4$ + $PhCH_3$	20.6	9.5			
α-MS + DHA	32.6	26.6	33.1		46.0

[a] Including ZPE correction. [b] Single point calculation using geometry structure of open-shell TS. [c] Full transition state optimization for closes-shell TS.

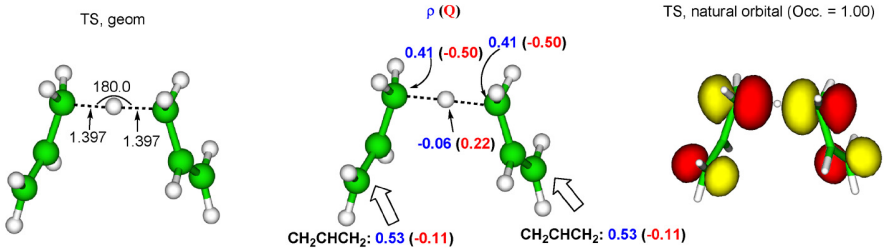

Figure S1. Key geometric features, group spin densities (ρ), natural bond orbital (NBO) charge densities (Q), and the singly occupied natural orbital (NO) for the identity HAT reactions of allyl•/propene.

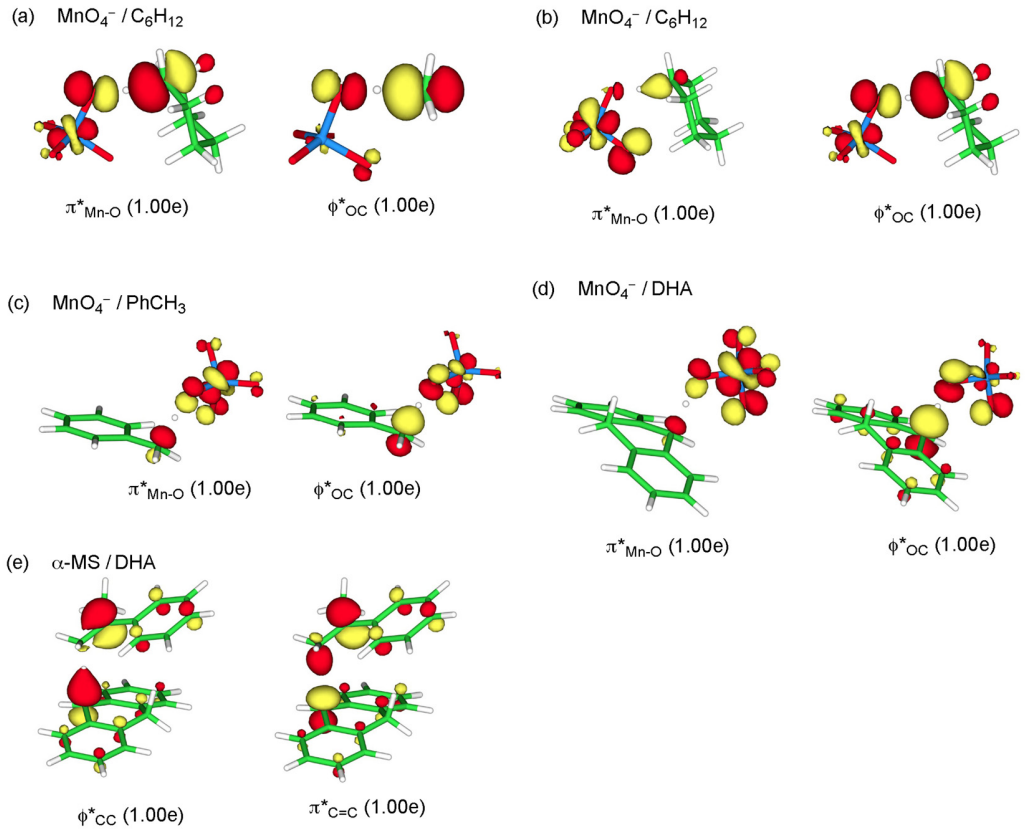

Figure S2. Natural orbital (NO) of the triplet TSs of nonidentity reactions.

A Comment about Potential Disparities in MCR Analyses of Experimental Data: Generally intrinsic and identity barriers obtained by MCR analyses of experimental data have uncertainties, due to errors in reaction energies, in work functions of reactants and products clusters, as well as in rate constants. Additionally, some disparities between the identity barriers derived in this work in Table 1 (and in ref. 21e) vs. data in ref. 32 originate from different equations used to link a given rate constant to the corresponding free energy barriers. Thus, we used uniformly the Eyring equation (with standard state concentrations of 1 M). On the other hand, ref. 32 uses in the MCR analysis the following equation:

$$k = Z \exp[-\Delta G^{\ddagger}/RT];\ Z = 10^{11}\ \text{L mol}^{-1}\text{s}^{-1} \qquad \text{(S.1)}$$

The two equations differ in the preexponential factor. In the Eyring formulation, it is 6.2×10^{12} s^{-1} at 298K, whereas for the above expression Z is 10^{11}. Because of the different preexponentials there will be

a difference in activation free energies derived from the two equaions by ca. 2.45 kcal mol^{-1}. For example, if we use the rate constant 5×10^{-11} $M^{-1}S^{-1}$ for the identity barrier of DHA (cited in ref. 32a,b) at 298K, we get 31.49 kcal mol^{-1} with the Eyring equation and 29.04 kcal mol^{-1} with the collision theory equation. One can debate which is the most appropriate preexponential to use. Some prefer ~6×10^{10} s^{-1} for reactions in solutions, others use Eyring's original formulation ($k_BT/h = 6.2\times10^{12}$ s^{-1} at 298K). Since the Eyring equation is the source of many free energy barriers in the literature, for consistency, we preferred using it uniformly.

This disparity carries over to the MCR analyses. Ref. 32 uses eq. S2 in terms of rate constants:

$$k_{12} = (k_{11}k_{22}K_{12}f_{12})^{1/2} \; ; \; \ln(f_{12}) = (\ln K_{12})^2/4\ln(k_{11}k_{22}/Z^2) \qquad \text{(S.2)}$$

While we used equations 2a and 2b in the text, which together can be written as follows:

$$\Delta G^{\ddagger}_{12} = \tfrac{1}{2}[\Delta G^{\ddagger}_{11} + \Delta G^{\ddagger}_{22}] + 0.5\Delta G_{12} + \Delta G_{12}^{\,2}/[8[\Delta G^{\ddagger}_{11} + \Delta G^{\ddagger}_{22}]];$$

$$\Delta G_0^{\ddagger} = \tfrac{1}{2}[\Delta G^{\ddagger}_{11} + \Delta G^{\ddagger}_{22}] \qquad \text{(S.3)}$$

Thus, for example, using equation S.3 for MnO_4^-/DHA, for which Eyring's $\Delta G^{\ddagger}_{12}$ = 18.7 kcal mol^{-1} (19 ±2 in ref. 15g) and ΔG_{12} = -5.7 kcal mol^{-1} (ref. 15g, 32d see also Table 1) along with the identity free energy barrier for DHA_{yl}•-radical/DHA converted by means of the Eyring equation from the rate constant 5×10^{-11} $M^{-1}S^{-1}$ (cited in ref. 32a,b), leads to an identity free energy barrier of 11.4 kcal mol^{-1} for MnO_4^-/MnO_4H^-• (Table 2). The corresponding MCR-based rate constant, 2×10^6 $M^{-1}s^{-1}$ (extracted in ref. 32 from eq. S.1) leads with the Eyring equation to a value of 8.9 kcal mol^{-1}. We note that equations S.2 and S.3 are identical, except for the representation. Thus, the source of this disparity is unclear; it might arise due to uncertainties in the $\ln(f_{12})$ term in eq. S.2. Our conclusion is that adherance to a single set of equations is advisable to get consistent identity barrier data. We used here the Eyring equation and equation 2 in the text.

A Comment about MCR Analyses of Theoretical Data: Equation S3 uses free energies. But one can perform MCR analyses of enthalpic or ZPE corrected barrier, as well. The simplest way to show that the Marcus equation reflects the "plasticity" behavior of potential energy barriers in general, is to start from a barrier given by the expression:

$E(x) = -4\Delta E_0^{\ddagger} x^2 + \Delta E_0^{\ddagger}$ (S.4)

This expression describes a quadratic barrier with a height given by $\Delta E_0^{\ddagger}$ and identical $E(x)$ values at x=−0.5 and x=0.5; hence a symmetric barrier. Adding a linear perturbation, $E'(x) = \Delta E_{12}(x + 0.5)$, which lowers the right-hand point (at x=0.5) by ΔE_{12}, changes the maximum of the potential energy curve and yields the following expression for the barrier after perturbation:

$\Delta E^{\ddagger}_{12} = \Delta E_0^{\ddagger} + 0.5\Delta E_{12} + \Delta E_{12}^2/[16\Delta E_0^{\ddagger}]$ (S.5)

This is precisely equation 2a in the text (or S3 herein), but written in terms of potential energies, *E*. Thus, the Marcus equation need not be associated with free energies or with a model of intersecting-parabolas with weak overlap. Indeed many theoretical works use ZPE corrected barriers and correlate them with the energy-based Marcus equation (e.g., J. M. Gonzales, W. D. Allen and H. F. Schaefer III, *J. Phys. Chem. A*, 2005, **109**, 10613; S. Wolfe, D. J. Mitchell and H. B. Schlegel, *J. Am. Chem. Soc.*, 1981, **103**, 7694; etc). The constancy of the so derived identity barriers works well in these cases, but there is no rule that identity barriers must be constant. Therefore our MCR analysis of the computational data, and the finding of variable identity barrier are not uncertainties of the MCR analysis, but ones that reflect the physical effect of HAT/PCET blending and hence the breakdown of transferability of identity barriers from one reaction to the other.

An Assessment of the Identity Barrier for the Reaction $MnO_4^-/MnO_4H^-\bullet$: In the literature (ref. 32a,b), this identity rate constant is estimated using MCR analysis of the rate constant for MnO_4^-/DHA (Table 1, entry 4), using an identity rate constant for $DHA_{yl}\bullet$-radical/DHA, which is in turn estimated using MCR analysis of the rate constant for the reaction, Fe^{III}(Hbim) + DHA. Since the so-estimated rate constant for $DHA_{yl}\bullet$-radical/DHA, was 5×10^{-11} $M^{-1}S^{-1}$, using eq. S2 this led to a large rate constant for $MnO_4^-/MnO_4H^-\bullet$ of 2×10^{6} $M^{-1}S^{-1}$ (as reported in ref. 32c), and hence a small free energy barrier.

Using the Eyring equation, the MCR-based rate constant, 5×10^{-11} $M^{-1}S^{-1}$, for $DHA_{yl}\bullet$-radical/DHA lead to a barrier of 31.5 kcal/mol. Since this looked too high, we tried estimating this barrier by comparison to analogous alkyl/alkane reactions, for which both computed and experimental barriers are known. Thus, the B3LYP/B1 barrier of the reaction $PhCH_2\bullet/PhCH_3$ is 16.5 kcal mol^{-1} (ref. 20), while the experimental enthalpic barrier is 18.7 kcal mol^{-1} (ref. 33), and the free energy barrier is $\Delta G^{\ddagger}(PhCH_2^{\bullet}/PhCH_3)$ = 23.4 kcal mol^{-1}, i.e., 4.7 kcal mol^{-1} higher than the enthalic barrier and 6.9 kcal

mol^{-1} higher than the computed barrier. Similarly, $\Delta G^{\ddagger}(CH_3^{\bullet}/CH_4)$ = 20 kcal mol^{-1} and is higher by 5.1 than the enthalpic barrier (ref. 31) and 5.5 than the computed barrier. Since the B3LYP barrier for DHA_{yl}•-radical/DHA is 17.2 kcal mol^{-1} (Table 2) using the highest increment (6.9 kcal mol^{-1}) we may expect a free energy barrier of ~24 kcal mol^{-1} for this reaction. Using this value, and the MCR analysis of the free energy barrier for MnO_4^-/DHA (Table 1, entry 4) predicts for MnO_4^-/MnO_4H^-• an identity free energy barrier of ~19 kcal mol^{-1}.

$TS_{CH3/CH4}$

C	-0.009708	0.064301	0.924375
H	-0.022949	0.136493	2.269424
H	0.995668	0.361749	0.634270
H	-0.778902	0.759680	0.595451
H	-0.237515	-0.974155	0.693877
C	-0.036189	0.208684	3.614473
H	0.733013	-0.486685	3.943397
H	0.191606	1.247144	3.844971
H	-1.041561	-0.088776	3.904578

$RC_{CH3/CH4}$

C	-0.000676	0.014746	0.027024
H	-0.013396	0.069908	1.116503
H	0.987675	0.294989	-0.340128
H	-0.747059	0.698026	-0.380763
H	-0.230037	-1.004100	-0.288538
C	-0.047926	0.272086	4.766970
H	0.751764	-0.452337	4.824891
H	0.181379	1.326569	4.711091
H	-1.076950	-0.057628	4.771127

$TS_{C6H11/C6H12}$ (axial)

C	-0.828507	0.219588	-0.229032
H	-0.844236	0.407203	0.847434
H	0.503177	-0.047984	-0.417889
C	-1.157815	1.458407	-1.045999
H	-0.466399	2.272540	-0.801822
H	-2.159906	1.819789	-0.761927
C	-1.614060	-1.020755	-0.621147
H	-1.238678	-1.898258	-0.083373
H	-2.661764	-0.897649	-0.300197
C	-1.146493	1.185428	-2.559250
H	-0.117262	0.994284	-2.886658
H	-1.485212	2.074511	-3.101336
C	-1.594934	-1.273977	-2.137507
H	-0.582697	-1.563857	-2.445785
H	-2.248579	-2.117445	-2.383287
C	-2.020291	-0.024026	-2.920891
H	-3.069637	0.205911	-2.692089
H	-1.972102	-0.217269	-3.997721
C	1.844862	-0.266256	-0.599053
H	1.938718	-0.069810	-1.669979
C	2.584801	0.752608	0.252756
H	3.653779	0.736245	-0.016374
H	2.234985	1.766079	0.027117
C	2.131868	-1.714243	-0.238492
H	3.159277	-1.964713	-0.550903
H	1.476229	-2.387275	-0.801735
C	2.455055	0.465971	1.757918
H	3.080589	1.162662	2.325693
H	1.420636	0.646402	2.074475
C	2.002553	-1.980504	1.270315
H	2.308243	-3.007448	1.496024
H	0.949546	-1.896238	1.566029
C	2.834967	-0.984131	2.089963
H	3.900466	-1.138222	1.872548
H	2.705668	-1.173255	3.160830

$RC_{C6H11/C6H12}$ (axial)

C	-1.102413	0.030527	-0.128656
H	-1.240597	-0.051240	0.954720
H	-0.023284	-0.054633	-0.312374
C	-1.592477	1.399619	-0.624077
H	-1.029896	2.202445	-0.135810
H	-2.642580	1.533697	-0.331990
C	-1.826444	-1.119946	-0.844021
H	-1.427862	-2.083675	-0.509906
H	-2.888079	-1.107837	-0.563109
C	-1.475499	1.522144	-2.150902
H	-0.414080	1.509629	-2.432211
H	-1.873926	2.485968	-2.485191
C	-1.709061	-0.997533	-2.370807
H	-0.658899	-1.130857	-2.662520
H	-2.271389	-1.800302	-2.859479
C	-2.199292	0.371468	-2.866159
H	-3.278490	0.455469	-2.681143
H	-2.062736	0.453471	-3.949696

C	3.815417	-1.041338	-0.743752
H	3.382655	-1.109375	-1.736250
C	4.356814	0.265244	-0.260887
H	5.426105	0.346126	-0.534570
H	3.859027	1.101830	-0.761118
C	4.165471	-2.290931	-0.002365
H	5.206716	-2.581693	-0.239137
H	3.541944	-3.127373	-0.333202
C	4.247978	0.408193	1.271689
H	4.787240	1.302222	1.601362
H	3.195554	0.553873	1.543315
C	4.060530	-2.108431	1.526286
H	4.468281	-2.988215	2.034734
H	3.002435	-2.041877	1.806827
C	4.784484	-0.837211	1.990955
H	5.859956	-0.937520	1.791099
H	4.679575	-0.719845	3.074588

$TS_{C6H11/C6H12}$ (equal)

H	-0.199495	-0.689419	0.046897
C	-0.148688	-0.600937	1.403596
H	0.655222	-1.302559	1.648921
C	0.190511	0.831264	1.778081
H	-0.505235	1.516707	1.275071
H	1.195620	1.096588	1.434719
C	0.076278	1.049589	3.302276
H	0.260587	2.101987	3.545708
H	0.857774	0.468396	3.807974
C	-1.299490	0.613814	3.827442
H	-2.070253	1.274262	3.408161
H	-1.344313	0.736669	4.914807
C	-1.620134	-0.838682	3.445169
H	-2.625750	-1.108741	3.786536
H	-0.922560	-1.511570	3.959969
C	-1.501548	-1.056104	1.921911
H	-2.294372	-0.480381	1.424113
H	-1.677379	-2.108581	1.676147
C	-0.272599	-0.799567	-1.307839
H	-1.287252	-1.186429	-1.448168
C	-0.086699	0.583542	-1.905832
H	-0.907090	1.247716	-1.615238
H	0.835820	1.031868	-1.512240
C	0.018697	0.515370	-3.444790
H	-0.946532	0.194698	-3.857006
H	0.217846	1.512960	-3.852089
C	1.111082	-0.469223	-3.887301
H	1.137396	-0.537268	-4.980078
H	2.091004	-0.083133	-3.576460
C	0.902127	-1.862383	-3.275693
H	-0.019284	-2.300781	-3.679718
H	1.720528	-2.531384	-3.564555
C	0.795093	-1.790158	-1.737486
H	0.590995	-2.784476	-1.326725
H	1.767870	-1.476636	-1.333474

$RC_{C6H11/C6H12}$ (equal)

H	0.082144	-0.684265	1.979049
C	-0.117740	-0.481383	3.036406
H	0.548673	-1.138418	3.610907
C	0.210799	0.982214	3.367689
H	-0.369025	1.639571	2.706237
H	1.266551	1.188898	3.162885
C	-0.122215	1.318481	4.829107
H	0.074567	2.377203	5.028235
H	0.544019	0.748401	5.490124
C	-1.580806	0.976669	5.168650
H	-2.247248	1.633722	4.594218
H	-1.780828	1.179565	6.226045
C	-1.909383	-0.486933	4.837406
H	-2.965122	-0.693579	5.042255
H	-1.329558	-1.144313	5.498842
C	-1.576324	-0.823155	3.375995
H	-2.242529	-0.253084	2.714953
H	-1.773106	-1.881870	3.176876
C	-0.432028	-1.370366	-3.281676
H	-1.222253	-1.737305	-2.635334
C	-0.333783	0.091872	-3.574354
H	-1.311106	0.574869	-3.477470
H	0.316542	0.576852	-2.821634
C	0.269893	0.365297	-4.967839
H	-0.463426	0.089491	-5.735184
H	0.464895	1.436207	-5.085730
C	1.556780	-0.441790	-5.189392
H	1.955852	-0.245326	-6.189979

H	2.322868	-0.106862	-4.476995
C	1.313725	-1.946154	-5.005264
H	0.613282	-2.292946	-5.774527
H	2.244580	-2.504388	-5.148949
C	0.725073	-2.256444	-3.612881
H	0.440325	-3.310852	-3.542527
H	1.527840	-2.112242	-2.864888

$TS_{DHAyl/DHA}$

C	-1.589787	2.273402	2.350772
H	-0.743024	2.626292	1.761917
C	-2.461447	3.342191	2.861010
C	-3.350411	3.069707	3.920689
C	-3.427511	1.667985	4.482585
H	-4.222301	1.126051	3.947204
H	-3.737573	1.698091	5.530974
C	-2.142339	0.883813	4.340618
C	-1.265064	1.179135	3.277019
C	-2.432759	4.633935	2.309231
H	-1.741951	4.847351	1.499487
C	-3.260224	5.638314	2.796005
H	-3.220886	6.631299	2.362332
C	-4.130713	5.367884	3.852885
H	-4.772541	6.148388	4.245544
C	-4.166627	4.089904	4.408244
H	-4.840853	3.881958	5.233487
C	-0.099928	0.409869	3.118162
H	0.574999	0.636392	2.299248
C	0.197424	-0.624919	3.995956
H	1.103567	-1.205216	3.862202
C	-0.666758	-0.906222	5.055866
H	-0.436722	-1.705579	5.751103
C	-1.825696	-0.149736	5.221645
H	-2.495922	-0.367567	6.047587
H	-2.282114	1.685194	1.314980
C	-2.933948	1.185051	0.209488
H	-3.234928	2.143435	-0.213815
C	-4.046868	0.384365	0.740399
C	-3.866040	-0.995328	0.967902
C	-2.515032	-1.621238	0.704528
H	-2.633131	-2.676434	0.442084
H	-1.939333	-1.605117	1.642586
C	-1.708494	-0.907256	-0.356563
C	-1.910800	0.471507	-0.569682
C	-5.288937	0.969406	1.040094
H	-5.428589	2.031292	0.865508
C	-6.333537	0.206813	1.547219
H	-7.287017	0.673277	1.768396
C	-6.155020	-1.161550	1.759427
H	-6.968294	-1.765481	2.145681
C	-4.926804	-1.751434	1.465883
H	-4.789685	-2.816086	1.628574
C	-1.119878	1.138237	-1.520531
H	-1.280200	2.198114	-1.691767
C	-0.153250	0.458079	-2.250767
H	0.444225	0.987177	-2.984702
C	0.035679	-0.909441	-2.045731
H	0.780533	-1.450098	-2.618455
C	-0.743768	-1.580748	-1.105234
H	-0.598983	-2.645450	-0.949704

$RC_{DHAyl/DHA}$

C	-1.145966	2.597148	3.062758
H	-0.409872	2.813484	2.295651
C	-2.137656	3.575594	3.356654
C	-3.121564	3.315756	4.348173
C	-3.177185	1.967636	5.030531
H	-4.072511	1.438202	4.670107
H	-3.339421	2.105623	6.105831
C	-1.980154	1.070925	4.808236
C	-1.024876	1.388464	3.805473
C	-2.159140	4.825068	2.689683
H	-1.410332	5.024055	1.929913
C	-3.106042	5.785009	3.000720
H	-3.103864	6.737339	2.482422
C	-4.061521	5.527329	3.990215
H	-4.801746	6.277666	4.242888
C	-4.059570	4.298707	4.650702
H	-4.807271	4.101251	5.413284
C	0.045540	0.489132	3.578134
H	0.771446	0.724974	2.806937
C	0.176222	-0.669119	4.324242
H	1.005081	-1.343064	4.138405
C	-0.758539	-0.965473	5.322915
H	-0.657857	-1.868138	5.914483
C	-1.824727	-0.095402	5.552121

H	-2.552336	-0.333531	6.322468
H	-2.673499	1.603354	0.694641
C	-3.158924	1.139289	-0.177139
H	-3.580921	1.955822	-0.767276
C	-4.253187	0.218417	0.320121
C	-3.897353	-1.072177	0.738249
C	-2.439964	-1.475888	0.665856
H	-2.341754	-2.563975	0.685019
H	-1.926225	-1.103368	1.565156
C	-1.755443	-0.900839	-0.556212
C	-2.111142	0.390367	-0.972760
C	-5.589699	0.616120	0.377378
H	-5.865289	1.612250	0.045561
C	-6.570578	-0.252230	0.853368
H	-7.605899	0.067790	0.890629
C	-6.217279	-1.534236	1.268941
H	-6.975579	-2.218940	1.632121
C	-4.885407	-1.939910	1.205739
H	-4.611203	-2.942164	1.520160
C	-1.496962	0.943828	-2.097501
H	-1.781733	1.938423	-2.426576
C	-0.528699	0.231336	-2.802959
H	-0.059803	0.671725	-3.675837
C	-0.174709	-1.050842	-2.388655
H	0.569760	-1.616046	-2.938248
C	-0.791463	-1.612424	-1.272005
H	-0.526430	-2.617259	-0.957885

$TS_{MnO4K/MnO4HK}$

Mn	-0.501196	0.338502	0.454300
O	0.081800	-0.410091	1.867987
O	0.466071	1.616588	0.219274
O	-0.304728	-0.745288	-0.709955
O	-1.989281	0.803781	0.659509
H	0.982532	0.130260	2.439156
O	1.932699	0.672101	2.921287
Mn	3.449985	-0.060416	2.677463
O	3.160070	-1.328713	1.712334
O	4.050301	-0.538210	4.050185
O	4.334407	1.040572	1.919703
K	1.147664	-2.511627	0.674776
K	2.385914	2.798020	1.416378

$RC_{MnO4K/MnO4HK}$

Mn	-0.230598	-0.038095	-0.130312
O	-0.166858	-0.370331	1.651292
O	1.367363	-0.220759	-0.516017
O	-1.091424	-1.194622	-0.760345
O	-0.616691	1.488897	-0.371964
H	0.307135	0.365835	2.081852
O	1.842818	1.616659	2.345949
Mn	3.423236	1.333408	2.516679
O	3.660155	-0.252151	2.611278
O	3.973270	2.044178	3.806577
O	4.146160	1.912114	1.208337
K	2.058314	-1.916198	1.386411
K	1.980482	2.381439	-0.321648

$TS_{MnO4-/MnO4H-}$

Mn	-0.826448	0.285421	0.392508
O	0.504970	-0.434696	1.131015
O	-0.329640	1.207836	-0.822895
O	-1.779178	-0.886288	-0.172899
O	-1.630431	1.157605	1.473149
H	1.422055	0.138136	1.659150
O	2.339102	0.711144	2.187436
Mn	3.670109	-0.009293	2.926345
O	4.473837	-0.882046	1.845988
O	3.172875	-0.931217	4.141955
O	4.623169	1.162252	3.491533

$TS_{Cl2CrO2/Cl2CrO2H}$

Cr	-0.025609	-0.122275	0.334082
O	0.207023	1.050982	1.452895
O	0.819037	-1.390282	0.595272
Cl	-2.086416	-0.664495	0.253878
Cl	0.499389	0.628512	-1.593040
H	0.891666	1.050339	2.430493
O	1.576245	1.055078	3.408120
Cr	1.797596	-0.107627	4.540157
O	0.941506	-1.370719	4.292754
Cl	1.278530	0.669554	6.458406

Cl	3.853315	-0.667716	4.627687

$RC_{Cl2CrO2/Cl2CrO2H}$

Cr	-0.529606	0.161163	0.417064
O	0.190535	0.741057	1.680231
O	-1.673422	-0.782326	0.860120
Cl	-1.345460	1.751911	-0.717420
Cl	0.861461	-0.935464	-0.740444
H	0.686192	0.999943	3.514920
O	1.003868	1.047860	4.436212
Cr	1.816762	-0.290193	5.168798
O	2.031549	-1.580270	4.349271
Cl	0.783618	-0.831020	6.976505
Cl	3.741873	0.362376	5.873265

$TS_{(CH3)2CO/(CH3)2COH}$

C	0.019426	-0.251005	-0.138508
C	1.491802	-0.474955	-0.031556
H	1.986828	-0.253613	-0.987076
H	1.937673	0.218663	0.698079
H	1.730580	-1.496160	0.267779
C	-0.973805	-1.270583	0.313635
H	-1.135614	-1.207462	1.401930
H	-1.937647	-1.096963	-0.169050
H	-0.636197	-2.289014	0.101433
O	-0.422185	0.885389	-0.549222
H	0.397507	1.704861	-0.841348
O	1.217168	2.524327	-1.133446
C	0.775517	3.660699	-1.544185
C	1.768708	4.680405	-1.996124
H	2.732612	4.506597	-1.513640
H	1.930331	4.617690	-3.084467
H	1.431148	5.698771	-1.783505
C	-0.696861	3.884561	-1.651245
H	-0.935668	4.905681	-1.950847
H	-1.142686	3.190730	-2.380702
H	-1.191910	3.663458	-0.695678

$RC_{(CH3)2CO/(CH3)2COH}$

C	0.018415	-0.307765	0.187971
C	1.474446	-0.632940	0.294808
H	1.823628	-1.242024	-0.559691
H	2.089527	0.272522	0.314528
H	1.679612	-1.200560	1.205844
C	-1.015858	-1.356485	0.418076
H	-0.804644	-1.921435	1.329330
H	-2.009271	-0.908776	0.508788
H	-1.060557	-2.078871	-0.417178
O	-0.352397	0.596362	-0.781285
H	0.365764	1.232060	-0.954675
O	1.400236	2.741976	-1.399690
C	0.878626	3.788625	-1.741213
C	1.716176	5.008063	-2.052610
H	2.772461	4.744463	-2.078023
H	1.414129	5.454357	-3.004384
H	1.551214	5.766014	-1.279112
C	-0.620722	3.927700	-1.875324
H	-0.969293	4.842162	-1.386954
H	-0.875349	4.017860	-2.937207
H	-1.129413	3.058770	-1.459748

$TS_{C6H7/C6H8}$

C	-0.215974	0.195255	-1.309412
H	-0.376848	0.141672	0.060161
H	0.865932	0.330181	-1.277005
C	-0.988553	1.357714	-1.753766
H	-0.584958	2.345885	-1.552400
C	-0.680622	-1.099534	-1.810919
H	-0.045369	-1.965648	-1.651371
C	-1.867440	-1.248943	-2.424871
H	-2.184283	-2.231543	-2.761575
C	-2.179359	1.239133	-2.366322
H	-2.730269	2.128177	-2.658403
C	-2.793574	-0.094318	-2.696253
H	-3.732099	-0.225155	-2.131459
H	-3.113381	-0.109479	-3.749376
C	-0.537548	0.099985	1.430476
H	-1.611321	0.290620	1.410095
C	-0.138946	-1.250126	1.833603
H	-0.815926	-2.069283	1.610336
C	0.291112	1.186299	1.958478
H	-0.061715	2.205696	1.831132

C	1.472625	0.962951	2.559494
H	2.066626	1.799045	2.916348
C	1.037210	-1.503905	2.433800
H	1.303781	-2.523463	2.695947
C	2.018764	-0.420232	2.789245
H	2.334656	-0.529239	3.837993
H	2.951050	-0.555460	2.215228

$RC_{C6H7/C6H8}$

C	-0.382310	0.218214	-1.786510
H	-0.226954	0.233067	-0.697966
H	0.625589	0.343298	-2.209597
C	-1.252524	1.375878	-2.195663
H	-0.905357	2.369985	-1.926587
C	-0.946633	-1.113294	-2.202446
H	-0.369356	-1.994970	-1.937164
C	-2.095349	-1.253301	-2.863328
H	-2.443203	-2.247469	-3.131313
C	-2.401368	1.237211	-2.856689
H	-2.979338	2.119193	-3.119832
C	-2.965051	-0.094950	-3.273285
H	-3.974327	-0.220057	-2.853454
H	-3.117330	-0.110603	-4.362796
C	-0.452079	0.135397	2.441863
H	-1.475546	0.359396	2.168192
C	-0.007050	-1.210006	2.500800
H	-0.706146	-2.006558	2.266523
C	0.452140	1.184677	2.746665
H	0.102552	2.211318	2.700772
C	1.746494	0.931539	3.094915
H	2.421148	1.749751	3.324306
C	1.275896	-1.521624	2.843678
H	1.594902	-2.557941	2.883342
C	2.288977	-0.465664	3.178330
H	2.704698	-0.648492	4.185573
H	3.171095	-0.567709	2.520878

$TS_{Ph(CH3)C=CH2/PhC(CH3)2}$

C	-0.506366	-0.190848	-0.119412
C	0.045719	-0.354829	1.175194
C	0.371033	-0.390894	-1.212427
C	1.379678	-0.687926	1.359501
C	1.707289	-0.722575	-1.023058
C	2.225459	-0.873503	0.262920
H	-0.578215	-0.220220	2.049409
H	0.001586	-0.283516	-2.223906
H	1.766294	-0.803639	2.366449
H	2.348609	-0.865331	-1.886135
H	3.267611	-1.132551	0.410040
C	-1.900520	0.165628	-0.332180
C	-2.427778	0.254559	-1.741514
H	-3.485495	0.521354	-1.743084
H	-1.893690	1.014052	-2.324261
H	-2.324899	-0.694257	-2.280988
C	-2.813512	0.321455	0.729691
H	-2.433932	0.561357	1.719617
H	-3.742642	0.838526	0.498425
H	-3.336449	-0.932436	1.030474
C	-3.957933	-2.107061	1.443583
H	-3.739928	-2.047216	2.507990
H	-4.979402	-1.820347	1.206612
C	-3.370635	-3.178622	0.741941
C	-2.160651	-3.846148	1.344063
H	-1.926626	-3.416670	2.319119
H	-2.323960	-4.921020	1.486149
H	-1.271655	-3.738564	0.712112
C	-3.816075	-3.584183	-0.581729
C	-3.179810	-4.642594	-1.274293
C	-4.895787	-2.951222	-1.246018
C	-3.599805	-5.044128	-2.536758
C	-5.310122	-3.353793	-2.507278
C	-4.668083	-4.405507	-3.165930
H	-2.346526	-5.160274	-0.817049
H	-5.417633	-2.131040	-0.769458
H	-3.088105	-5.861449	-3.033533
H	-6.141299	-2.844379	-2.983151
H	-4.994595	-4.718624	-4.150896

$RC_{Ph(CH3)C=CH2/PhC(CH3)2}$

C	0.166165	0.169951	-0.175061
C	0.577541	-0.068246	1.167883
C	0.857545	-0.553632	-1.188785
C	1.597244	-0.958573	1.466352

C	1.874813	-1.442809	-0.878586
C	2.256602	-1.656221	0.449498
H	0.089045	0.458141	1.978157
H	0.586158	-0.411275	-2.227278
H	1.885249	-1.112676	2.500867
H	2.378845	-1.976518	-1.677351
H	3.053289	-2.351362	0.687399
C	-0.882731	1.085960	-0.487923
C	-1.278271	1.339188	-1.915707
H	-2.068434	2.088556	-1.979601
H	-0.434596	1.696860	-2.519724
H	-1.647978	0.429985	-2.408391
C	-1.611771	1.818633	0.603152
H	-0.944768	2.481877	1.170486
H	-2.415044	2.434715	0.196571
H	-2.059535	1.131366	1.331786
C	-2.551156	-2.960814	1.974110
H	-1.582097	-2.489987	1.853138
H	-2.971374	-2.966799	2.973119
C	-3.180504	-3.528052	0.936258
C	-2.537011	-3.564223	-0.430569
H	-1.612597	-2.985139	-0.439686
H	-2.289439	-4.588172	-0.729629
H	-3.210160	-3.162810	-1.194740
C	-4.523318	-4.153360	1.086066
C	-4.898831	-5.263236	0.313061
C	-5.461812	-3.648016	2.001236
C	-6.147152	-5.861942	0.469546
C	-6.710008	-4.242347	2.156406
C	-7.058975	-5.356259	1.393075
H	-4.205276	-5.678010	-0.408437
H	-5.215837	-2.765577	2.580172
H	-6.406534	-6.725444	-0.133255
H	-7.417316	-3.827227	2.866166
H	-8.032832	-5.817930	1.510881

$TS_{MnO4-/C6H12}$

Mn	-0.026406	0.004340	-0.045880
O	-0.001062	-0.004701	1.680135
O	1.560564	0.022024	-0.405235
O	-0.697431	-1.341376	-0.574903
O	-0.724038	1.342095	-0.560482
H	1.053894	0.002321	2.152488
C	2.169000	0.007141	3.003445
H	1.561240	-0.002383	3.913427
C	2.964311	-1.268359	2.810710
H	2.288284	-2.129785	2.777034
H	3.606326	-1.418433	3.699851
C	3.853615	-1.237756	1.558725
H	3.211344	-1.255267	0.673249
H	4.491277	-2.130396	1.534166
C	4.712959	0.034747	1.514534
H	5.317704	0.044285	0.600179
H	5.419669	0.035706	2.359288
C	3.834018	1.293327	1.572250
H	3.191614	1.310418	0.686846
H	4.457903	2.195876	1.557329
C	2.944350	1.296787	2.824296
H	2.255091	2.147963	2.799554
H	3.583883	1.447415	3.715131

$TS_{MnO4-/C6H12}(OS)$

Mn	-0.105734	0.060132	-0.023845
O	-0.396224	0.304382	1.532215
O	1.455250	0.277204	-0.309452
O	-0.507219	-1.442881	-0.405504
O	-0.962034	1.086240	-0.899786
H	1.155186	-1.234915	2.943715
C	1.759772	-1.979680	3.473184
H	1.712639	-1.725851	4.539634
C	1.159351	-3.374486	3.237792
H	0.109122	-3.386284	3.550053
H	1.684594	-4.109439	3.867320
C	1.271071	-3.794117	1.763861
H	0.647791	-3.134180	1.150266
H	0.882711	-4.811703	1.630924
C	2.723565	-3.716839	1.267895
H	2.768206	-3.967681	0.202235
H	3.330218	-4.468991	1.795786
C	3.325400	-2.322415	1.502216
H	2.799960	-1.590201	0.879203
H	4.376683	-2.308558	1.188238
C	3.211963	-1.902854	2.976016
H	3.596766	-0.885202	3.105534

H	3.843396	-2.561048	3.592783

$IH_{MnO4-/C6H12}$

Mn	-0.143008	0.000483	-0.255441
O	-0.351722	-0.003122	1.540334
O	1.488957	-0.004989	-0.344664
O	-0.748232	-1.352490	-0.843703
O	-0.738706	1.360620	-0.836889
H	0.538361	-0.006919	1.921288
C	2.522486	-0.010098	3.371501
H	1.662494	-0.012824	4.034558
C	3.211516	-1.299064	3.057751
H	2.503683	-2.132932	3.107113
H	3.976957	-1.504200	3.834190
C	3.910622	-1.268255	1.683015
H	3.148073	-1.275001	0.897718
H	4.527793	-2.166831	1.563403
C	4.764110	-0.002719	1.519773
H	5.234260	0.000146	0.530277
H	5.580328	-0.003159	2.259311
C	3.906902	1.259581	1.688544
H	3.144449	1.267615	0.903161
H	4.521450	2.160475	1.572965
C	3.207631	1.282289	3.063354
H	2.497289	2.113786	3.116319
H	3.972430	1.486339	3.840713

$TS_{MnO4-/C6H12}$(CS)

Mn	-0.136100	-0.009080	0.194186
O	-0.331345	-0.005441	1.900255
O	1.497757	0.002742	0.273328
O	-0.678752	-1.362272	-0.442378
O	-0.697965	1.332456	-0.450336
H	0.697402	0.002436	2.223120
C	2.142151	0.015469	2.790773
H	1.555775	0.013010	3.717768
C	2.937115	-1.265337	2.654156
H	2.257640	-2.115583	2.527636
H	3.474382	-1.450076	3.606630
C	3.968106	-1.238890	1.516917
H	3.432355	-1.272602	0.565820
H	4.608147	-2.128754	1.576920
C	4.824519	0.034565	1.566670
H	5.542090	0.038306	0.736853
H	5.419358	0.042068	2.493621
C	3.946899	1.293159	1.509874
H	3.410539	1.312454	0.558716
H	4.571779	2.194048	1.564825
C	2.915401	1.308740	2.646950
H	2.221650	2.146611	2.515415
H	3.449206	1.507961	3.598424

$TS_{MnO4-/PhCH3}$(OS)

Mn	-0.086311	0.029005	0.043102
O	0.013455	-0.012183	1.747178
O	1.478337	0.052986	-0.369306
O	-0.807953	1.367678	-0.426721
O	-0.782537	-1.296682	-0.493910
H	1.116043	-0.044903	2.113965
C	2.457557	0.014420	2.520486
H	2.342575	0.588939	3.439381
H	2.877315	0.579563	1.695211
C	2.948333	-1.346605	2.681526
C	3.347054	-2.110073	1.561298
H	3.245121	-1.666348	0.576656
C	3.013646	-1.967733	3.946969
H	2.698195	-1.408344	4.822642
C	3.812279	-3.410075	1.709220
H	4.106504	-3.975022	0.830118
C	3.477942	-3.271216	4.090963
H	3.520406	-3.720812	5.078584
C	3.886095	-4.002495	2.973962
H	4.243177	-5.021090	3.084370

$RC_{MnO4-/PhCH3}$

Mn	-0.155752	0.026659	-0.626832
O	-0.384310	0.343820	0.928108
O	1.126189	-0.925997	-0.783651
O	0.092467	1.391462	-1.419184
O	-1.444654	-0.707737	-1.218944
H	1.276390	-0.008044	2.542452
C	2.171411	-0.069806	3.166622

H	1.896734	0.147776	4.203187
H	2.847456	0.726099	2.832135
C	2.842868	-1.416657	3.050968
C	2.777011	-2.143403	1.853954
H	2.216472	-1.744547	1.011760
C	3.561848	-1.963142	4.121499
H	3.615300	-1.416730	5.059301
C	3.421692	-3.374200	1.737134
H	3.354840	-3.920047	0.801720
C	4.206060	-3.195056	4.006046
H	4.755310	-3.599219	4.851033
C	4.139157	-3.906568	2.808963
H	4.635841	-4.866992	2.714426

$IH_{MnO4-/PhCH3}$

Mn	0.044034	0.281926	-0.340564
O	-1.690308	0.025374	0.105712
O	0.594128	-1.248001	-0.192247
O	0.727763	1.224326	0.754974
O	0.115701	0.772784	-1.852882
H	-1.771778	-0.918346	0.285585
C	2.810737	0.028632	3.104737
H	3.184712	0.696384	3.874234
H	2.121657	0.426582	2.365930
C	3.220993	-1.316110	3.080631
C	2.740689	-2.211136	2.076624
H	2.045918	-1.843348	1.323631
C	4.128140	-1.839969	4.049687
H	4.506247	-1.177496	4.822897
C	3.152511	-3.533536	2.059770
H	2.774062	-4.193326	1.285725
C	4.527854	-3.165315	4.017322
H	5.219385	-3.538786	4.766743
C	4.044949	-4.026108	3.022328
H	4.360084	-5.064043	2.998307

$TS_{MnO4-/PhCH3}$(CS)

Mn	-0.184544	0.053448	0.203683
O	-0.057708	-0.020788	1.920792
O	1.403267	0.081697	-0.102566
O	-0.886879	1.403384	-0.250003
O	-0.859958	-1.263939	-0.367410
H	0.972729	-0.056540	2.124667
C	2.605833	0.017608	2.350429
H	2.402887	0.624602	3.230489
H	3.018843	0.550228	1.507408
C	3.021178	-1.340574	2.569938
C	3.552199	-2.129802	1.518462
H	3.600188	-1.696295	0.525805
C	2.907090	-1.960625	3.839281
H	2.485850	-1.391005	4.662200
C	3.966834	-3.435581	1.734563
H	4.365269	-4.012693	0.905398
C	3.323395	-3.268895	4.049091
H	3.224492	-3.710325	5.036594
C	3.863136	-4.020663	3.001758
H	4.183129	-5.044231	3.165116

$TS_{MnO4-/DHA}$(OS)

Mn	-0.413650	0.008665	0.213877
O	-0.171379	-0.623838	1.760595
O	0.970778	0.779811	-0.072405
O	-1.627227	1.034597	0.228747
O	-0.618046	-1.170685	-0.831473
H	0.894251	-0.358732	2.226942
C	2.142733	-0.025059	2.728819
H	2.519128	0.568505	1.901144
C	2.827096	-1.312053	2.912660
C	3.610031	-1.883230	1.894161
H	3.683595	-1.367595	0.942299
C	4.272554	-3.089752	2.088924
H	4.869073	-3.512870	1.287071
C	4.172522	-3.753779	3.313202
H	4.693385	-4.691820	3.474328
C	3.389753	-3.202243	4.328171
H	3.300744	-3.718530	5.280531
C	2.707153	-2.001836	4.138318
C	1.788264	-1.434563	5.197607
H	0.772679	-1.816588	5.005933
H	2.071414	-1.800612	6.189775
C	1.727697	0.076894	5.184617
C	1.858508	0.744221	3.947576
C	1.497920	0.810240	6.347507

H	1.411845	0.287111	7.296407
C	1.364979	2.198743	6.308827
H	1.180036	2.754837	7.221903
C	1.465873	2.861631	5.084020
H	1.354066	3.940146	5.037714
C	1.712728	2.142309	3.920352
H	1.788731	2.655954	2.967576

$RC_{MnO4-/DHA}$

Mn	0.247169	0.713655	-0.643945
O	-0.004518	1.489321	0.739166
O	1.040741	-0.647433	-0.334867
O	1.114417	1.629108	-1.621694
O	-1.152960	0.374042	-1.330472
H	0.283301	-1.275827	3.261698
C	1.213933	-0.703389	3.120110
H	1.124371	-0.239264	2.136964
C	2.380288	-1.666142	3.164610
C	2.939903	-2.187933	1.994886
H	2.529874	-1.880814	1.037276
C	4.008602	-3.080713	2.064744
H	4.437201	-3.478637	1.150834
C	4.532926	-3.450332	3.303245
H	5.371553	-4.136987	3.360280
C	3.983059	-2.923579	4.471363
H	4.396128	-3.200408	5.437647
C	2.906002	-2.036703	4.411411
C	2.271723	-1.458107	5.659757
H	1.391068	-2.066556	5.920855
H	2.956676	-1.533084	6.509613
C	1.826170	-0.023951	5.459223
C	1.304600	0.342586	4.209547
C	1.916147	0.928302	6.476854
H	2.329974	0.644778	7.440871
C	1.484493	2.236740	6.263027
H	1.560243	2.969907	7.059760
C	0.968402	2.599673	5.019020
H	0.640681	3.618621	4.841283
C	0.883909	1.658091	3.994242
H	0.499002	1.929917	3.015810

$IH_{MnO4-/DHA}$

Mn	0.308467	0.768660	-0.496941
O	-1.318892	0.032113	-0.769326
O	1.166552	-0.574452	-0.138802
O	0.236427	1.727350	0.782084
O	0.807776	1.423370	-1.857329
H	-1.201817	-0.915970	-0.638003
C	2.008183	-0.267872	3.106753
H	1.608127	0.002311	2.134746
C	2.696970	-1.507034	3.241426
C	2.814902	-2.388671	2.136712
H	2.392099	-2.071461	1.187686
C	3.440671	-3.616087	2.279044
H	3.521457	-4.281426	1.425626
C	3.961658	-4.003628	3.520579
H	4.444352	-4.968569	3.635587
C	3.859082	-3.140027	4.613433
H	4.270679	-3.439845	5.574094
C	3.244012	-1.896699	4.494217
C	3.209280	-0.935264	5.662816
H	2.983368	-1.479440	6.587924
H	4.227235	-0.536335	5.805340
C	2.265253	0.238440	5.510779
C	1.746272	0.568695	4.228851
C	1.943543	1.037795	6.604275
H	2.335196	0.779555	7.585128
C	1.133767	2.166699	6.461524
H	0.894646	2.775465	7.327284
C	0.635995	2.507436	5.197151
H	0.009534	3.385474	5.079152
C	0.932988	1.722837	4.095099
H	0.547478	1.963456	3.108559

$TS_{MnO4-/DHA}$(CS)

Mn	-0.426832	-0.010673	0.258178
O	-0.165206	-0.649626	1.804607
O	0.957661	0.761291	-0.004895
O	-1.642368	1.008406	0.281806
O	-0.626448	-1.180451	-0.794588
H	0.842469	-0.381765	2.214444
C	2.198454	-0.002643	2.730219
H	2.558237	0.586816	1.894728

C	2.850783	-1.297224	2.905553
C	3.637601	-1.876194	1.891410
H	3.728857	-1.356721	0.943073
C	4.282193	-3.091752	2.086293
H	4.880847	-3.517934	1.287428
C	4.163640	-3.761699	3.306155
H	4.671033	-4.707057	3.467150
C	3.377141	-3.204515	4.316161
H	3.271658	-3.724964	5.264747
C	2.710238	-1.996332	4.126912
C	1.780031	-1.428326	5.175841
H	0.764315	-1.801566	4.965191
H	2.044085	-1.803310	6.170075
C	1.729322	0.083512	5.171658
C	1.882088	0.756067	3.936858
C	1.482565	0.811546	6.333257
H	1.381046	0.283222	7.277913
C	1.349470	2.200935	6.300715
H	1.149931	2.752416	7.213455
C	1.468300	2.868764	5.079724
H	1.356199	3.947549	5.036517
C	1.734191	2.156261	3.916710
H	1.825733	2.675843	2.968432

$TS_{\alpha\text{-MS/DHA}}$

C	-0.157651	3.243879	-0.084973
C	-1.305730	2.408577	-0.085534
H	-1.427662	1.658116	-0.856166
C	-0.066401	4.196046	0.963941
H	0.791044	4.853900	1.017235
C	-2.296309	2.536385	0.879205
H	-3.162248	1.884165	0.841667
C	-1.058914	4.315730	1.925710
H	-0.956056	5.059172	2.708817
C	-2.184982	3.490262	1.892324
H	-2.960243	3.586949	2.643600
C	0.869164	3.147876	-1.095465
C	2.101511	4.006289	-0.980105
H	1.853099	5.073262	-1.047241
H	2.620016	3.860599	-0.025972
H	2.808263	3.782049	-1.779997
C	0.795735	2.210645	-2.180091
H	-0.204404	1.918723	-2.500937
H	1.412976	2.480834	-3.038333
H	-0.199668	0.230794	0.939582
C	0.436610	-0.671112	0.884630
H	0.207911	-1.245512	1.787439
C	0.037608	-1.446707	-0.348031
C	-1.051037	-2.317222	-0.332293
H	-1.583588	-2.483232	0.599538
C	-1.467924	-2.973751	-1.489796
H	-2.316560	-3.647468	-1.456696
C	-0.783510	-2.760405	-2.689228
H	-1.099466	-3.267926	-3.593985
C	0.310460	-1.907303	-2.719509
H	0.853442	-1.755006	-3.647111
C	0.745547	-1.241240	-1.555658
C	1.899611	-0.366151	-1.567352
H	2.510627	-0.373956	-2.466087
H	1.265867	1.134407	-1.860780
C	2.567049	-0.052502	-0.324558
C	1.877496	-0.219676	0.899927
C	2.524402	0.084564	2.097202
H	1.995578	-0.054043	3.035348
C	3.830535	0.569802	2.107943
H	4.316198	0.800732	3.049265
C	4.512276	0.750531	0.900289
H	5.530839	1.122829	0.901138
C	3.887835	0.441670	-0.298356
H	4.420427	0.567740	-1.235893

$RC_{\alpha\text{-MS/DHA}}$

C	-0.434176	3.622998	-0.317008
C	-1.519352	2.774814	-0.597141
H	-1.522657	2.197270	-1.513883
C	-0.442592	4.309172	0.907802
H	0.378850	4.966545	1.164948
C	-2.578073	2.640100	0.295036
H	-3.398997	1.973457	0.054772
C	-1.503639	4.177253	1.801324
H	-1.488269	4.727540	2.735722
C	-2.578132	3.344207	1.499136
H	-3.401589	3.237126	2.196192
C	0.689321	3.784230	-1.280693

C	2.053246	4.117968	-0.721800
H	2.065139	5.111489	-0.261972
H	2.354295	3.402375	0.049114
H	2.806019	4.113002	-1.511432
C	0.507209	3.653619	-2.602096
H	-0.466523	3.461123	-3.036333
H	1.335520	3.759276	-3.293665
H	0.129676	0.549446	0.809505
C	0.590022	-0.440905	0.943950
H	0.246842	-0.806432	1.915033
C	0.109595	-1.352786	-0.165228
C	-0.977535	-2.212387	0.004866
H	-1.488077	-2.243539	0.962511
C	-1.409530	-3.030571	-1.037264
H	-2.254391	-3.694327	-0.890789
C	-0.745342	-2.999431	-2.262097
H	-1.069246	-3.638995	-3.075623
C	0.346348	-2.150741	-2.435155
H	0.871545	-2.134474	-3.385316
C	0.778378	-1.322096	-1.397654
C	1.952019	-0.379768	-1.562852
H	2.586738	-0.702095	-2.392272
H	1.570749	0.615806	-1.836895
C	2.765538	-0.255084	-0.292046
C	2.095888	-0.283868	0.939805
C	2.828573	-0.164546	2.122615
H	2.310990	-0.197549	3.076458
C	4.213159	-0.009097	2.091416
H	4.769566	0.080390	3.017817
C	4.878695	0.018038	0.867185
H	5.956950	0.127924	0.833736
C	4.154080	-0.109071	-0.316417
H	4.673186	-0.099392	-1.270027

$IH_{\alpha\text{-MS/DHA}}$

C	-0.234969	3.413875	-0.027682
C	-1.402543	2.666672	-0.358028
H	-1.460482	2.157008	-1.311364
C	-0.226780	4.044326	1.250266
H	0.636038	4.622748	1.555402
C	-2.472918	2.568732	0.517904
H	-3.344908	1.990990	0.230063
C	-1.303135	3.940547	2.117329
H	-1.261887	4.438297	3.080477
C	-2.438153	3.204083	1.763070
H	-3.278153	3.127057	2.443666
C	0.870824	3.521330	-0.923476
C	2.115256	4.259425	-0.516722
H	1.909463	5.309141	-0.270221
H	2.583290	3.814812	0.371121
H	2.857670	4.249256	-1.315856
C	0.842302	2.859126	-2.271234
H	-0.096031	3.041169	-2.805818
H	1.657842	3.218998	-2.901107
H	-0.003331	0.304170	0.833861
C	0.584674	-0.626619	0.822827
H	0.373300	-1.109214	1.783997
C	0.071684	-1.492651	-0.305324
C	-1.193648	-2.069319	-0.233326
H	-1.790961	-1.924289	0.661966
C	-1.709108	-2.822899	-1.288180
H	-2.696579	-3.262937	-1.208667
C	-0.946597	-3.007074	-2.447493
H	-1.342374	-3.590276	-3.271490
C	0.316640	-2.449023	-2.537756
H	0.915605	-2.597669	-3.430500
C	0.857516	-1.686030	-1.473522
C	2.171797	-1.142958	-1.545290
H	2.751947	-1.299597	-2.448922
H	0.953179	1.767645	-2.192480
C	2.785269	-0.481155	-0.444578
C	2.048678	-0.256560	0.750107
C	2.678521	0.348655	1.834399
H	2.114960	0.516246	2.747379
C	4.013251	0.748987	1.767704
H	4.482933	1.215778	2.626000
C	4.741969	0.543497	0.590026
H	5.779566	0.853104	0.531822
C	4.137939	-0.062435	-0.497468
H	4.702241	-0.233894	-1.408530