Supporting information

Mechanism of fatty acid decarboxylation catalyzed by a non-heme iron oxidase (UndA): a QM/MM study

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Table S1. Calculated imaginary frequencies of involved transition states (cm^{-1}).

	Imaginary frequency
$^5TS1_{E\text{-}M\text{-}2}$	-1304.0
$^5TS1_{E\text{-}M\text{-}1}$	-1316.8
$^5TS2_{E\text{-}M\text{-}2}$	-272.8
$^5TS1_{E\text{-}M\text{-}3}$	-1026.3
$^5TS1_{E\text{-}M\text{-}4}$	-1064.1

Table S2. Calculated relative electronic energies and Gibbs free energies (kcal/mol) with the ZPE correction of the involved species.

	ΔE	Δ(E+ZPE)	ΔG	Δ(G+ZPE)
$^5R_{E\text{-}D\text{-}1}$	-11.2	-11.2	-11.4	-11.3
$^5R_{E\text{-}D\text{-}2}$	-0.1	-1.7	-2.1	-3.7
$^5R_{E\text{-}M\text{-}1}$	0.0	0.0	0.0	0
$^5TS1_{E\text{-}M\text{-}1}$	28.1	24.0	27.8	23.7
$^5IM1_{E\text{-}M\text{-}1}$	8.3	8.6	7.7	8.0
$^5R_{E\text{-}M\text{-}2}$	13.3	13.0	14.0	13.7
$^5TS1_{E\text{-}M\text{-}2}$	27.8	24.3	26.8	23.3
$^5IM1_{E\text{-}M\text{-}2}$	8.3	8.6	7.7	8.0
$^5TS2_{E\text{-}M\text{-}2}$	26.0	23.8	24.6	22.4

$^5P_{E\text{-}M\text{-}2}$	-13.3	-9.6	-14.7	-10.9
$^5R_{E\text{-}M\text{-}3}$	17.4	17.0	15.9	15.5
$^5TS1_{E\text{-}M\text{-}3}$	34.3	30.5	34.1	30.3
$^5IM1_{E\text{-}M\text{-}3}$	28.5	28.0	27.3	26.8
$^5R_{E\text{-}M\text{-}4}$	17.8	17.0	16.8	16.0
$^5TS1_{E\text{-}M\text{-}4}$	33.0	30.2	33.0	30.2
$^5IM1_{E\text{-}M\text{-}4}$	27.9	28.7	27.9	28.7
$^5R_{S\text{-}D}$	4.6	3.8	2.9	2.1
$^5R_{S\text{-}M}$	-2.1	-2.1	-2.0	-2.0

Table S3. The spin densities on selected atoms (group) of involved species.

	Fe	O1	O2	Sub
$^{os}R_{E\text{-}D\text{-}1}$	-1.11	0.47	0.60	0.01
$^3R_{E\text{-}D\text{-}1}$	1.09	0.40	0.55	-0.01
$^7R_{E\text{-}D\text{-}1}$	4.06	0.75	0.70	0.20
$^5R_{E\text{-}D\text{-}1}$	4.17	-0.21	-0.50	0.24
$^5R_{E\text{-}D\text{-}2}$	4.19	-0.25	-0.51	0.25
$^5R_{E\text{-}M\text{-}1}$	2.85	0.50	0.58	0.12
$^5R_{E\text{-}M\text{-}2}$	2.87	0.41	0.58	0.18
$^5R_{E\text{-}M\text{-}3}$	2.83	0.44	0.57	0.02
$^5R_{E\text{-}M\text{-}4}$	2.95	0.32	0.50	0.24
$^5R_{S\text{-}D}$	4.15	-0.36	-0.30	0.24
$^5R_{S\text{-}M}$	2.63	0.66	0.71	0.05
$^5TS1_{E\text{-}M\text{-}2}$	2.90	0.03	0.35	0.75
$^5IM1_{E\text{-}M\text{-}2}$	2.85	0.05	0.00	1.14
$^5TS2_{E\text{-}M\text{-}2}$	2.88	0.02	-0.01	1.13
$^5P_{E\text{-}M\text{-}2}$	3.69	0.11	0.02	0.00
$^5R_{O\text{-}D}$	3.28	0.43		0.07
$^5R_{O\text{-}M}$	3.15	0.57		0.09
$^5TS1_{O\text{-}M}$	2.87	0.46		0.49
$^5IM1_{O\text{-}M}$	2.80	0.14		1.14

Table S4. ΔE^i and $\Delta E^{i\text{-}0}$ values (kcal/mol) of three individual residues (Glu159, Trp190 and His201) toward the H-abstraction step of $^5R_{E\text{-}M\text{-}2}$.

	ΔE^i	$\Delta E^{i\text{-}0}$
Glu159	12.4	-2.0
Trp190	14.1	-0.3
His201	14.3	-0.1

Table S5. Relative energies (kcal/mol) of involved species in H-abstraction using $^5R_{E\text{-}M\text{-}1}$ as the

reactant model with different QM regions.

	$^{5}R_{E\text{-}M\text{-}1}$	$^{5}TS1_{E\text{-}M\text{-}1}$	$^{5}IM1_{E\text{-}M\text{-}1}$
QM region A	0.0	28.1	8.3
Large QM region	0.0	27.3	13.6

Table S6. The absolute total energies, QM energies and MM energies of involved species (a.u.).

	Absolute energy	QM energy	MM energy
$^{cs}R_{E\text{-}D\text{-}1}$	-2941.716899	-2834.234980	-107.481920
$^{os}R_{E\text{-}D\text{-}1}$	-2941.745084	-2834.267078	-107.478007
$^{3}R_{E\text{-}D\text{-}1}$	-2941.741591	-2834.264527	-107.477064
$^{7}R_{E\text{-}D\text{-}1}$	-2941.753825	-2834.273837	-107.479988
$^{5}R_{E\text{-}D\text{-}1}$	-2941.752865	-2834.275005	-107.477861
$^{5}R_{E\text{-}D\text{-}2}$	-2941.735084	-2834.260789	-107.474295
$^{5}R_{E\text{-}M\text{-}1}$	-2941.719549	-2834.235297	-107.484253
$^{5}R_{E\text{-}M\text{-}2}$	-2941.709864	-2834.229509	-107.480354
$^{5}R_{E\text{-}M\text{-}3}$	-2941.703633	-2834.225506	-107.478128
$^{5}R_{E\text{-}M\text{-}4}$	-2941.703729	-2834.216119	-107.487609
$^{5}R_{S\text{-}D}$	-2941.727118	-2834.245863	-107.481255
$^{5}R_{S\text{-}M}$	-2941.735803	-2834.255720	-107.480082
$^{5}TS1_{E\text{-}M\text{-}2}$	-2941.672379	-2834.198263	-107.474116
$^{5}IM1_{E\text{-}M\text{-}2}$	-2941.705657	-2834.229023	-107.476634
$^{5}TS2_{E\text{-}M\text{-}2}$	-2941.690543	-2834.214909	-107.475634
$^{5}P_{E\text{-}M\text{-}2}$	-2941.758864	-2834.289352	-107.469512
$^{5}TS1_{E\text{-}M\text{-}1}$	-2941.671809	-2834.192121	-107.479688
$^{5}TS1_{E\text{-}M\text{-}3}$	-2941.676309	-2834.209595	-107.466714
$^{5}IM1_{E\text{-}M\text{-}3}$	-2941.684302	-2834.220210	-107.464093
$^{5}TS1_{E\text{-}M\text{-}4}$	-2941.675303	-2834.190879	-107.484424
$^{5}IM1_{E\text{-}M\text{-}4}$	-2941.684093	-2834.201844	-107.482249
$^{5}R_{O\text{-}D}$	-2908.534902	-2759.142594	-149.392308
$^{5}R_{O\text{-}M}$	-2908.496779	-2759.090898	-149.405881
$^{5}TS1_{O\text{-}M}$	-2908.450605	-2759.039522	-149.411082
$^{5}IM1_{O\text{-}M}$	-2908.484374	-2759.072176	-149.412198

Table S7. Natural charges of selected atoms (group) of optimized species.

	Fe	O1	O2	Sub
$^{os}R_{E\text{-}D\text{-}1}$	1.23	-0.26	-0.25	-0.51
$^{3}R_{E\text{-}D\text{-}1}$	1.25	-0.29	-0.27	-0.50
$^{7}R_{E\text{-}D\text{-}1}$	1.64	-0.28	-0.20	-0.67

$^5R_{E\text{-}D\text{-}1}$	1.70	-0.38	-0.24	-0.63
$^5R_{E\text{-}D\text{-}2}$	1.71	-0.38	-0.27	-0.63
$^5R_{E\text{-}M\text{-}1}$	1.44	-0.41	-0.28	-0.60
$^5R_{E\text{-}M\text{-}2}$	1.46	-0.41	-0.25	-0.64
$^5R_{E\text{-}M\text{-}3}$	1.46	-0.26	-0.29	-0.59
$^5R_{E\text{-}M\text{-}4}$	1.46	-0.31	-0.22	-0.65
$^5R_{S\text{-}D}$	1.63	-0.27	-0.27	-0.64
$^5R_{S\text{-}M}$	1.36	-0.28	-0.25	-0.60
$^5TS1_{E\text{-}M\text{-}2}$	1.47	-0.51	-0.41	-0.32
$^5IM1_{E\text{-}M\text{-}2}$	1.46	-0.58	-0.57	-0.16
$^5TS2_{E\text{-}M\text{-}2}$	1.42	-0.44	-0.51	-0.21
$^5P_{E\text{-}M\text{-}2}$	1.39	-0.72	-0.58	0.53
$^5TS1_{E\text{-}M\text{-}1}$	1.47	-0.51	-0.43	-0.30
$^5IM1_{E\text{-}M\text{-}1}$	1.46	-0.58	-0.57	-0.16
$^5TS1_{E\text{-}M\text{-}3}$	1.45	-0.49	-0.41	-0.30
$^5IM1_{E\text{-}M\text{-}3}$	1.45	-0.51	-0.54	-0.17
$^5TS1_{E\text{-}M\text{-}4}$	1.47	-0.42	-0.38	-0.32
$^5IM1_{E\text{-}M\text{-}4}$	1.47	-0.44	-0.52	-0.17
$^5R_{O\text{-}D}$	1.51	-0.67		-0.55
$^5R_{O\text{-}M}$	1.49	-0.64		-0.64
$^5TS1_{O\text{-}M}$	1.45	-0.79		-0.44
$^5IM1_{O\text{-}M}$	1.46	-1.05		0.21

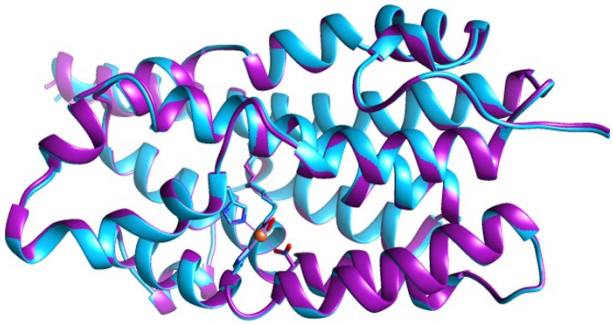

Figure S1. Overlap of chains A (purple) and B (blue). Both chains were derived from the crystal structure of PfUndA (PDB ID: 4WWZ).

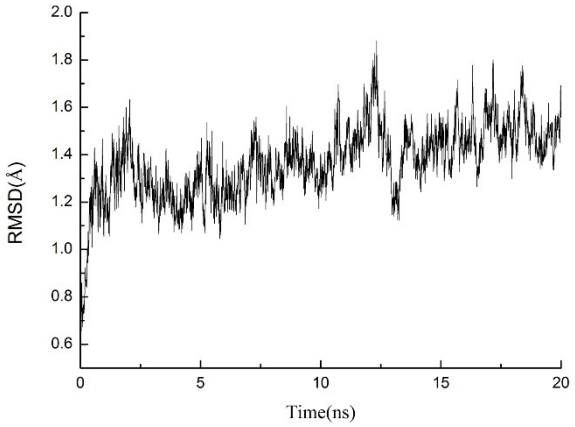

Figure S2. RMSDs of the backbone atoms of UndA in complex with the substrate (lauric acid) in 20 ns MD simulations.

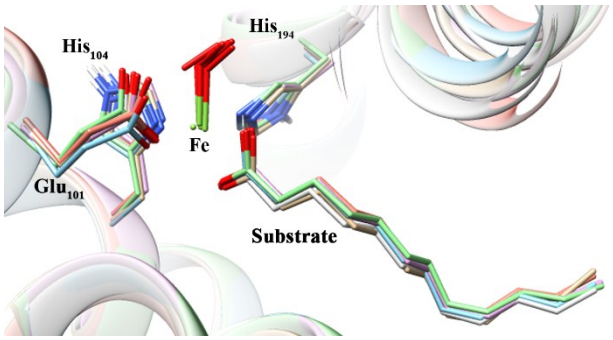

Figure S3. Overlap of active site pockets of six QM/MM-optimized reactants, which were derived from the MD trajectory from 15 to 20 ns with an interval of 1 ns.

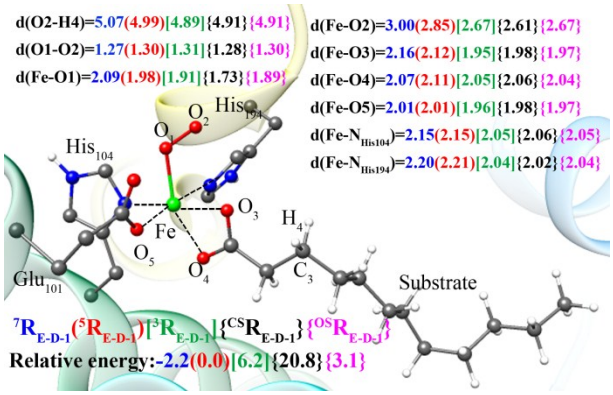

Figure S4. Optimized structures of reactant $R_{E\text{-}D\text{-}1}$ at different spin states. All distances are given in Å. The energy of the $^5R_{E\text{-}D\text{-}1}$ was set to zero (kcal/mol).

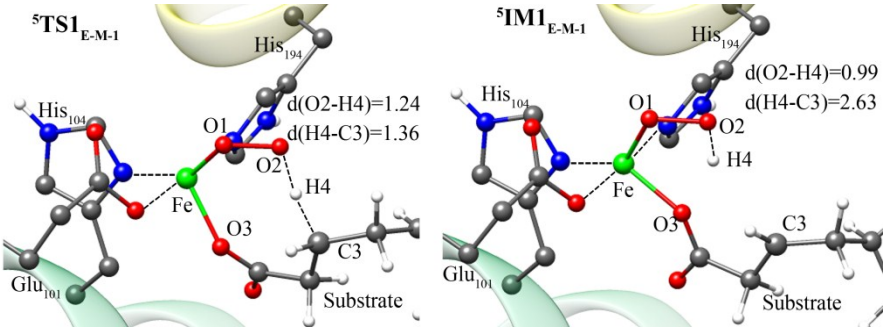

Figure S5. Optimized structures of ^{5}TS1$_{E\text{-}M\text{-}1}$ and ^{5}IM1$_{E\text{-}M\text{-}1}$ for H-abstraction using ^{5}R$_{E\text{-}M\text{-}1}$ as the reactant. All distances are given in Å.

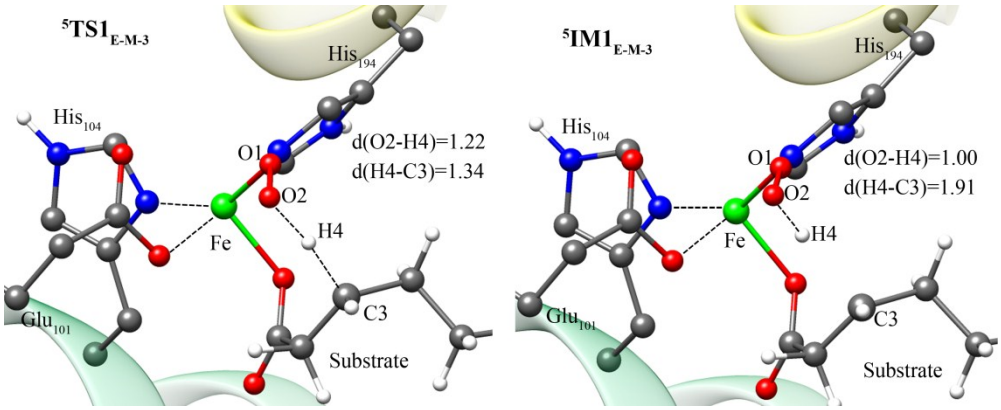

Figure S6. Optimized structures of ^{5}TS1$_{E\text{-}M\text{-}3}$ and ^{5}IM1$_{E\text{-}M\text{-}3}$ for H-abstraction using ^{5}R$_{E\text{-}M\text{-}3}$ as the reactant. All distances are given in Å.

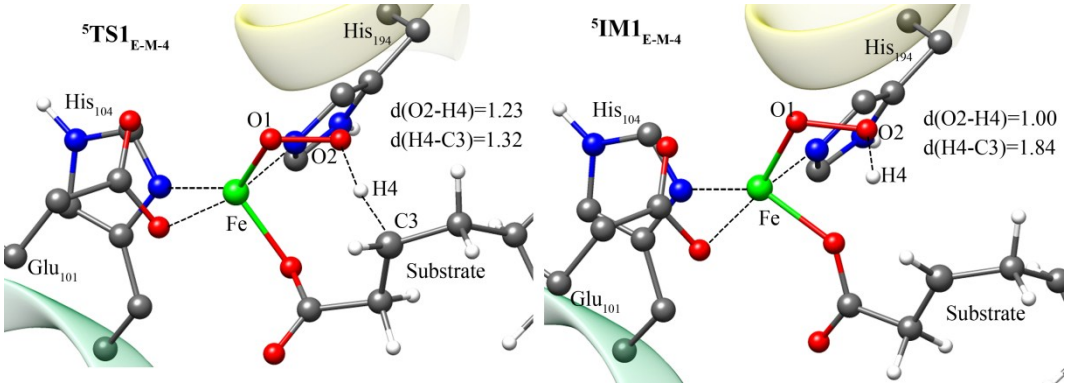

Figure S7. Optimized structures of ^{5}TS1$_{E\text{-}M\text{-}4}$ and ^{5}IM1$_{E\text{-}M\text{-}4}$ of H-abstraction using ^{5}R$_{E\text{-}M\text{-}4}$ as the reactant. All distances are given in Å.

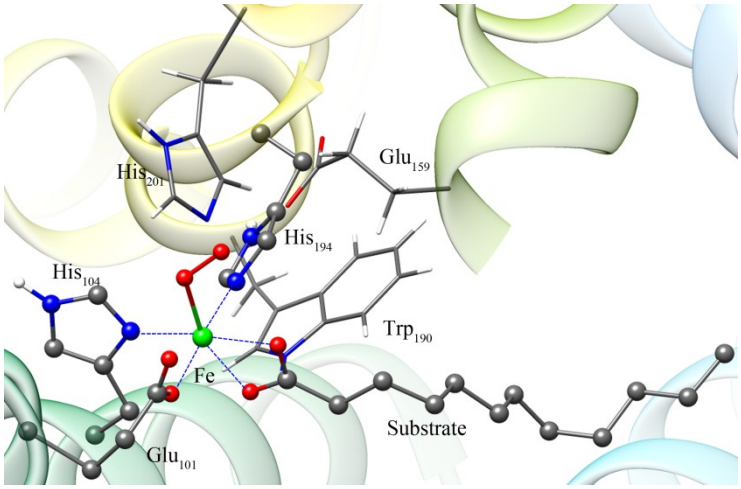

Figure S8. Three surrounding residues (Glu159, Trp190 and His201) outside the QM region, which are shown in stick model.

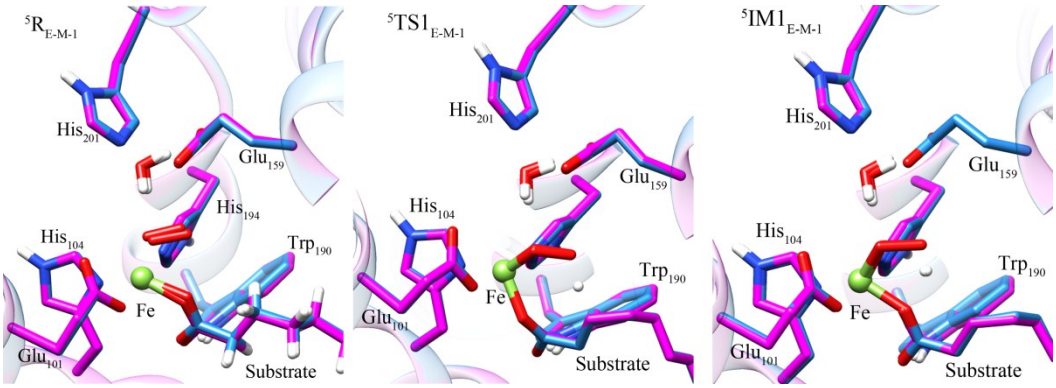

Figure S9. Overlap of QM/MM-optimized active site pockets of $^{5}R_{E\text{-}M\text{-}1}$, $^{5}TS1_{E\text{-}M\text{-}1}$ and $^{5}IM1_{E\text{-}M\text{-}1}$ using QM region A and large QM region. The purple represent the optimized structures using a large QM region, which includes the residues Glu159, Trp190, His201 and one water molecule.

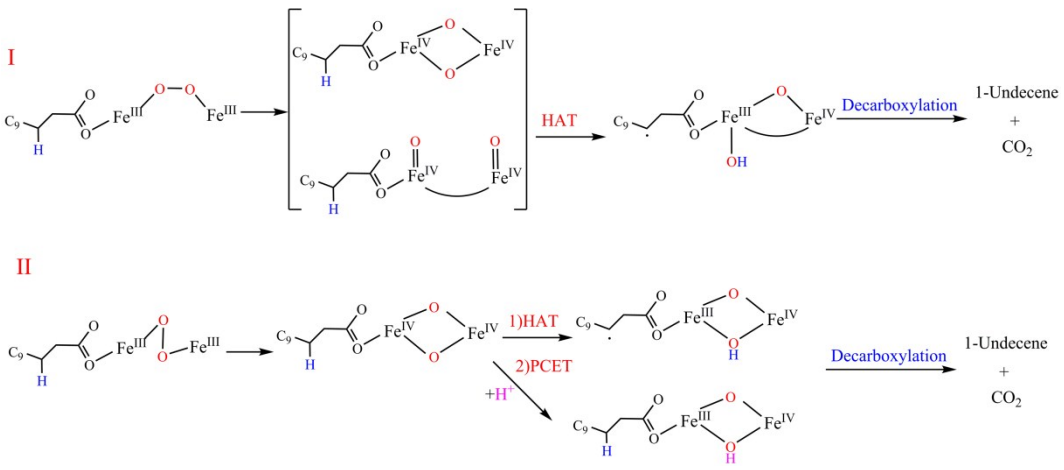

Figure S10. Two proposed mechanisms for the UndA-catalyzed decarboxylation of fatty acid. Path I was proposed by Manley et al. (*J. Am. Chem. Soc*. 2019, **141**, 8684), and Path II was suggested by Zhang et al. (*J. Am. Chem. Soc*.2019, **141**, 14510).

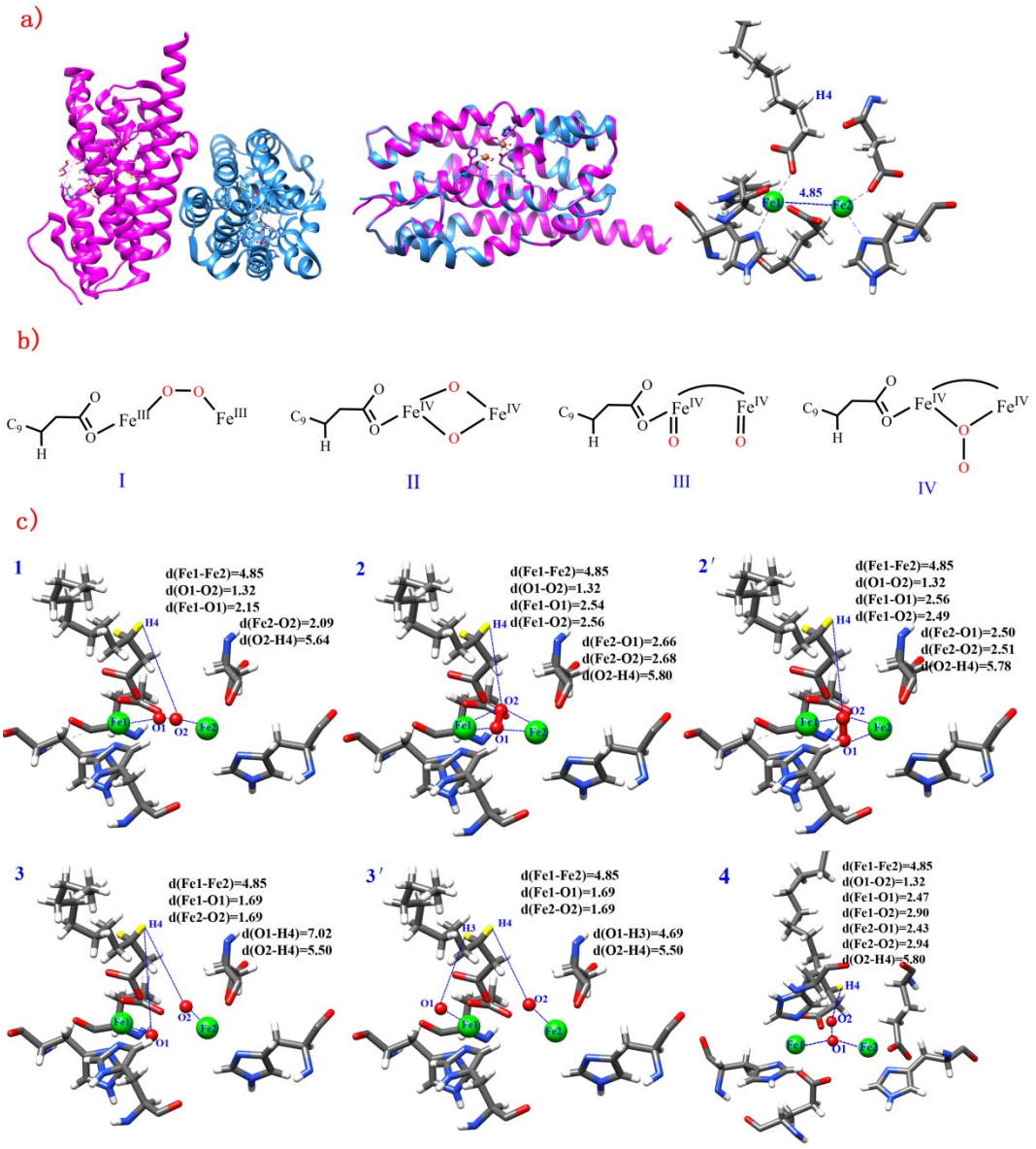

Figure S11. (a) Crystal structure of PfUndA from *Pseudomonas fluorescens* Pf-5 (PDB ID: 6P5Q), overlap of two chains, and the active site of one chain (chain A). (b) Four possible binding modes of dioxygen in UndA or nonheme diiron enzymes proposed in the literatures. Modes I and II were proposed by Zhang et al. (*J. Am. Chem. Soc*. 2019, **141**, 14510), III was suggested by Manley et al. (*J. Am. Chem. Soc*. 2019, 141, 8684), and IV was proposed by Fox et al. (*Nature* 2017, 544, 191−195). (c) Constructed models of Fe_2 (III/III) complexes and Fe_2(IV/ IV) intermediates based on the crystal structure (PDB ID: 6P5Q). Noted that the two oxygen atoms were manually added without changing the positions of any coordinated residues, the substrate and iron atoms. Thus, these structures were only used to analyze the possibility of βH-abstraction. Key distances are shown in Å.

Cartesian coordinates of QM regions of optimized species:

$^{1}R_{E\text{-}D\text{-}1}$

C	2.008000	11.850000	0.028000
H	2.656000	12.407000	0.672000
H	1.126000	11.570000	0.565000
C	2.734000	10.585000	-0.460000
H	3.682000	10.820000	-0.951000
H	3.010000	10.006000	0.433000
C	2.007000	9.595000	-1.387000
O	0.719000	9.500000	-1.252000
O	2.695000	8.935000	-2.179000
C	-2.347000	11.343000	-1.229000
H	-1.643000	11.500000	-0.439000
H	-2.767000	10.363000	-1.142000
N	-0.995000	10.398000	-3.168000
C	-1.647000	11.475000	-2.562000
C	-0.477000	10.855000	-4.306000
H	0.089000	10.272000	-5.015000
N	-0.752000	12.159000	-4.469000
H	-0.371000	12.733000	-5.237000
C	-1.487000	12.572000	-3.382000
H	-1.832000	13.589000	-3.300000
C	-3.279000	5.199000	-6.070000
H	-4.327000	4.984000	-6.034000
H	-2.724000	4.304000	-5.882000
N	-3.786000	7.266000	-4.673000
H	-4.744000	7.365000	-5.017000
C	-2.942000	6.227000	-5.023000
C	-3.149000	8.075000	-3.803000
H	-3.597000	8.943000	-3.347000
N	-1.924000	7.615000	-3.568000
C	-1.792000	6.449000	-4.306000
H	-0.887000	5.866000	-4.280000
C	-1.036000	7.022000	-0.734000
O	-1.628000	8.158000	-0.819000
O	-0.143000	6.784000	-1.614000
C	-1.396000	6.033000	0.340000
H	-2.492000	6.020000	0.386000
H	-1.070000	6.461000	1.298000
C	-0.812000	4.625000	0.158000
H	0.273000	4.675000	0.283000
H	-0.987000	4.283000	-0.869000
C	-1.414000	3.610000	1.145000

H	-1.466000	4.063000	2.145000
H	-0.733000	2.755000	1.234000
C	-2.805000	3.116000	0.720000
H	-2.708000	2.496000	-0.183000
H	-3.422000	3.977000	0.425000
C	-3.570000	2.355000	1.806000
H	-3.589000	2.972000	2.715000
H	-3.026000	1.439000	2.070000
C	-5.017000	2.031000	1.403000
H	-5.020000	1.289000	0.593000
H	-5.471000	2.939000	0.983000
C	-5.893000	1.561000	2.575000
H	-6.940000	1.523000	2.248000
H	-5.847000	2.330000	3.357000
C	-5.521000	0.195000	3.172000
H	-6.027000	0.074000	4.140000
H	-4.446000	0.163000	3.394000
C	-5.898000	-0.997000	2.282000
H	-5.472000	-0.873000	1.276000
H	-6.990000	-1.011000	2.150000
C	-5.431000	-2.335000	2.861000
H	-5.792000	-2.426000	3.894000
H	-4.334000	-2.334000	2.913000
C	-5.890000	-3.544000	2.053000
H	-5.506000	-3.510000	1.026000
H	-6.985000	-3.583000	1.996000
H	-5.546000	-4.482000	2.503000
Fe	-0.479000	8.522000	-2.492000
O	0.655000	8.422000	-3.795000
O	1.054000	7.270000	-4.190000

$^{3}R_{E\text{-}D\text{-}1}$

C	2.015000	11.865000	0.038000
H	2.652000	12.440000	0.677000
H	1.136000	11.577000	0.576000
C	2.762000	10.607000	-0.433000
H	3.705000	10.855000	-0.928000
H	3.055000	10.050000	0.468000
C	2.074000	9.573000	-1.341000
O	0.774000	9.483000	-1.251000
O	2.795000	8.862000	-2.047000
C	-2.342000	11.346000	-1.221000
H	-1.639000	11.507000	-0.431000
H	-2.758000	10.364000	-1.134000

N	-0.975000	10.407000	-3.156000
C	-1.641000	11.480000	-2.554000
C	-0.457000	10.863000	-4.295000
H	0.118000	10.280000	-4.995000
N	-0.744000	12.163000	-4.461000
H	-0.365000	12.737000	-5.230000
C	-1.487000	12.575000	-3.377000
H	-1.842000	13.588000	-3.299000
C	-3.254000	5.221000	-6.065000
H	-4.299000	4.995000	-6.026000
H	-2.690000	4.332000	-5.872000
N	-3.787000	7.278000	-4.659000
H	-4.750000	7.362000	-4.993000
C	-2.926000	6.259000	-5.025000
C	-3.153000	8.099000	-3.797000
H	-3.614000	8.953000	-3.328000
N	-1.914000	7.666000	-3.585000
C	-1.768000	6.508000	-4.331000
H	-0.849000	5.948000	-4.324000
C	-1.029000	7.034000	-0.727000
O	-1.622000	8.166000	-0.810000
O	-0.130000	6.823000	-1.612000
C	-1.382000	6.031000	0.333000
H	-2.477000	6.018000	0.390000
H	-1.045000	6.446000	1.293000
C	-0.801000	4.623000	0.129000
H	0.285000	4.670000	0.246000
H	-0.985000	4.293000	-0.900000
C	-1.397000	3.600000	1.112000
H	-1.434000	4.041000	2.119000
H	-0.719000	2.742000	1.182000
C	-2.796000	3.118000	0.699000
H	-2.713000	2.508000	-0.211000
H	-3.413000	3.984000	0.421000
C	-3.553000	2.349000	1.786000
H	-3.563000	2.960000	2.700000
H	-3.008000	1.431000	2.040000
C	-5.004000	2.031000	1.393000
H	-5.015000	1.289000	0.582000
H	-5.458000	2.940000	0.976000
C	-5.876000	1.563000	2.569000
H	-6.924000	1.527000	2.245000
H	-5.826000	2.335000	3.349000
C	-5.506000	0.197000	3.168000

H	-6.009000	0.081000	4.138000
H	-4.429000	0.162000	3.388000
C	-5.890000	-0.995000	2.282000
H	-5.466000	-0.875000	1.275000
H	-6.982000	-1.004000	2.153000
C	-5.429000	-2.334000	2.862000
H	-5.789000	-2.424000	3.896000
H	-4.332000	-2.339000	2.913000
C	-5.894000	-3.542000	2.055000
H	-5.511000	-3.510000	1.028000
H	-6.989000	-3.575000	1.999000
H	-5.555000	-4.482000	2.505000
Fe	-0.466000	8.555000	-2.452000
O	0.714000	8.481000	-3.951000
O	1.131000	7.261000	-4.159000

$^{7}R_{E\text{-}D\text{-}1}$

C	2.073000	11.948000	0.088000
H	2.700000	12.540000	0.721000
H	1.202000	11.646000	0.631000
C	2.845000	10.701000	-0.378000
H	3.789000	10.956000	-0.865000
H	3.136000	10.144000	0.524000
C	2.154000	9.675000	-1.284000
O	0.852000	9.607000	-1.205000
O	2.854000	8.953000	-2.002000
C	-2.388000	11.472000	-1.208000
H	-1.681000	11.616000	-0.418000
H	-2.808000	10.490000	-1.136000
N	-1.087000	10.526000	-3.138000
C	-1.693000	11.626000	-2.540000
C	-0.540000	10.952000	-4.275000
H	0.007000	10.337000	-4.975000
N	-0.765000	12.264000	-4.445000
H	-0.365000	12.819000	-5.218000
C	-1.489000	12.714000	-3.361000
H	-1.797000	13.743000	-3.286000
C	-3.283000	5.179000	-6.096000
H	-4.325000	4.939000	-6.074000
H	-2.709000	4.296000	-5.903000
N	-3.869000	7.212000	-4.683000
H	-4.825000	7.289000	-5.042000
C	-2.984000	6.211000	-5.043000

C	-3.260000	8.039000	-3.811000
H	-3.749000	8.882000	-3.349000
N	-2.017000	7.631000	-3.577000
C	-1.842000	6.481000	-4.330000
H	-0.914000	5.933000	-4.315000
C	-0.922000	6.841000	-0.652000
O	-1.520000	7.986000	-0.629000
O	-0.057000	6.648000	-1.559000
C	-1.291000	5.813000	0.380000
H	-2.386000	5.826000	0.435000
H	-0.953000	6.200000	1.351000
C	-0.751000	4.399000	0.154000
H	0.336000	4.407000	0.274000
H	-0.942000	4.088000	-0.881000
C	-1.388000	3.392000	1.125000
H	-1.403000	3.827000	2.135000
H	-0.754000	2.503000	1.187000
C	-2.810000	2.984000	0.714000
H	-2.761000	2.370000	-0.197000
H	-3.383000	3.880000	0.437000
C	-3.601000	2.253000	1.802000
H	-3.594000	2.871000	2.711000
H	-3.089000	1.318000	2.065000
C	-5.059000	1.982000	1.404000
H	-5.091000	1.247000	0.587000
H	-5.487000	2.907000	0.995000
C	-5.944000	1.530000	2.577000
H	-6.990000	1.496000	2.245000
H	-5.894000	2.308000	3.350000
C	-5.584000	0.169000	3.190000
H	-6.116000	0.051000	4.144000
H	-4.515000	0.143000	3.443000
C	-5.930000	-1.029000	2.297000
H	-5.497000	-0.899000	1.296000
H	-7.020000	-1.063000	2.155000
C	-5.444000	-2.358000	2.881000
H	-5.806000	-2.453000	3.914000
H	-4.348000	-2.339000	2.935000
C	-5.881000	-3.575000	2.075000
H	-5.496000	-3.536000	1.049000
H	-6.975000	-3.630000	2.016000
H	-5.525000	-4.508000	2.526000
Fe	-0.505000	8.624000	-2.318000
O	0.761000	8.302000	-3.951000

O	1.228000	7.161000	-4.276000

$^{5}R_{E\text{-}D\text{-}1}$

C	2.06600000	11.95300000	0.10500000
H	2.70700000	12.53900000	0.77200000
H	1.17900000	11.66400000	0.67500000
C	2.84200000	10.70500000	-0.34600000
H	3.78900000	10.95700000	-0.82900000
H	3.12600000	10.15400000	0.56200000
C	2.16300000	9.67000000	-1.25000000
O	0.85800000	9.59100000	-1.17800000
O	2.87000000	8.94700000	-1.95800000
C	-2.35900000	11.43900000	-1.22000000
H	-1.66100000	11.57600000	-0.38800000
H	-2.76200000	10.42500000	-1.14500000
N	-1.03900000	10.49500000	-3.14900000
C	-1.66200000	11.58900000	-2.55200000
C	-0.49600000	10.92600000	-4.28800000
H	0.06200000	10.31600000	-4.98200000
N	-0.73800000	12.23500000	-4.45800000
H	-0.34400000	12.79500000	-5.23200000
C	-1.47000000	12.67600000	-3.37600000
H	-1.79200000	13.70100000	-3.30300000
C	-3.28900000	5.17500000	-6.09300000
H	-4.35100000	4.91500000	-6.11600000
H	-2.70600000	4.27300000	-5.88900000
N	-3.85300000	7.20200000	-4.65800000
H	-4.81300000	7.28600000	-5.00500000
C	-2.97800000	6.20000000	-5.03700000
C	-3.23200000	8.01500000	-3.78100000
H	-3.71200000	8.85400000	-3.30300000
N	-1.98900000	7.59800000	-3.56600000
C	-1.82700000	6.45600000	-4.33400000
H	-0.90200000	5.90300000	-4.33400000
C	-0.92300000	6.88500000	-0.66700000
O	-1.50900000	8.03100000	-0.68200000
O	-0.03400000	6.67300000	-1.55300000
C	-1.31300000	5.86500000	0.36500000
H	-2.40900000	5.87600000	0.39900000
H	-0.99300000	6.25800000	1.33900000
C	-0.76300000	4.45000000	0.15500000
H	0.32300000	4.47000000	0.28000000
H	-0.94700000	4.12900000	-0.87800000

C	-1.39300000	3.44400000	1.13100000
H	-1.41500000	3.88400000	2.13800000
H	-0.74800000	2.56200000	1.20000000
C	-2.80800000	3.01500000	0.71800000
H	-2.74800000	2.40300000	-0.19300000
H	-3.39400000	3.90300000	0.44100000
C	-3.59100000	2.27100000	1.80300000
H	-3.58500000	2.88200000	2.71700000
H	-3.07300000	1.33700000	2.05800000
C	-5.04800000	1.99400000	1.40700000
H	-5.07900000	1.25800000	0.59100000
H	-5.48000000	2.91800000	0.99700000
C	-5.93100000	1.53900000	2.58000000
H	-6.97800000	1.50700000	2.25000000
H	-5.88100000	2.31600000	3.35600000
C	-5.57100000	0.17600000	3.18900000
H	-6.09800000	0.05800000	4.14600000
H	-4.50100000	0.14800000	3.43700000
C	-5.92400000	-1.01900000	2.29500000
H	-5.49000000	-0.88800000	1.29400000
H	-7.01400000	-1.04700000	2.15300000
C	-5.44400000	-2.35100000	2.87600000
H	-5.80900000	-2.44800000	3.90800000
H	-4.34800000	-2.33700000	2.93300000
C	-5.88500000	-3.56400000	2.06400000
H	-5.49700000	-3.52200000	1.03900000
H	-6.97900000	-3.61400000	2.00200000
H	-5.53300000	-4.49900000	2.51300000
Fe	-0.40100000	8.58500000	-2.38400000
O	0.79600000	8.32800000	-3.93900000
O	1.16700000	7.12200000	-4.26400000

$^{5}R_{E\text{-}D\text{-}2}$

C	2.06600000	11.93300000	0.11600000
H	2.69900000	12.53900000	0.77500000
H	1.18100000	11.64600000	0.68800000
C	2.86000000	10.68700000	-0.30000000
H	3.79600000	10.94000000	-0.80600000
H	3.17600000	10.18000000	0.62300000
C	2.21000000	9.58900000	-1.14700000
O	0.90000000	9.53800000	-1.17200000
O	2.94700000	8.78400000	-1.72200000
C	-2.34100000	11.35300000	-1.25300000

H	-1.64600000	11.49000000	-0.41800000
H	-2.75400000	10.34300000	-1.16900000
N	-0.96600000	10.39700000	-3.15600000
C	-1.63000000	11.48500000	-2.58100000
C	-0.41900000	10.83100000	-4.29300000
H	0.18100000	10.23700000	-4.96700000
N	-0.69500000	12.13000000	-4.48200000
H	-0.30700000	12.69600000	-5.25500000
C	-1.45600000	12.56400000	-3.41700000
H	-1.80600000	13.58200000	-3.36100000
C	-3.24000000	5.14200000	-6.10800000
H	-4.30200000	4.87900000	-6.13600000
H	-2.65700000	4.23900000	-5.90600000
N	-3.76500000	7.22100000	-4.72700000
H	-4.71300000	7.33600000	-5.09800000
C	-2.93300000	6.15800000	-5.04100000
C	-3.13600000	8.02000000	-3.84200000
H	-3.57900000	8.90600000	-3.41700000
N	-1.93100000	7.53600000	-3.55600000
C	-1.80900000	6.36100000	-4.28000000
H	-0.93600000	5.73500000	-4.20200000
C	-0.90900000	6.82900000	-0.64700000
O	-1.46100000	7.98900000	-0.69600000
O	-0.01300000	6.57500000	-1.51500000
C	-1.33600000	5.83700000	0.39500000
H	-2.43300000	5.85400000	0.39900000
H	-1.04000000	6.24800000	1.37100000
C	-0.78700000	4.41700000	0.22500000
H	0.29500000	4.43500000	0.38500000
H	-0.93900000	4.08000000	-0.80800000
C	-1.45100000	3.42800000	1.19600000
H	-1.50600000	3.88400000	2.19400000
H	-0.81000000	2.54700000	1.30000000
C	-2.85300000	2.99300000	0.74500000
H	-2.76500000	2.37100000	-0.15800000
H	-3.43300000	3.87600000	0.44200000
C	-3.65600000	2.25700000	1.81900000
H	-3.67800000	2.87900000	2.72500000
H	-3.13600000	1.33100000	2.09800000
C	-5.10100000	1.95900000	1.39300000
H	-5.10400000	1.21700000	0.58300000
H	-5.53500000	2.87400000	0.96800000
C	-6.00000000	1.50200000	2.55300000
H	-7.03900000	1.44800000	2.20400000

H	-5.97500000	2.28700000	3.32000000
C	-5.62800000	0.15100000	3.18300000
H	-6.17000000	0.03500000	4.13200000
H	-4.56200000	0.14100000	3.44900000
C	-5.94900000	-1.05800000	2.29600000
H	-5.51500000	-0.92600000	1.29600000
H	-7.03800000	-1.11300000	2.15000000
C	-5.44100000	-2.37400000	2.89000000
H	-5.79700000	-2.46400000	3.92500000
H	-4.34500000	-2.33800000	2.93800000
C	-5.86500000	-3.60500000	2.09700000
H	-5.48600000	-3.57000000	1.06900000
H	-6.95900000	-3.67400000	2.04500000
H	-5.49400000	-4.52800000	2.55500000
Fe	-0.30400000	8.49500000	-2.38500000
O	0.93500000	7.75300000	-3.79800000
O	1.68000000	8.63800000	-4.42000000

$^{5}R_{E\text{-}M\text{-}1}$

C	1.99900000	11.93200000	-0.05500000
H	2.71400000	12.40200000	0.62900000
H	1.11100000	11.66600000	0.52300000
C	2.63900000	10.65900000	-0.65800000
H	3.60100000	10.88200000	-1.12600000
H	2.82700000	9.96400000	0.16800000
C	1.78800000	9.94300000	-1.70900000
O	0.67100000	9.41200000	-1.25100000
O	2.12400000	9.92300000	-2.89400000
C	-2.25000000	11.43600000	-1.24800000
H	-1.54500000	11.63500000	-0.43400000
H	-2.63600000	10.42400000	-1.09100000
N	-1.01700000	10.35500000	-3.19000000
C	-1.56200000	11.49700000	-2.59200000
C	-0.44700000	10.73900000	-4.33500000
H	0.07700000	10.10000000	-5.03300000
N	-0.60400000	12.05900000	-4.51200000
H	-0.19700000	12.60100000	-5.29300000
C	-1.30000000	12.55700000	-3.42900000
H	-1.55200000	13.60200000	-3.35900000
C	-3.26200000	5.24600000	-6.13600000
H	-4.33000000	5.01600000	-6.17400000
H	-2.70900000	4.33000000	-5.91300000

N	-3.81700000	7.24600000	-4.64000000
H	-4.79100000	7.32200000	-4.94900000
C	-2.94000000	6.27300000	-5.08500000
C	-3.18500000	8.03600000	-3.75300000
H	-3.66000000	8.83700000	-3.21100000
N	-1.92300000	7.63400000	-3.60800000
C	-1.76800000	6.52600000	-4.42600000
H	-0.84500000	5.97700000	-4.46800000
C	-1.67400000	7.24500000	-0.28000000
O	-0.69900000	7.10500000	-1.12300000
O	-2.43600000	8.23400000	-0.29900000
C	-1.80700000	6.13800000	0.74200000
H	-2.87900000	6.00200000	0.90800000
H	-1.40800000	6.53200000	1.68600000
C	-1.10800000	4.81300000	0.39800000
H	-0.02800000	4.94200000	0.51500000
H	-1.27500000	4.57200000	-0.66000000
C	-1.61400000	3.65500000	1.27400000
H	-1.65800000	3.99000000	2.31900000
H	-0.89100000	2.83100000	1.24700000
C	-2.99300000	3.14900000	0.82900000
H	-2.88900000	2.60300000	-0.12100000
H	-3.64200000	4.00800000	0.61000000
C	-3.72700000	2.28500000	1.85600000
H	-3.76900000	2.83900000	2.80400000
H	-3.15000000	1.37300000	2.06100000
C	-5.16000000	1.93900000	1.42300000
H	-5.13700000	1.20400000	0.60600000
H	-5.62400000	2.84300000	1.00500000
C	-6.04600000	1.44700000	2.57700000
H	-7.08500000	1.36700000	2.22900000
H	-6.03900000	2.22800000	3.34800000
C	-5.63600000	0.10300000	3.19700000
H	-6.15900000	-0.03000000	4.15400000
H	-4.56600000	0.11600000	3.44300000
C	-5.94600000	-1.10800000	2.30900000
H	-5.53300000	-0.96100000	1.30100000
H	-7.03600000	-1.18600000	2.18300000
C	-5.39900000	-2.41500000	2.88700000
H	-5.73000000	-2.51400000	3.93000000
H	-4.30300000	-2.35900000	2.91100000
C	-5.82000000	-3.65100000	2.10300000
H	-5.46600000	-3.60900000	1.06500000
H	-6.91300000	-3.73800000	2.07700000

H	-5.42300000	-4.57000000	2.55000000
Fe	-0.52900000	8.48700000	-2.42400000
O	0.94100000	7.48900000	-3.40200000
O	0.82700000	6.18700000	-3.22600000

$^{5}TS1_{E\text{-}M\text{-}1}$

C	2.09400000	11.82500000	-0.27100000
H	2.80500000	12.29100000	0.41900000
H	1.23400000	11.48400000	0.30700000
C	2.77700000	10.62600000	-0.97300000
H	3.66300000	10.92800000	-1.53800000
H	3.11500000	9.94000000	-0.18800000
C	1.86800000	9.82500000	-1.90900000
O	0.82000000	9.32400000	-1.32700000
O	2.11200000	9.68800000	-3.11600000
C	-2.35200000	11.28700000	-1.14100000
H	-1.64800000	11.49200000	-0.32700000
H	-2.76200000	10.28600000	-0.96900000
N	-1.10700000	10.18300000	-3.06800000
C	-1.65400000	11.32800000	-2.48100000
C	-0.54400000	10.56000000	-4.21800000
H	-0.00900000	9.92300000	-4.90800000
N	-0.70500000	11.87800000	-4.40800000
H	-0.30300000	12.41600000	-5.19400000
C	-1.40000000	12.38300000	-3.32900000
H	-1.65800000	13.42800000	-3.27300000
C	-3.33600000	5.19200000	-6.12200000
H	-4.41100000	5.00300000	-6.18300000
H	-2.82100000	4.24900000	-5.91800000
N	-3.86600000	7.11500000	-4.51300000
H	-4.84200000	7.21500000	-4.80400000
C	-2.99300000	6.17300000	-5.03300000
C	-3.21700000	7.85700000	-3.59700000
H	-3.68500000	8.62400000	-3.00200000
N	-1.94800000	7.45200000	-3.49500000
C	-1.81000000	6.39400000	-4.38100000
H	-0.89700000	5.83800000	-4.46500000
C	-2.16100000	7.29200000	-0.03900000
O	-1.09700000	7.84900000	-0.54500000
O	-3.25100000	7.85200000	0.02100000
C	-1.93600000	5.90200000	0.54800000
H	-2.85600000	5.33600000	0.40400000
H	-1.83900000	6.03500000	1.63800000
C	-0.70800000	5.15700000	0.07100000

H	0.22300000	5.59900000	0.43200000
H	-0.39300000	5.48700000	-1.20700000
C	-0.71900000	3.63800000	0.14400000
H	-0.41100000	3.36800000	1.16900000
H	0.08600000	3.24500000	-0.48900000
C	-2.06500000	2.94400000	-0.17200000
H	-1.87400000	2.01600000	-0.72000000
H	-2.64000000	3.56700000	-0.86900000
C	-2.91600000	2.63100000	1.07600000
H	-2.97000000	3.51700000	1.72500000
H	-2.39700000	1.86500000	1.66900000
C	-4.34900000	2.17800000	0.75400000
H	-4.31900000	1.29600000	0.09700000
H	-4.83600000	2.97100000	0.17000000
C	-5.22000000	1.89000000	1.99300000
H	-6.27700000	1.94500000	1.70100000
H	-5.07500000	2.69900000	2.72000000
C	-4.98000000	0.53300000	2.68100000
H	-5.41300000	0.57000000	3.69000000
H	-3.90300000	0.36700000	2.82800000
C	-5.58800000	-0.66600000	1.93700000
H	-5.17900000	-0.72800000	0.91800000
H	-6.67000000	-0.50200000	1.82100000
C	-5.35100000	-2.00200000	2.65300000
H	-5.74600000	-1.93900000	3.67600000
H	-4.26900000	-2.16800000	2.74900000
C	-5.97700000	-3.20300000	1.94100000
H	-5.57000000	-3.32300000	0.93000000
H	-7.06400000	-3.08900000	1.85100000
H	-5.78500000	-4.13400000	2.48600000
Fe	-0.51400000	8.32100000	-2.31600000
O	0.66400000	6.86000000	-2.53000000
O	0.04500000	5.60100000	-2.36000000

^{5}IM1$_{E\text{-}M\text{-}1}$

C	1.99000000	11.82800000	-0.17500000
H	2.70700000	12.28200000	0.51600000
H	1.10700000	11.53600000	0.39900000
C	2.63300000	10.58100000	-0.82700000
H	3.55900000	10.83100000	-1.35200000
H	2.89500000	9.88900000	-0.01800000
C	1.73400000	9.83100000	-1.81000000
O	0.65600000	9.30100000	-1.28300000

O	1.99300000	9.76700000	-3.01400000
C	-2.34800000	11.31900000	-1.13900000
H	-1.63700000	11.52700000	-0.33300000
H	-2.74700000	10.31500000	-0.95900000
N	-1.16700000	10.20500000	-3.10400000
C	-1.67000000	11.35700000	-2.48900000
C	-0.61100000	10.58500000	-4.25900000
H	-0.11100000	9.94300000	-4.97100000
N	-0.73700000	11.90900000	-4.42300000
H	-0.32800000	12.44800000	-5.20600000
C	-1.39900000	12.41600000	-3.32500000
H	-1.62900000	13.46600000	-3.25000000
C	-3.31600000	5.17700000	-6.17600000
H	-4.38900000	4.97900000	-6.22800000
H	-2.78900000	4.24400000	-5.96700000
N	-3.83800000	7.14400000	-4.63100000
H	-4.81300000	7.24000000	-4.93300000
C	-2.97100000	6.17900000	-5.11000000
C	-3.18800000	7.92000000	-3.74700000
H	-3.64900000	8.71800000	-3.19000000
N	-1.92200000	7.51000000	-3.63300000
C	-1.78400000	6.41800000	-4.47300000
H	-0.87000000	5.86000000	-4.52500000
C	-1.84200000	7.07300000	-0.01400000
O	-0.92900000	7.09700000	-0.94300000
O	-2.64100000	7.99700000	0.17200000
C	-1.81800000	5.81900000	0.87000000
H	-2.84900000	5.46700000	0.96400000
H	-1.54400000	6.18300000	1.87600000
C	-0.88300000	4.73700000	0.43600000
H	0.15300000	5.03400000	0.30000000
H	-0.12200000	5.84600000	-1.82000000
C	-1.13600000	3.27000000	0.60300000
H	-0.83400000	2.95500000	1.62000000
H	-0.44100000	2.73700000	-0.05900000
C	-2.58100000	2.77700000	0.35000000
H	-2.54500000	1.81600000	-0.17600000
H	-3.08500000	3.45800000	-0.34700000
C	-3.43000000	2.59900000	1.61400000
H	-3.42000000	3.51900000	2.21600000
H	-2.95500000	1.83100000	2.24000000
C	-4.88500000	2.20800000	1.31500000
H	-4.89700000	1.38700000	0.58300000
H	-5.38300000	3.05500000	0.82400000

C	-5.69100000	1.80700000	2.56300000
H	-6.76200000	1.83900000	2.32500000
H	-5.53800000	2.56900000	3.33800000
C	-5.36300000	0.41300000	3.12800000
H	-5.77200000	0.33300000	4.14500000
H	-4.27500000	0.29900000	3.24000000
C	-5.91500000	-0.75000000	2.29200000
H	-5.54900000	-0.68000000	1.25800000
H	-7.01000000	-0.66100000	2.23300000
C	-5.54200000	-2.12400000	2.85900000
H	-5.90300000	-2.19800000	3.89500000
H	-4.44800000	-2.20500000	2.90600000
C	-6.08900000	-3.29400000	2.04300000
H	-5.69600000	-3.28300000	1.02000000
H	-7.18400000	-3.25700000	1.97900000
H	-5.81500000	-4.25700000	2.49000000
Fe	-0.53900000	8.33500000	-2.42700000
O	0.79400000	7.07100000	-2.94800000
O	0.37200000	5.70300000	-2.66900000

$^{5}R_{E\text{-}M\text{-}2}$

C	2.07300000	11.88800000	-0.18600000
H	2.79200000	12.36100000	0.49100000
H	1.20800000	11.57800000	0.40300000
C	2.73600000	10.65900000	-0.85100000
H	3.65100000	10.92400000	-1.38600000
H	3.01900000	9.96600000	-0.04900000
C	1.83500000	9.89400000	-1.82000000
O	0.74000000	9.43200000	-1.27300000
O	2.11000000	9.76100000	-3.01700000
C	-2.33300000	11.33800000	-1.15600000
H	-1.62800000	11.53400000	-0.34200000
H	-2.73600000	10.33100000	-0.99700000
N	-1.08800000	10.26800000	-3.09800000
C	-1.64400000	11.40300000	-2.50100000
C	-0.53500000	10.65400000	-4.25000000
H	-0.00500000	10.02400000	-4.95100000
N	-0.71300000	11.97100000	-4.43100000
H	-0.31400000	12.51400000	-5.21600000
C	-1.40600000	12.46400000	-3.34500000
H	-1.67700000	13.50500000	-3.28200000
C	-3.26900000	5.22700000	-6.08800000
H	-4.34100000	5.01800000	-6.13500000

H	-2.73500000	4.29400000	-5.88600000
N	-3.84700000	7.10800000	-4.45100000
H	-4.82800000	7.17600000	-4.73000000
C	-2.94000000	6.21700000	-5.00100000
C	-3.22200000	7.85900000	-3.52600000
H	-3.71900000	8.58600000	-2.90400000
N	-1.93400000	7.51200000	-3.44900000
C	-1.75800000	6.47800000	-4.36000000
H	-0.82000000	5.97100000	-4.47700000
C	-2.04800000	7.17400000	-0.10800000
O	-0.93100000	7.61000000	-0.64400000
O	-3.09000000	7.82800000	-0.14100000
C	-1.92200000	5.82800000	0.59200000
H	-2.91700000	5.37900000	0.58100000
H	-1.68400000	6.01900000	1.64700000
C	-0.86800000	4.89100000	-0.01800000
H	0.12600000	5.26900000	0.24100000
H	-0.92000000	4.95100000	-1.10800000
C	-0.99200000	3.42800000	0.43000000
H	-0.80700000	3.36000000	1.51100000
H	-0.18100000	2.86100000	-0.04200000
C	-2.35700000	2.78100000	0.09300000
H	-2.20500000	1.81700000	-0.40300000
H	-2.87500000	3.39400000	-0.65800000
C	-3.26900000	2.56700000	1.30900000
H	-3.33000000	3.49100000	1.90200000
H	-2.79500000	1.82600000	1.96700000
C	-4.68800000	2.11500000	0.94100000
H	-4.63000000	1.24200000	0.27300000
H	-5.16800000	2.91000000	0.35300000
C	-5.58000000	1.79000000	2.15300000
H	-6.62800000	1.78200000	1.82900000
H	-5.49900000	2.60600000	2.88200000
C	-5.27900000	0.44600000	2.84100000
H	-5.75200000	0.43800000	3.83200000
H	-4.19900000	0.35100000	3.02800000
C	-5.77100000	-0.77900000	2.05600000
H	-5.33100000	-0.78400000	1.04900000
H	-6.85800000	-0.69800000	1.91200000
C	-5.44300000	-2.10800000	2.74500000
H	-5.85000000	-2.09900000	3.76600000
H	-4.35300000	-2.19600000	2.84700000
C	-5.97200000	-3.33200000	1.99800000
H	-5.54600000	-3.39700000	0.98900000

H	-7.06300000	-3.29100000	1.89500000
H	-5.72200000	-4.26100000	2.52200000
Fe	-0.53300000	8.42800000	-2.29500000
O	0.87100000	7.18300000	-2.94100000
O	0.51700000	5.94900000	-2.64700000

$^{5}TS1_{E\text{-}M\text{-}2}$

C	2.13100000	11.85400000	-0.26900000
H	2.85700000	12.32900000	0.39900000
H	1.28300000	11.53100000	0.33500000
C	2.79900000	10.64400000	-0.96600000
H	3.68500000	10.93600000	-1.53400000
H	3.13300000	9.95900000	-0.17700000
C	1.88500000	9.84200000	-1.89800000
O	0.84100000	9.33600000	-1.31000000
O	2.11900000	9.71000000	-3.10600000
C	-2.35400000	11.28100000	-1.11200000
H	-1.65500000	11.48200000	-0.29300000
H	-2.76600000	10.27900000	-0.94400000
N	-1.10200000	10.18200000	-3.03700000
C	-1.65400000	11.32500000	-2.45100000
C	-0.54400000	10.55700000	-4.19100000
H	-0.00500000	9.92100000	-4.87800000
N	-0.71300000	11.87400000	-4.38300000
H	-0.31400000	12.41100000	-5.17200000
C	-1.40700000	12.37800000	-3.30300000
H	-1.67100000	13.42200000	-3.25200000
C	-3.32800000	5.20300000	-6.10900000
H	-4.40200000	5.01500000	-6.16900000
H	-2.81300000	4.26100000	-5.90500000
N	-3.86200000	7.11200000	-4.48400000
H	-4.84100000	7.20700000	-4.76500000
C	-2.98300000	6.18500000	-5.01900000
C	-3.21400000	7.85200000	-3.56500000
H	-3.68500000	8.60700000	-2.95600000
N	-1.94000000	7.45900000	-3.47500000
C	-1.79800000	6.41100000	-4.37300000
H	-0.88100000	5.86500000	-4.47300000
C	-2.17200000	7.27300000	-0.08000000
O	-1.08200000	7.84500000	-0.51700000
O	-3.26600000	7.82700000	-0.08100000
C	-1.97100000	5.87400000	0.49700000
H	-2.88500000	5.31500000	0.29400000
H	-1.92700000	5.98400000	1.59200000

C	-0.72400000	5.13600000	0.05600000
H	0.18500000	5.56500000	0.48000000
H	-0.39100000	5.47800000	-1.20000000
C	-0.74300000	3.61300000	0.12900000
H	-0.44100000	3.33800000	1.15300000
H	0.06500000	3.22700000	-0.50700000
C	-2.08100000	2.91700000	-0.20400000
H	-1.87900000	1.97500000	-0.72400000
H	-2.64400000	3.51900000	-0.93000000
C	-2.95100000	2.62300000	1.03400000
H	-3.02400000	3.51900000	1.66500000
H	-2.43200000	1.87400000	1.64700000
C	-4.37100000	2.14300000	0.69800000
H	-4.31700000	1.24700000	0.06400000
H	-4.86100000	2.91400000	0.08800000
C	-5.25400000	1.86900000	1.93200000
H	-6.30800000	1.90600000	1.62900000
H	-5.12400000	2.69200000	2.64600000
C	-5.00200000	0.52600000	2.64300000
H	-5.43700000	0.57300000	3.65100000
H	-3.92400000	0.37400000	2.79300000
C	-5.59700000	-0.68900000	1.91400000
H	-5.18300000	-0.76200000	0.89800000
H	-6.67900000	-0.53400000	1.79000000
C	-5.35300000	-2.01100000	2.65100000
H	-5.75000000	-1.93400000	3.67300000
H	-4.27000000	-2.16900000	2.75100000
C	-5.97300000	-3.22600000	1.95800000
H	-5.56400000	-3.36000000	0.94900000
H	-7.06000000	-3.11700000	1.86500000
H	-5.77800000	-4.14700000	2.51800000
Fe	-0.50500000	8.33000000	-2.29300000
O	0.67500000	6.86500000	-2.51200000
O	0.05900000	5.60700000	-2.36100000

$^{5}TS2_{E\text{-}M\text{-}1}$

C	1.99200000	11.82900000	-0.17600000
H	2.70800000	12.28300000	0.51700000
H	1.10900000	11.53500000	0.39800000
C	2.63800000	10.58400000	-0.82800000
H	3.56400000	10.83500000	-1.35200000
H	2.89800000	9.89000000	-0.02100000
C	1.73900000	9.83800000	-1.81400000

O	0.65900000	9.30900000	-1.29000000
O	1.99800000	9.77700000	-3.02000000
C	-2.34600000	11.32200000	-1.14600000
H	-1.63400000	11.52900000	-0.34000000
H	-2.74400000	10.31800000	-0.96800000
N	-1.16600000	10.21700000	-3.11800000
C	-1.67000000	11.36500000	-2.49700000
C	-0.61200000	10.60000000	-4.27200000
H	-0.11200000	9.96000000	-4.98600000
N	-0.73900000	11.92400000	-4.43100000
H	-0.33000000	12.46400000	-5.21300000
C	-1.40000000	12.42700000	-3.33000000
H	-1.63000000	13.47700000	-3.25100000
C	-3.31700000	5.17600000	-6.17700000
H	-4.39000000	4.97600000	-6.22800000
H	-2.78800000	4.24300000	-5.96700000
N	-3.83700000	7.14400000	-4.63400000
H	-4.81300000	7.23800000	-4.93200000
C	-2.97100000	6.17900000	-5.11400000
C	-3.18400000	7.92400000	-3.75600000
H	-3.64400000	8.72300000	-3.19800000
N	-1.91700000	7.51800000	-3.64700000
C	-1.78200000	6.42100000	-4.48200000
H	-0.86700000	5.86400000	-4.53500000
C	-1.87000000	7.16600000	-0.06600000
O	-0.94500000	7.13800000	-0.96100000
O	-2.67200000	8.07500000	0.12200000
C	-1.82800000	5.72700000	0.95500000
H	-2.86200000	5.38700000	1.02400000
H	-1.54600000	6.13700000	1.93600000
C	-0.88300000	4.70000000	0.47400000
H	0.14600000	5.01900000	0.32800000
H	-0.12500000	5.85800000	-1.81700000
C	-1.12800000	3.23100000	0.60900000
H	-0.82400000	2.90600000	1.62100000
H	-0.43900000	2.70400000	-0.06400000
C	-2.57900000	2.75800000	0.35300000
H	-2.55400000	1.80100000	-0.18200000
H	-3.07600000	3.45200000	-0.33500000
C	-3.42900000	2.58100000	1.61800000
H	-3.41000000	3.49900000	2.22300000
H	-2.96000000	1.80700000	2.24100000
C	-4.88600000	2.20300000	1.31600000
H	-4.90200000	1.38400000	0.58400000

H	-5.37900000	3.05400000	0.82700000
C	-5.69300000	1.80500000	2.56400000
H	-6.76400000	1.84100000	2.32700000
H	-5.53700000	2.56500000	3.34000000
C	-5.36600000	0.41100000	3.12900000
H	-5.77500000	0.33000000	4.14500000
H	-4.27900000	0.29600000	3.24100000
C	-5.91700000	-0.75200000	2.29100000
H	-5.55000000	-0.68100000	1.25800000
H	-7.01200000	-0.66400000	2.23100000
C	-5.54300000	-2.12500000	2.85900000
H	-5.90400000	-2.20000000	3.89400000
H	-4.44800000	-2.20400000	2.90600000
C	-6.08800000	-3.29600000	2.04300000
H	-5.69500000	-3.28500000	1.01900000
H	-7.18300000	-3.26000000	1.97900000
H	-5.81300000	-4.25800000	2.49000000
Fe	-0.52600000	8.35400000	-2.45800000
O	0.80200000	7.07000000	-2.95300000
O	0.36800000	5.70500000	-2.66200000

$^{5}P_{E\text{-}M\text{-}2}$

C	2.01100000	11.92400000	-0.08900000
H	2.78100000	12.39000000	0.53500000
H	1.14500000	11.71800000	0.54400000
C	2.55000000	10.59600000	-0.66600000
H	3.43700000	10.75200000	-1.28600000
H	2.85700000	9.97300000	0.18300000
C	1.53400000	9.79700000	-1.47800000
O	0.44900000	9.37700000	-0.93400000
O	1.75200000	9.57300000	-2.70100000
C	-2.22300000	11.41600000	-1.47200000
H	-1.50800000	11.50600000	-0.64800000
H	-2.65000000	10.40900000	-1.41700000
N	-0.96300000	10.47700000	-3.45800000
C	-1.54000000	11.57300000	-2.81400000
C	-0.40600000	10.93800000	-4.57600000
H	0.12600000	10.34500000	-5.31000000
N	-0.59500000	12.26300000	-4.69300000
H	-0.19600000	12.84000000	-5.45100000
C	-1.30700000	12.68700000	-3.59100000
H	-1.58700000	13.72100000	-3.47100000
C	-3.38400000	5.19300000	-6.15900000

H	-4.45400000	4.98500000	-6.24200000
H	-2.85700000	4.26200000	-5.93600000
N	-3.92200000	7.20600000	-4.67400000
H	-4.87500000	7.32600000	-5.02600000
C	-3.07200000	6.19400000	-5.08100000
C	-3.28200000	7.97100000	-3.76500000
H	-3.74200000	8.81200000	-3.27000000
N	-2.05000000	7.51400000	-3.55500000
C	-1.92000000	6.39900000	-4.37200000
H	-1.01700000	5.81700000	-4.37300000
C	-1.17700000	7.01300000	0.36900000
O	-0.44300000	6.41000000	-0.30700000
O	-1.90900000	7.64700000	1.02300000
C	-1.57100000	4.49100000	2.13700000
H	-2.65100000	4.48200000	2.24700000
H	-1.02500000	5.06500000	2.88000000
C	-0.94300000	3.78600000	1.19500000
H	0.14600000	3.82200000	1.16000000
H	0.01300000	5.74200000	-1.94600000
C	-1.57000000	2.92600000	0.13200000
H	-1.07800000	1.94800000	0.17000000
H	-1.28300000	3.33000000	-0.85200000
C	-3.09300000	2.75700000	0.17900000
H	-3.41400000	2.28100000	-0.75700000
H	-3.56200000	3.75000000	0.18900000
C	-3.66300000	1.95500000	1.35700000
H	-3.30700000	2.37500000	2.30500000
H	-3.27400000	0.92800000	1.32000000
C	-5.20100000	1.95000000	1.34500000
H	-5.56100000	1.30000000	0.53500000
H	-5.55600000	2.95900000	1.09700000
C	-5.84400000	1.54600000	2.68100000
H	-6.93700000	1.58800000	2.57300000
H	-5.58800000	2.30800000	3.42900000
C	-5.45000000	0.16300000	3.21600000
H	-5.86300000	0.04000000	4.22700000
H	-4.35800000	0.11300000	3.33500000
C	-5.92000000	-1.01200000	2.35200000
H	-5.56300000	-0.89300000	1.31900000
H	-7.01900000	-1.00600000	2.29700000
C	-5.43800000	-2.36200000	2.89000000
H	-5.76300000	-2.47200000	3.93400000
H	-4.33900000	-2.36400000	2.90500000
C	-5.92400000	-3.55500000	2.07600000

H	-5.56500000	-3.50600000	1.04100000
H	-7.02100000	-3.58700000	2.04500000
H	-5.57500000	-4.50200000	2.50200000
Fe	-0.23500000	8.51400000	-2.82300000
O	0.90400000	6.93400000	-3.16000000
O	0.45300000	5.58300000	-2.79600000

$^{5}R_{E\text{-}M\text{-}3}$

C	1.92600000	11.83500000	-0.01500000
H	2.57900000	12.36700000	0.68600000
H	1.02000000	11.56700000	0.53100000
C	2.66200000	10.57100000	-0.48600000
H	3.60900000	10.81000000	-0.97900000
H	2.94700000	10.01700000	0.42000000
C	1.97900000	9.52500000	-1.38300000
O	0.68700000	9.35000000	-1.24700000
O	2.71100000	8.85800000	-2.12400000
C	-2.33900000	11.43500000	-1.27800000
H	-1.63500000	11.60000000	-0.45500000
H	-2.72300000	10.41700000	-1.17100000
N	-1.10000000	10.45900000	-3.26100000
C	-1.65300000	11.56800000	-2.62000000
C	-0.55300000	10.89000000	-4.39600000
H	-0.05800000	10.27400000	-5.13500000
N	-0.72300000	12.21700000	-4.52600000
H	-0.31700000	12.77900000	-5.29100000
C	-1.41200000	12.66500000	-3.41800000
H	-1.67400000	13.70400000	-3.30900000
C	-3.32200000	5.08900000	-6.17400000
H	-4.39000000	4.86300000	-6.23100000
H	-2.77100000	4.16600000	-5.97200000
N	-3.88200000	7.05500000	-4.64500000
H	-4.85500000	7.14500000	-4.95200000
C	-3.00300000	6.09300000	-5.10300000
C	-3.23400000	7.86800000	-3.78800000
H	-3.70100000	8.67000000	-3.24100000
N	-1.96300000	7.48800000	-3.67800000
C	-1.81600000	6.36800000	-4.47400000
H	-0.89300000	5.82100000	-4.53200000
C	-1.70600000	7.66000000	0.05700000
O	-1.77800000	8.16700000	-1.17000000
O	-2.50700000	8.02800000	0.90300000
C	-0.60200000	6.66900000	0.36600000

H	-0.72300000	6.38300000	1.41200000
H	0.33500000	7.23200000	0.28300000
C	-0.51600000	5.42700000	-0.52900000
H	0.36900000	4.85500000	-0.21900000
H	-0.35000000	5.74600000	-1.56700000
C	-1.74800000	4.52000000	-0.49500000
H	-1.63500000	3.75300000	-1.27300000
H	-2.61800000	5.12400000	-0.78500000
C	-2.03200000	3.82800000	0.84600000
H	-1.13800000	3.27400000	1.16600000
H	-2.23000000	4.57200000	1.62900000
C	-3.22300000	2.86700000	0.74200000
H	-3.00700000	2.11700000	-0.03400000
H	-4.10700000	3.42000000	0.39500000
C	-3.59000000	2.15200000	2.04400000
H	-2.69800000	1.65600000	2.45400000
H	-3.90000000	2.89200000	2.79400000
C	-4.69500000	1.10700000	1.85100000
H	-4.33800000	0.36200000	1.12800000
H	-5.57800000	1.57700000	1.39400000
C	-5.10600000	0.41100000	3.15600000
H	-4.19700000	0.13500000	3.70800000
H	-5.63200000	1.13400000	3.79300000
C	-5.26800000	-1.96800000	2.18800000
H	-6.91700000	-0.59000000	2.48000000
H	-6.24500000	-1.23100000	3.96900000
C	-5.97000000	-0.84900000	2.97600000
H	-5.17100000	-1.68000000	1.13400000
H	-4.24100000	-2.08200000	2.56400000
C	-5.97900000	-3.32000000	2.26900000
H	-5.46900000	-4.07400000	1.66100000
H	-7.01500000	-3.24800000	1.91500000
H	-6.00800000	-3.68800000	3.30000000
Fe	-0.56600000	8.49900000	-2.52900000
O	0.68700000	8.31000000	-3.94000000
O	0.91300000	7.06600000	-3.58700000

$^{5}TS1_{E\text{-}M\text{-}3}$

C	2.00800000	11.72700000	-0.31300000
H	2.81300000	12.14000000	0.30300000
H	1.17000000	11.51400000	0.34800000
C	2.50500000	10.42300000	-0.98200000
H	3.36300000	10.60400000	-1.63400000
H	2.84800000	9.76400000	-0.17500000

C	1.47900000	9.62500000	-1.79400000
O	0.38800000	9.26600000	-1.18800000
O	1.69500000	9.33900000	-2.98600000
C	-2.40400000	11.34100000	-1.13000000
H	-1.69200000	11.54400000	-0.32300000
H	-2.79700000	10.33600000	-0.95800000
N	-1.28700000	10.25400000	-3.12700000
C	-1.73700000	11.40600000	-2.48200000
C	-0.73500000	10.63500000	-4.28000000
H	-0.27400000	9.98600000	-5.01100000
N	-0.80700000	11.96800000	-4.41500000
H	-0.38700000	12.50100000	-5.19500000
C	-1.43500000	12.47600000	-3.29600000
H	-1.62200000	13.53200000	-3.19400000
C	-3.42700000	5.06100000	-6.23800000
H	-4.49900000	4.86300000	-6.31900000
H	-2.90400000	4.13300000	-5.99400000
N	-3.90300000	7.19600000	-4.93900000
H	-4.85600000	7.31400000	-5.30400000
C	-3.10200000	6.10000000	-5.20400000
C	-3.23700000	8.04600000	-4.14500000
H	-3.64800000	8.96000000	-3.74900000
N	-2.03100000	7.55400000	-3.87300000
C	-1.94600000	6.32600000	-4.50500000
H	-1.08700000	5.68800000	-4.40400000
C	-1.98000000	7.81000000	0.15900000
O	-2.11700000	7.68400000	-1.14100000
O	-2.54900000	8.69000000	0.80000000
C	-1.00200000	6.87600000	0.87500000
H	-1.42100000	6.65300000	1.86500000
H	-0.13300000	7.51000000	1.08200000
C	-0.52700000	5.59800000	0.22100000
H	0.27900000	5.13900000	0.80400000
H	0.23700000	6.00300000	-0.79700000
C	-1.54200000	4.58300000	-0.24400000
H	-1.07900000	3.85800000	-0.92500000
H	-2.34000000	5.09000000	-0.79200000
C	-2.11100000	3.82300000	0.98100000
H	-1.28500000	3.29900000	1.47800000
H	-2.49900000	4.54200000	1.71300000
C	-3.21700000	2.81600000	0.64500000
H	-2.83500000	2.06900000	-0.06500000
H	-4.04900000	3.32700000	0.14300000
C	-3.73700000	2.11600000	1.90700000

H	-2.88300000	1.68900000	2.45200000
H	-4.18000000	2.86500000	2.57900000
C	-4.75300000	1.00000000	1.64500000
H	-4.27800000	0.23400000	1.01900000
H	-5.60400000	1.38900000	1.06800000
C	-5.26200000	0.37100000	2.95200000
H	-4.39700000	0.15400000	3.59700000
H	-5.85800000	1.11800000	3.49300000
C	-5.28900000	-2.05800000	2.11700000
H	-6.99100000	-0.71900000	2.20900000
H	-6.41300000	-1.25200000	3.77800000
C	-6.07700000	-0.92100000	2.78600000
H	-5.15500000	-1.84300000	1.04900000
H	-4.27700000	-2.09700000	2.54500000
C	-5.94500000	-3.43000000	2.27200000
H	-5.38900000	-4.20300000	1.73100000
H	-6.97200000	-3.42400000	1.88500000
H	-5.99000000	-3.72600000	3.32500000
Fe	-0.84300000	8.32600000	-2.45700000
O	0.14800000	6.77700000	-2.69600000
O	0.99900000	6.45400000	-1.63300000

^{5}IM1$_{E\text{-}M\text{-}3}$

C	2.00400000	11.73500000	-0.31000000
H	2.81000000	12.14700000	0.30700000
H	1.16600000	11.52100000	0.35100000
C	2.50200000	10.43300000	-0.98200000
H	3.36200000	10.61800000	-1.63100000
H	2.84300000	9.76900000	-0.17800000
C	1.47700000	9.64300000	-1.80400000
O	0.39200000	9.25800000	-1.19500000
O	1.68300000	9.39400000	-3.00300000
C	-2.40600000	11.34500000	-1.13200000
H	-1.69500000	11.54800000	-0.32500000
H	-2.80000000	10.34000000	-0.95800000
N	-1.29100000	10.25200000	-3.12900000
C	-1.73900000	11.40600000	-2.48400000
C	-0.73900000	10.63200000	-4.28200000
H	-0.27800000	9.98200000	-5.01100000
N	-0.81200000	11.96500000	-4.42000000
H	-0.39300000	12.49700000	-5.20000000
C	-1.43800000	12.47400000	-3.30000000
H	-1.62600000	13.53000000	-3.20000000
C	-3.41100000	5.06100000	-6.23600000

H	-4.48300000	4.86000000	-6.31400000
H	-2.88400000	4.13500000	-5.99400000
N	-3.89400000	7.19000000	-4.93000000
H	-4.84700000	7.30600000	-5.29300000
C	-3.08700000	6.09900000	-5.20100000
C	-3.23300000	8.03800000	-4.13100000
H	-3.64800000	8.94700000	-3.72700000
N	-2.02400000	7.55000000	-3.86100000
C	-1.93200000	6.32700000	-4.50200000
H	-1.06800000	5.69400000	-4.40800000
C	-1.99800000	7.84600000	0.16600000
O	-2.11400000	7.70800000	-1.13300000
O	-2.57100000	8.73800000	0.78700000
C	-1.04300000	6.91200000	0.91500000
H	-1.47300000	6.75400000	1.91400000
H	-0.15900000	7.53300000	1.10300000
C	-0.61400000	5.60200000	0.33000000
H	0.28100000	5.17900000	0.79000000
H	0.62700000	6.23200000	-0.98300000
C	-1.60500000	4.59800000	-0.15500000
H	-1.13700000	3.89500000	-0.85600000
H	-2.41300000	5.10800000	-0.68700000
C	-2.16900000	3.80500000	1.05100000
H	-1.34000000	3.27800000	1.54200000
H	-2.56000000	4.51100000	1.79500000
C	-3.26800000	2.80000000	0.69300000
H	-2.87900000	2.06400000	-0.02500000
H	-4.09800000	3.31800000	0.19200000
C	-3.79000000	2.08800000	1.94400000
H	-2.93500000	1.65800000	2.48700000
H	-4.23300000	2.83000000	2.62200000
C	-4.80200000	0.97300000	1.67300000
H	-4.32400000	0.21400000	1.04000000
H	-5.65400000	1.36400000	1.09900000
C	-5.30500000	0.33400000	2.97600000
H	-4.43700000	0.12100000	3.61800000
H	-5.90500000	1.07400000	3.52100000
C	-5.30700000	-2.08600000	2.12600000
H	-7.02400000	-0.76500000	2.22700000
H	-6.44000000	-1.30400000	3.79200000
C	-6.10800000	-0.96300000	2.80300000
H	-5.17500000	-1.86300000	1.05900000
H	-4.29400000	-2.11700000	2.55400000
C	-5.94900000	-3.46500000	2.27200000

H	-5.38700000	-4.22900000	1.72600000
H	-6.97700000	-3.46400000	1.88700000
H	-5.99100000	-3.76800000	3.32300000
Fe	-0.83300000	8.33000000	-2.45700000
O	0.16800000	6.81000000	-2.72600000
O	1.18600000	6.55400000	-1.74200000

$^{5}R_{E\text{-}M\text{-}4}$

C	2.04000000	11.88200000	-0.23500000
H	2.85400000	12.32200000	0.35200000
H	1.21800000	11.67900000	0.44900000
C	2.53800000	10.56900000	-0.88300000
H	3.39800000	10.74200000	-1.53500000
H	2.87400000	9.91500000	-0.07000000
C	1.50200000	9.78700000	-1.69700000
O	0.44900000	9.37200000	-1.04600000
O	1.66100000	9.58100000	-2.90900000
C	-2.45500000	11.37900000	-0.95600000
H	-1.74800000	11.60700000	-0.15400000
H	-2.84600000	10.37500000	-0.76700000
N	-1.37700000	10.22300000	-2.92400000
C	-1.79600000	11.39900000	-2.30900000
C	-0.84700000	10.56000000	-4.10000000
H	-0.41000000	9.88200000	-4.82000000
N	-0.91000000	11.88900000	-4.27700000
H	-0.48900000	12.40600000	-5.06600000
C	-1.50200000	12.44000000	-3.16000000
H	-1.67600000	13.50100000	-3.09000000
C	-3.30100000	5.11900000	-6.16100000
H	-4.36800000	4.88800000	-6.21000000
H	-2.74700000	4.20400000	-5.93600000
N	-3.78200000	7.25000000	-4.86100000
H	-4.72000000	7.38400000	-5.25600000
C	-2.99000000	6.14400000	-5.10600000
C	-3.16300000	8.04400000	-3.97000000
H	-3.58600000	8.95300000	-3.57800000
N	-1.99400000	7.51700000	-3.61700000
C	-1.89000000	6.31500000	-4.30400000
H	-1.09500000	5.61600000	-4.09200000
C	-1.82300000	7.18500000	0.47000000
O	-1.93000000	7.52700000	-0.81400000
O	-1.66200000	8.00300000	1.36300000
C	-2.00900000	5.71200000	0.80300000

H	-3.05900000	5.47000000	0.60100000
H	-1.85000000	5.61600000	1.88000000
C	-1.11800000	4.71900000	0.04700000
H	-0.06800000	5.00500000	0.17700000
H	-1.33600000	4.78400000	-1.02400000
C	-1.30300000	3.26800000	0.51600000
H	-1.03600000	3.19600000	1.57900000
H	-0.57000000	2.65100000	-0.01800000
C	-2.72900000	2.70600000	0.29800000
H	-2.67900000	1.74900000	-0.23600000
H	-3.29200000	3.37200000	-0.37000000
C	-3.53600000	2.49900000	1.58700000
H	-3.50800000	3.41300000	2.19700000
H	-3.04000000	1.72500000	2.18800000
C	-4.99900000	2.11600000	1.32500000
H	-5.03700000	1.30000000	0.58900000
H	-5.50300000	2.97000000	0.85200000
C	-5.77800000	1.71700000	2.59000000
H	-6.85400000	1.73400000	2.37100000
H	-5.61700000	2.48700000	3.35500000
C	-5.42200000	0.33300000	3.16000000
H	-5.84000000	0.24200000	4.17300000
H	-4.33300000	0.24600000	3.28300000
C	-5.93500000	-0.84300000	2.31800000
H	-5.57100000	-0.75600000	1.28400000
H	-7.03200000	-0.79100000	2.25900000
C	-5.51500000	-2.20600000	2.87700000
H	-5.86800000	-2.29700000	3.91300000
H	-4.41800000	-2.25000000	2.91700000
C	-6.02600000	-3.38800000	2.05700000
H	-5.63900000	-3.35800000	1.03100000
H	-7.12200000	-3.38500000	1.99800000
H	-5.72000000	-4.34400000	2.49600000
Fe	-0.82900000	8.34700000	-2.13200000
O	0.62500000	7.08200000	-2.38600000
O	0.19700000	5.86100000	-2.41400000

$^{5}TS1_{E\text{-}M\text{-}4}$

C	2.08900000	11.85600000	-0.19700000
H	2.88700000	12.33100000	0.38500000
H	1.26800000	11.64000000	0.48600000
C	2.62300000	10.54500000	-0.81600000
H	3.45300000	10.72300000	-1.50500000
H	3.02100000	9.94200000	0.01000000

C	1.59500000	9.66300000	-1.53300000
O	0.51600000	9.36200000	-0.87900000
O	1.80400000	9.25000000	-2.68900000
C	-2.38200000	11.33100000	-1.04600000
H	-1.68100000	11.54800000	-0.23400000
H	-2.78600000	10.33100000	-0.86300000
N	-1.20700000	10.15400000	-2.94500000
C	-1.69600000	11.33500000	-2.39000000
C	-0.65100000	10.47000000	-4.11300000
H	-0.17900000	9.78200000	-4.80100000
N	-0.75600000	11.79200000	-4.34200000
H	-0.35100000	12.29200000	-5.15000000
C	-1.41200000	12.35800000	-3.26700000
H	-1.62500000	13.41500000	-3.23600000
C	-3.36400000	5.11900000	-6.18600000
H	-4.43200000	4.89500000	-6.27100000
H	-2.82300000	4.19600000	-5.96200000
N	-3.84700000	7.23700000	-4.85400000
H	-4.77600000	7.39300000	-5.25900000
C	-3.06900000	6.12200000	-5.10800000
C	-3.22300000	8.00200000	-3.94000000
H	-3.63300000	8.91600000	-3.54300000
N	-2.07300000	7.44500000	-3.57600000
C	-1.97900000	6.26100000	-4.28800000
H	-1.17400000	5.56400000	-4.13300000
C	-1.78700000	7.20300000	0.58100000
O	-1.99600000	7.66400000	-0.65000000
O	-1.50700000	7.91400000	1.52900000
C	-1.97000000	5.70100000	0.76000000
H	-2.89500000	5.39500000	0.26600000
H	-2.08500000	5.52400000	1.83800000
C	-0.80300000	4.87100000	0.27800000
H	0.14600000	5.18200000	0.72300000
H	-0.52500000	5.30000000	-0.98400000
C	-0.94500000	3.35900000	0.19400000
H	-0.57100000	2.94600000	1.14600000
H	-0.23400000	2.99000000	-0.55800000
C	-2.35400000	2.79500000	-0.07900000
H	-2.26100000	1.84800000	-0.62200000
H	-2.89200000	3.45600000	-0.76800000
C	-3.19100000	2.55800000	1.19000000
H	-3.18500000	3.45300000	1.82600000
H	-2.70000000	1.77200000	1.78100000
C	-4.64900000	2.17000000	0.90300000

H	-4.67100000	1.30800000	0.22000000
H	-5.12800000	2.99600000	0.36000000
C	-5.47400000	1.86300000	2.16700000
H	-6.54000000	1.90400000	1.91200000
H	-5.31500000	2.66900000	2.89600000
C	-5.19000000	0.50400000	2.83100000
H	-5.62100000	0.50900000	3.84200000
H	-4.10800000	0.36900000	2.97500000
C	-5.75900000	-0.70200000	2.06800000
H	-5.35800000	-0.72500000	1.04400000
H	-6.84700000	-0.57900000	1.96500000
C	-5.45800000	-2.04200000	2.74900000
H	-5.85200000	-2.02500000	3.77500000
H	-4.36900000	-2.15900000	2.83800000
C	-6.02600000	-3.25200000	2.00600000
H	-5.61200000	-3.32800000	0.99400000
H	-7.11700000	-3.18500000	1.91400000
H	-5.79400000	-4.18700000	2.52800000
Fe	-0.78000000	8.22100000	-1.99200000
O	0.45500000	6.77300000	-2.16100000
O	-0.22600000	5.54300000	-2.10500000

^{5}IM1$_{E\text{-}M\text{-}4}$

C	2.04700000	11.86600000	-0.14300000
H	2.81200000	12.33000000	0.48800000
H	1.19700000	11.60200000	0.49100000
C	2.62200000	10.58800000	-0.79700000
H	3.44400000	10.80000000	-1.48700000
H	3.03400000	9.96600000	0.00700000
C	1.58300000	9.74100000	-1.51200000
O	0.55000000	9.34400000	-0.85700000
O	1.69800000	9.42400000	-2.72600000
C	-2.28300000	11.34800000	-1.17000000
H	-1.57700000	11.55300000	-0.35900000
H	-2.67200000	10.33900000	-1.00000000
N	-1.03800000	10.26700000	-3.10800000
C	-1.60100000	11.40300000	-2.51900000
C	-0.50800000	10.65400000	-4.26900000
H	0.01100000	10.02200000	-4.97700000
N	-0.69500000	11.97000000	-4.46100000
H	-0.31000000	12.51100000	-5.25300000
C	-1.38100000	12.46400000	-3.37100000
H	-1.65700000	13.50400000	-3.31100000
C	-3.38700000	5.17800000	-6.19600000

H	-4.46100000	4.99100000	-6.26500000
H	-2.87300000	4.24100000	-5.96900000
N	-3.86200000	7.23200000	-4.75100000
H	-4.82400000	7.35100000	-5.08100000
C	-3.04000000	6.19100000	-5.14100000
C	-3.18300000	8.02700000	-3.90000000
H	-3.61000000	8.89200000	-3.41800000
N	-1.95200000	7.55800000	-3.71900000
C	-1.86200000	6.40500000	-4.47700000
H	-0.97600000	5.79800000	-4.47700000
C	-1.75900000	7.07200000	0.02200000
O	-1.02700000	7.01700000	-1.06600000
O	-2.42900000	8.05600000	0.33200000
C	-1.72700000	5.79800000	0.87700000
H	-2.75900000	5.44200000	0.95200000
H	-1.46200000	6.13100000	1.89400000
C	-0.80000000	4.72800000	0.40400000
H	0.24300000	5.01700000	0.29500000
H	-0.18400000	5.73400000	-1.88700000
C	-1.07400000	3.25600000	0.43100000
H	-0.70000000	2.83200000	1.38200000
H	-0.43900000	2.78800000	-0.33300000
C	-2.53800000	2.80000000	0.23600000
H	-2.53900000	1.85100000	-0.31400000
H	-3.05800000	3.50700000	-0.42200000
C	-3.34000000	2.60300000	1.52900000
H	-3.29400000	3.50600000	2.15400000
H	-2.85500000	1.81100000	2.11700000
C	-4.81100000	2.24300000	1.26800000
H	-4.86000000	1.42900000	0.53000000
H	-5.30400000	3.10500000	0.79800000
C	-5.59800000	1.84800000	2.53100000
H	-6.67300000	1.90000000	2.31400000
H	-5.42000000	2.60300000	3.30700000
C	-5.28400000	0.44700000	3.08800000
H	-5.69000000	0.37000000	4.10600000
H	-4.19700000	0.31900000	3.19700000
C	-5.85300000	-0.70800000	2.25100000
H	-5.47800000	-0.64900000	1.21900000
H	-6.94500000	-0.59800000	2.18300000
C	-5.51200000	-2.08800000	2.82600000
H	-5.88100000	-2.15200000	3.85800000
H	-4.41900000	-2.19000000	2.88100000
C	-6.07500000	-3.25200000	2.01000000

H	-5.67700000	-3.25000000	0.98800000
H	-7.16800000	-3.19700000	1.94100000
H	-5.81800000	-4.21600000	2.46100000
Fe	-0.38700000	8.28800000	-2.38600000
O	0.81600000	6.90800000	-3.01800000
O	0.41100000	5.56000000	-2.66100000

$^{5}R_{S\text{-}D}$

C	2.06800000	11.90600000	0.07600000
H	2.69700000	12.49500000	0.75400000
H	1.18200000	11.60300000	0.63800000
C	2.87000000	10.67400000	-0.37200000
H	3.81300000	10.94700000	-0.85100000
H	3.16600000	10.13400000	0.53800000
C	2.23200000	9.61100000	-1.27400000
O	0.93200000	9.50300000	-1.24800000
O	2.98300000	8.88600000	-1.93800000
C	-2.35500000	11.38900000	-1.17700000
H	-1.65400000	11.53500000	-0.34800000
H	-2.75000000	10.37300000	-1.09400000
N	-1.07300000	10.45500000	-3.16000000
C	-1.67100000	11.54100000	-2.51700000
C	-0.58600000	10.92000000	-4.31200000
H	-0.07800000	10.34200000	-5.06800000
N	-0.82400000	12.23500000	-4.44000000
H	-0.44000000	12.80900000	-5.20600000
C	-1.50400000	12.65100000	-3.31700000
H	-1.81300000	13.67600000	-3.20700000
C	-3.25800000	5.13100000	-6.14600000
H	-4.32500000	4.89100000	-6.16900000
H	-2.69300000	4.21800000	-5.94600000
N	-3.74400000	7.21000000	-4.75200000
H	-4.70400000	7.32300000	-5.09100000
C	-2.92200000	6.14900000	-5.09200000
C	-3.08100000	8.02100000	-3.90500000
H	-3.50600000	8.90800000	-3.46400000
N	-1.86100000	7.54500000	-3.67200000
C	-1.76400000	6.36500000	-4.38900000
H	-0.88100000	5.74900000	-4.35600000
C	-1.00000000	6.93000000	-0.65700000
O	-1.54500000	8.08500000	-0.78000000
O	-0.06900000	6.63000000	-1.47300000
C	-1.45300000	5.96700000	0.40600000

H	-2.54900000	5.96100000	0.37300000
H	-1.19400000	6.41000000	1.37700000
C	-0.86500000	4.55500000	0.28700000
H	0.21100000	4.60800000	0.47300000
H	-0.98000000	4.19200000	-0.74100000
C	-1.52100000	3.56200000	1.25800000
H	-1.62500000	4.03500000	2.24500000
H	-0.85200000	2.70700000	1.40200000
C	-2.88900000	3.06100000	0.77300000
H	-2.74900000	2.42800000	-0.11400000
H	-3.49600000	3.91400000	0.43600000
C	-3.69300000	2.31100000	1.83800000
H	-3.75100000	2.94100000	2.73600000
H	-3.15100000	1.40400000	2.13600000
C	-5.12000000	1.96700000	1.38700000
H	-5.08700000	1.21700000	0.58500000
H	-5.57200000	2.86500000	0.94500000
C	-6.02600000	1.49600000	2.53600000
H	-7.06100000	1.42500000	2.17500000
H	-6.02300000	2.28300000	3.30200000
C	-5.64100000	0.15200000	3.17200000
H	-6.17900000	0.03300000	4.12200000
H	-4.57400000	0.15300000	3.43500000
C	-5.95400000	-1.06200000	2.28900000
H	-5.52200000	-0.92900000	1.28700000
H	-7.04200000	-1.12500000	2.14500000
C	-5.43600000	-2.37300000	2.88500000
H	-5.78800000	-2.46300000	3.92200000
H	-4.34000000	-2.33100000	2.93100000
C	-5.85500000	-3.60800000	2.09700000
H	-5.47900000	-3.57400000	1.06700000
H	-6.94800000	-3.68400000	2.04800000
H	-5.47800000	-4.52900000	2.55600000
Fe	-0.27700000	8.46600000	-2.48800000
O	1.08600000	8.73800000	-4.19900000
O	1.04800000	7.49900000	-3.77400000

$^{5}R_{S\text{-}M}$

C	2.00500000	11.86300000	0.04800000
H	2.65400000	12.42200000	0.73100000
H	1.11000000	11.58500000	0.60900000
C	2.76100000	10.60700000	-0.41200000
H	3.71200000	10.85500000	-0.89200000
H	3.04200000	10.04900000	0.49200000

C	2.09300000	9.57000000	-1.33100000
O	0.78700000	9.53000000	-1.32500000
O	2.83200000	8.83000000	-1.98900000
C	-2.33400000	11.36800000	-1.22700000
H	-1.63000000	11.51500000	-0.40200000
H	-2.73100000	10.35400000	-1.13600000
N	-1.01200000	10.44600000	-3.20800000
C	-1.64700000	11.51600000	-2.56700000
C	-0.52600000	10.92000000	-4.35600000
H	0.00500000	10.35500000	-5.10400000
N	-0.80000000	12.22600000	-4.48600000
H	-0.42100000	12.80900000	-5.25000000
C	-1.50100000	12.62500000	-3.37200000
H	-1.83900000	13.64200000	-3.26500000
C	-3.20900000	5.18500000	-6.10600000
H	-4.27300000	4.92900000	-6.11100000
H	-2.62800000	4.28300000	-5.89600000
N	-3.70300000	7.29400000	-4.75700000
H	-4.66300000	7.39500000	-5.09900000
C	-2.88000000	6.22200000	-5.06600000
C	-3.05300000	8.11900000	-3.91700000
H	-3.48100000	9.01200000	-3.49300000
N	-1.84000000	7.63800000	-3.65400000
C	-1.73500000	6.44000000	-4.34400000
H	-0.85300000	5.82700000	-4.28700000
C	-1.14300000	7.06400000	-0.66600000
O	-1.78600000	8.15300000	-0.74300000
O	-0.19400000	6.85100000	-1.50500000
C	-1.47800000	6.03300000	0.38400000
H	-2.57300000	5.99200000	0.42200000
H	-1.16800000	6.45200000	1.35100000
C	-0.86200000	4.64200000	0.18900000
H	0.22000000	4.71100000	0.32300000
H	-1.02300000	4.30600000	-0.84400000
C	-1.45300000	3.60600000	1.16100000
H	-1.51700000	4.04900000	2.16500000
H	-0.76200000	2.76100000	1.24800000
C	-2.83600000	3.09800000	0.72500000
H	-2.72500000	2.47200000	-0.17200000
H	-3.45800000	3.95100000	0.41700000
C	-3.60500000	2.33800000	1.80900000
H	-3.62800000	2.95700000	2.71700000
H	-3.06000000	1.42300000	2.07800000
C	-5.05000000	2.01200000	1.40300000

H	-5.05100000	1.26800000	0.59400000
H	-5.50400000	2.91900000	0.98000000
C	-5.92900000	1.54400000	2.57300000
H	-6.97500000	1.50000000	2.24300000
H	-5.88800000	2.31800000	3.35100000
C	-5.55500000	0.18200000	3.17900000
H	-6.06700000	0.06300000	4.14300000
H	-4.48100000	0.15800000	3.41000000
C	-5.91800000	-1.01400000	2.29000000
H	-5.49400000	-0.88600000	1.28500000
H	-7.00900000	-1.04100000	2.15900000
C	-5.43500000	-2.34600000	2.86900000
H	-5.79300000	-2.44200000	3.90300000
H	-4.33800000	-2.33300000	2.91900000
C	-5.88200000	-3.56000000	2.06100000
H	-5.50000000	-3.52000000	1.03400000
H	-6.97700000	-3.60900000	2.00600000
H	-5.52900000	-4.49500000	2.50900000
Fe	-0.38100000	8.53600000	-2.55800000
O	0.99400000	8.69600000	-4.22100000
O	1.02100000	7.45100000	-3.82300000

$^{5}R_{O\text{-}D}$

C	1.62200000	6.15600000	10.22400000
H	2.15200000	5.76400000	11.09900000
H	0.67300000	5.61700000	10.14000000
C	2.47700000	5.90200000	8.97600000
H	3.46000000	6.36700000	9.05200000
H	2.66600000	4.82000000	8.92900000
C	1.93100000	6.29600000	7.59600000
O	0.67900000	6.01000000	7.36000000
O	2.73100000	6.79600000	6.79900000
C	-2.50600000	7.04200000	8.89600000
H	-1.89700000	6.38000000	9.51700000
H	-2.85100000	6.44000000	8.05400000
N	-1.10900000	8.18600000	7.11900000
C	-1.70400000	8.21300000	8.37900000
C	-0.46800000	9.34100000	6.96800000
H	0.10800000	9.63000000	6.10300000
N	-0.61700000	10.11300000	8.05900000
H	-0.14700000	11.01400000	8.21300000
C	-1.39000000	9.42000000	8.96600000
H	-1.64200000	9.85000000	9.92200000
C	-2.87600000	8.08400000	0.94800000

H	-3.91800000	8.03700000	0.62100000
H	-2.26700000	7.43300000	0.31700000
N	-3.62200000	7.90200000	3.37300000
H	-4.55600000	8.27600000	3.19200000
C	-2.69500000	7.66700000	2.37400000
C	-3.09500000	7.53100000	4.55600000
H	-3.62100000	7.56900000	5.49600000
N	-1.86200000	7.07900000	4.37000000
C	-1.60600000	7.14500000	3.01800000
H	-0.67200000	6.80700000	2.60400000
C	-1.20600000	4.27800000	5.44300000
O	-1.75800000	5.10000000	6.25700000
O	-0.17500000	4.69600000	4.82000000
C	-1.75900000	2.90100000	5.22100000
H	-2.84900000	2.99900000	5.13500000
H	-1.59000000	2.33900000	6.15000000
C	-1.13900000	2.17900000	4.01700000
H	-0.07500000	2.03900000	4.21400000
H	-1.19200000	2.82800000	3.13400000
C	-1.81400000	0.83700000	3.70000000
H	-2.05400000	0.30900000	4.63500000
H	-1.10300000	0.19300000	3.16800000
C	-3.08500000	1.00500000	2.85600000
H	-2.81000000	1.39100000	1.86400000
H	-3.72300000	1.77700000	3.31200000
C	-3.92000000	-0.26700000	2.71700000
H	-4.08700000	-0.68600000	3.72000000
H	-3.34900000	-1.02300000	2.16300000
C	-5.28500000	-0.02400000	2.05900000
H	-5.15200000	0.24400000	1.00300000
H	-5.74900000	0.85000000	2.53600000
C	-6.24400000	-1.21400000	2.20400000
H	-7.24600000	-0.91800000	1.86700000
H	-6.32900000	-1.43500000	3.27700000
C	-5.83000000	-2.48200000	1.44600000
H	-6.42100000	-3.33500000	1.80700000
H	-4.78400000	-2.73000000	1.67100000
C	-6.01800000	-2.37100000	-0.07100000
H	-5.56900000	-1.44100000	-0.44600000
H	-7.09400000	-2.29300000	-0.28600000
C	-5.42600000	-3.55600000	-0.83500000
H	-5.77900000	-4.49100000	-0.38100000
H	-4.33500000	-3.54600000	-0.71200000
C	-5.77600000	-3.54300000	-2.32100000

H	-5.38600000	-2.65000000	-2.82300000
H	-6.86300000	-3.55000000	-2.46300000
H	-5.37000000	-4.41900000	-2.83800000
Fe	-0.41700000	6.54800000	5.77700000
O	0.66800000	7.42100000	4.92200000

$^{5}R_{O\text{-}M}$

C	1.52000000	6.36000000	9.93600000
H	2.05500000	5.92900000	10.78800000
H	0.58000000	5.82000000	9.82800000
C	2.37300000	6.13700000	8.67800000
H	3.32500000	6.67400000	8.70200000
H	2.63900000	5.07100000	8.67900000
C	1.77600000	6.37200000	7.28900000
O	0.49600000	6.16800000	7.16000000
O	2.54700000	6.66800000	6.36100000
C	-2.62500000	7.31600000	8.79300000
H	-1.99900000	6.60800000	9.34200000
H	-2.98900000	6.76600000	7.92800000
N	-1.24200000	8.48400000	7.04700000
C	-1.83800000	8.50300000	8.30900000
C	-0.59400000	9.63600000	6.89400000
H	-0.04000000	9.93100000	6.01500000
N	-0.74200000	10.40100000	7.98800000
H	-0.27900000	11.30900000	8.12900000
C	-1.51800000	9.70600000	8.89600000
H	-1.76200000	10.12600000	9.85900000
C	-2.98500000	8.13300000	0.85400000
H	-4.02500000	8.13500000	0.51800000
H	-2.39200000	7.48500000	0.20600000
N	-3.81400000	7.80100000	3.23300000
H	-4.75500000	8.15200000	3.03700000
C	-2.83000000	7.67800000	2.27200000
C	-3.31000000	7.44300000	4.42800000
H	-3.87500000	7.39600000	5.34400000
N	-2.03200000	7.10700000	4.28200000
C	-1.72500000	7.23100000	2.94500000
H	-0.75500000	6.97900000	2.55600000
C	-1.85700000	4.44400000	7.08200000
O	-2.00800000	5.54700000	6.37100000
O	-2.27700000	4.32400000	8.23000000
C	-1.11100000	3.29200000	6.42700000
H	-1.64300000	2.37400000	6.69600000
H	-0.17400000	3.26600000	6.99100000

C	-0.80400000	3.34800000	4.93000000
H	0.03500000	2.66800000	4.74100000
H	-0.43800000	4.34800000	4.66600000
C	-1.96600000	2.96900000	4.00300000
H	-1.75600000	3.35500000	2.99600000
H	-2.87500000	3.48400000	4.34500000
C	-2.24000000	1.46000000	3.89900000
H	-2.52200000	1.05400000	4.88100000
H	-1.31100000	0.94300000	3.62000000
C	-3.33400000	1.13000000	2.87400000
H	-3.00900000	1.47300000	1.88100000
H	-4.24000000	1.70600000	3.11400000
C	-3.71400000	-0.35300000	2.80400000
H	-4.07700000	-0.68300000	3.78700000
H	-2.81600000	-0.95300000	2.59400000
C	-4.77400000	-0.65300000	1.73400000
H	-4.36100000	-0.38700000	0.75300000
H	-5.64800000	-0.00400000	1.88400000
C	-5.22300000	-2.12200000	1.73500000
H	-5.78900000	-2.31900000	2.65600000
H	-4.33000000	-2.76100000	1.78900000
C	-5.26300000	-2.47900000	-0.80500000
H	-4.25400000	-2.88000000	-0.63200000
H	-5.12400000	-1.43000000	-1.09500000
C	-6.04700000	-2.56200000	0.51400000
H	-6.96600000	-1.96300000	0.44100000
H	-6.36900000	-3.60000000	0.67000000
C	-5.89500000	-3.24200000	-1.97000000
H	-5.92600000	-4.31700000	-1.76400000
H	-5.32800000	-3.09200000	-2.89500000
H	-6.92300000	-2.91300000	-2.16000000
Fe	-0.71600000	6.83000000	5.80100000
O	0.40400000	7.62700000	4.90300000

$^{5}TS1_{O\text{-}M}$

C	1.59800000	6.38400000	9.97400000
H	2.20900000	5.96500000	10.78000000
H	0.68000000	5.80400000	9.90900000
C	2.36900000	6.24800000	8.64700000
H	3.33500000	6.75900000	8.66500000
H	2.58000000	5.17800000	8.52000000
C	1.64300000	6.68800000	7.37600000
O	0.40800000	6.31100000	7.28100000
O	2.23800000	7.35200000	6.50900000

C	-2.58500000	7.17600000	8.86400000
H	-1.95500000	6.51700000	9.46500000
H	-2.92700000	6.57500000	8.02100000
N	-1.31100000	8.33100000	7.03300000
C	-1.81800000	8.35500000	8.33100000
C	-0.67200000	9.48300000	6.83300000
H	-0.17100000	9.78100000	5.92300000
N	-0.74000000	10.25200000	7.93300000
H	-0.26700000	11.15900000	8.04800000
C	-1.45700000	9.56100000	8.89100000
H	-1.64200000	9.98900000	9.86300000
C	-3.09800000	8.16600000	0.91500000
H	-4.14900000	8.17200000	0.61500000
H	-2.54000000	7.45800000	0.30200000
N	-3.73400000	8.25300000	3.37700000
H	-4.66200000	8.64500000	3.19300000
C	-2.89400000	7.82800000	2.36300000
C	-3.14700000	8.02700000	4.56100000
H	-3.59800000	8.22100000	5.52000000
N	-1.95500000	7.46900000	4.36500000
C	-1.80200000	7.30800000	3.00100000
H	-0.94300000	6.82400000	2.57300000
C	-2.01400000	4.35700000	6.99100000
O	-2.28400000	5.42500000	6.28400000
O	-2.41400000	4.17900000	8.14500000
C	-1.10200000	3.29400000	6.37500000
H	-1.52600000	2.31500000	6.63900000
H	-0.17500000	3.37500000	6.95300000
C	-0.78900000	3.34800000	4.89600000
H	0.12300000	2.78700000	4.66500000
H	-0.38000000	4.55400000	4.68700000
C	-1.90700000	3.05400000	3.92100000
H	-1.65000000	3.45000000	2.92800000
H	-2.81300000	3.57500000	4.25300000
C	-2.20000000	1.54300000	3.79200000
H	-2.49000000	1.14300000	4.77300000
H	-1.27700000	1.01500000	3.51300000
C	-3.30200000	1.23400000	2.76800000
H	-2.97300000	1.56500000	1.77300000
H	-4.19600000	1.82600000	3.01000000
C	-3.68800000	-0.24900000	2.71600000
H	-4.04200000	-0.56700000	3.70700000
H	-2.79300000	-0.85400000	2.50800000
C	-4.75700000	-0.56900000	1.66200000

H	-4.34800000	-0.33300000	0.67100000
H	-5.62600000	0.09100000	1.79800000
C	-5.21700000	-2.03400000	1.70600000
H	-5.78300000	-2.20000000	2.63300000
H	-4.33000000	-2.68000000	1.77500000
C	-5.26500000	-2.46100000	-0.82200000
H	-4.26000000	-2.86600000	-0.63800000
H	-5.11900000	-1.42200000	-1.14200000
C	-6.04900000	-2.50000000	0.49900000
H	-6.96200000	-1.89300000	0.41100000
H	-6.38300000	-3.53000000	0.68400000
C	-5.90300000	-3.25200000	-1.96500000
H	-5.93800000	-4.32100000	-1.73100000
H	-5.33800000	-3.13000000	-2.89500000
H	-6.93100000	-2.92400000	-2.16100000
Fe	-0.77800000	6.71500000	5.82300000
O	0.04600000	5.72900000	4.65000000

^{5}IM1$_{O\text{-}M}$

C	1.54700000	6.35700000	10.06000000
H	2.17600000	5.95800000	10.86200000
H	0.62100000	5.78400000	10.04300000
C	2.27300000	6.15800000	8.71500000
H	3.25600000	6.63600000	8.70400000
H	2.42900000	5.07800000	8.61000000
C	1.52400000	6.62400000	7.46700000
O	0.34900000	6.09600000	7.29200000
O	2.04500000	7.45100000	6.69800000
C	-2.53200000	7.26200000	8.83500000
H	-1.91200000	6.58600000	9.42800000
H	-2.88300000	6.66600000	7.99400000
N	-1.17000000	8.36900000	7.02600000
C	-1.74300000	8.42600000	8.29900000
C	-0.53300000	9.51900000	6.82500000
H	0.00200000	9.80000000	5.93000000
N	-0.66100000	10.31800000	7.89800000
H	-0.20500000	11.23400000	8.01100000
C	-1.41800000	9.64900000	8.84000000
H	-1.65100000	10.09800000	9.79300000
C	-3.06600000	8.16600000	0.96200000
H	-4.11200000	8.16600000	0.64500000
H	-2.49400000	7.46900000	0.34800000
N	-3.77800000	8.13000000	3.40800000
H	-4.70800000	8.51200000	3.21800000

C	-2.88800000	7.80000000	2.40600000
C	-3.22800000	7.83600000	4.60200000
H	-3.72900000	7.94100000	5.55000000
N	-2.01200000	7.33600000	4.41800000
C	-1.79800000	7.28600000	3.05400000
H	-0.89400000	6.89100000	2.62900000
C	-2.01400000	4.38100000	7.07500000
O	-2.21000000	5.42900000	6.30800000
O	-2.37900000	4.30100000	8.24700000
C	-1.25400000	3.19900000	6.45900000
H	-1.80900000	2.29800000	6.76500000
H	-0.32300000	3.18300000	7.02900000
C	-0.96800000	3.19300000	4.99600000
H	0.07000000	3.05300000	4.69700000
H	-0.03800000	5.28000000	4.20000000
C	-2.03100000	2.89000000	3.99600000
H	-1.78400000	3.34000000	3.02300000
H	-2.97700000	3.34000000	4.33000000
C	-2.26800000	1.37400000	3.78500000
H	-2.53600000	0.91300000	4.74500000
H	-1.32800000	0.89700000	3.47400000
C	-3.36600000	1.09200000	2.75100000
H	-3.03100000	1.43600000	1.76200000
H	-4.25600000	1.69000000	2.99800000
C	-3.76800000	-0.38300000	2.67800000
H	-4.13400000	-0.70600000	3.66200000
H	-2.87800000	-0.99600000	2.47100000
C	-4.83100000	-0.67700000	1.61300000
H	-4.41300000	-0.43100000	0.62800000
H	-5.69500000	-0.01200000	1.75200000
C	-5.29800000	-2.13900000	1.63900000
H	-5.88400000	-2.30900000	2.55200000
H	-4.41400000	-2.78700000	1.72600000
C	-5.28900000	-2.52500000	-0.89200000
H	-4.28000000	-2.91500000	-0.69500000
H	-5.15300000	-1.48000000	-1.19600000
C	-6.09900000	-2.59600000	0.41100000
H	-7.01800000	-2.00100000	0.31400000
H	-6.41900000	-3.63400000	0.57300000
C	-5.89400000	-3.30900000	-2.05700000
H	-5.90800000	-4.38300000	-1.84300000
H	-5.32000000	-3.15800000	-2.97700000
H	-6.92600000	-2.99900000	-2.25800000
Fe	-0.75900000	6.68900000	5.85100000

O	0.37700000	6.09300000	4.54200000