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A theoretical study into a *trans*-dioxo Mn^{V} porphyrin complex that does not follow oxygen rebound mechanism in C-H bond activation reactions

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Electronic Supplementary Information

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Methods

Electronic energy calculations. Density functional theory (DFT)[S1] was applied using the B3LYP functional[S2] as implemented in the Gaussian 09 (G09) package.[S3] The geometries were optimized using the LACVP basis set, which uses Los Alamos ECP on transition metals[S4] (slightly tweaked as implemented in the Jaguar program, used by us due to historical reasons),[S5] and 6-31G on the rest of the atoms.[S6] The stationary states were confirmed by frequency calculations, and the transition states were connected with the ground states on both sides by performing IRC calculations and continuing relaxing the geometry down to ground state from the end geometry obtained by IRC. The high molecular charge (3+) made it necessary to perform the optimizations in solvent to avoid artificial results (*vide infra*).[S7] The solvent (acetonitrile) effects were included using CPCM model with UFF cavity, per G09 default.[S8] Single-point energy evaluations on the optimized geometry were done with the Def2-TZVPP basis set,[S9] obtained from EMSL Basis Set Library.[S10] This resulting electronic energy (ΔE) was used throughout the text as the final energy due to sufficient accuracy (*vide infra*). The Mulliken spin densities are also taken from Def2-TZVPP calculations, unless otherwise noted.

Free energy calculations. Free energy calculations were done and presented in the ESI tables below, albeit not used in the text (*vide infra*). Dispersion effects were calculated using DFT-D3 program.[S11] MECP was found using a shell program to G09 that iterates to the same energy and geometry for two different spin states.[S12]

In previous trials, we have found that using gas-phase optimizations in HAT reactions for highly charged species (2+ and above) can cause a hydride transfer (i.e. one proton and two electrons) rather than a net hydrogen atom transfer from the substrate to the metal-oxo species, possibly due to self-interaction errors (SIE). Most of the time, performing optimizations in solvent avoids these artificial results;[S7] hence the solvent effects were included during optimizations. However, in doing so, other problems may arise. Adding thermal contributions then becomes in principle inaccurate since the standard solvent models are parameterized to yield good solvation free energies. This means that thermal effects are already included, to a certain extent, in the obtained electronic energies, hence possibly double counting the thermal contributions[S13] (the same consideration applies to the dispersion correction as well). On the other hand, gas-phase frequency calculations on the so obtained structure may not be meaningful either since the structure may not be in a stationary point without the solvent. This leaves us in principle with no easily available options to calculate in a uniform manner the free energies and at the same time avoid SIE, for highly charge systems, unless one is prepared to enlarge the model system to include counter ions,[S14] which may be more time consuming and sometimes leading to 'reactions' between the transition metal complex and the counter ions, which may or may not be realistic.

Assuming though that the above described errors are negligible, the free energies (ΔG) can still be calculated by adding zero-point vibration energy (ΔZ_0), thermal corrections to Z_0 (ΔE(Thermal)) and entropy (-TΔS). Relatively recent consensus is that dispersion effects are needed as well (ΔDisp). Also, if the energy of separated reactants in solvent is evaluated, there is a correction factor of RT•ln(24.5) due to change of standard states (either subtracted from the complexed states or added to the non-complexed states, depending on the reference state).[S15] In C-H activation

reactions, tunnelling is an issue as well,[S16] but is ignored in the current study since its magnitude is not likely to affect the main conclusions. If using separated reactants as the reference point, it is our experience that ΔDisp are usually large, but is roughly cancelled out by -TΔS. At the same time, ΔZ_0 + RT•ln(24.5) is roughly cancelled out by thermal corrections to Z_0 and complexation energy together. Hence, basing the relative energies on ΔE with the complexed reactants as the reference point gives as many times the same values (within some error margins) as free energies ΔG with the separated reactants as the reference point, as evidenced by many, many early days DFT ΔE calculations that gave surprisingly good agreement with experiments without any corrections. Therefore, we use throughout this study the electronic energies (Δ*E*) without any correction factors (except for solvent modelling, which is included by default on all calculations) due to its simplicity, both in calculation and analysis. Our approach is ultimately validated by the good agreement with experiments, within the expected error margins (±3 kcal mol^{-1}).

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Tables

Table S1. Relative energies of the [(Por)OMn^{V}O]$^{-}$ species in different spin states, in kcal/mol.

Multiplicity	Frequency	ΔLACVP	ΔDef2-TZVPP	**ΔE**[a]	ΔZ$_0$	ΔE(Thermal)[b]	-TΔS[b]	ΔDisp	**ΔG**[c]
1	63.1139	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
3 (a)	49.7236	1.70	+6.00	**7.71**	-0.64	+0.22	-1.23	+0.35	**6.40**
3 (b)	*i*982.1234	37.44	----[d]	**37.44**	-4.29	+0.22	-1.11	+0.27	**32.54**
3 (c)	*i*876.3514	18.06	----[d]	**18.06**	-1.74	+0.14	-1.17	+0.24	**15.53**
3 (d)	*i*188.9488	15.82	----[d]	**15.82**	-1.81	+0.10	-0.93	+0.37	**13.55**
3 (e)	58.8815	11.91	+8.41	**20.32**	-1.41	+0.42	-1.57	+0.40	**18.15**
5 (a)	52.0186	38.67	----[d]	**38.67**	-3.31	+0.54	-2.20	+0.57	**34.27**
5 (b)	188.744	3.88	+6.74	**10.62**	-0.73	+0.27	-1.66	+0.39	**8.88**

[a] Electronic energy as sum of the two previous columns. [b] T = 298.15 K. [c] Sum of the five previous columns, but not used in the text due to added uncertainty (see Methods section). [d] Deemed unnecessary calculations due to either not being a ground state (imaginary frequencies present) or too high ΔLACVP energy to be a realistic alternative.

Table S2. Relative singlet-triplet energy difference (^{3}ΔE-^{1}ΔE) for the [(Por)OMn^{V}O]$^{-}$ species using different functionals, in kcal/mol.

Functional (X)	$^{3}\Delta E_{[X/\Delta Def2\text{-}TZVPP//B3LYP/LACVP]}$ - $^{1}\Delta E_{[X/\Delta Def2\text{-}TZVPP//B3LYP/LACVP]}$
B3LYP	7.71
BLYP	26.30
BP86	28.94
M11L	20.71
OLYP	24.18
B3LYP*	14.96
PW91PW91	28.53

Table S3. Relative quartet-doublet energy difference (^{4}ΔE-^{2}ΔE) for the [(Por)OMn^{IV}OH]$^{-}$ species using different functionals, in kcal/mol.

Functional (X)	$^{4}\Delta E_{[X/\Delta Def2\text{-}TZVPP//B3LYP/LACVP]}$ - $^{2}\Delta E_{[X/\Delta Def2\text{-}TZVPP//B3LYP/LACVP]}$
B3LYP	-9.67
BLYP	-2.36
BP86	-2.50
M11L	-1.70
OLYP	-9.38
B3LYP*	-9.44
PW91PW91	-4.36

Table S4. Relative energies for the C-H activation reaction of xanthene by $[(TF_4TMAP)OMn^{V}O]^{3+}$ (**1**), in kcal/mol.

	ΔLACVP	ΔDef2-TZVPP	**ΔE**[a]	ΔZ_0	ΔE(Thermal)[b]	-TΔS[b]	ΔDisp	RT•ln(24.5)[c]	**ΔG**[d]
Mult = 1									
Reactant	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00		**0.00**
TS_{C-H}	9.58	+7.44	**17.02**	-4.59	-0.28	+3.59	-6.60		**9.14**
Intermediate	-16.60	+1.22	**-15.38**	-2.81	+0.55	-0.10	+1.71		**-16.02**
$Mn^{IV}OH$ + C•	-14.92	+0.00	**-14.92**	-3.08	-1.00	-9.75	+7.03	+1.89	**-19.84**
TS_{reb}	-3.41	+5.00	**1.60**	-2.93	-0.19	+3.72	-8.28		**-6.09**
Product	-24.05	+1.95	**-22.10**	-0.25	-0.23	+3.84	-11.69		**-30.43**
Mult = 3 (a)									
Reactant	3.60	+5.94	**9.54**	-0.61	+0.17	-0.63	-0.43		**8.03**
TS_{C-H}	7.23	+6.19	**13.42**	-3.81	-0.42	+3.04	-6.04		**6.19**
Intermediate	-21.58	-1.29	**-22.87**	-1.92	+0.31	-0.27	+0.67		**-24.07**
$Mn^{IV}OH$ + C•	-19.29	-2.92	**-22.21**	-2.18	-1.19	-9.70	+6.93	+1.89	**-26.46**
TS_{reb}	-9.53	+1.19	**-8.34**	-2.70	-0.16	+3.15	-7.21		**-15.26**
Product	-32.37	+2.10	**-30.26**	-0.28	-0.25	+2.94	-11.29		**-39.15**
Mult = 3 (b)									
Reactant	11.74	+10.58	**22.31**	-1.39	+0.40	-1.35	+0.46		**20.44**
TS_{C-H}	14.99	+8.64	**23.63**	-4.06	-0.27	+2.76	-6.06		**16.00**
Intermediate	-15.88	+1.43	**-14.44**	-2.72	+0.54	-1.47	-1.17		**-19.26**
$Mn^{IV}OH$ + C•	-14.92	+0.00	**-14.92**	-3.08	-1.00	-9.75	+7.03	+1.89	**-19.84**
TS_{reb}	-6.58	+2.01	**-4.57**	-2.10	-0.30	+3.64	-7.68		**-11.01**
Product	-35.11	+3.68	**-31.44**	+0.51	-0.34	+3.43	-10.62		**-38.46**
Mult = 5									
Reactant	5.67	+6.88	**12.55**	-0.73	+0.22	-1.16	-0.45		**10.42**
TS_{C-H}	8.88	+6.94	**15.81**	-3.73	-0.40	+2.53	-5.81		**8.42**
Intermediate	-21.88	-1.01	**-22.89**	-1.85	+0.27	+0.93	+0.33		**-23.21**
$Mn^{IV}OH$ + C•	-19.29	-2.92	**-22.21**	-2.18	-1.19	-9.70	+6.93	+1.89	**-26.46**
TS_{reb}	-8.93	+1.57	**-7.35**	-3.13	-0.17	+3.04	-7.23		**-14.85**
Product	-31.91	+2.73	**-29.18**	-0.45	-0.19	+2.69	-11.94		**-39.07**
MECP									
Mult 1 ⇔ 3									
MECP1	5.40	+5.42	**10.82**						
MECP2	9.59	+6.70	**16.29**						

[a] Electronic energy as sum of the two previous columns. [b] T = 298.15 K. [c] Correction for change of standard state for dissociation in solvent. [d] Free energy as sum of the six previous columns, but not used in the text due to added uncertainty (see Methods section).

Table S5. Relative energies for the hydroxylation reaction of xanthene cation by $[(TF_4TMAP)(CH_3CN)Mn^{III}OH]^{4+}$, in kcal/mol.[a]

	ΔLACVP	ΔDef2-TZVPP	**ΔE**[b]	ΔZ$_0$	ΔE(Thermal)[c]	-TΔS[c]	ΔDisp	RT•ln(24.5)[d]	**ΔG**[e]
$Mn^{III}OH + C^+$	1.51	-3.24	**-1.73**	-0.14	-1.53	-9.98	+11.07	+1.89	**-0.42**
Intermediate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00		**0.00**
TS_{reb}	4.85	+2.09	**6.94**	+0.07	-0.73	+3.86	-4.72		**5.42**
Product	0.15	+2.08	**2.24**	+2.05	-0.89	+4.24	-5.67		**1.96**

[a] The calculated system multiplicity is triplet. [b] Electronic energy as sum of the two previous columns. [c] T = 298.15 K. [d] Correction for change of standard state for dissociation in solvent. [e] Sum of the six previous columns, but not used in the text due to added uncertainty (see Methods section).

Table S6. Mulliken spin density distribution of the $[(Por)OMn^VO]^-$ species in different spin states.[a]

Multiplicity	Mn	O^1	O^2	4xN	Porphyrin
1	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**
3 (a)	**2.59**	**0.54**	**-0.95**	**-0.19**	**0.00**
3 (b)[b]	-0.13	0.08	0.08	0.74	1.23
3 (c)[b]	0.42	0.77	0.77	0.10	-0.07
3 (d)[b]	0.04	0.96	0.96	0.10	-0.07
3 (e)	1.30	-0.31	1.01	-0.07	0.07
5 (a)[b]	2.47	0.64	-0.87	0.56	1.20
5 (b)	**2.58**	**0.55**	**1.00**	**-0.14**	**0.01**

[a] The energetically lowest configuration in each spin state is marked in bold. [b] Spin densities are taken from LACVP calculations as larger basis set calculations were deemed unnecessary for these species.

Table S7. Mulliken spin density distribution for the $[(Por)OMn^VO]^-$ species in triplet states.[a]

Functional	Mn	O^1	O^2	4xN	Porphyrin
B3LYP	2.59	0.54	-0.95	-0.19	0.00
BLYP	2.28	0.43	-0.58	-0.18	0.05
BP86	2.31	0.43	-0.57	-0.21	0.05
M11L	2.41	0.72	-0.92	-0.25	0.05
OLYP	2.47	0.47	-0.73	-0.25	0.04
B3LYP*	2.55	0.55	-0.91	-0.19	0.01
PW91PW91	2.33	0.43	-0.60	-0.22	0.05

[a] Spin densities are triplet structure spin densities (the singlet spin densities are all closed shells) taken from X/Def2-TZVPP//B3LYP/LACVP calculations, where X is the investigated functional.

Table S8. Mulliken spin density distribution for the [(Por)OMn^{IV}OH]$^{-}$ species using different functionals.

Multiplicity	Functional	Mn	O^1	O^2	4xN	Porphyrin
2	B3LYP	1.65	-0.59	0.03	-0.16	0.06
	BLYP[a]	0.82	0.22	-0.02	-0.06	0.04
	BP86[a]	0.82	0.22	-0.01	-0.07	0.05
	M11L	1.72	-0.66	0.06	-0.21	0.09
	OLYP[a]	0.95	0.12	-0.03	-0.10	0.06
	B3LYP*	1.43	-0.37	0.02	-0.13	0.06
	PW91PW91[a]	0.88	0.16	-0.02	-0.08	0.05
4	B3LYP	2.64	0.51	0.02	-0.17	0.00
	BLYP	2.52	0.58	0.04	-0.18	0.04
	BP86	2.57	0.57	0.03	-0.22	0.05
	M11L	2.46	0.70	0.03	-0.26	0.07
	OLYP	2.64	0.56	0.02	-0.25	0.03
	B3LYP*	2.57	0.57	0.03	-0.22	0.04
	PW91PW91	2.62	0.53	0.02	-0.18	0.01

[a] The spin densities are somewhat different from the B3LYP one, indicating that the orbital mixing is a bit different. However, despite trials, no other spin density distributions were obtained, prompting us to conclude that this is most likely the lowest energy spin density distribution for the given functional.

Table S9. Mulliken spin density distribution for the C-H activation reaction of xanthene by $[(TF_4TMAP)OMn^{V}O]^{3+}$ (**1**).

	Mn	$O_{inactive}$	O_{active}	4xN	Substrate	Porphyrin	4 x $C_6F_4N(Me)_3$
Mult = 1							
Reactant	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TS	1.42	-0.52	-0.49	-0.15	-0.31	0.05	0.00
Intermediate	1.62	-0.57	0.04	-0.15	-0.99	0.05	0.00
$Mn^{IV}OH$ + C•	1.62	-0.57	0.04	-0.15	-0.99	0.06	0.00
TS_{reb}	1.58	-0.59	0.03	-0.17	-0.56	-0.26	-0.01
Product	0.94	-0.07	0.00	-0.14	0.00	-0.72	-0.01
Mult = 3 (a)							
Reactant	2.56	0.59	-0.95	-0.19	0.00	0.00	0.00
TS	2.58	0.55	-0.66	-0.19	-0.29	0.00	0.00
Intermediate	2.60	0.55	0.01	-0.17	-0.99	0.00	0.00
$Mn^{IV}OH$ + C•	2.59	0.55	0.02	-0.17	-1.00	0.00	0.00
TS_{reb}	2.61	0.50	-0.01	-0.21	-0.66	-0.23	-0.01
Product	2.68	0.44	-0.01	-0.30	0.00	-0.78	-0.03
Mult = 3 (b)							
Reactant	1.45	-0.42	1.03	-0.10	0.00	0.06	0.00
TS	1.44	-0.42	0.76	-0.10	0.28	0.05	0.00
Intermediate	1.62	-0.57	0.05	-0.15	1.00	0.05	0.00
$Mn^{IV}OH$ + C•	1.62	-0.57	0.04	-0.15	1.01	0.06	0.00
TS_{reb}	1.35	-0.05	-0.05	-0.11	0.81	0.03	0.00
Product	1.61	0.45	-0.01	-0.06	0.00	0.01	0.00
Mult = 5							
Reactant	2.53	0.60	1.00	-0.14	0.00	0.00	0.00
TS_{C-H}	2.55	0.59	0.73	-0.14	0.29	-0.01	0.00
Intermediate	2.60	0.55	0.01	-0.17	1.01	0.00	0.00
$Mn^{IV}OH$ + C•	2.59	0.55	0.02	-0.17	1.00	0.00	0.00
TS_{reb}	2.64	0.55	0.02	-0.16	0.77	0.17	0.01
Product	2.66	0.48	-0.01	-0.07	0.00	0.89	0.04
MECP Mult 1 ⇔ 3							
MECP1 (Mult = 1)	1.34	-0.43	-0.79	-0.15	-0.01	0.04	0.00
MECP1 (Mult = 3)	2.47	0.59	-0.86	-0.19	0.00	-0.01	0.00
MECP2 (Mult = 1)	1.42	-0.52	-0.49	-0.15	-0.31	0.05	0.00
MECP2 (Mult = 3)	2.51	0.54	-0.53	-0.18	-0.32	-0.02	0.00

Table S10. Mulliken spin density distribution for the hydroxylation reaction of xanthene cation by $[(TF_4TMAP)(CH_3CN)Mn^{III}OH]^{4+}$ (**2**).

	Mn	CH_3CN	O	4xN	Substrate	Porphyrin	4 x $C_6F_4N(Me)_3$
$Mn^{III}OH$ + C^+	1.97	-0.01	0.07	-0.16	0.01	0.11	0.00
Intermediate	1.99	-0.01	0.06	-0.15	0.01	0.10	0.00
TS_{reb}	2.01	-0.01	0.03	-0.16	0.01	0.12	0.00
Product	2.03	-0.01	0.00	-0.16	0.00	0.14	0.00

Table S11. Selected geometries for the [(Por)OMn^{V}O]$^{-}$ species in different spin states, in Å.[a]

Multiplicity	Mn-O^{1}	Mn-O^{2}	Mn-N^{1}	Mn-N^{2}	Mn-N^{3}	Mn-N^{4}
1	**1.65**	**1.65**	**2.06**	**2.06**	**2.06**	**2.06**
3 (a)	**1.72**	**1.95**	**2.05**	**2.04**	**2.05**	**2.04**
3 (b)	1.65	1.65	2.07	2.07	2.07	2.07
3 (c)	1.75	1.75	2.05	2.05	2.05	2.05
3 (d)	1.80	1.80	2.06	2.04	2.06	2.04
3 (e)	1.72	1.94	2.04	2.05	2.04	2.05
5 (a)	1.72	1.93	2.06	2.05	2.06	2.05
5 (b)	**1.72**	**1.99**	**2.04**	**2.05**	**2.04**	**2.05**

[a] The energetically lowest configuration in each spin state is marked in bold.

Table S12. Selected geometries for the [(Por)OMn^{IV}OH]$^{-}$ species, in Å and °.

Multiplicity	Mn-O	Mn-OH	Mn-N^{1}	Mn-N^{2}	Mn-N^{3}	Mn-N^{4}	O-H	Mn-O-H
2	1.74	1.92	2.05	2.05	2.05	2.05	0.98	110.25
4	1.72	1.99	2.04	2.05	2.05	2.05	0.98	109.35

Table S13. Selected geometries for the C-H activation reaction of xanthene by $[(TF_4TMAP)OMn^{V}O]^{3+}$ (**1**), in Å and °.

	$Mn\text{-}O_{inactive}$	$Mn\text{-}O_{active}$	$O_{active}\text{-}H_{subs}$	$H_{subs}\text{-}C_{subs}$	$O_{active}\text{-}C_{subs}$	$Mn\text{-}O_{active}\text{-}H_{subs}$	$Mn\text{-}O_{active}\text{-}C_{subs}$
Mult = 1							
Reactant	1.65	1.65	2.31	1.10	3.41	145.94	146.03
TS	1.73	1.82	1.38	1.22	2.60	125.71	127.17
Intermediate	1.74	1.91	0.98	4.62	4.27	112.57	142.01
$Mn^{IV}OH + C\bullet$	1.74	1.90	0.98	----	----	112.61	----
TS_{reb}	1.73	1.98	0.98	2.52	2.22	109.99	137.79
Product	1.63	2.30	0.98	2.07	1.50	108.31	139.49
Mult = 3 (a)							
Reactant	1.71	1.94	2.21	1.10	3.31	136.48	137.24
TS	1.71	1.95	1.40	1.21	2.61	124.16	125.37
Intermediate	1.71	1.98	0.98	3.38	3.24	111.63	157.04
$Mn^{IV}OH + C\bullet$	1.71	1.97	0.98	----	----	111.50	----
TS_{reb}	1.70	2.03	0.98	2.59	2.31	110.83	137.93
Product	1.68	2.28	0.98	2.08	1.51	110.12	138.11
Mult = 3 (b)							
Reactant	1.72	1.94	2.26	1.10	3.36	143.27	143.18
TS	1.71	1.94	1.46	1.19	2.65	124.14	125.90
Intermediate	1.74	1.90	0.98	2.77	3.63	113.98	135.08
$Mn^{IV}OH + C\bullet$	1.74	1.90	0.98	----	----	112.61	----
TS_{reb}	1.69	2.00	0.98	2.57	2.41	110.03	134.61
Product	1.72	2.32	0.98	2.07	1.50	108.37	139.88
Mult = 5							
Reactant	1.72	1.98	2.20	1.10	3.30	135.87	136.72
TS	1.72	1.98	1.42	1.20	2.62	124.54	125.77
Intermediate	1.71	1.98	0.98	3.41	3.25	111.48	157.74
$Mn^{IV}OH + C\bullet$	1.71	1.97	0.98	----	----	111.50	----
TS_{reb}	1.70	2.04	0.98	2.59	2.31	110.11	141.16
Product	1.67	2.26	0.98	2.08	1.51	108.96	138.63

Table S14. Selected geometries for the hydroxylation reaction of xanthene cation by $[(TF_4TMAP)(CH_3CN)Mn^{III}OH]^{4+}$ (**2**), in Å and °.

	$Mn\text{-}NCCH_3$	Mn-O	$O\text{-}H_{subs}$	$H_{subs}\text{-}C_{subs}$	$O_{active}\text{-}C_{subs}$	$Mn\text{-}O_{active}\text{-}H_{subs}$	$Mn\text{-}O_{active}\text{-}C_{subs}$
$Mn^{III}OH$	2.15	1.82	0.98	----	----	113.49	----
Intermediate	2.13	1.83	0.98	3.45	3.02	113.57	137.91
TS_{reb}	2.09	1.88	0.98	2.48	2.05	112.03	141.86
Product	2.00	1.98	0.98	2.12	1.56	111.01	137.92

Coordinates

Coordinates are given in xyz-file format, with system total charge/multiplicity given within parenthesis in the comment line.

Xanthene(•)(+)

```
24
(0/1) Xanthene
C 2.00460 4.69149 -4.48259
C 1.45833 5.16586 -5.69468
C 0.77631 4.28213 -6.54748
C 0.64667 2.93115 -6.18016
C 1.86165 3.33568 -4.13749
C 1.18098 2.42907 -4.97744
O -0.05245 2.11506 -7.09612
C -0.22895 0.74473 -6.80499
C 1.03387 0.96479 -4.59320
C 0.26882 0.15334 -5.62740
C -0.93611 0.00546 -7.76949
C -1.15812 -1.36580 -7.56038
C -0.67169 -1.98592 -6.38924
C 0.03304 -1.22503 -5.43949
H -1.29894 0.50840 -8.66105
H -1.70385 -1.94356 -8.30148
H -0.84028 -3.04602 -6.22133
H 0.40864 -1.70219 -4.53636
H 0.52751 0.88967 -3.62004
H 2.02976 0.52308 -4.44418
H 0.34638 4.61936 -7.48606
H 1.56254 6.21135 -5.97204
H 2.53333 5.36963 -3.81852
H 2.28273 2.96915 -3.20328

23
(0/2) Xanthene (-H) radical
C 0.39364 5.52775 -4.67081
C -0.47236 5.45642 -5.78909
C -0.65668 4.23122 -6.46152
C 0.02439 3.09708 -6.00944
C 1.07083 4.38518 -4.22663
C 0.90664 3.12975 -4.88470
O -0.19485 1.89874 -6.71726
C 0.45643 0.71447 -6.31904
C 1.57029 1.92802 -4.47888
C 1.34529 0.71143 -5.19915
C 0.18895 -0.43564 -7.06754
C 0.81501 -1.64746 -6.71156
C 1.70211 -1.68948 -5.60840
C 1.96259 -0.53107 -4.86562
H -0.49469 -0.37862 -7.90922
H 0.61421 -2.54709 -7.28627
H 2.18217 -2.62591 -5.33760
H 2.64321 -0.56368 -4.01811
H 2.24235 1.93866 -3.62601
H -1.31515 4.15202 -7.32128
H -0.99656 6.34378 -6.13220
H 0.53273 6.47432 -4.15569
H 1.73574 4.44022 -3.36788

23
(1/1) Xanthene (-H) cation
C 0.40896 5.49996 -4.66018
C -0.46233 5.42251 -5.78911
C -0.66300 4.22067 -6.47559
C 0.01902 3.08141 -6.02365
C 1.08145 4.36982 -4.21692
C 0.90284 3.11947 -4.89282
O -0.18403 1.89924 -6.70529
C 0.44445 0.73024 -6.32845
C 1.55191 1.92778 -4.50278
C 1.33823 0.72158 -5.20496
C 0.17688 -0.42524 -7.07723
C 0.81180 -1.61352 -6.70201
C 1.70816 -1.66138 -5.59123
C 1.96911 -0.51549 -4.85321
H -0.50441 -0.38085 -7.91927
H 0.61858 -2.51980 -7.26798
H 2.18257 -2.60115 -5.32987
H 2.64779 -0.53781 -4.00589
H 2.22447 1.93849 -3.64883
H -1.32257 4.15372 -7.33329
H -0.98083 6.31649 -6.12218
H 0.54019 6.44974 -4.15304
H 1.74705 4.41423 -3.36010
```

$[(Por)OMn^{V}O]^{-}$

```
39
(-1/1)
Mn -0.00280 -0.00291 -0.14704
O -0.02636 -0.02324 1.50222
O 0.01929 0.01792 -1.79632
N 1.11283 1.72598 -0.11130
N -1.73208 1.11320 -0.15666
N -1.11884 -1.73174 -0.18285
N 1.72591 -1.11877 -0.13740
C 2.49606 1.81199 -0.09423
C 2.89392 3.21701 -0.07502
C 1.73633 3.96365 -0.08093
C 0.62060 3.02178 -0.10411
H 1.63253 5.04111 -0.07130
H 3.91807 3.56715 -0.05956
C 3.38364 0.72716 -0.09562
C -3.02779 0.62123 -0.17855
C -3.96976 1.73715 -0.17650
C -3.22321 2.89458 -0.15348
C -1.81817 2.49641 -0.14125
C -0.73346 3.38383 -0.11731
H -3.57340 3.91880 -0.14520
H -5.04719 1.63355 -0.19063
C -0.62672 -3.02755 -0.19017
C -1.74250 -3.96936 -0.21385
C -2.90002 -3.22262 -0.22024
C -2.50207 -1.81762 -0.20031
C -3.38967 -0.73280 -0.19872
H -3.92420 -3.57268 -0.23625
H -1.63878 -5.04683 -0.22364
C 3.02166 -0.62684 -0.11535
C 3.96355 -1.74278 -0.11650
C 3.21698 -2.90019 -0.13934
C 1.81197 -2.50203 -0.15242
C 0.72735 -3.38953 -0.17659
H 3.56714 -3.92443 -0.14701
H 5.04098 -1.63920 -0.10195
H -0.96251 4.44621 -0.10837
H -4.45196 -0.96170 -0.21403
H 0.95649 -4.45183 -0.18535
H 4.44589 0.95600 -0.08044

39
(-1/3) Species a
Mn -0.00435 -0.00385 -0.05635
O -0.02717 -0.02347 1.65889
O 0.02129 0.01888 -2.00218
N 1.10620 1.71698 -0.08425
N -1.71551 1.10257 -0.17294
N -1.11302 -1.72328 -0.15271
N 1.70975 -1.10786 -0.15499
C 2.49146 1.80794 -0.07305
C 2.88895 3.21082 -0.05292
C 1.73280 3.95702 -0.05922
C 0.61849 3.01693 -0.08343
H 1.62692 5.03400 -0.05325
H 3.91377 3.55824 -0.04079
C 3.38031 0.72898 -0.09453
C -3.01731 0.61430 -0.19482
C -3.95478 1.72845 -0.20346
C -3.20845 2.88522 -0.18016
C -1.80707 2.48987 -0.15738
C -0.73069 3.38192 -0.11638
H -3.55673 3.90977 -0.17675
H -5.03165 1.62337 -0.22270
C -0.62517 -3.02309 -0.16807
C -1.73949 -3.96317 -0.19195
C -2.89562 -3.21694 -0.19829
C -2.49810 -1.81408 -0.17805
C -3.38646 -0.73467 -0.19747
H -3.92035 -3.56425 -0.21871
H -1.63350 -5.04006 -0.20610
C 3.01158 -0.61958 -0.13238
C 3.94929 -1.73350 -0.14359
C 3.20296 -2.89028 -0.16652
C 1.80134 -2.49520 -0.16959
C 0.72451 -3.38764 -0.17567
H 3.55137 -3.91472 -0.17869
H 5.02627 -1.62833 -0.13340
H -0.96221 4.44312 -0.11184
H -4.44854 -0.96127 -0.21771
H 0.95611 -4.44875 -0.18905
H 4.44250 0.95566 -0.08313

39
(-1/3) Species b
Mn -0.00303 -0.00283 -0.14703
O -0.02579 -0.02331 1.50545
O 0.01952 0.01771 -1.79951
N 1.12232 1.73185 -0.11125
N -1.74319 1.11453 -0.15663
N -1.12846 -1.73751 -0.18281
N 1.73701 -1.12015 -0.13742
C 2.49641 1.82905 -0.09386
C 2.89407 3.22646 -0.07408
C 1.72777 3.97674 -0.08081
C 0.62450 3.04326 -0.10383
H 1.62660 5.05455 -0.07119
H 3.91720 3.57858 -0.05811
C 3.39281 0.72906 -0.09535
C -3.03528 0.63656 -0.17838
C -3.97390 1.74582 -0.17693
C -3.22087 2.90998 -0.15383
C -1.83055 2.51424 -0.14125
C -0.73433 3.38734 -0.11736
H -3.57348 3.93347 -0.14596
H -5.05122 1.64454 -0.19129
C -0.63067 -3.04893 -0.19021
C -1.73394 -3.98239 -0.21375
C -2.90024 -3.23210 -0.21959
C -2.50255 -1.83468 -0.20021
C -3.39896 -0.73469 -0.19867
H -3.92338 -3.58420 -0.23525
H -1.63279 -5.06019 -0.22371
C 3.02912 -0.64218 -0.11564
C 3.96772 -1.75145 -0.11683
C 3.21468 -2.91560 -0.14035
C 1.82437 -2.51986 -0.15273
C 0.72816 -3.39299 -0.17661
H 3.56728 -3.93909 -0.14835
H 5.04504 -1.65018 -0.10227
H -0.96384 4.45121 -0.10857
H -4.46114 -0.96355 -0.21399
H 0.95771 -4.45685 -0.18552
H 4.45500 0.95790 -0.07989

39
(-1/3) Species c
Mn -0.00308 -0.00283 -0.14708
O -0.02589 -0.02309 1.60196
O 0.01970 0.01753 -1.89602
N 1.12854 1.70808 -0.11304
N -1.73892 1.08983 -0.15637
N -1.13471 -1.71372 -0.18100
N 1.73275 -1.09547 -0.13768
C 2.51256 1.81076 -0.09456
C 2.89834 3.21801 -0.07373
C 1.73387 3.95354 -0.08102
C 0.62700 3.00180 -0.10494
H 1.61937 5.02995 -0.07111
H 3.91937 3.57705 -0.05688
C 3.40581 0.73208 -0.09545
C -3.04237 0.61302 -0.17849
C -3.97398 1.73612 -0.17712
C -3.21628 2.88607 -0.15415
C -1.81528 2.47506 -0.14132
C -0.72811 3.35918 -0.11773
H -3.55607 3.91384 -0.14632
H -5.05226 1.64214 -0.19165
C -0.63317 -3.00744 -0.18907
C -1.74003 -3.95917 -0.21391
C -2.90452 -3.22366 -0.21938
C -2.51873 -1.81640 -0.19947
C -3.41198 -0.73772 -0.19853
H -3.92556 -3.58270 -0.23553
H -1.62552 -5.03558 -0.22448
C 3.03620 -0.61866 -0.11553
C 3.96781 -1.74176 -0.11641
C 3.21012 -2.89170 -0.14039
C 1.80911 -2.48070 -0.15270
C 0.72194 -3.36483 -0.17633
H 3.54991 -3.91946 -0.14858
H 5.04608 -1.64779 -0.10150
H -0.95757 4.42159 -0.10870
H -4.47415 -0.96653 -0.21435
H 0.95141 -4.42723 -0.18566
H 4.46797 0.96088 -0.07933

39
(-1/3) Species d
Mn -0.00309 -0.00282 -0.14716
O -0.04564 -0.03529 1.65129
O 0.03954 0.02967 -1.94534
N 1.10521 1.72877 -0.10651
N -1.72413 1.09435 -0.15743
N -1.11138 -1.73439 -0.18765
N 1.71796 -1.10000 -0.13655
C 2.48851 1.82790 -0.09029
C 2.88151 3.23455 -0.07181
C 1.72035 3.97467 -0.07886
C 0.61127 3.02466 -0.10095
H 1.61000 5.05151 -0.06995
H 3.90402 3.58955 -0.05579
C 3.37984 0.74726 -0.09317
C -3.02352 0.60030 -0.17952
C -3.96645 1.71149 -0.17847
C -3.22370 2.87186 -0.15380
C -1.81969 2.48090 -0.14162
C -0.74397 3.37800 -0.11643
H -3.57765 3.89471 -0.14486
H -5.04345 1.60441 -0.19445
C -0.61744 -3.03029 -0.19317
C -1.72652 -3.98030 -0.21526
C -2.88768 -3.24018 -0.22232
C -2.49468 -1.83354 -0.20384
C -3.38602 -0.75290 -0.20088
H -3.91019 -3.59519 -0.23832
H -1.61617 -5.05715 -0.22415
C 3.01734 -0.60594 -0.11445
C 3.96028 -1.71713 -0.11544
C 3.21753 -2.87750 -0.14008
C 1.81352 -2.48654 -0.15232
C 0.73779 -3.38364 -0.17759
H 3.57148 -3.90035 -0.14897
H 5.03727 -1.61004 -0.09943
H -0.98297 4.43817 -0.10867
H -4.44824 -0.98208 -0.21536
H 0.97679 -4.44381 -0.18532
H 4.44206 0.97644 -0.07867

39
(-1/3) Species e
Mn -0.00454 -0.00430 -0.03207
O -0.02707 -0.02337 1.68732
O 0.02286 0.01486 -1.97543
N 1.09206 1.71182 -0.14669
N -1.73194 1.10021 -0.09058
N -1.09750 -1.71652 -0.21572
N 1.72394 -1.10735 -0.06900
C 2.47928 1.81256 -0.12988
C 2.87041 3.21566 -0.13222
C 1.70894 3.95767 -0.13809
C 0.60029 3.01307 -0.13951
H 1.60055 5.03465 -0.13505
H 3.89304 3.57031 -0.12341
C 3.37777 0.73870 -0.09009
C -3.02948 0.60811 -0.13281
C -3.97685 1.71792 -0.13642
C -3.23574 2.87820 -0.11121
C -1.83056 2.48496 -0.09227
C -0.75206 3.37688 -0.11145
H -3.58931 3.90124 -0.11438
H -5.05341 1.60878 -0.16399
C -0.60562 -3.01774 -0.22630
C -1.71360 -3.96174 -0.27708
C -2.87507 -3.21970 -0.28491
C -2.48463 -1.81715 -0.23920
C -3.38420 -0.74423 -0.19857
H -3.89744 -3.57417 -0.31163
H -1.60506 -5.03854 -0.29621
C 3.02190 -0.61471 -0.06581
C 3.96946 -1.72439 -0.07279
C 3.22833 -2.88469 -0.09585
C 1.82298 -2.49155 -0.10291
C 0.74567 -3.38246 -0.17176
H 3.58217 -3.90743 -0.11610
H 5.04634 -1.61488 -0.07049
H -0.98221 4.43892 -0.11067
H -4.44422 -0.98194 -0.22578
H 0.97616 -4.44424 -0.19081
H 4.43806 0.97667 -0.08375

39
(-1/5) Species a
Mn -0.00466 -0.00400 -0.03625
O -0.02831 -0.02398 1.68101
O 0.02229 0.01944 -1.96580
N 1.11238 1.72683 -0.06727
N -1.72061 1.10573 -0.16842
N -1.11970 -1.73346 -0.13665
N 1.71472 -1.11121 -0.15009
C 2.49944 1.82483 -0.06170
C 2.89704 3.20323 -0.05178
C 1.72262 3.96133 -0.05929
C 0.63047 3.03136 -0.07291
H 1.62107 5.03867 -0.06063
H 3.92052 3.55455 -0.04614
C 3.38932 0.71568 -0.08397
C -3.02979 0.61972 -0.19643
C -3.96693 1.73919 -0.22320
C -3.22291 2.89233 -0.20084
C -1.81717 2.49896 -0.15968
C -0.74659 3.38477 -0.10755
H -3.57058 3.91695 -0.20988
H -5.04340 1.63390 -0.25410
C -0.63741 -3.03773 -0.15829
C -1.72930 -3.96750 -0.19150
C -2.90377 -3.20946 -0.19673
C -2.50644 -1.83128 -0.16764
C -3.39580 -0.72167 -0.18733
H -3.92699 -3.56058 -0.22315
H -1.62743 -5.04462 -0.21262
C 3.02406 -0.62505 -0.13348
C 3.96192 -1.74382 -0.16327
C 3.21793 -2.89696 -0.18725
C 1.81149 -2.50430 -0.17190
C 0.74013 -3.39073 -0.16673
H 3.56607 -3.92115 -0.21219
H 5.03880 -1.63819 -0.16485
H -0.97947 4.44638 -0.10379
H -4.45881 -0.94723 -0.20760
H 0.97303 -4.45226 -0.18111
H 4.45243 0.94138 -0.07256

39
(-1/5) Species b
Mn -0.00443 -0.00416 -0.03757
O -0.02681 -0.02168 1.68142
O 0.02177 0.01506 -2.02594
N 1.09883 1.70500 -0.13806
N -1.72449 1.10701 -0.11248
N -1.10444 -1.71008 -0.20376
N 1.71723 -1.11358 -0.09258
C 2.48705 1.79777 -0.12373
C 2.88196 3.19897 -0.12410
C 1.72525 3.94540 -0.12911
C 0.61135 3.00830 -0.13190
H 1.61978 5.02237 -0.12786
H 3.90659 3.54690 -0.11790
C 3.38096 0.72305 -0.09509
C -3.02439 0.62025 -0.14399
C -3.96497 1.73423 -0.13778
C -3.21899 2.89028 -0.11271
C -1.81630 2.49226 -0.10408
C -0.73643 3.37982 -0.11316
H -3.56636 3.91517 -0.10733
H -5.04181 1.62841 -0.15663
C -0.61689 -3.01332 -0.21478
C -1.73025 -3.94990 -0.26170
C -2.88691 -3.20340 -0.26962
C -2.49254 -1.80267 -0.22770
C -3.38719 -0.72859 -0.19806
H -3.91127 -3.55108 -0.29733
H -1.62462 -5.02667 -0.28172
C 3.01732 -0.62655 -0.08086
C 3.95781 -1.74065 -0.07834
C 3.21176 -2.89673 -0.09935
C 1.80915 -2.49858 -0.11511
C 0.73014 -3.38546 -0.17131
H 3.55917 -3.92156 -0.11058
H 5.03475 -1.63467 -0.06888
H -0.96121 4.44245 -0.10921
H -4.44774 -0.96174 -0.22157
H 0.95518 -4.44792 -0.18652
H 4.44171 0.95636 -0.08662
```

1 + xanthene

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(3/1) Reactants
Mn -0.23970 0.17766 0.01356
O -0.05490 -0.23786 1.59594
O -0.43633 0.59830 -1.56860
N 1.12248 1.70008 0.25111
N -1.76355 1.46018 0.53273
N -1.60311 -1.34461 -0.22499
N 1.28174 -1.10382 -0.50549
C 2.49173 1.61782 0.06179
C 3.10076 2.91955 0.32697
C 2.08595 3.77379 0.67175
C 0.84448 3.00365 0.62540
H 2.17135 4.82027 0.92688
H 4.15451 3.14935 0.26114
C 3.19942 0.46488 -0.32356
C -3.10897 1.14684 0.62441
C -3.85881 2.32981 1.04257
C -2.95168 3.34567 1.19530
C -1.63613 2.79604 0.87257
C -0.43131 3.52166 0.91496
H -3.15344 4.36107 1.50472
H -4.92606 2.37641 1.20480
C -1.32682 -2.64562 -0.60921
C -2.56827 -3.41552 -0.65668
C -3.58148 -2.56390 -0.30135
C -2.97149 -1.26362 -0.02945
C -3.67885 -0.11257 0.36369
H -4.63485 -2.79475 -0.23362
H -2.65446 -4.46007 -0.91939
C 2.62853 -0.79332 -0.58790
C 3.37812 -1.97617 -1.00608
C 2.46943 -2.98883 -1.17036
C 1.15359 -2.43794 -0.85269
C -0.05163 -3.16216 -0.90273
H 2.67075 -4.00310 -1.48369
H 4.44631 -2.02517 -1.16113
C -0.51413 4.96739 1.30163
C -5.16508 -0.24042 0.51392
C 0.03130 -4.60493 -1.30048
C 4.68775 0.58330 -0.46015
C 5.56728 0.20088 0.56091
C 6.95257 0.30469 0.43510
C 7.56855 0.80022 -0.73460
C 6.69084 1.19080 -1.76429
C 5.30110 1.07914 -1.61402
F 5.06010 -0.29663 1.74929
F 7.71984 -0.10244 1.52013
N 9.06882 0.87125 -0.80331
F 7.13003 1.69889 -2.97587
F 4.51279 1.48138 -2.68116
C 9.62501 1.41107 -2.13600
C 9.59341 1.81364 0.30537
C 9.65866 -0.54807 -0.62638
H 10.74269 -0.46512 -0.70958
H 9.38934 -0.93792 0.35206
H 9.26131 -1.18207 -1.41983
H 10.68007 1.84683 0.21941
H 9.16673 2.80374 0.14092
H 9.30859 1.42627 1.28068
H 10.71059 1.40590 -2.03766
H 9.32132 0.75762 -2.95158
H 9.26962 2.42650 -2.29653
C 0.41594 -5.60856 -0.40628
C 0.50326 -6.96365 -0.75591
C 0.20061 -7.40166 -2.05938
C -0.18479 -6.39091 -2.96652
C -0.26510 -5.04861 -2.59578
F 0.72542 -5.26986 0.90112
F 0.89835 -7.82542 0.25392
F -0.50184 -6.70553 -4.28257
F -0.64426 -4.13163 -3.56309
N 0.25797 -8.82973 -2.52739
C 0.68864 -9.84498 -1.44931
C -1.14561 -9.27067 -3.00646
C 1.28275 -8.95259 -3.68002
H 0.68058 -10.82213 -1.93258
H 1.69237 -9.60959 -1.10128
H -0.02221 -9.83061 -0.62569
H 1.33204 -10.00405 -3.96443
H 0.95583 -8.35252 -4.52569
H 2.25096 -8.61044 -3.31299
H -1.07329 -10.31255 -3.32021
H -1.83768 -9.17167 -2.16924
H -1.45885 -8.65131 -3.84340
C -5.76318 -0.76866 1.66525
C -7.14556 -0.89860 1.79987
C -8.04274 -0.50684 0.78271
C -7.44922 0.02873 -0.37670
C -6.05682 0.15111 -0.48906
F -4.96793 -1.18087 2.72125
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N -9.52025 -0.69008 0.99245
F -8.18390 0.45788 -1.47000
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C -10.39561 -0.23088 -0.19067
C -9.82524 -2.19181 1.20528
C -9.97590 0.13118 2.22128
H -11.42913 -0.40963 0.10601
H -10.23802 0.83010 -0.37270
H -10.15371 -0.81976 -1.07348
H -10.90497 -2.29443 1.31901
H -9.47973 -2.73545 0.32518
H -9.32048 -2.54471 2.10137
H -11.04773 -0.02865 2.34272
H -9.44704 -0.20992 3.10781
H -9.76647 1.18322 2.02450
C -0.20662 5.42203 2.59068
C -0.28528 6.76754 2.95019
C -0.67890 7.77036 2.03783
C -0.99270 7.32104 0.74088
C -0.90752 5.96303 0.40225
F 0.18274 4.51432 3.56134
F 0.04201 7.09373 4.26101
N -0.73286 9.20235 2.49422
F -1.39683 8.17397 -0.27301
F -1.22755 5.61320 -0.89975
C -1.16959 10.20833 1.40995
C -1.75017 9.33472 3.65239
C 0.67368 9.64757 2.96071
H -1.80026 10.38892 3.92631
H -2.72005 8.98620 3.29576
H -1.41585 8.74402 4.50181
H -1.15695 11.18985 1.88415
H -0.46422 10.18508 0.58179
H -2.17589 9.97129 1.07066
H 0.60295 10.69192 3.26657
H 0.99253 9.03510 3.80054
H 1.36055 9.54213 2.11997
C 1.97590 4.69760 -4.46753
C 1.43977 5.17040 -5.68461
C 0.78252 4.28059 -6.55085
C 0.66890 2.92607 -6.19170
C 1.84954 3.33781 -4.13116
C 1.19485 2.42454 -4.98486
O -0.00470 2.10359 -7.12195
C -0.20523 0.73864 -6.81805
C 1.07025 0.95561 -4.61224
C 0.28362 0.15091 -5.63467
C -0.92577 0.00300 -7.77515
C -1.17350 -1.36199 -7.55185
C -0.70138 -1.97768 -6.37269
C 0.01777 -1.21984 -5.43102
H -1.27956 0.50336 -8.67188
H -1.72951 -1.93706 -8.28749
H -0.89140 -3.03175 -6.19076
H 0.38145 -1.69507 -4.52231
H 0.59343 0.86201 -3.62509
H 2.07623 0.52214 -4.50306
H 0.35959 4.61628 -7.49322
H 1.53158 6.21886 -5.95532
H 2.48528 5.38018 -3.79276
H 2.26516 2.97267 -3.19428

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(3/1) C-H Transition State
Mn -0.25743 0.20037 -0.20840
O -0.06712 -0.22804 1.46044
O -0.62016 0.63241 -1.93562
N 1.10525 1.71069 -0.01247
N -1.76977 1.49259 0.31901
N -1.63407 -1.31353 -0.41040
N 1.23875 -1.08407 -0.74554
C 2.47790 1.61890 -0.19032
C 3.09898 2.91094 0.08367
C 2.09109 3.77326 0.42972
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H 2.18738 4.81785 0.68827
H 4.15508 3.13111 0.02284
C 3.17752 0.45888 -0.56772
C -3.11667 1.18958 0.43363
C -3.85609 2.37756 0.85637
C -2.94190 3.38884 0.99403
C -1.63465 2.83008 0.65333
C -0.42411 3.54612 0.68446
H -3.13442 4.40544 1.30525
H -4.92077 2.42966 1.03357
C -1.37330 -2.62267 -0.78095
C -2.61798 -3.38937 -0.79363
C -3.62104 -2.52785 -0.43532
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C -3.69689 -0.06910 0.19572
H -4.67398 -2.75308 -0.34554
H -2.71421 -4.43808 -1.03492
C 2.59220 -0.79295 -0.82844
C 3.33007 -1.98552 -1.23332
C 2.41134 -2.99180 -1.38376
C 1.10252 -2.42621 -1.06856
C -0.10498 -3.14928 -1.08778
H 2.60383 -4.01048 -1.68788
H 4.39745 -2.04583 -1.39028
C -0.48302 4.98313 1.10590
C -5.18150 -0.18921 0.36680
C -0.03661 -4.60030 -1.45556
C 4.67006 0.55655 -0.67421
C 5.52108 0.16736 0.36869
C 6.91014 0.25490 0.27613
C 7.56037 0.73767 -0.88048
C 6.71183 1.13427 -1.93201
C 5.31774 1.04061 -1.81393
F 4.98002 -0.31862 1.54683
F 7.64628 -0.15413 1.38195
N 9.06255 0.79158 -0.91395
F 7.18488 1.63181 -3.13516
F 4.56147 1.44951 -2.90173
C 9.65508 1.31286 -2.23826
C 9.57174 1.73706 0.19931
C 9.63320 -0.63195 -0.71013
H 10.71971 -0.56020 -0.76687
H 9.33604 -1.01052 0.26465
H 9.24982 -1.26947 -1.50756
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H 9.16780 2.73276 0.01283
H 9.25197 1.36516 1.16985
H 10.73797 1.29708 -2.11539
H 9.36264 0.65499 -3.05450
H 9.31407 2.33025 -2.41652
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C 0.50575 -6.94253 -0.89858
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C -0.45523 -5.08219 -2.70328
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H -10.18772 -0.76464 -1.16007
H -10.91583 -2.22727 1.24949
H -9.50349 -2.67593 0.24083
H -9.32251 -2.47663 2.01390
H -11.04344 0.04712 2.25994
H -9.43676 -0.14022 3.01102
H -9.75852 1.25100 1.92599
C -0.08625 5.40604 2.38203
C -0.12859 6.74269 2.77765
C -0.57214 7.77055 1.91751
C -0.98420 7.35321 0.63757
C -0.93532 6.00285 0.26265
F 0.35802 4.47339 3.30468
F 0.28612 7.03438 4.07186
N -0.57395 9.19275 2.40680
F -1.45269 8.23177 -0.32570
F -1.34990 5.68841 -1.02171
C -1.05619 10.22828 1.37071
C -1.51579 9.31844 3.62745
C 0.86573 9.60647 2.79574
H -1.51153 10.36349 3.93928
H -2.51755 9.01685 3.31880
H -1.15398 8.68708 4.43556
H -0.98823 11.20057 1.85888
H -0.40668 10.20295 0.49801
H -2.08801 10.02068 1.09469
H 0.82921 10.64410 3.12919
H 1.22589 8.97036 3.60040
H 1.49870 9.51112 1.91266
C 0.84429 5.03528 -3.89465
C 0.00460 5.22709 -5.01449
C -0.44401 4.11839 -5.75300
C -0.05387 2.82995 -5.35514
C 1.21842 3.73627 -3.51268
C 0.77133 2.60303 -4.23005
O -0.52828 1.76172 -6.14670
C 0.05380 0.48577 -5.98675
C 1.09509 1.20550 -3.80593
C 0.88163 0.18677 -4.88027
C -0.23291 -0.45682 -6.98659
C 0.32709 -1.74285 -6.89479
C 1.17285 -2.06795 -5.81083
C 1.44163 -1.10996 -4.81916
H -0.87461 -0.17559 -7.81625
H 0.11231 -2.48068 -7.66304
H 1.61416 -3.05847 -5.74310
H 2.08935 -1.36294 -3.98313
H 0.31539 0.92870 -2.90499
H 2.07163 1.12007 -3.32139
H -1.07842 4.23760 -6.62623
H -0.29126 6.22923 -5.31267
H 1.19917 5.89147 -3.32768
H 1.86039 3.58999 -2.64735

151
(3/1) Intermediate
Mn 0.13309 0.09142 1.04550
O 0.28149 -0.46004 2.68501
O -0.03553 0.69142 -0.75838
N 1.45399 1.62279 1.38931
N -1.41458 1.32083 1.58020
N -1.19351 -1.40114 0.60082
N 1.68367 -1.12153 0.47900
C 2.83183 1.57885 1.23105
C 3.41468 2.86328 1.60802
C 2.38024 3.67185 2.00217
C 1.15431 2.89094 1.86761
H 2.44407 4.69583 2.34114
H 4.46446 3.11670 1.57341
C 3.56925 0.46849 0.78066
C -2.76339 0.99879 1.57114
C -3.54665 2.13941 2.03854
C -2.65914 3.14452 2.32225
C -1.32437 2.63042 2.02712
C -0.13437 3.36710 2.16887
H -2.88801 4.13165 2.69722
H -4.62190 2.16877 2.14082
C -0.89030 -2.67750 0.15530
C -2.11893 -3.45238 -0.00329
C -3.15738 -2.63022 0.34854
C -2.57237 -1.34727 0.73171
C -3.30973 -0.23516 1.17611
H -4.21062 -2.87173 0.34906
H -2.18127 -4.48055 -0.32970
C 3.02742 -0.78213 0.43449
C 3.81028 -1.92467 -0.02986
C 2.92627 -2.94424 -0.26799
C 1.59353 -2.43548 0.04759
O 0.40266 -3.16966 -0.09968
H 3.15511 -3.93586 -0.63100
H 4.88334 -1.94738 -0.15446
C -0.25319 4.77535 2.66790
C -4.80173 -0.37525 1.23072
C 0.52394 -4.58345 -0.58083
C 5.05419 0.63415 0.65752
C 5.91944 0.55058 1.75631
C 7.30006 0.71308 1.63842
C 7.92595 0.97881 0.40110
C 7.06380 1.05784 -0.70932
C 5.67942 0.88957 -0.56654
F 5.40356 0.28958 3.01464
F 8.05335 0.59878 2.80102
N 9.41838 1.15083 0.35099
F 7.51288 1.30903 -1.99533
F 4.90726 0.99682 -1.71352
C 9.98302 1.45389 -1.05166
C 9.82913 2.33844 1.25368
C 10.10328 -0.15141 0.82817
H 11.18094 -0.00080 0.75691
H 9.82241 -0.35656 1.85846
H 9.78756 -0.96236 0.17076
H 10.90950 2.45707 1.16754
H 9.31623 3.23177 0.89530
H 9.55877 2.12599 2.28503
H 11.06062 1.56458 -0.92854
H 9.76712 0.62365 -1.72091
H 9.55299 2.37963 -1.42907
C 0.92162 -5.62974 0.25726
C 1.05601 -6.95740 -0.17319
C 0.79028 -7.32248 -1.50691
C 0.38748 -6.26919 -2.35640
C 0.25890 -4.95546 -1.90564
F 1.19752 -5.36519 1.58937
F 1.45909 -7.86804 0.78987
F 0.10881 -6.50960 -3.69686
F -0.13073 -3.99230 -2.82200
N 0.91446 -8.71279 -2.06522
C 1.35348 -9.77966 -1.04225
C -0.45523 -9.17416 -2.61626
C 1.97605 -8.72200 -3.18986
H 1.38538 -10.72551 -1.58357
H 2.34273 -9.53550 -0.65952
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H 2.05557 -9.74580 -3.55668
H 1.66325 -8.06114 -3.99466
H 2.92455 -8.39374 -2.76370
H -0.32843 -10.18710 -2.99936
H -1.17323 -9.16316 -1.79556
H -0.77212 -8.51081 -3.41723
C -5.46737 -0.95151 2.32004
C -6.85537 -1.08563 2.36537
C -7.69008 -0.65089 1.31311
C -7.02821 -0.06646 0.21604
C -5.63184 0.05893 0.19316
F -4.73651 -1.40887 3.40378
F -7.39857 -1.67254 3.50214
N -9.17785 -0.83634 1.42668
F -7.69627 0.41313 -0.89884
F -5.06566 0.64122 -0.92953
C -9.98108 -0.33102 0.21132
C -9.50119 -2.34315 1.56568
C -9.70340 -0.05901 2.65653
H -11.02991 -0.52327 0.43751
H -9.81721 0.73659 0.08058
H -9.68373 -0.88409 -0.67761
H -10.58566 -2.44021 1.62840
H -9.12246 -2.85512 0.68020
H -9.03956 -2.73621 2.46825
H -10.78332 -0.20434 2.69882
H -9.23996 -0.44626 3.56069
H -9.46565 0.99660 2.51998
C 0.01357 5.13044 3.99677
C -0.11113 6.43907 4.46356
C -0.51169 7.50362 3.62728
C -0.77818 7.15574 2.28911
C -0.64744 5.83306 1.84248
F 0.40322 4.15559 4.90000
F 0.16966 6.66226 5.80651
N -0.63328 8.88703 4.20292
F -1.17898 8.07910 1.33731
F -0.92403 5.58548 0.50727
C -1.07236 9.96685 3.19362
C -1.69363 8.88384 5.32877
C 0.73772 9.33973 4.75798
H -1.77172 9.90336 5.70759
H -2.64288 8.56146 4.89977
H -1.38051 8.21336 6.12546
H -1.10240 10.90614 3.74630
H -0.34479 10.03190 2.38727
H -2.06246 9.72849 2.80931
H 0.61234 10.34752 5.15492
H 1.05526 8.66539 5.54947
H 1.45443 9.33906 3.93607
C 2.39231 0.49959 -4.22729
C 2.83844 0.44676 -5.57064
C 1.95413 0.04603 -6.59293
C 0.64094 -0.29722 -6.25832
C 1.07365 0.15636 -3.89993
C 0.15719 -0.25729 -4.91382
O -0.20321 -0.69114 -7.31689
C -1.53930 -1.05323 -7.05596
C -1.20032 -0.62746 -4.64688
C -2.05553 -1.02852 -5.72247
C -2.31720 -1.43132 -8.15437
C -3.66111 -1.80469 -7.94903
C -4.20730 -1.79394 -6.64246
C -3.41888 -1.41281 -5.54930
H -1.87614 -1.43192 -9.14664
H -4.27404 -2.10001 -8.79584
H -5.24348 -2.08277 -6.48850
H -3.83865 -1.40390 -4.54612
H 0.32762 1.59297 -0.89083
H -1.57923 -0.60169 -3.62963
H 2.27211 -0.00102 -7.63018
H 3.86175 0.71487 -5.81848
H 3.07934 0.80986 -3.44463
H 0.72665 0.20478 -2.86739

151
(3/1) Reb Transition State
Mn -0.07818 0.24977 -0.24969
O 0.07729 -0.23276 1.40779

O -0.33850 0.91386 -2.09370
N 1.25867 1.79463 0.00450
N -1.60183 1.51389 0.25172
N -1.42241 -1.25254 -0.63168
N 1.44192 -0.97986 -0.82659
C 2.64290 1.72509 -0.13915
C 3.23347 3.01638 0.14985
C 2.20078 3.86801 0.48078
C 0.97429 3.09508 0.40233
H 2.27692 4.91449 0.73893
H 4.28543 3.25948 0.09744
C 3.36858 0.56963 -0.51047
C -2.95845 1.18839 0.30968
C -3.72565 2.35484 0.73549
C -2.83424 3.37701 0.92536
C -1.50459 2.85086 0.61621
C -0.31717 3.59712 0.69287
H -3.05441 4.38327 1.25181
H -4.79705 2.38833 0.87488
C -1.14185 -2.54859 -1.03194
C -2.36693 -3.32654 -1.08919
C -3.39459 -2.48485 -0.71789
C -2.80008 -1.19612 -0.42829
C -3.51424 -0.05848 0.00434
H -4.44467 -2.73118 -0.64694
H -2.44559 -4.37020 -1.35753
C 2.80593 -0.66749 -0.84496
C 3.57029 -1.83843 -1.25954
C 2.67331 -2.84603 -1.49319
C 1.34196 -2.31379 -1.20699
C 0.15437 -3.05808 -1.30380
H 2.89317 -3.84691 -1.83563
H 4.64490 -1.88787 -1.36200
C -0.41979 5.02778 1.11209
C -4.99948 -0.20705 0.14749
C 0.26447 -4.49910 -1.67982
C 4.86339 0.67343 -0.48590
C 5.57861 0.71933 0.72087
C 6.96773 0.82672 0.77085
C 7.76339 0.89620 -0.39361
C 7.05716 0.84134 -1.60994
C 5.65889 0.73441 -1.63445
F 4.89828 0.64107 1.92503
F 7.55616 0.86226 2.03045
N 9.25484 1.03216 -0.26063
F 7.68252 0.89428 -2.84578
F 5.05682 0.70525 -2.88482
C 10.01302 1.10518 -1.60083
C 9.58497 2.33834 0.49946
C 9.82345 -0.18885 0.49956
H 10.90542 -0.06469 0.55453
H 9.40131 -0.22705 1.50078
H 9.57047 -1.08822 -0.06266
H 10.67056 2.40787 0.57602
H 9.18718 3.17516 -0.07579
H 9.14341 2.30726 1.49258
H 11.06973 1.20011 -1.35022
H 9.84519 0.19139 -2.16691
H 9.68207 1.97736 -2.16081
C 0.81884 -5.46074 -0.82361
C 0.93493 -6.81931 -1.14671
C 0.48354 -7.31832 -2.38399
C -0.08660 -6.35868 -3.24872
C -0.18706 -5.01104 -2.90617
F 1.26766 -5.07630 0.43165
F 1.50142 -7.62690 -0.17194
F -0.56770 -6.73345 -4.49942
F -0.74074 -4.15329 -3.84578
N 0.56615 -8.75360 -2.82357
C 1.22702 -9.69637 -1.79886
C -0.85927 -9.29885 -3.07099
C 1.40857 -8.85451 -4.11670
H 1.22975 -10.68801 -2.25114
H 2.24782 -9.37053 -1.60767
H 0.64232 -9.70599 -0.88145
H 1.46151 -9.90843 -4.39224
H 0.93140 -8.28608 -4.91099
H 2.40480 -8.46475 -3.90575
H -0.76434 -10.34137 -3.37728
H -1.41808 -9.22310 -2.13761
H -1.34009 -8.72178 -3.85748
C -5.59551 -0.72540 1.30442
C -6.97585 -0.87983 1.43385
C -7.87446 -0.52362 0.40488
C -7.28389 0.00135 -0.76072
C -5.89314 0.14699 -0.86751
F -4.80009 -1.10404 2.37348
F -7.44580 -1.40907 2.63088
N -9.34951 -0.73289 0.60931
F -8.02094 0.39652 -1.86609
F -5.40108 0.66412 -2.05610
C -10.22732 -0.30848 -0.58461
C -9.62500 -2.23698 0.84267
C -9.82921 0.09691 1.82283
H -11.25884 -0.50263 -0.29039
H -10.08927 0.75258 -0.78160
H -9.96948 -0.90531 -1.45739
H -10.70266 -2.36033 0.95581
H -9.26635 -2.78610 -0.02873
H -9.11514 -2.56680 1.74462
H -10.89757 -0.08585 1.94298
H -9.29592 -0.21684 2.71673
H -9.64404 1.15015 1.60928
C -0.00179 5.48223 2.37212
C -0.09374 6.81813 2.76126
C -0.61937 7.81820 1.91430
C -1.03827 7.37433 0.64524
C -0.93319 6.02641 0.27542
F 0.50991 4.57985 3.29132
F 0.35248 7.13926 4.03935
N -0.69228 9.23782 2.40443
F -1.56315 8.22628 -0.31473
F -1.35286 5.69159 -1.00378
C -1.30507 10.22976 1.39634
C -1.57475 9.30483 3.67303
C 0.73418 9.74774 2.71514
H -1.62808 10.34959 3.98065
H -2.56716 8.93151 3.41778
H -1.12835 8.70641 4.46315
H -1.29910 11.20486 1.88338
H -0.69626 10.25854 0.49533
H -2.32695 9.93327 1.16747
H 0.64918 10.78171 3.05210
H 1.17854 9.13626 3.49704
H 1.32201 9.69156 1.79823
C 2.98960 2.59369 -4.76021
C 2.36621 3.56619 -5.58257
C 1.01434 3.43155 -5.94111
C 0.29653 2.32280 -5.47240
C 2.25983 1.49669 -4.29387
C 0.88862 1.33178 -4.63849
O -1.04289 2.22481 -5.86810
C -1.78556 1.08468 -5.53553
C 0.08895 0.23076 -4.16500
C -1.23474 0.06592 -4.70782
C -3.07977 0.99985 -6.06660
C -3.85704 -0.13488 -5.78002
C -3.33331 -1.17622 -4.97326
C -2.04212 -1.07607 -4.44705
H -3.45590 1.80344 -6.69170
H -4.86149 -0.21416 -6.18605
H -3.93959 -2.05258 -4.76345
H -1.64137 -1.86754 -3.82222
H 0.06818 1.80209 -2.19115
H 0.56648 -0.59922 -3.66109
H 0.51915 4.16067 -6.57449
H 2.93437 4.41966 -5.94139
H 4.03505 2.70360 -4.48889
H 2.73127 0.75576 -3.65602

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(3/1) Hydroxylated Product
Mn 0.08902 -0.18949 0.74362
O 0.23143 -0.63959 2.30421
O -0.25560 0.54935 -1.41166
N 1.42002 1.37951 0.90934
N -1.43739 1.11164 1.01040
N -1.26555 -1.67198 0.30954
N 1.57158 -1.33900 0.01469
C 2.80393 1.31449 0.79925
C 3.39177 2.59657 1.10241
C 2.34697 3.45743 1.39572
C 1.13100 2.69410 1.27111
H 2.41540 4.50432 1.65583
H 4.44537 2.83584 1.07451
C 3.52854 0.16588 0.38293
C -2.80232 0.79430 1.07988
C -3.57008 1.98844 1.42321
C -2.68224 3.01687 1.56913
C -1.34741 2.47681 1.33271
C -0.17339 3.21090 1.46347
H -2.90665 4.04322 1.82319
H -4.64343 2.03028 1.54100
C -0.98277 -2.97415 -0.09491
C -2.19116 -3.75814 -0.13183
C -3.22640 -2.91676 0.24357
C -2.63987 -1.62638 0.50975
C -3.36551 -0.46335 0.87754
H -4.27544 -3.16617 0.31685
H -2.26428 -4.80307 -0.39789
C 2.94108 -1.03514 -0.01326
C 3.69539 -2.19803 -0.47513
C 2.79811 -3.19939 -0.71166
C 1.47295 -2.68377 -0.38325
C 0.31056 -3.44736 -0.43087
H 3.01132 -4.19507 -1.07344
H 4.76779 -2.24279 -0.59671
C -0.28397 4.65641 1.83807
C -4.84594 -0.60896 1.03430
C 0.42080 -4.87469 -0.86641
C 5.01931 0.26241 0.39778
C 5.74840 0.31138 1.59705
C 7.13750 0.42015 1.63299
C 7.92255 0.48867 0.46088
C 7.20348 0.43436 -0.74823
C 5.80552 0.32761 -0.75871
F 5.08166 0.22988 2.80910
F 7.73892 0.45474 2.88715
N 9.41521 0.62410 0.57946
F 7.81672 0.49266 -1.99053
F 5.18963 0.30854 -2.00327
C 10.16028 0.69488 -0.76794
C 9.75335 1.93097 1.33428
C 9.99085 -0.59586 1.33582
H 11.07352 -0.47294 1.37895
H 9.57931 -0.63165 2.34152
H 9.73067 -1.49612 0.77831
H 10.83962 1.99987 1.40111
H 9.35099 2.76708 0.76117
H 9.32044 1.90182 2.33129
H 11.21969 0.78762 -0.52796
H 9.98482 -0.21857 -1.33232
H 9.82565 1.56760 -1.32479
C 0.90804 -5.88496 -0.03014
C 1.00950 -7.22971 -0.41422
C 0.61222 -7.65459 -1.69646
C 0.11355 -6.64054 -2.54310
C 0.02540 -5.30854 -2.13958
F 1.30900 -5.56658 1.25861
F 1.51142 -8.09640 0.54418
F -0.31184 -6.94315 -3.83233
F -0.46283 -4.38956 -3.05521
N 0.67969 -9.06976 -2.20057
C 1.26425 -10.07926 -1.19299
C -0.74668 -9.56084 -2.54183
C 1.58449 -9.13306 -3.45375
H 1.25349 -11.04913 -1.69032
H 2.28622 -9.79830 -0.94564
H 0.64146 -10.10942 -0.30177
H 1.63206 -10.17522 -3.77088
H 1.15926 -8.52189 -4.24576
H 2.57615 -8.77349 -3.17641
H -0.66691 -10.59208 -2.88825
H -1.35042 -9.50837 -1.63503
H -1.17046 -8.93641 -3.32490
C -5.42994 -1.17063 2.17871
C -6.80853 -1.32500 2.32274
C -7.72132 -0.93173 1.31980
C -7.14500 -0.36623 0.16617
C -5.75592 -0.21740 0.04635
F -4.62294 -1.58549 3.22585
F -7.26407 -1.88711 3.51091
N -9.19402 -1.14220 1.53865
F -7.89621 0.06782 -0.91536
F -5.28167 0.33938 -1.13223
C -10.08538 -0.68872 0.36571
C -9.47309 -2.65023 1.74172
C -9.65344 -0.33887 2.77745
H -11.11359 -0.89037 0.66625
H -9.94954 0.37676 0.19297
H -9.83718 -1.26380 -0.52451
H -10.55022 -2.77152 1.86199
H -9.12461 -3.18186 0.85541
H -8.95662 -3.00146 2.63166
H -10.72018 -0.52205 2.91086
H -9.10648 -0.67400 3.65533
H -9.46886 0.71869 2.58513
C -0.21691 5.10055 3.16529
C -0.31298 6.44833 3.51263
C -0.47798 7.46621 2.54814
C -0.54394 7.02906 1.21136
C -0.44667 5.66824 0.88699
F -0.05819 4.17992 4.18809
F -0.24356 6.76233 4.86581
N -0.57542 8.89799 2.99668
F -0.70650 7.89615 0.14228
F -0.51868 5.33185 -0.45607
C -0.73776 9.91808 1.85204
C -1.80913 9.06646 3.91394
C 0.71414 9.29339 3.75394
H -1.86158 10.11641 4.20342
H -2.69643 8.78191 3.34729
H -1.69737 8.44170 4.79695
H -0.78636 10.90028 2.32285
H 0.12315 9.86493 1.18838
H -1.65963 9.71660 1.31035
H 0.61602 10.34062 4.04179
H 0.82412 8.67181 4.63896
H 1.56027 9.16027 3.07890
C 3.01048 2.38263 -3.75652
C 2.41981 3.24696 -4.70657
C 1.07650 3.07653 -5.07463
C 0.33077 2.04329 -4.48035
C 2.24364 1.36506 -3.16884
C 0.88597 1.18440 -3.51065
O -0.99877 1.91027 -4.92000
C -1.72666 0.76832 -4.54038
C 0.04196 0.13073 -2.82553
C -1.24876 -0.13735 -3.57055
C -2.95786 0.57919 -5.19295
C -3.72739 -0.55232 -4.88382
C -3.26162 -1.48853 -3.93267
C -2.03486 -1.27577 -3.28650
H -3.28578 1.30596 -5.92979
H -4.67885 -0.70911 -5.38465
H -3.85344 -2.36904 -3.69990
H -1.68172 -1.98654 -2.54593
H -0.90254 1.28590 -1.38508
H 0.61162 -0.78737 -2.66671
H 0.60418 3.71577 -5.81421
H 3.00620 4.03979 -5.16293
H 4.05371 2.50442 -3.48065
H 2.69289 0.70747 -2.43084

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(3/3) Reactants
Mn -0.11748 -0.23366 0.86438
O 0.10419 -0.66931 2.50535
O -0.38737 0.27096 -0.99150
N 1.24045 1.28894 1.02803
N -1.63016 1.06250 1.30503
N -1.48783 -1.72767 0.59483
N 1.36852 -1.47799 0.22960
C 2.61406 1.19994 0.85757
C 3.22756 2.49864 1.11486
C 2.21395 3.36607 1.42331
C 0.96940 2.60548 1.37031
H 2.30051 4.41695 1.65787
H 4.28391 2.71815 1.06016
C 3.31550 0.05121 0.46140
C -2.97678 0.75237 1.44442
C -3.71646 1.94452 1.83871
C -2.81017 2.96770 1.93126
C -1.50277 2.41305 1.60228
C -0.30233 3.14119 1.62645
H -3.00681 3.99304 2.20850
H -4.77966 1.99220 2.02398
C -1.22748 -3.02426 0.17700
C -2.46484 -3.79852 0.17561
C -3.46402 -2.95798 0.58738
C -2.85075 -1.65860 0.84227
C -3.55331 -0.51114 1.24121
H -4.51244 -3.19243 0.70016
H -2.55628 -4.83986 -0.09675
C 2.72401 -1.18463 0.15575
C 3.45556 -2.35827 -0.30418
C 2.53544 -3.35373 -0.50199
C 1.23033 -2.80526 -0.15554
C 0.02966 -3.53222 -0.18620
H 2.72260 -4.35837 -0.85199
H 4.52259 -2.41168 -0.46407
C -0.38587 4.59955 1.95981
C -5.03098 -0.64436 1.45216
C 0.09277 -4.96272 -0.62704
C 4.80692 0.15069 0.35052
C 5.66043 -0.23541 1.39215
C 7.04914 -0.14695 1.29448
C 7.69451 0.33399 0.13445
C 6.84256 0.72702 -0.91577
C 5.44886 0.63226 -0.79351
F 5.12256 -0.72104 2.57147
F 7.78906 -0.55385 2.39813
N 9.19654 0.38952 0.09631
F 7.31150 1.22243 -2.12106
F 4.68713 1.03779 -1.87814
C 9.78491 0.90978 -1.23036
C 9.70796 1.33716 1.20686
C 9.76921 -1.03330 0.30020
H 10.85546 -0.96042 0.23999
H 9.47553 -1.41094 1.27638
H 9.38398 -1.67212 -0.49529
H 10.79698 1.35163 1.14865
H 9.30209 2.33205 1.02032
H 9.39200 0.96617 2.17898
H 10.86812 0.89545 -1.11019
H 9.49128 0.25036 -2.04488
H 9.44233 1.92658 -1.40904
C 0.51839 -5.99327 0.21654
C 0.56799 -7.33944 -0.17297
C 0.18102 -7.73927 -1.46638
C -0.23850 -6.69983 -2.32468
C -0.27949 -5.36693 -1.91570
F 0.90430 -5.69291 1.51280
F 1.01020 -8.23166 0.78956
F -0.63193 -6.97523 -3.62860
F -0.70044 -4.42020 -2.83462
N 0.18204 -9.15655 -1.96994
C 0.64320 -10.20662 -0.93852
C -1.25454 -9.55624 -2.38445
C 1.14078 -9.27640 -3.17835
H 0.58269 -11.17195 -1.44130
H 1.66997 -10.00487 -0.64039
H -0.02210 -10.19280 -0.07751
H 1.13314 -10.31822 -3.50052
H 0.79529 -8.63462 -3.98531
H 2.14012 -8.98574 -2.85221
H -1.22062 -10.59144 -2.72560
H -1.90070 -9.46291 -1.51073
H -1.59705 -8.91089 -3.18952
C -5.57598 -1.12411 2.64994
C -6.95037 -1.25819 2.84650
C -7.89116 -0.92517 1.84808
C -7.35095 -0.43757 0.64256
C -5.96543 -0.30693 0.46872
F -4.73438 -1.47864 3.69032
F -7.36954 -1.73702 4.08182
N -9.35758 -1.10264 2.12982
F -8.13383 -0.06306 -0.43683
F -5.52124 0.17433 -0.75189
C -10.28464 -0.73034 0.95566
C -9.64857 -2.58612 2.45914
C -9.76406 -0.20019 3.31819
H -11.30204 -0.92271 1.29697
H -10.16481 0.32372 0.71447
H -10.05437 -1.35699 0.09614
H -10.71897 -2.67455 2.64781
H -9.36117 -3.18908 1.59731
H -9.09005 -2.88359 3.34297
H -10.83485 -0.33012 3.47722
H -9.21622 -0.49897 4.20888
H -9.54039 0.83374 3.05291
C -0.09892 5.10244 3.23545
C -0.17789 6.46145 3.54022
C -0.55304 7.42908 2.58327
C -0.84454 6.93083 1.29890
C -0.75845 5.56046 1.01509
F 0.27125 4.23183 4.24634
F 0.13083 6.83722 4.84189
N -0.60932 8.87778 2.98249
F -1.22610 7.74434 0.24499
F -1.05434 5.16099 -0.27828
C -1.03017 9.83977 1.85333
C -1.64181 9.05604 4.12103
C 0.79259 9.33884 3.44808
H -1.69736 10.12041 4.35098
H -2.60613 8.69081 3.76603
H -1.31804 8.50137 4.99832
H -1.02469 10.83961 2.28767
H -0.31251 9.78318 1.03741
H -2.03138 9.58854 1.50939
H 0.71989 10.39380 3.71449
H 1.10170 8.75726 4.31324
H 1.48806 9.20284 2.61876
C 1.41982 4.79768 -3.42587
C 0.98336 5.14264 -4.72305
C 0.71118 4.13204 -5.66057
C 0.88038 2.78595 -5.29220
C 1.58095 3.44342 -3.08189
C 1.31795 2.41053 -4.00668
O 0.58474 1.83694 -6.29608
O 0.68936 0.46028 -5.99687
C 1.49868 0.95135 -3.62161
C 1.11767 -0.00647 -4.73845
O 0.33758 -0.41548 -7.03880
C 0.40967 -1.80269 -6.82727
C 0.83038 -2.30079 -5.57537
C 1.17793 -1.40351 -4.54958
H 0.01468 -0.00401 -7.99070
H 0.13890 -2.48582 -7.62789
H 0.88533 -3.37210 -5.40286
H 1.50325 -1.78680 -3.58425
H 0.89468 0.73418 -2.72596
H 2.54549 0.77784 -3.33121
H 0.37249 4.36828 -6.66513
H 0.85535 6.18544 -5.00085
H 1.63201 5.57391 -2.69570
H 1.91809 3.17711 -2.08206

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(3/3) C-H Transition State
Mn -0.25654 0.18025 -0.13921
O -0.03944 -0.24426 1.50734
O -0.66238 0.64426 -1.99402
N 1.09919 1.69979 -0.00055
N -1.76690 1.47487 0.34706

N -1.63236 -1.31333 -0.38499
N 1.23276 -1.08231 -0.73316
C 2.47329 1.61014 -0.17999
C 3.08957 2.90376 0.08724
C 2.08099 3.76523 0.42884
C 0.83545 3.00778 0.38195
H 2.17330 4.81140 0.68118
H 4.14516 3.12413 0.02317
C 3.17613 0.45510 -0.55635
C -3.11468 1.17202 0.47135
C -3.84878 2.35938 0.89677
C -2.93527 3.37116 1.02388
C -1.63109 2.81589 0.67548
C -0.42779 3.53803 0.69396
H -3.12445 4.38876 1.33284
H -4.91211 2.40915 1.08094
C -1.37051 -2.62128 -0.76646
C -2.61280 -3.38747 -0.77806
C -3.61533 -2.53155 -0.40901
C -2.99869 -1.23209 -0.16193
C -3.69890 -0.08181 0.23469
H -4.66744 -2.75785 -0.31565
H -2.70597 -4.43419 -1.02779
C 2.58782 -0.79240 -0.81654
C 3.32143 -1.98384 -1.22577
C 2.40187 -2.98729 -1.38025
C 1.09499 -2.42340 -1.06298
C -0.10836 -3.14756 -1.08319
H 2.59027 -4.00537 -1.68808
H 4.38853 -2.04292 -1.38319
C -0.48912 4.97769 1.10423
C -5.18196 -0.20377 0.41083
C -0.04273 -4.59627 -1.45945
C 4.66804 0.55316 -0.66344
C 5.51807 0.16685 0.38122
C 6.90711 0.25470 0.28877
C 7.55739 0.73470 -0.86896
C 6.70929 1.12814 -1.92205
C 5.31513 1.03431 -1.80459
F 4.97595 -0.31633 1.55963
F 7.64265 -0.15115 1.39575
N 9.05951 0.78947 -0.90187
F 7.18241 1.62277 -3.12601
F 4.55868 1.44000 -2.89297
C 9.65244 1.30758 -2.22735
C 9.56762 1.73821 0.20927
C 9.63095 -0.63325 -0.69401
H 10.71745 -0.56066 -0.74976
H 9.33317 -1.00977 0.28136
H 9.24900 -1.27294 -1.49037
H 10.65690 1.75147 0.15534
H 9.16356 2.73328 0.01980
H 9.24740 1.36888 1.18064
H 10.73526 1.29254 -2.10393
H 9.36071 0.64735 -3.04191
H 9.31117 2.32440 -2.40842
C 0.40191 -5.58438 -0.57530
C 0.45700 -6.94679 -0.90244
C 0.05656 -7.40925 -2.17069
C -0.38509 -6.41388 -3.06899
C -0.43303 -5.06406 -2.72121
F 0.80072 -5.22293 0.70150
F 0.91876 -7.78996 0.09470
F -0.79298 -6.75177 -4.35365
F -0.87852 -4.16597 -3.67618
N 0.06672 -8.84742 -2.61064
C 0.54945 -9.84398 -1.53711
C -1.36999 -9.28103 -2.98896
C 1.01373 -9.00934 -3.82330
H 0.48917 -10.83304 -1.99128
H 1.57870 -9.62140 -1.26327
H -0.10508 -9.79144 -0.66945
H 1.02620 -10.06616 -4.09209
H 0.64459 -8.41714 -4.65729
H 2.00991 -8.67954 -3.52556
H -1.32826 -10.32967 -3.28532
H -2.00527 -9.15724 -2.11111
H -1.73066 -8.67519 -3.81647
C -5.76281 -0.72288 1.57495
C -7.14315 -0.85150 1.73036
C -8.05472 -0.46748 0.72310
C -7.47827 0.05983 -0.44863
C -6.08768 0.18128 -0.58208
F -4.95196 -1.12788 2.62154
F -7.59872 -1.38293 2.93089
N -9.52903 -0.64989 0.95482
F -8.22852 0.48108 -1.53412
F -5.60764 0.70154 -1.77282
C -10.42118 -0.19978 -0.21928
C -9.83003 -2.15019 1.18298
C -9.96775 0.18000 2.18405
H -11.45019 -0.37894 0.09246
H -10.26846 0.86040 -0.41002
H -10.18981 -0.79352 -1.10165
H -10.90791 -2.25261 1.31307
H -9.49687 -2.70022 0.30211
H -9.31227 -2.49623 2.07430
H -11.03868 0.02466 2.31822
H -9.43013 -0.15822 3.06642
H -9.75668 1.23017 1.97916
C -0.09574 5.41024 2.37795
C -0.14041 6.75004 2.76256
C -0.58320 7.77027 1.89299
C -0.99129 7.34269 0.61517
C -0.93987 5.98948 0.25088
F 0.34787 4.48491 3.30774
F 0.27141 7.05239 4.05488
N -0.58812 9.19623 2.37110
F -1.45852 8.21281 -0.35589
F -1.35116 5.66325 -1.03122
C -1.07034 10.22301 1.32615
C -1.53205 9.32967 3.58949
C 0.85052 9.61521 2.75864
H -1.53265 10.37771 3.89108
H -2.53213 9.02062 3.28275
H -1.16846 8.70783 4.40414
H -1.00480 11.19909 1.80702
H -0.41908 10.19198 0.45496
H -2.10135 10.01173 1.04990
H 0.81198 10.65545 3.08357
H 1.21057 8.98623 3.56893
H 1.48466 9.51366 1.87709
C 0.87208 5.05368 -3.92497
C 0.05563 5.24893 -5.06064
C -0.38334 4.14133 -5.80717
C -0.00734 2.85125 -5.40096
C 1.23238 3.75214 -3.53565
C 0.79366 2.62119 -4.26018
O -0.47336 1.78388 -6.20051
C 0.11330 0.50918 -6.03789
C 1.10040 1.21900 -3.82585
C 0.91752 0.20597 -4.91625
C -0.14694 -0.42732 -7.05069
C 0.41697 -1.71181 -6.95653
C 1.24088 -2.04039 -5.85758
C 1.48331 -1.08734 -4.85335
H -0.77198 -0.14292 -7.89200
H 0.22206 -2.44485 -7.73466
H 1.68622 -3.02899 -5.78723
H 2.11509 -1.34334 -4.00595
H 0.30633 0.94451 -2.95929
H 2.07175 1.13455 -3.33057
H -1.00006 4.26294 -6.69274
H -0.22983 6.25219 -5.36527
H 1.22039 5.90817 -3.35126
H 1.85713 3.60352 -2.65807

151
(3/3) Intermediate
Mn 0.02489 -0.41455 0.85841
O 0.22757 -0.77551 2.52007
O -0.19189 0.02247 -1.06241
N 1.42542 1.06338 0.92292
N -1.44241 0.95116 1.27959
N -1.40107 -1.86329 0.64008
N 1.47013 -1.76572 0.33641
C 2.79281 0.91782 0.74004
C 3.45521 2.20158 0.94210
C 2.47877 3.11386 1.24056
C 1.20666 2.39933 1.22616
H 2.60997 4.16330 1.45989
H 4.51842 2.37973 0.87328
C 3.45486 -0.27505 0.40936
C -2.80137 0.70292 1.40162
C -3.50003 1.93929 1.73769
C -2.55463 2.92731 1.80542
C -1.26505 2.30513 1.52115
C -0.03912 2.98894 1.49696
H -2.71622 3.97363 2.01994
H -4.56374 2.03785 1.89827
C -1.18524 -3.19875 0.32244
C -2.45100 -3.92133 0.35286
C -3.42266 -3.01732 0.69164
C -2.76440 -1.72989 0.87412
C -3.42501 -0.54193 1.22531
H -4.48069 -3.20499 0.80256
H -2.58030 -4.97473 0.15170
C 2.82844 -1.51584 0.21516
C 3.52231 -2.74047 -0.17060
C 2.57282 -3.72074 -0.28101
C 1.28723 -3.10774 0.03868
C 0.05777 -3.78543 0.03372
H 2.72663 -4.75172 -0.56429
H 4.58441 -2.83345 -0.34500
C -0.05733 4.45892 1.78398
C -4.90775 -0.61030 1.42980
C 0.07145 -5.24539 -0.30114
C 4.94351 -0.21698 0.25030
C 5.82181 -0.60898 1.26876
C 7.20810 -0.54452 1.12907
C 7.82620 -0.08272 -0.05323
C 6.94972 0.30894 -1.08352
C 5.55887 0.23791 -0.91950
F 5.31240 -1.06943 2.47089
F 7.97370 -0.95291 2.21457
N 9.32703 -0.03757 -0.13026
F 7.39150 0.78055 -2.30867
F 4.77201 0.64034 -1.98751
C 9.88645 0.47188 -1.47359
C 9.87013 0.91515 0.96074
C 9.89712 -1.46186 0.06834
H 10.98215 -1.39425 -0.01646
H 9.62355 -1.83281 1.05291
H 9.49070 -2.10259 -0.71505
H 10.95704 0.92613 0.87329
H 9.46146 1.90974 0.77858
H 9.57966 0.55149 1.94349
H 10.97219 0.45191 -1.37879
H 9.57043 -0.19043 -2.27710
H 9.54608 1.48995 -1.64975
C 0.47583 -6.22360 0.61267
C 0.49085 -7.59510 0.32133
C 0.08916 -8.07733 -0.93905
C -0.31487 -7.09256 -1.86624
C -0.32202 -5.73314 -1.55448
F 0.87594 -5.84156 1.88303
F 0.91731 -8.42605 1.34412
F -0.72171 -7.45098 -3.14573
F -0.72726 -4.84619 -2.53752
N 0.06266 -9.52567 -1.34328
C 0.50856 -10.50780 -0.24123
C -1.38184 -9.92891 -1.72349
C 1.01426 -9.74488 -2.54342
H 0.42821 -11.50602 -0.67176
H 1.53977 -10.30351 0.03908
H -0.15348 -10.41809 0.61768
H 0.98774 -10.80597 -2.79403
H 0.67643 -9.15362 -3.39118
H 2.01948 -9.44946 -2.24082
H -1.36470 -10.98380 -1.99905
H -2.01914 -9.77191 -0.85264
H -1.72158 -9.33049 -2.56513
C -5.47804 -1.06654 2.62528
C -6.85749 -1.13535 2.81878
C -7.77955 -0.75235 1.82082
C -7.21415 -0.28870 0.61739
C -5.82355 -0.22726 0.44547
F -4.65698 -1.46150 3.66765
F -7.30163 -1.59717 4.05186
N -9.25308 -0.85240 2.10318
F -7.97613 0.12868 -0.46136
F -5.35477 0.23381 -0.77440
C -10.15843 -0.42281 0.93195
C -9.62438 -2.31960 2.42356
C -9.61165 0.06141 3.29887
H -11.18479 -0.56199 1.27207
H -9.98093 0.62435 0.69628
H -9.96260 -1.05571 0.06867
H -10.69556 -2.34735 2.62610
H -9.38408 -2.93044 1.55301
H -9.07216 -2.65692 3.29703
H -10.68904 -0.00795 3.45148
H -9.08709 -0.27825 4.18887
H -9.32670 1.08333 3.04632
C -0.19102 4.97640 3.07920
C -0.19357 6.34621 3.34307
C -0.06055 7.31232 2.32215
C 0.06440 6.80012 1.01639
C 0.06330 5.41913 0.77463
F -0.30999 4.11075 4.15348
F -0.32557 6.73482 4.67094
N -0.05252 8.77172 2.68416
F 0.19140 7.60797 -0.10143
F 0.18305 5.00703 -0.54295
C 0.10546 9.72665 1.48358
C -1.38553 9.14504 3.37367
C 1.13472 9.06235 3.63337
H -1.35155 10.21327 3.58983
H -2.20269 8.91961 2.68788
H -1.48959 8.58060 4.29714
H 0.11194 10.73624 1.89470
H 1.04672 9.52352 0.97663
H -0.73674 9.60668 0.80483
H 1.10851 10.12597 3.87297
H 1.03013 8.47503 4.54237
H 2.05851 8.80969 3.11192
C -3.42543 3.06735 -3.29336
C -3.59201 3.81926 -4.48208
C -2.54596 3.88933 -5.42554
C -1.35168 3.20965 -5.16863
C -2.22420 2.39018 -3.04631
C -1.14576 2.44230 -3.98056
O -0.33785 3.30927 -6.14296
C 0.89264 2.64879 -5.94871
C 0.10144 1.76698 -3.77608
C 1.12772 1.87406 -4.76937
C 1.84990 2.79217 -6.95726
C 3.09894 2.15295 -6.81534
C 3.37046 1.37897 -5.66104
C 2.40332 1.24249 -4.65669
H 1.61858 3.39174 -7.83268
H 3.84985 2.25775 -7.59337
H 4.33449 0.88877 -5.55488
H 2.61327 0.64807 -3.77073
H -0.93388 -0.47762 -1.46569
H 0.24486 1.17769 -2.86953
H -2.65129 4.45894 -6.34413
H -4.52449 4.34342 -4.67207
H -4.23530 3.01598 -2.57040
H -2.08659 1.80834 -2.13819

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(3/3) Reb Transition State
Mn -0.29025 0.01476 -0.02312
O -0.02578 -0.35018 1.62105
O -0.65551 0.36581 -1.99294
N 1.08626 1.53046 -0.00410
N -1.77865 1.36140 0.41859
N -1.70111 -1.44583 -0.22540
N 1.16759 -1.28201 -0.63267
C 2.46421 1.40008 -0.15802
C 3.10950 2.68316 0.11148
C 2.12206 3.57501 0.42395
C 0.85212 2.85439 0.36025
H 2.24314 4.61515 0.68958
H 4.17234 2.87311 0.07723
C 3.14572 0.22770 -0.50028
C -3.13462 1.08820 0.57802
C -3.84047 2.29970 0.93625
C -2.90341 3.31001 0.99224
C -1.61948 2.71769 0.67995
C -0.38921 3.41854 0.67128
H -3.08053 4.35121 1.21995
H -4.90157 2.38155 1.12249
C -1.47062 -2.76546 -0.60524
C -2.72655 -3.51203 -0.56407
C -3.70239 -2.64166 -0.16346
C -3.06315 -1.34492 0.04688
C -3.73747 -0.17967 0.42184
H -4.75410 -2.85173 -0.03144
H -2.84271 -4.55919 -0.80390
C 2.52353 -1.01638 -0.76322
C 3.21370 -2.20367 -1.22386
C 2.26427 -3.19421 -1.36281
C 0.99124 -2.61616 -0.98460
C -0.23615 -3.31512 -0.96422
H 2.42253 -4.20809 -1.70081
H 4.27133 -2.27768 -1.43328
C -0.41878 4.85968 1.07050
C -5.21220 -0.27212 0.65989
C -0.21005 -4.75972 -1.35566
C 4.63827 0.27638 -0.56265
C 5.44398 -0.32709 0.41541
C 6.83663 -0.27570 0.38145
C 7.54480 0.38550 -0.64608
C 6.74649 0.98561 -1.63850
C 5.34703 0.92247 -1.58185
F 4.85196 -0.98281 1.48242
F 7.51938 -0.89737 1.42142
N 9.04746 0.41456 -0.60591
F 7.27809 1.66355 -2.72435
F 4.64857 1.53248 -2.61504
C 9.70318 1.16654 -1.78084
C 9.51245 1.12902 0.68516
H 9.59550 -1.03096 -0.64863
H 10.68400 -0.97006 -0.62588
H 9.23591 -1.58584 0.21446
H 9.25868 -1.49532 -1.57604
H 10.60210 1.16849 0.66609
H 9.09455 2.13648 0.68461
H 9.17500 0.57060 1.55504
H 10.78000 1.10172 -1.62392
H 9.43304 0.68614 -2.71876
H 9.38616 2.20756 -1.76977
C 0.24409 -5.76730 -0.49808
C 0.26996 -7.12589 -0.84367
C -0.16967 -7.56603 -2.10707
C -0.61924 -6.55213 -2.98015
C -0.63847 -5.20659 -2.61333
F 0.68197 -5.43072 0.77325
F 0.74374 -7.98986 0.13093
F -1.06022 -6.86700 -4.26070
F -1.09248 -4.29028 -3.54792
N -0.18613 -8.99762 -2.56792
C 0.30123 -10.01559 -1.51720
C -1.63334 -9.40898 -2.92955
C 0.73913 -9.15325 -3.79748
H 0.21604 -10.99767 -1.98249
H 1.33900 -9.81250 -1.26108
H -0.33492 -9.96379 -0.63593
H 0.72589 -10.20422 -4.08876
H 0.37013 -8.53585 -4.61318
H 1.74617 -8.85026 -3.50772
H -1.60747 -10.45226 -3.24591
H -2.25228 -9.29509 -2.03886
H -2.00177 -8.78443 -3.73942
C -5.75198 -0.75089 1.86130
C -7.12594 -0.83144 2.08817
C -8.07531 -0.44040 1.11953
C -7.54202 0.04461 -0.09025
C -6.15683 0.11982 -0.29433
F -4.90485 -1.15388 2.88034
F -7.53717 -1.30937 3.32748
N -9.54097 -0.55179 1.43653
F -8.33376 0.47133 -1.14468
F -5.72394 0.60232 -1.51955
C -10.47736 -0.12053 0.29077
C -9.89621 -2.02303 1.75548
C -9.87401 0.35288 2.64591
H -11.49441 -0.27429 0.65220
H -10.31640 0.93068 0.06135
H -10.29414 -0.74247 -0.58307
H -10.96138 -2.05811 1.98650
H -9.67620 -2.62564 0.87375
H -9.31918 -2.36446 2.61105
H -10.94626 0.27526 2.82801
H -9.32204 0.01307 3.51918
H -9.60347 1.37799 2.39008
C -0.62893 5.27024 2.39584
C -0.65887 6.61213 2.77302
C -0.48325 7.66353 1.84639
C -0.27110 7.26277 0.51361
C -0.24297 5.90680 0.15897
F -0.79373 4.31990 3.39012
F -0.86334 6.88734 4.12096
N -0.53122 9.08689 2.32744
F -0.08576 8.16273 -0.52385
F -0.04156 5.61315 -1.18254
C -0.34317 10.14042 1.21807
C -1.90721 9.37165 2.97321
C 0.59856 9.32317 3.35631
H -1.90814 10.41443 3.29219
H -2.67883 9.20102 2.22196
H -2.05104 8.71953 3.83113
H -0.39795 11.11370 1.70617
H 0.63168 10.01036 0.75259
H -1.14213 10.04534 0.48497
H 0.53921 10.36451 3.67455
H 0.45977 8.66485 4.21060
H 1.55224 9.12607 2.86584
C -3.11564 4.02577 -3.52031
C -3.76601 3.59192 -4.70287
C -3.17185 2.61489 -5.52104
C -1.93346 2.07869 -5.14558
C -1.88238 3.47883 -3.15376
C -1.25607 2.48321 -3.95820
O -1.37647 1.11817 -5.99994
C -0.09688 0.60809 -5.73849
C -0.00016 1.87319 -3.61688
C 0.61496 0.98486 -4.56327
C 0.43594 -0.27438 -6.68653
C 1.72212 -0.80225 -6.47574
C 2.46278 -0.44112 -5.32237
C 1.91608 0.43673 -4.38108
H -0.14598 -0.53113 -7.56612
H 2.14822 -1.48599 -7.20442
H 3.45710 -0.85099 -5.17013
H 2.47859 0.71031 -3.49384
H -1.61679 0.48309 -2.15425
H 0.57517 2.25345 -2.78390
H -3.64771 2.27365 -6.43495
H -4.72531 4.01708 -4.98383
H -3.58042 4.78419 -2.89694
H -1.38210 3.80740 -2.24839

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(3/3) Hydroxylated Product
Mn 0.08291 -0.17959 0.63565
O 0.32224 -0.57763 2.24699
O -0.34711 0.24443 -1.56112
N 1.44091 1.33544 0.61698
N -1.39769 1.17657 1.05850
N -1.33559 -1.60936 0.27978
N 1.52178 -1.48022 -0.02688
C 2.82927 1.20159 0.44728

C 3.47715 2.47886 0.72120
C 2.49995 3.36744 1.06939
C 1.22483 2.65601 1.02253
H 2.62979 4.40239 1.35082
H 4.53979 2.66665 0.66710
C 3.50548 0.03678 0.10410
C -2.76573 0.91217 1.17348
C -3.46221 2.10251 1.57316
C -2.51183 3.10493 1.70160
C -1.23656 2.51897 1.38633
C 0.00181 3.21990 1.38326
H -2.68533 4.13663 1.97125
H -4.52701 2.18795 1.73643
C -1.11485 -2.94464 -0.07122
C -2.38199 -3.67088 -0.04874
C -3.35606 -2.78505 0.31740
C -2.71352 -1.49547 0.53687
C -3.37833 -0.34438 0.93795
H -4.41217 -2.98476 0.43020
H -2.50617 -4.72005 -0.27427
C 2.88919 -1.21549 -0.14911
C 3.57773 -2.39377 -0.59398
C 2.62423 -3.39117 -0.73719
C 1.35616 -2.81858 -0.37194
C 0.11826 -3.52189 -0.37389
H 2.78674 -4.40343 -1.07780
H 4.63651 -2.46902 -0.79730
C -0.02224 4.65160 1.80130
C -4.85808 -0.42633 1.15044
C 0.15547 -4.97281 -0.71580
C 4.99837 0.08593 0.02724
C 5.81402 -0.46009 1.02939
C 7.20632 -0.41844 0.97188
C 7.90123 0.17430 -0.10533
C 7.09177 0.71915 -1.11996
C 5.69269 0.66697 -1.03886
F 5.23374 -1.04976 2.14024
F 7.90281 -0.98351 2.03503
N 9.40471 0.18429 -0.09627
F 7.61048 1.32773 -2.25216
F 4.97988 1.21939 -2.09380
C 10.04652 0.85799 -1.32494
C 9.90728 0.96205 1.14298
C 9.93081 -1.26977 -0.06972
H 11.02017 -1.22499 -0.08093
H 9.58729 -1.76755 0.83382
H 9.56168 -1.78176 -0.95906
H 10.99677 0.98246 1.09926
H 9.50483 1.97475 1.09527
H 9.57963 0.45842 2.04914
H 11.12509 0.79393 -1.17995
H 9.75762 0.32309 -2.22739
H 9.73711 1.89992 -1.37318
C 0.72201 -5.93475 0.13183
C 0.77925 -7.30179 -0.16919
C 0.25447 -7.80892 -1.37459
C -0.31766 -6.84664 -2.23440
C -0.36221 -5.49020 -1.91398
F 1.24094 -5.54110 1.35640
F 1.36654 -8.10907 0.79384
F -0.85596 -7.22724 -3.46004
F -0.92812 -4.63135 -2.84446
N 0.27150 -9.25387 -1.78863
C 0.91749 -10.20304 -0.76055
C -1.17738 -9.75290 -1.99632
C 1.08006 -9.40735 -3.09755
H 0.85678 -11.20422 -1.18695
H 1.95879 -9.92478 -0.60894
H 0.36162 -10.16038 0.17384
H 1.08791 -10.46705 -3.35584
H 0.60530 -8.83438 -3.89041
H 2.09416 -9.05022 -2.91532
H -1.12317 -10.80169 -2.29101
H -1.71237 -9.64760 -1.05198
H -1.65701 -9.17085 -2.77949
C -5.42151 -0.89034 2.34644
C -6.79967 -0.96084 2.55002
C -7.72940 -0.56951 1.56272
C -7.17219 -0.09595 0.35922
C -5.78291 -0.03268 0.17829
F -4.59500 -1.29430 3.38208
F -7.23554 -1.43191 3.78370
N -9.20105 -0.67060 1.85520
F -7.94297 0.33061 -0.71094
F -5.32548 0.44088 -1.04160
C -10.11461 -0.23484 0.69296
C -9.57096 -2.13891 2.17068
C -9.54986 0.23738 3.05770
H -11.13868 -0.37716 1.03875
H -9.93976 0.81384 0.46215
H -9.92356 -0.86204 -0.17549
H -10.64061 -2.16750 2.38117
H -9.33742 -2.74521 1.29506
H -9.01222 -2.48115 3.03803
H -10.62588 0.16730 3.21965
H -9.01704 -0.10596 3.94139
H -9.26727 1.26047 2.80704
C -0.23578 5.05163 3.12995
C -0.26908 6.38974 3.51912
C -0.09486 7.45031 2.60239
C 0.11880 7.06138 1.26607
C 0.14892 5.70908 0.89882
F -0.39838 4.09244 4.11686
F -0.47323 6.65289 4.87031
N -0.14706 8.86914 3.09630
F 0.29890 7.97231 0.23623
F 0.34186 5.42877 -0.44704
C 0.03857 9.93282 1.99672
C -1.52403 9.14419 3.74363
C 0.98134 9.09980 4.12755
H -1.52782 10.18337 4.07423
H -2.29434 8.98001 2.98957
H -1.66750 8.48225 4.59407
H -0.02071 10.90169 2.49304
H 1.01461 9.81026 1.53174
H -0.75865 9.84083 1.26142
H 0.91931 10.13822 4.45478
H 0.84410 8.43351 4.97588
H 1.93566 8.90952 3.63561
C -2.92588 3.67333 -2.66882
C -3.50556 3.37158 -3.92241
C -2.91130 2.41724 -4.76173
C -1.74172 1.76455 -4.33394
C -1.76403 3.00295 -2.25822
C -1.15762 2.02576 -3.07740
O -1.18417 0.84245 -5.23784
C 0.10594 0.34265 -4.98396
C 0.05447 1.25010 -2.60894
C 0.75928 0.55339 -3.75240
C 0.71024 -0.36862 -6.03543
C 2.01089 -0.86599 -5.86338
C 2.70130 -0.64292 -4.65009
C 2.07419 0.05940 -3.61004
H 0.16576 -0.51005 -6.96395
H 2.48878 -1.41337 -6.67122
H 3.71338 -1.01576 -4.52248
H 2.59959 0.22480 -2.67450
H -0.98827 -0.40980 -1.91179
H 0.74067 1.88377 -2.04316
H -3.32682 2.17944 -5.73609
H -4.40745 3.88462 -4.24486
H -3.37995 4.42027 -2.02417
H -1.32255 3.22431 -1.29140

151
(3/3x) Reactants
Mn -0.24772 0.15717 0.14265
O -0.04898 -0.28854 1.78759
O -0.48219 0.67211 -1.71336
N 1.10620 1.68219 0.34791
N -1.77020 1.45890 0.52178
N -1.61071 -1.34594 -0.14617
N 1.24160 -1.06976 -0.51705
C 2.47715 1.60920 0.15001
C 3.08748 2.90806 0.42051
C 2.07248 3.76196 0.76328
C 0.83222 2.99215 0.71019
H 2.15572 4.80995 1.01253
H 4.14076 3.13835 0.34936
C 3.17881 0.47271 -0.28338
C -3.12279 1.15311 0.61101
C -3.87347 2.33889 1.00520
C -2.96586 3.35499 1.15921
C -1.65056 2.80064 0.86198
C -0.44655 3.52178 0.95244
H -3.16991 4.37213 1.46085
H -4.94176 2.38850 1.15862
C -1.34117 -2.64451 -0.55231
C -2.58026 -3.41571 -0.60367
C -3.59339 -2.56720 -0.24280
C -2.98313 -1.26955 0.03546
C -3.69558 -0.11181 0.39114
H -4.64770 -2.79602 -0.18407
H -2.66567 -4.45645 -0.88121
C 2.59470 -0.76629 -0.59969
C 3.33896 -1.93675 -1.04834
C 2.42875 -2.94763 -1.22179
C 1.11986 -2.40540 -0.87854
C -0.07469 -3.14681 -0.89257
H 2.62786 -3.95738 -1.55052
H 4.40619 -1.98348 -1.21017
C -0.53521 4.96824 1.33252
C -5.18178 -0.23639 0.53832
C 0.01191 -4.58585 -1.30357
C 4.66733 0.58792 -0.42152
C 5.54575 0.21293 0.60309
C 6.93124 0.31410 0.47691
C 7.54805 0.79989 -0.69647
C 6.67123 1.18298 -1.72972
C 5.28130 1.07343 -1.57929
F 5.03716 -0.27691 1.79394
F 7.69765 -0.08602 1.56507
N 9.04842 0.87010 -0.76469
F 7.11133 1.68216 -2.94460
F 4.49329 1.46997 -2.64867
C 9.60569 1.39863 -2.10144
C 9.57230 1.82129 0.33679
C 9.63817 -0.54767 -0.57578
H 10.72237 -0.46482 -0.65694
H 9.36670 -0.93052 0.40480
H 9.24301 -1.18750 -1.36561
H 10.65916 1.85243 0.25235
H 9.14695 2.81041 0.16337
H 9.28559 1.44256 1.31495
H 10.69120 1.39380 -2.00249
H 9.30228 0.73828 -2.91152
H 9.25089 2.41282 -2.27079
C 0.39427 -5.59617 -0.41618
C 0.48667 -6.94790 -0.77740
C 0.19084 -7.37495 -2.08607
C -0.19300 -6.35729 -2.98611
C -0.27791 -5.01841 -2.60388
F 0.69923 -5.26727 0.89466
F 0.88039 -7.81740 0.22623
F -0.50486 -6.66123 -4.30587
F -0.65734 -4.09370 -3.56357
N 0.25329 -8.79881 -2.56603
C 0.68324 -9.82238 -1.49547
C -1.14777 -9.23858 -3.05328
C 1.28205 -8.90979 -3.71626
H 0.67936 -10.79523 -1.98743
H 1.68527 -9.58725 -1.14229
H -0.03024 -9.81743 -0.67404
H 1.33142 -9.95812 -4.01201
H 0.95882 -8.30032 -4.55659
H 2.24918 -8.57276 -3.34184
H -1.07241 -10.27783 -3.37486
H -1.84273 -9.14735 -2.21759
H -1.45936 -8.61326 -3.88641
C -5.78184 -0.76966 1.68655
C -7.16437 -0.89929 1.81916
C -8.06029 -0.50306 0.80264
C -7.46505 0.03748 -0.35357
C -6.07254 0.16009 -0.46381
F -4.98843 -1.18556 2.74257
F -7.63875 -1.44282 3.00711
N -9.53804 -0.68690 1.00985
F -8.19822 0.47090 -1.44621
F -5.57466 0.69236 -1.64225
C -10.41176 -0.22452 -0.17326
C -9.84353 -2.18923 1.21808
C -9.99526 0.13092 2.24039
H -11.44567 -0.40444 0.12131
H -10.25422 0.83702 -0.35201
H -10.16834 -0.81082 -1.05739
H -10.92345 -2.29190 1.32999
H -9.49689 -2.73048 0.33695
H -9.34017 -2.54472 2.11392
H -11.06709 -0.02987 2.36059
H -9.46687 -0.21215 3.12646
H -9.78635 1.18360 2.04650
C -0.23802 5.42909 2.62197
C -0.32350 6.77566 2.97571
C -0.71398 7.77384 2.05701
C -1.01631 7.31866 0.75935
C -0.92432 5.95976 0.42645
F 0.14525 4.52636 3.59976
F -0.00706 7.10761 4.28773
N -0.77699 9.20708 2.50803
F -1.41456 8.16665 -0.26097
F -1.23170 5.60475 -0.87727
C -1.21128 10.20736 1.41760
C -1.80261 9.33879 3.65890
O 0.62455 9.65975 2.98217
H -1.86052 10.39385 3.92787
H -2.76799 8.98313 3.29725
H -1.47065 8.75369 4.51308
H -1.20620 11.19055 1.88850
H -0.50068 10.18445 0.59395
H -2.21440 9.96453 1.07296
H 0.54754 10.70476 3.28424
H 0.94059 9.05119 3.82593
H 1.31718 9.55471 2.14615
C 2.09095 4.65866 -4.56670
C 1.62693 5.10620 -5.82238
C 0.99445 4.20495 -6.69524
C 0.83421 2.86403 -6.30439
C 1.91915 3.31196 -4.19916
C 1.29001 2.38711 -5.05956
O 0.18881 2.02856 -7.24307
C -0.06358 0.67969 -6.90740
C 1.11845 0.93195 -4.65412
C 0.35636 0.11652 -5.68626
C -0.76143 -0.06623 -7.87333
C -1.05620 -1.41663 -7.62046
C -0.65348 -2.00748 -6.40344
C 0.04374 -1.23961 -5.45343
H -1.06178 0.41499 -8.79954
H -1.59516 -1.99956 -8.36260
H -0.88048 -3.04997 -6.19862
H 0.35363 -1.69538 -4.51534
H 0.59917 0.87750 -3.68492
H 2.10935 0.48078 -4.49163
H 0.62573 4.52160 -7.66653
H 1.75477 6.14422 -6.11761
H 2.57981 5.35059 -3.88629
H 2.27956 2.96584 -3.23272

151
(3/3x) C-H Transition State
Mn -0.26553 0.17768 -0.12349
O 0.00022 -0.23720 1.51557
O -0.64928 0.63907 -1.96684
N 1.09386 1.70236 0.00302
N -1.77724 1.46899 0.35903
N -1.63947 -1.31644 -0.36528
N 1.23002 -1.08367 -0.72590
C 2.46654 1.61600 -0.17954
C 3.08343 2.91272 0.08010
C 2.07324 3.77420 0.42101
C 0.82952 3.01058 0.38000
H 2.16529 4.82179 0.66845
H 4.13840 3.13633 0.01300
C 3.16940 0.45765 -0.55308
C -3.12528 1.16954 0.48345
C -3.86241 2.36027 0.89682
C -2.94862 3.37401 1.01717
C -1.64349 2.81407 0.67638
C -0.43838 3.53686 0.69141
H -3.14059 4.39423 1.31631
H -4.92624 2.41299 1.07874
C -1.37747 -2.62324 -0.75495
C -2.61904 -3.39200 -0.77305
C -3.62337 -2.53848 -0.39955
C -3.00610 -1.23998 -0.14453
C -3.70709 -0.08856 0.25353
H -4.67538 -2.76764 -0.30898
H -2.71301 -4.43723 -1.02952
C 2.58341 -0.79297 -0.81425
C 3.31974 -1.98251 -1.22991
C 2.40030 -2.98761 -1.38357
C 1.09400 -2.42315 -1.05845
C -0.11293 -3.14637 -1.07545
H 2.59009 -4.00452 -1.69516
H 4.38644 -2.04118 -1.39200
C -0.50201 4.97869 1.09566
C -5.19040 -0.21185 0.42906
C -0.04780 -4.59369 -1.45924
C 4.66225 0.55542 -0.65598
C 5.50888 0.16511 0.39021
C 6.89836 0.25166 0.30337
C 7.55370 0.73418 -0.85045
C 6.70965 1.13193 -1.90512
C 5.31499 1.03957 -1.79269
F 4.96270 -0.32092 1.56593
F 7.62963 -0.15799 1.41214
N 9.05604 0.78663 -0.87812
F 7.18772 1.62960 -3.10615
F 4.56401 1.44994 -2.88355
C 9.65397 1.30688 -2.20043
C 9.56194 1.73183 0.23692
C 9.62466 -0.63735 -0.67154
H 10.71143 -0.56652 -0.72428
H 9.32361 -1.01522 0.30231
H 9.24380 -1.27500 -1.47006
H 10.65146 1.74328 0.18706
H 9.16042 2.72811 0.04838
H 9.23736 1.36078 1.20620
H 10.73638 1.28998 -2.07368
H 9.36370 0.64910 -3.01753
H 9.31462 2.32455 -2.38027
C 0.40157 -5.58661 -0.58281
C 0.45711 -6.94718 -0.91747
C 0.05204 -7.40346 -2.18651
C -0.39414 -6.40354 -3.07750
C -0.44234 -5.05579 -2.72193
F 0.80497 -5.23236 0.69491
F 0.92380 -7.79549 0.07337
F -0.80630 -6.73500 -4.36278
F -0.89204 -4.15337 -3.67127
N 0.06244 -8.83915 -2.63459
C 0.55035 -9.84098 -1.56848
C -1.37495 -9.27247 -3.01042
C 1.00545 -8.99330 -3.85120
H 0.48931 -10.82763 -2.02781
H 1.58046 -9.61874 -1.29756
H -0.10076 -9.79383 -0.69794
H 1.01681 -10.04833 -4.12704
H 0.63390 -8.39548 -4.68011
H 2.00269 -8.66579 -3.55439
H -1.33300 -10.31931 -3.31308
H -2.00737 -9.15460 -2.12969
H -1.73926 -8.66222 -3.83306
C -5.77198 -0.73547 1.59091
C -7.15230 -0.86508 1.74590
C -8.06408 -0.47780 0.74010
C -7.48743 0.05368 -0.42965
C -6.09689 0.17617 -0.56222
F -4.96172 -1.14391 2.63702
F -7.60805 -1.40052 2.94490
N -9.53841 -0.66134 0.97107
F -8.23785 0.47821 -1.51409
F -5.61759 0.70033 -1.75191
C -10.43035 -0.20796 -0.20185
C -9.83916 -2.16231 1.19471
C -9.97760 0.16466 2.20265
H -11.45945 -0.38830 0.10893
H -10.27779 0.85282 -0.38939
H -10.19850 -0.79889 -1.08597
H -10.91709 -2.26542 1.32400
H -9.50543 -2.70971 0.31241
H -9.32167 -2.51076 2.08515
H -11.04819 0.00735 2.33734
H -9.43874 -0.17497 3.08373
H -9.76830 1.21568 2.00031
C -0.10887 5.41748 2.36743
C -0.15468 6.75870 2.74681
C -0.59884 7.77511 1.87350
C -1.00644 7.34182 0.59740
C -0.95354 5.98718 0.23868
F 0.33563 4.49674 3.30175
F 0.25705 7.06675 4.03810
N -0.60544 9.20290 2.34623
F -1.47430 8.20789 -0.37734
F -1.36372 5.65618 -1.04292
C -1.08953 10.22480 1.29752
C -1.54896 9.33963 3.56447
C 0.83273 9.62533 2.73135
H -1.55211 10.38900 3.86142
H -2.54841 9.02657 3.25972
H -1.18338 8.72231 4.38166
H -1.02524 11.20294 1.77434
H -0.43854 10.19104 0.42624
H -2.12032 10.01087 1.02249
H 0.79314 10.66672 3.05250
H 1.19418 8.99972 3.54363
H 1.46637 9.52136 1.84971
C 0.91121 5.05220 -3.91707
C 0.10648 5.25136 -5.06062
C -0.32576 4.14675 -5.81482
C 0.04565 2.85488 -5.40903
C 1.26700 3.74943 -3.52853
C 0.83562 2.62128 -4.26165
O -0.41316 1.79176 -6.21720
C 0.15914 0.51238 -6.04596
C 1.14195 1.21694 -3.82672
C 0.95209 0.20338 -4.91830
C -0.10306 -0.42398 -7.05879
C 0.44701 -1.71351 -6.95744
C 1.25887 -2.04838 -5.85119
C 1.50340 -1.09565 -4.84747
H -0.71908 -0.13516 -7.90518
H 0.25057 -2.44632 -7.73538
H 1.69295 -3.04151 -5.77511
H 2.12511 -1.35627 -3.99408
H 0.37209 0.94734 -2.96443
H 2.12150 1.13416 -3.34704
H -0.93397 4.27139 -6.70578
H -0.17540 6.25574 -5.36486
H 1.25385 5.90471 -3.33708
H 1.88211 3.59754 -2.64477

151
(3/3x) Intermediate
Mn -0.25677 0.09360 -0.02144
O -0.02704 -0.33450 1.64810
O -0.52031 0.55691 -1.84701
N 1.11979 1.60703 0.13321
N -1.74973 1.39378 0.50337
N -1.64092 -1.39227 -0.27246
N 1.23813 -1.19826 -0.56452
C 2.49280 1.50511 -0.03871
C 3.12148 2.79766 0.21771
C 2.11796 3.67196 0.54663
C 0.86663 2.92040 0.50199

H 2.21916 4.71884 0.79439
H 4.17948 3.00950 0.15888
C 3.18539 0.33591 -0.40122
C -3.10002 1.10314 0.61815
C -3.83120 2.30147 1.02257
C -2.91137 3.31093 1.13745
C -1.60791 2.73900 0.80732
C -0.39796 3.45610 0.80691
H -3.09836 4.33608 1.42325
H -4.89582 2.36339 1.19700
C -1.39199 -2.69627 -0.66991
C -2.64233 -3.45275 -0.69810
C -3.63752 -2.59282 -0.31359
C -3.00498 -1.30297 -0.04647
C -3.69164 -0.14809 0.36983
H -4.69158 -2.81233 -0.22182
H -2.74668 -4.49486 -0.96391
C 2.59210 -0.91316 -0.65650
C 3.31913 -2.10308 -1.09057
C 2.39169 -3.09753 -1.26232
C 1.08882 -2.52804 -0.92805
C -0.12828 -3.23142 -0.98157
H 2.57350 -4.11000 -1.59295
H 4.38521 -2.16771 -1.25482
C -0.46127 4.91040 1.16519
C -5.17627 -0.25798 0.54702
C -0.07877 -4.66700 -1.40794
C 4.67684 0.42642 -0.52239
C 5.53702 0.03585 0.51232
C 6.92535 0.11838 0.40543
C 7.56529 0.59746 -0.75836
C 6.70767 0.99358 -1.80276
C 5.31463 0.90467 -1.67030
F 5.00637 -0.44594 1.69692
F 7.67117 -0.29167 1.50433
N 9.06719 0.64921 -0.80538
F 7.17080 1.48534 -3.01214
F 4.54825 1.31095 -2.75278
C 9.64924 1.16943 -2.13475
C 9.58702 1.59493 0.30274
C 9.63786 -0.77490 -0.60601
H 10.72394 -0.70442 -0.67237
H 9.34886 -1.15263 0.37154
H 9.24648 -1.41215 -1.39979
H 10.67565 1.60759 0.23791
H 9.18162 2.59062 0.11938
H 9.27632 1.22384 1.27651
H 10.73310 1.15288 -2.02053
H 9.34991 0.51138 -2.94826
H 9.30775 2.18710 -2.31062
C 0.34117 -5.69465 -0.55759
C 0.38120 -7.04423 -0.93613
C -0.01039 -7.45233 -2.22552
C -0.42574 -6.41690 -3.09068
C -0.45667 -5.08063 -2.69245
F 0.72969 -5.38829 0.73703
F 0.81849 -7.93207 0.03332
F -0.82271 -6.70036 -4.39227
F -0.87021 -4.13896 -3.62042
N -0.01673 -8.87320 -2.71894
C 0.44128 -9.91763 -1.68064
C -1.45536 -9.26978 -3.12851
C 0.93955 -9.00594 -3.92782
H 0.37607 -10.88642 -2.17615
H 1.46919 -9.71789 -1.38514
H -0.22273 -9.89446 -0.81885
H 0.92821 -10.05029 -4.24173
H 0.59470 -8.36948 -4.73926
H 1.94029 -8.71550 -3.60580
H -1.42609 -10.30719 -3.46333
H -2.09955 -9.16850 -2.25423
H -1.79682 -8.62803 -3.93691
C -5.76006 -0.76816 1.71365
C -7.14131 -0.87914 1.87451
C -8.05188 -0.48530 0.87018
C -7.47294 0.03022 -0.30553
C -6.08136 0.13364 -0.44399
F -4.95121 -1.18044 2.75934
F -7.59960 -1.40030 3.07886
N -9.52787 -0.64001 1.11138
F -8.22218 0.45886 -1.38925
F -5.59978 0.64556 -1.63816
C -10.41857 -0.18035 -0.05994
C -9.85627 -2.13238 1.35092
C -9.94359 0.20508 2.33814
H -11.44868 -0.34231 0.25765
H -10.25024 0.87654 -0.25580
H -10.20070 -0.78071 -0.94113
H -10.93449 -2.21240 1.49333
H -9.54432 -2.69358 0.46944
H -9.33573 -2.48454 2.23819
H -11.01829 0.07917 2.47269
H -9.41495 -0.14534 3.22125
H -9.70395 1.24861 2.13038
C -0.15716 5.38806 2.44657
C -0.21901 6.74203 2.77671
C -0.59403 7.73056 1.84126
C -0.90142 7.25851 0.55082
C -0.83198 5.89264 0.24193
F 0.21423 4.49609 3.43867
F 0.10613 7.09160 4.08206
N -0.63521 9.17205 2.26814
F -1.28487 8.09517 -0.48457
F -1.14516 5.51975 -1.05577
C -1.05996 10.15884 1.16195
C -1.65431 9.33737 3.42074
C 0.77426 9.61388 2.72876
H -1.69898 10.39786 3.67008
H -2.62535 8.98596 3.07015
H -1.32536 8.76466 4.28440
H -1.04273 11.14985 1.61582
H -0.35088 10.11361 0.33791
H -2.06627 9.92179 0.82273
H 0.71178 10.66404 3.01609
H 1.08703 9.01362 3.57972
H 1.46119 9.48824 1.89075
C 0.39169 5.52686 -4.66941
C -0.47261 5.45591 -5.78901
C -0.65604 4.23104 -6.46193
C 0.02463 3.09687 -6.00925
C 1.06834 4.38426 -4.22496
C 0.90585 3.12931 -4.88403
O -0.19351 1.89903 -6.71772
C 0.45782 0.71495 -6.31966
C 1.57052 1.92797 -4.47848
C 1.34611 0.71171 -5.20010
C 0.18955 -0.43516 -7.06793
C 0.81414 -1.64716 -6.71097
C 1.70037 -1.68921 -5.60710
C 1.96197 -0.53087 -4.86531
H -0.49376 -0.37774 -7.90982
H 0.61267 -2.54687 -7.28530
H 2.17890 -2.62615 -5.33512
H 2.64152 -0.56342 -4.01707
H 0.18702 1.12428 -2.22031
H 2.25495 1.94128 -3.63583
H -1.31333 4.15199 -7.32257
H -0.99659 6.34324 -6.13256
H 0.53067 6.47339 -4.15436
H 1.73242 4.43889 -3.36541

151
(3/3x) Reb Transition State
Mn -0.21542 0.07054 -0.09139
O 0.00263 -0.39635 1.52165
O -0.49009 0.43079 -2.03640
N 1.21010 1.54159 0.00036
N -1.67632 1.42867 0.34914
N -1.65774 -1.37552 -0.33365
N 1.23376 -1.25504 -0.70617
C 2.58177 1.38973 -0.14062
C 3.25154 2.66252 0.12214
C 2.27218 3.57778 0.40922
C 0.99573 2.86901 0.33971
H 2.40472 4.62239 0.65303
H 4.31784 2.83571 0.09714
C 3.23871 0.19229 -0.48348
C -3.03173 1.17951 0.50213
C -3.72409 2.41225 0.87244
C -2.77425 3.39847 0.94281
C -1.49164 2.77607 0.61975
C -0.25617 3.45080 0.61046
H -2.93078 4.43924 1.18846
H -4.78610 2.51715 1.04381
C -1.44476 -2.68961 -0.71285
C -2.70959 -3.42710 -0.68024
C -3.67637 -2.54141 -0.28329
C -3.01229 -1.25304 -0.07715
C -3.66020 -0.06711 0.31776
H -4.72774 -2.74479 -0.13731
H -2.83991 -4.47423 -0.91396
C 2.60020 -1.02991 -0.76910
C 3.28588 -2.25095 -1.18945
C 2.32118 -3.20789 -1.36983
C 1.03728 -2.58462 -1.05009
C -0.20167 -3.25325 -1.06043
H 2.46747 -4.22860 -1.69311
H 4.35032 -2.35916 -1.34320
C -0.27706 4.91360 0.94054
C -5.13649 -0.13826 0.56039
C -0.20047 -4.69765 -1.46230
C 4.73672 0.20783 -0.51247
C 5.50378 -0.37440 0.50730
C 6.89823 -0.36375 0.49994
C 7.64356 0.23524 -0.53857
C 6.88269 0.82198 -1.56765
C 5.48104 0.79993 -1.53704
F 4.87069 -0.97647 1.58213
F 7.54276 -0.96849 1.57310
N 9.14577 0.21202 -0.47752
F 7.45367 1.44638 -2.66495
F 4.81933 1.39566 -2.60075
C 9.84477 0.89361 -1.67027
C 9.62060 0.95537 0.79348
C 9.64076 -1.25310 -0.46253
H 10.72999 -1.23050 -0.41749
H 9.24261 -1.76696 0.40896
H 9.30752 -1.73345 -1.38312
H 10.71114 0.95439 0.78711
H 9.24019 1.97687 0.75205
H 9.25260 0.44104 1.67800
H 10.91593 0.79612 -1.49288
H 9.57115 0.38513 -2.59242
H 9.56577 1.94466 -1.70602
C 0.20589 -5.72278 -0.60235
C 0.20272 -7.07916 -0.95784
C -0.22046 -7.49800 -2.23377
C -0.62548 -6.46619 -3.10788
C -0.61508 -5.12318 -2.73154
F 0.62569 -5.40652 0.68039
F 0.63245 -7.96230 0.01969
F -1.05063 -6.76014 -4.39855
F -1.02473 -4.18752 -3.66729
N -0.26271 -8.92495 -2.70678
C 0.18313 -9.96310 -1.65734
C -1.71246 -9.29865 -3.09724
C 0.67919 -9.09349 -3.92229
H 0.09097 -10.93804 -2.13616
H 1.21819 -9.78139 -1.37587
H -0.47083 -9.91067 -0.78913
H 0.64114 -10.14075 -4.22454
H 0.34161 -8.45808 -4.73771
H 1.68905 -8.82215 -3.61217
H -1.70546 -10.34007 -3.42051
H -2.34506 -9.17593 -2.21743
H -2.05094 -8.66000 -3.90925
C -5.68793 -0.12921 1.84920
C -7.06122 -0.20574 2.08065
C -8.00015 -0.30388 1.03096
C -7.45578 -0.30755 -0.26761
C -6.07171 -0.22535 -0.47612
F -4.85223 -0.05765 2.95179
F -7.48240 -0.18590 3.40559
N -9.46538 -0.39530 1.35758
F -8.23540 -0.38498 -1.41071
F -5.63209 -0.22147 -1.79106
C -10.38721 -0.51757 0.12794
C -9.72492 -1.64940 2.22633
C -9.90702 0.87821 2.11578
H -11.40398 -0.59103 0.51404
H -10.28864 0.36965 -0.49426
H -10.13396 -1.41605 -0.43155
H -10.79546 -1.69253 2.42880
H -9.40787 -2.52753 1.66313
H -9.17376 -1.56972 3.16005
H -10.97570 0.78804 2.31433
H -9.35829 0.95434 3.05145
H -9.70899 1.74075 1.47880
C -0.19383 5.39381 2.25348
C -0.23122 6.75468 2.55831
C -0.35652 7.74781 1.56258
C -0.43455 7.27321 0.23909
C -0.39312 5.90020 -0.04253
F -0.07494 4.49812 3.30294
F -0.14642 7.10675 3.90056
N -0.40903 9.19485 1.96792
F -0.55958 8.11218 -0.85635
F -0.48147 5.52236 -1.37379
C -0.54189 10.18498 0.79334
C -1.63749 9.42613 2.87968
C 0.89121 9.57455 2.71460
H -1.66417 10.48649 3.13194
H -2.53260 9.14321 2.32469
H -1.53927 8.83111 3.78457
H -0.56636 11.18129 1.23557
H 0.31922 10.09126 0.13441
H -1.46723 9.99127 0.25479
H 0.82401 10.63272 2.96952
H 0.98194 8.97751 3.61848
H 1.73345 9.39564 2.04545
C -4.28016 3.03152 -3.37812
C -4.62341 2.58464 -4.67882
C -3.62847 2.10335 -5.54701
C -2.30029 2.06998 -5.10293
C -2.95117 2.98831 -2.94692
C -1.92006 2.49940 -3.79848
O -1.34439 1.59735 -6.01308
C 0.01526 1.62459 -5.67490
C -0.54206 2.41989 -3.40022
C 0.43983 2.04258 -4.37967
C 0.91938 1.22831 -6.66864
C 2.29534 1.24775 -6.38303
C 2.75478 1.66272 -5.10795
C 1.84156 2.05102 -4.12293
H 0.54517 0.91885 -7.63943
H 3.00703 0.94483 -7.14567
H 3.81880 1.67390 -4.89476
H 2.19192 2.36353 -3.14299
H 0.29907 0.14480 -2.54609
H -0.22990 2.83239 -2.45093
H -3.86577 1.76408 -6.55040
H -5.65717 2.61694 -5.01084
H -5.05437 3.40699 -2.71516
H -2.68829 3.32548 -1.94903

151
(3/3x) Hydroxylated Product
Mn 0.12471 -0.19627 0.72946
O 0.36365 -0.62809 2.37255
O -0.32515 0.24658 -1.50655
N 1.50653 1.31270 0.73564
N -1.35154 1.16569 1.14611
N -1.31267 -1.61930 0.35796
N 1.55820 -1.48963 0.03656
C 2.87808 1.18242 0.55475
C 3.54092 2.45760 0.81826
C 2.56121 3.35445 1.15804
C 1.29196 2.63311 1.11451
H 2.68950 4.39492 1.42128
H 4.60378 2.64400 0.76005
C 3.54306 -0.00485 0.19281
C -2.71019 0.91038 1.26464
C -3.41433 2.12435 1.67500
C -2.46987 3.11063 1.79625
C -1.18138 2.50652 1.46076
C 0.04600 3.19411 1.44626
H -2.63339 4.14134 2.07774
H -4.47877 2.21583 1.83942
C -1.09972 -2.93985 -0.02039
C -2.36456 -3.66984 -0.01760
C -3.33854 -2.78136 0.36103
C -2.67837 -1.50026 0.59461
C -3.33173 -0.32695 1.01303
H -4.39462 -2.98082 0.47590
H -2.49447 -4.71497 -0.26043
C 2.91947 -1.23968 -0.06569
C 3.61946 -2.44663 -0.50370
C 2.66958 -3.42102 -0.66439
C 1.38163 -2.82026 -0.31859
C 0.15060 -3.50166 -0.34308
H 2.82639 -4.43743 -0.99646
H 4.68188 -2.53303 -0.68315
C 0.02016 4.64718 1.81614
C -4.81755 -0.39964 1.20069
C 0.16714 -4.94530 -0.74456
C 5.03957 0.03962 0.11571
C 5.85055 -0.48222 1.13355
C 7.24349 -0.44110 1.08098
C 7.94175 0.13045 -0.00478
C 7.13604 0.65445 -1.03363
C 5.73685 0.60318 -0.95676
F 5.26466 -1.05385 2.25077
F 7.93550 -0.98907 2.15524
N 9.44530 0.13675 0.00650
F 7.65833 1.24257 -2.17440
F 5.02731 1.13922 -2.02175
C 10.09082 0.79035 -1.23124
C 9.94914 0.93102 1.23489
C 9.96658 -1.31860 0.05570
H 11.05607 -1.27753 0.04543
H 9.62017 -1.80118 0.96640
H 9.59710 -1.84280 -0.82637
H 11.03881 0.94440 1.19300
H 9.55265 1.94509 1.17080
H 9.61699 0.44336 2.14805
H 11.16888 0.72933 -1.08145
H 9.80540 0.24024 -2.12569
H 9.78098 1.83112 -1.29803
C 0.58734 -5.96454 0.11603
C 0.60008 -7.32131 -0.23765
C 0.17923 -7.74712 -1.51202
C -0.23852 -6.72133 -2.38727
C -0.24362 -5.37783 -2.01283
F 1.00484 -5.64196 1.39794
F 1.04218 -8.19794 0.74026
F -0.66091 -7.02210 -3.67734
F -0.66343 -4.44839 -2.95061
N 0.15076 -9.17554 -1.98198
C 0.60750 -10.20717 -0.93070
C -1.29586 -9.56420 -2.36965
C 1.09279 -9.33733 -3.19821
H 0.52211 -11.18414 -1.40664
H 1.64175 -10.01652 -0.65203
H -0.04499 -10.15755 -0.06124
H 1.06686 -10.38599 -3.49681
H 0.74648 -8.70875 -4.01528
H 2.09986 -9.05288 -2.89075
H -1.27942 -10.60628 -2.69045
H -1.92840 -9.44541 -1.48923
H -1.64146 -8.93077 -3.18273
C -5.41143 -0.59865 2.45372
C -6.79389 -0.66912 2.62697
C -7.69665 -0.53982 1.54960
C -7.10801 -0.33730 0.28655
C -5.71551 -0.27362 0.13648
F -4.61113 -0.74229 3.57506
F -7.26144 -0.87840 3.91954
N -9.17477 -0.62402 1.81068
F -7.85007 -0.18680 -0.87401
F -5.22598 -0.06563 -1.14373
C -10.06053 -0.45778 0.55934
C -9.51515 -2.01039 2.40602
C -9.59082 0.49845 2.79054
H -11.09138 -0.54645 0.90310
H -9.89653 0.52510 0.12153
H -9.83672 -1.24586 -0.15644
H -10.59240 -2.03766 2.57234
H -9.22035 -2.77370 1.68446
H -8.98981 -2.14486 3.34856
H -10.66718 0.41465 2.94452
H -9.06814 0.37313 3.73558
H -9.34328 1.45771 2.33404
C 0.09713 5.09206 3.14193
C 0.05461 6.44414 3.48342
C -0.06889 7.46358 2.51449
C -0.14191 7.02472 1.17854
C -0.09671 5.66005 0.85995
F 0.21607 4.16878 4.16731
F 0.13219 6.76013 4.83511
N -0.12523 8.89922 2.95782
F -0.26650 7.89290 0.10595
F -0.18471 5.31888 -0.48112
C -0.24980 9.92076 1.80952
C -1.36022 9.10556 3.86632
C 1.16964 9.25932 3.72352
H -1.38697 10.15827 4.14897
H -1.25141 8.84026 3.29626
H -1.26983 8.48416 4.75418
H -0.27674 10.90461 2.27853
H 0.61540 9.84389 1.15381
H -1.17166 9.74288 1.25985
H 1.10096 10.31074 4.00476
H 1.25348 8.63966 4.61269
H 2.01667 9.09684 3.05610
C -3.39530 3.22782 -2.62202
C -3.89570 2.86803 -3.89423
C -3.14218 2.03866 -4.73831
C -1.89244 1.56830 -4.29771
C -2.15005 2.73923 -2.19908
C -1.38034 1.89009 -3.02400
O -1.18235 0.76408 -5.20720
C 0.16036 0.44992 -4.92837
C -0.07016 1.30353 -2.54113
C 0.74950 0.73331 -3.67983
C 0.88229 -0.15401 -5.97285
C 2.23605 -0.46585 -5.77512
C 2.86079 -0.16558 -4.54304
C 2.11705 0.42712 -3.51124
H 0.38383 -0.35825 -6.91547
H 2.80401 -0.92933 -6.57719
H 3.91207 -0.39363 -4.39389
H 2.59216 0.65004 -2.56079
H -0.93898 -0.44173 -1.84064
H 0.50678 2.03369 -1.96888
H -3.49690 1.75999 -5.72584
H -4.86130 3.23922 -4.22667
H -3.97398 3.87846 -1.97276
H -1.76738 3.00330 -1.21779

151
(3/5) Reactants
Mn -0.12196 -0.23725 0.88044
O 0.09880 -0.67604 2.52774
O -0.39174 0.27711 -1.00727
N 1.23684 1.28546 1.04720
N -1.63369 1.06088 1.29422
N -1.49240 -1.73176 0.60748
N 1.35899 -1.47352 0.23104
C 2.61128 1.19488 0.88525
C 3.22567 2.49192 1.14792
C 2.21110 3.36158 1.44724
C 0.96586 2.60313 1.38400
H 2.29767 4.41276 1.68051
H 4.28277 2.70954 1.10023
C 3.31089 0.04782 0.48163

C -2.98232 0.75279 1.42889
C -3.72389 1.94878 1.80663
C -2.81811 2.97229 1.89607
C -1.50852 2.41452 1.58275
C -0.30843 3.14189 1.62020
H -3.01614 3.99993 2.16352
H -4.78811 1.99816 1.98521
C -1.23246 -3.02743 0.18705
C -2.46846 -3.80349 0.18891
C -3.46785 -2.96387 0.60247
C -2.85529 -1.66372 0.85434
C -3.55884 -0.51256 1.24061
H -4.51605 -3.19898 0.71597
H -2.55928 -4.84467 -0.08434
C 2.71575 -1.18141 0.15886
C 3.44555 -2.35071 -0.31404
C 2.52480 -3.34378 -0.51923
C 1.22089 -2.79883 -0.16380
C 0.02318 -3.53002 -0.18798
H 2.71056 -4.34549 -0.87822
H 4.51232 -2.40291 -0.47585
C -0.39455 4.60235 1.94314
C -5.03691 -0.64376 1.44927
C 0.08717 -4.95862 -0.63494
C 4.80310 0.14352 0.37780
C 5.65081 -0.24281 1.42410
C 7.04019 -0.15743 1.33284
C 7.69212 0.32031 0.17513
C 6.84595 0.71354 -0.87968
C 5.45153 0.62194 -0.76384
F 5.10632 -0.72599 2.60137
F 7.77404 -0.56408 2.44064
N 9.19442 0.37291 0.14397
F 7.32146 1.20638 -2.08344
F 4.69575 1.02794 -1.85245
C 9.78974 0.88929 -1.18112
C 9.70259 1.32166 1.25509
C 9.76371 -1.05042 0.35361
H 10.85037 -0.97929 0.29896
H 9.46442 -1.42574 1.32898
H 9.38177 -1.69032 -0.44260
H 10.79198 1.33279 1.20282
H 9.30069 2.31733 1.06421
H 9.38024 0.95378 2.22631
H 10.87238 0.87283 -1.05634
H 9.49811 0.22893 -1.99560
H 9.45008 1.90645 -1.36334
C 0.51426 -5.99226 0.20402
C 0.56341 -7.33693 -0.19074
C 0.17457 -7.73180 -1.48511
C -0.24598 -6.68909 -2.33892
C -0.28678 -5.35780 -1.92465
F 0.90243 -5.69668 1.50068
F 1.00719 -8.23276 0.76771
F -0.64102 -6.95948 -3.64341
F -0.70971 -4.40756 -2.83898
N 0.17461 -9.14720 -1.99392
C 0.63630 -10.20126 -0.96682
C -1.26250 -9.54477 -2.40870
C 1.13226 -9.26298 -3.20357
H 0.57492 -11.16471 -1.47309
H 1.66344 -10.00103 -0.66898
H -0.02814 -10.19044 -0.10509
H 1.12264 -10.30328 -3.53059
H 0.78728 -8.61687 -4.00729
H 2.13231 -8.97559 -2.87672
H -1.22933 -10.57879 -2.75351
H -1.90799 -9.45423 -1.53418
H -1.60534 -8.89644 -3.21122
C -5.58418 -1.12292 2.64631
C -6.95894 -1.25648 2.84055
C -7.89795 -0.92343 1.84046
C -7.35552 -0.43643 0.63570
C -5.96968 -0.30640 0.46413
F -4.74455 -1.47704 3.68845
F -7.38034 -1.73491 4.07526
N -9.36489 -1.10052 2.11972
F -8.13643 -0.06241 -0.44529
F -5.52332 0.17348 -0.75627
C -10.28986 -0.72782 0.94404
C -9.65670 -2.58397 2.44840
C -9.77326 -0.19816 3.30751
H -11.30791 -0.91946 1.28383
H -10.16899 0.32613 0.70286
H -10.05866 -1.35476 0.08500
H -10.72745 -2.67228 2.63514
H -9.36785 -3.18692 1.58704
H -9.09978 -2.88156 3.33319
H -10.84432 -0.32808 3.46473
H -9.22694 -0.49703 4.19908
H -9.54911 0.83579 3.04271
C -0.11508 5.11488 3.21663
C -0.19380 6.47640 3.51020
C -0.56129 7.43710 2.54337
C -0.84582 6.92911 1.26123
C -0.76006 5.55647 0.98877
F 0.24748 4.25178 4.23673
F 0.10763 6.86190 4.81072
N -0.61614 8.88918 2.93012
F -1.21897 7.73472 0.19826
F -1.04761 5.14764 -0.30359
C -1.02819 9.84225 1.79036
C -1.65496 9.08000 4.06071
C 0.78447 9.35032 3.39958
H -1.70429 10.14576 4.28574
H -2.61948 8.72064 3.70024
H -1.34157 8.52680 4.94267
H -1.02490 10.84571 2.21630
H -0.30491 9.77819 0.97996
H -2.02718 9.58864 1.44180
H 0.71378 10.40812 3.65495
H 1.08646 8.77641 4.27238
H 1.48431 9.20382 2.57571
C 1.46399 4.79276 -3.40742
C 1.03742 5.14310 -4.70643
C 0.76485 4.13607 -5.64770
C 0.92376 2.78824 -5.28116
C 1.61481 3.43682 -3.06531
C 1.35129 2.40740 -3.99382
O 0.62859 1.84313 -6.28887
C 0.72336 0.46522 -5.99202
C 1.52036 0.94640 -3.61054
C 1.14107 -0.00668 -4.73194
C 0.37312 -0.40619 -7.03810
C 0.43588 -1.79427 -6.82924
C 0.84581 -2.29750 -5.57583
C 1.19196 -1.40447 -4.54583
H 0.05863 0.00924 -7.99110
H 0.16628 -2.47406 -7.63308
H 0.89355 -3.36949 -5.40540
H 1.50903 -1.79177 -3.57935
H 0.90851 0.73139 -2.71940
H 2.56407 0.76580 -3.31341
H 0.43363 4.37641 -6.65378
H 0.91735 6.18722 -4.98278
H 1.67641 5.56616 -2.67431
H 1.94413 3.16648 -2.06396

151
(3/5) C-H Transition State
Mn -0.25905 0.17476 -0.11855
O 0.01244 -0.24500 1.52638
O -0.65316 0.64612 -2.00198
N 1.09512 1.69718 0.00747
N -1.77024 1.46473 0.36391
N -1.63533 -1.31350 -0.36602
N 1.22969 -1.08470 -0.72295
C 2.46928 1.60787 -0.17159
C 3.08469 2.90334 0.09005
C 2.07535 3.76547 0.42728
C 0.83066 3.00610 0.38385
H 2.16641 4.81291 0.67477
H 4.14011 3.12422 0.02495
C 3.17282 0.45261 -0.54551
C -3.11856 1.16379 0.49443
C -3.85142 2.35293 0.91450
C -2.93780 3.36578 1.03127
C -1.63463 2.80922 0.68301
C -0.43338 3.53453 0.69491
H -3.12639 4.38552 1.33338
H -4.91417 2.40338 1.10169
C -1.37320 -2.61985 -0.75698
C -2.61430 -3.38711 -0.77010
C -3.61715 -2.53558 -0.39212
C -3.00210 -1.23735 -0.13909
C -3.70333 -0.09015 0.26282
H -4.66861 -2.76401 -0.29675
H -2.70660 -4.43224 -1.02665
C 2.58464 -0.79461 -0.80660
C 3.31797 -1.98483 -1.22082
C 2.39801 -2.98723 -1.37899
C 1.09164 -2.42369 -1.05825
C -0.11265 -3.14591 -1.07950
H 2.58554 -4.00410 -1.69130
H 4.38492 -2.04339 -1.37947
C -0.49727 4.97652 1.09682
C -5.18570 -0.21333 0.44218
C -0.04950 -4.59243 -1.46471
C 4.66500 0.55011 -0.64997
C 5.51243 0.16315 0.39663
C 6.90175 0.24982 0.30735
C 7.55509 0.72908 -0.84897
C 6.70966 1.12323 -1.90393
C 5.31515 1.03071 -1.78959
F 4.96727 -0.31956 1.57384
F 7.63443 -0.15642 1.41609
N 9.05734 0.78243 -0.87859
F 7.18584 1.61736 -3.10688
F 4.56170 1.43705 -2.87982
C 9.65352 1.29939 -2.20306
C 9.56395 1.73110 0.23331
C 9.62711 -0.64068 -0.66878
H 10.71379 -0.56898 -0.72213
H 9.32686 -1.01649 0.30610
H 9.24647 -1.28049 -1.46566
H 10.65339 1.74283 0.18212
H 9.16174 2.72663 0.04236
H 9.24077 1.36269 1.20406
H 10.73607 1.28328 -2.07747
H 9.36271 0.63915 -3.01795
H 9.31363 2.31647 -2.38527
C 0.39325 -5.58689 -0.58684
C 0.44649 -6.94720 -0.92297
C 0.04598 -7.40068 -2.19441
C -0.39334 -6.39873 -3.08655
C -0.43942 -5.05117 -2.72988
F 0.79214 -5.23430 0.69240
F 0.90656 -7.79768 0.06873
F -0.80074 -6.72755 -4.37371
F -0.88273 -4.14594 -3.67911
N 0.05400 -8.83599 -2.64369
C 0.53381 -9.84070 -1.57644
C -1.38305 -9.26450 -3.02654
C 1.00188 -8.99197 -3.85644
H 0.47218 -10.82647 -2.03760
H 1.56317 -9.62192 -1.29994
H -0.12145 -9.79312 -0.70902
H 1.01109 -10.04685 -4.13291
H 0.63560 -8.39250 -4.68650
H 1.99883 -8.66777 -3.55520
H -1.34271 -10.31120 -3.32980
H -2.01931 -9.14541 -2.14874
H -1.74165 -8.65264 -3.85050
C -5.76394 -0.73268 1.60744
C -7.14396 -0.86168 1.76564
C -8.05768 -0.47803 0.76020
C -7.48380 0.04913 -0.41286
C -6.09356 0.17111 -0.54907
F -4.95081 -1.13738 2.65235
F -7.59697 -1.39289 2.96722
N -9.53152 -0.66026 0.99509
F -8.23636 0.46991 -1.49692
F -5.61604 0.69132 -1.74082
C -10.42612 -0.21076 -0.17740
C -9.83225 -2.16037 1.22482
C -9.96751 0.17041 2.22476
H -11.45445 -0.39015 0.13646
H -10.27412 0.84941 -0.36878
H -10.19631 -0.80467 -1.06005
H -10.90986 -2.26252 1.35739
H -9.50119 -2.71100 0.34355
H -9.31257 -2.50597 2.11518
H -11.03834 0.01598 2.36074
H -9.42867 -0.16797 3.10634
H -9.75594 1.22035 2.01919
C -0.10640 5.41681 2.36862
C -0.15234 6.75888 2.74508
C -0.59428 7.77361 1.86867
C -0.99964 7.33824 0.59259
C -0.94673 5.98290 0.23647
F 0.33613 4.49730 3.30464
F 0.25727 7.06918 4.03619
N -0.60086 9.20236 2.33838
F -1.46547 8.20236 -0.38447
F -1.35515 5.64870 -1.04451
C -1.08244 10.22259 1.28673
C -1.54636 9.34210 3.55488
C 0.83705 9.62466 2.72498
H -1.55017 10.39227 3.84887
H -2.54527 9.02792 3.24952
H -1.18182 8.72717 4.37433
H -1.01846 11.20154 1.76193
H -0.42977 10.18692 0.41678
H -2.11284 10.00885 1.01012
H 0.79754 10.66683 3.04354
H 1.19665 9.00081 3.53944
H 1.47212 9.51815 1.84469
C 0.89822 5.05862 -3.93836
C 0.09079 5.25594 -5.08007
C -0.34397 4.14947 -5.83071
C 0.02717 2.85848 -5.42267
C 1.25391 3.75614 -3.54765
C 0.81932 2.62641 -4.27633
O -0.43512 1.79255 -6.22642
C 0.14697 0.51618 -6.05972
C 1.12172 1.22283 -3.83957
C 0.94234 0.21046 -4.93268
C -0.10913 -0.41946 -7.07447
C 0.44983 -1.70580 -6.97650
C 1.26480 -2.03709 -5.87174
C 1.50332 -1.08461 -4.86590
H -0.72745 -0.13298 -7.92004
H 0.25793 -2.43818 -7.75601
H 1.70631 -3.02718 -5.79813
H 2.12808 -1.34270 -4.01389
H 0.33193 0.95030 -2.97916
H 2.09456 1.13877 -3.34687
H -0.95401 4.27257 -6.72070
H -0.19107 6.25982 -5.38605
H 1.24333 5.91212 -3.36121
H 1.87163 3.60590 -2.66533

151
(3/5) Intermediate
Mn 0.14015 -0.07376 0.96327
O 0.29501 -0.58581 2.59032
O -0.04774 0.50747 -0.92003
N 1.44178 1.47524 1.24820
N -1.41744 1.16421 1.44091
N -1.17268 -1.57074 0.52711
N 1.69291 -1.27283 0.38262
C 2.81928 1.44354 1.07002
C 3.39272 2.72923 1.44868
C 2.35808 3.52466 1.86483
C 1.13612 2.74085 1.73403
H 2.41881 4.54102 2.22568
H 4.44023 2.98936 1.40509
C 3.56367 0.34363 0.61367
C -2.76634 0.84606 1.39757
C -3.55627 1.99135 1.83911
C -2.67370 2.99224 2.14668
C -1.33395 2.47337 1.89011
C -0.14997 3.21254 2.04230
H -2.90758 3.98598 2.50014
H -4.63387 2.02423 1.90794
C -0.85705 -2.86581 0.14203
C -2.08065 -3.64578 -0.00757
C -3.12691 -2.81000 0.27896
C -2.55566 -1.51192 0.62209
C -3.30618 -0.39038 1.00988
H -4.17978 -3.05103 0.26145
H -2.13347 -4.68671 -0.29138
C 3.03090 -0.91769 0.30547
C 3.82152 -2.06767 -0.12224
C 2.95042 -3.10972 -0.29595
C 1.61563 -2.60698 0.01537
C 0.43646 -3.36305 -0.08381
H 3.18643 -4.11414 -0.61609
H 4.89248 -2.07791 -0.26347
C -0.27228 4.61607 2.55102
C -4.79854 -0.52775 1.02517
C 0.57334 -4.80276 -0.47388
C 5.04284 0.52623 0.45809
C 5.93134 0.46413 1.53931
C 7.30665 0.64486 1.39055
C 7.90193 0.90868 0.13785
C 7.01634 0.96185 -0.95552
C 5.63763 0.77577 -0.78219
F 5.44493 0.20806 2.81008
F 8.08570 0.55231 2.53765
N 9.38963 1.10614 0.05504
F 7.43519 1.20218 -2.25352
F 4.83996 0.85599 -1.91333
C 9.91784 1.41360 -1.36076
C 9.80033 2.30548 0.94238
C 10.10646 -0.18151 0.52447
H 11.17952 -0.01374 0.42773
H 9.85267 -0.38385 1.56240
H 9.78941 -1.00243 -0.11975
H 10.87836 2.43336 0.84073
H 9.27469 3.19073 0.58258
H 9.54597 2.09974 1.97904
H 10.99526 1.54771 -1.26144
H 9.70506 0.57586 -2.02148
H 9.45951 2.32840 -1.73205
C 0.97480 -5.78559 0.43620
C 1.12599 -7.13769 0.09745
C 0.87585 -7.59371 -1.21094
C 0.46765 -6.60495 -2.13205
C 0.32263 -5.26490 -1.77241
F 1.23850 -5.42772 1.74845
F 1.52834 -7.97714 1.12302
F 0.19581 -6.93931 -3.45334
F -0.07030 -4.37005 -2.75321
N 1.01447 -9.01825 -1.67151
C 1.47237 -10.00563 -0.57917
C -0.35325 -9.53015 -2.18114
C 2.07017 -9.09516 -2.79998
H 1.52441 -10.98421 -1.05697
H 2.45566 -9.71705 -0.21260
H 0.74478 -10.02266 0.22956
H 2.17241 -10.14374 -3.08115
H 1.73658 -8.51089 -3.65402
H 3.01336 -8.71014 -2.41109
H -0.22079 -10.56710 -2.49113
H -1.06842 -9.46623 -1.36034
H -0.67850 -8.92769 -3.02590
C -5.49359 -1.10827 2.09369
C -6.88242 -1.24081 2.10082
C -7.68805 -0.80010 1.02855
C -6.99656 -0.21029 -0.04716
C -5.60002 -0.08676 -0.03162
F -4.79247 -1.57039 3.19455
F -7.45624 -1.83288 3.21928
N -9.17834 -0.98542 1.10048
F -7.63318 0.27645 -1.17670
F -5.00275 0.49985 -1.13683
C -9.94763 -0.47418 -0.13422
C -9.50646 -2.49267 1.22414
C -9.73712 -0.21360 2.31929
H -11.00179 -0.67191 0.05992
H -9.78426 0.59501 -0.25231
H -9.62236 -1.01971 -1.01795
H -10.59228 -2.58861 1.25836
H -9.10576 -3.00158 0.34665
H -9.06907 -2.89041 2.13666
H -10.81834 -0.35558 2.32910
H -9.30141 -0.60790 3.23419
H -9.49190 0.84190 2.19618
C -0.45842 4.90820 3.90853
C -0.57695 6.21399 4.38490
C -0.51920 7.33676 3.53114
C -0.33188 7.05130 2.16498
C -0.21320 5.73074 1.70871
F -0.52287 3.87501 4.82798
F -0.75613 6.37539 5.75350
N -0.66124 8.71545 4.11416
F -0.25789 8.03602 1.19342
F -0.04146 5.54350 0.34661
C -0.57787 9.86007 3.08379
C -2.04066 8.84373 4.80275
C 0.47167 8.96632 5.13704
H -2.11391 9.85580 5.20240
H -2.81318 8.67089 4.05274
H -2.11696 8.11950 5.61025
H -0.69400 10.78626 3.64681
H 0.39332 9.84228 2.59315
H -1.38296 9.76122 2.35865
H 0.34171 9.97704 5.52497
H 0.40203 8.24435 5.94695
H 1.42600 8.87646 4.61735
C 2.91388 0.25434 -4.82384
C 2.89603 0.22714 -6.23984
C 1.66646 0.21949 -6.93097
C 0.47527 0.23960 -6.19960
C 1.71388 0.27322 -4.10110
C 0.45301 0.26714 -4.77091
O -0.72714 0.23148 -6.93585
C -1.96544 0.25148 -6.26180
C -0.80139 0.28932 -4.07882
C -2.01886 0.28107 -4.83266
C -3.11524 0.24129 -7.05680
C -4.38105 0.26068 -6.43525
C -4.47507 0.29003 -5.02267
C -3.31585 0.30000 -4.23601
H -3.01749 0.21887 -8.13815
H -5.28081 0.25314 -7.04398
H -5.45221 0.30514 -4.54734
H -3.39016 0.32162 -3.15156
H 0.37379 1.38096 -1.07032
H -0.80502 0.31178 -2.98891
H 1.62869 0.19885 -8.01612
H 3.82759 0.21225 -6.79876
H 3.86350 0.26053 -4.29567
H 1.71389 0.29102 -3.01379

151
(3/5) Reb Transition State
Mn -0.07582 0.24220 -0.18230
O 0.07558 -0.26647 1.43494
O -0.29052 0.88454 -2.10346
N 1.25209 1.78096 0.05835
N -1.60816 1.52282 0.26617
N -1.41406 -1.24443 -0.61299
N 1.45479 -0.99195 -0.78341
C 2.64081 1.70742 -0.08317
C 3.22728 3.00099 0.20783
C 2.19730 3.85162 0.53193
C 0.96592 3.08316 0.45182
H 2.27190 4.89881 0.78593
H 4.27939 3.24219 0.15661
C 3.37155 0.56507 -0.45697
C -2.96368 1.19232 0.32647
C -3.72773 2.34906 0.76281
C -2.83521 3.37325 0.95847

C -1.51042 2.85386 0.64166
C -0.31768 3.59778 0.72933
H -3.05465 4.37522 1.29739
H -4.79844 2.37903 0.90636
C -1.13025 -2.53745 -1.02024
C -2.36205 -3.30831 -1.09266
C -3.38841 -2.46975 -0.72635
C -2.79757 -1.18220 -0.42066
C -3.51563 -0.05657 0.01178
H -4.43987 -2.71226 -0.66867
H -2.43979 -4.34962 -1.36851
C 2.81737 -0.67665 -0.79413
C 3.58144 -1.84096 -1.20856
C 2.68231 -2.84855 -1.45135
C 1.35356 -2.31806 -1.16973
C 0.15822 -3.05892 -1.28392
H 2.90214 -3.84705 -1.79988
H 4.65632 -1.88949 -1.30627
C -0.41869 5.02814 1.14300
C -5.00091 -0.20713 0.15016
C 0.26408 -4.49693 -1.66122
C 4.86605 0.67704 -0.44320
C 5.59195 0.70566 0.75685
C 6.98159 0.81421 0.79355
C 7.76463 0.89938 -0.37817
C 7.04597 0.86324 -1.58808
C 5.64747 0.75632 -1.59974
F 4.92279 0.61202 1.96572
F 7.58203 0.83708 2.04724
N 9.25745 1.03318 -0.25856
F 7.65817 0.93470 -2.82909
F 5.03074 0.74487 -2.84270
C 10.00290 1.11549 -1.60538
C 9.59482 2.33330 0.50879
C 9.83321 -0.19400 0.48681
H 10.91573 -0.07057 0.53106
H 9.42201 -0.23931 1.49219
H 9.57396 -1.08920 -0.07915
H 10.68113 2.40411 0.57246
H 9.18844 3.17440 -0.05409
H 9.16560 2.29254 1.50705
H 11.06229 1.20426 -1.36406
H 9.82627 0.20729 -2.17787
H 9.67008 1.99389 -2.15418
C 0.84639 -5.45640 -0.81921
C 0.96119 -6.81410 -1.14387
C 0.47924 -7.31819 -2.36796
C -0.11549 -6.36153 -3.21965
C -0.21439 -5.01431 -2.87626
F 1.32140 -5.06973 0.42590
F 1.55610 -7.61774 -0.18259
F -0.61930 -6.73897 -4.46083
F -0.79202 -4.16012 -3.80546
N 0.55703 -8.75366 -2.80704
C 1.23097 -9.69515 -1.78980
C -0.87020 -9.30243 -3.03579
C 1.38229 -8.85362 -4.11097
H 1.22456 -10.68805 -2.23937
H 2.25519 -9.37159 -1.61430
H 0.65953 -9.70089 -0.86379
H 1.42723 -9.90667 -4.39151
H 0.89696 -8.27988 -4.89662
H 2.38263 -8.46858 -3.91114
H -0.77604 -10.34511 -3.34179
H -1.41743 -9.22707 -2.09558
H -1.36256 -8.72807 -3.81697
C -5.59894 -0.72299 1.30686
C -6.97983 -0.87548 1.43312
C -7.87548 -0.51848 0.40186
C -7.28196 0.00482 -0.76303
C -5.89079 0.14861 -0.86724
F -4.80559 -1.10192 2.37687
F -7.45272 -1.40385 2.62894
N -9.35120 -0.72555 0.60328
F -8.01584 0.40011 -1.87005
F -5.39451 0.66453 -2.05413
C -10.22615 -0.29957 -0.59230
C -9.62929 -2.22938 0.83588
C -9.83212 0.10493 1.81603
H -11.25849 -0.49167 -0.29969
H -10.08574 0.76122 -0.78910
H -9.96811 -0.89709 -1.46454
H -10.70738 -2.35110 0.94650
H -9.26948 -2.77892 -0.03478
H -9.12203 -2.56003 1.73900
H -10.90103 -0.07616 1.93366
H -9.30145 -0.20988 2.71111
H -9.64477 1.15789 1.60304
C 0.01804 5.49300 2.39342
C -0.07770 6.83005 2.77727
C -0.62632 7.82175 1.93502
C -1.06388 7.36781 0.67558
C -0.95521 6.01916 0.31073
F 0.55219 4.59941 3.30851
F 0.38658 7.16068 4.04639
N -0.70310 9.24293 2.41945
F -1.61056 8.21083 -0.28002
F -1.39316 5.67500 -0.95967
C -1.33841 10.22489 1.41552
C -1.56693 9.30885 3.70084
C 0.72329 9.76611 2.70721
H -1.62120 10.35416 4.00657
H -2.56093 8.92958 3.46145
H -1.10539 8.71500 4.48572
H -1.33507 11.20212 1.89821
H -0.74166 10.25547 0.50637
H -2.36040 9.91786 1.20139
H 0.63411 10.80097 3.04027
H 1.18390 9.16242 3.48575
H 1.29830 9.71004 1.78225
C 2.99307 2.59415 -4.83250
C 2.37615 3.55908 -5.66915
C 1.02999 3.41571 -6.04630
C 0.31185 2.30552 -5.58253
C 2.26384 1.49473 -4.37193
C 0.89820 1.31925 -4.73713
O -1.02247 2.19956 -5.99248
C -1.77309 1.07004 -5.64388
C 0.10171 0.21464 -4.27919
C -1.22465 0.05653 -4.80586
C -3.07052 0.98855 -6.16635
C -3.85556 -0.13585 -5.85913
C -3.33645 -1.17014 -5.03955
C -2.04168 -1.07468 -4.52252
H -3.44441 1.78673 -6.79964
H -4.86311 -0.21220 -6.25789
H -3.95002 -2.03732 -4.81336
H -1.64324 -1.86094 -3.88923
H 0.12387 1.76836 -2.21232
H 0.56877 -0.60205 -3.74615
H 0.53978 4.14018 -6.68879
H 2.94475 4.41406 -6.02359
H 4.03351 2.71299 -4.54587
H 2.73009 0.76002 -3.72291

151
(3/5) Hydroxylated Product
Mn 0.07693 -0.16434 0.67110
O 0.21080 -0.62038 2.27492
O -0.24878 0.56118 -1.44967
N 1.39635 1.39171 0.85654
N -1.46696 1.14764 0.98023
N -1.26734 -1.64641 0.23464
N 1.58828 -1.36780 0.01830
C 2.78802 1.32021 0.73154
C 3.36509 2.61428 0.95702
C 2.31911 3.48472 1.22766
C 1.10531 2.71596 1.17870
H 2.38964 4.54490 1.42248
H 4.41625 2.85795 0.89852
C 3.52451 0.15433 0.39261
C -2.82574 0.80348 1.09457
C -3.58409 1.96860 1.53206
C -2.69960 2.99906 1.68665
C -1.37164 2.49167 1.35008
C -0.19617 3.24007 1.42817
H -2.92085 4.00333 2.01768
H -4.65026 1.99154 1.70707
C -0.98517 -2.94569 -0.17757
C -2.19906 -3.71355 -0.24195
C -3.23509 -2.86964 0.13426
C -2.65123 -1.59248 0.42923
C -3.37686 -0.44545 0.84322
H -4.28615 -3.11427 0.19082
H -2.27628 -4.75446 -0.52043
C 2.96058 -1.06931 0.05117
C 3.72233 -2.25194 -0.33277
C 2.82641 -3.24921 -0.59469
C 1.48979 -2.71204 -0.35157
C 0.31417 -3.45247 -0.46564
H 3.04713 -4.25410 -0.92402
H 4.79922 -2.31025 -0.39662
C -0.29970 4.67600 1.81117
C -4.85544 -0.60756 1.01162
C 0.41113 -4.87623 -0.90094
C 5.01542 0.26167 0.43632
C 5.71800 0.34187 1.64893
C 7.10598 0.45544 1.70979
C 7.91300 0.50226 0.55148
C 7.21933 0.41619 -0.67023
C 5.82209 0.30184 -0.70617
F 5.02569 0.28810 2.84749
F 7.68315 0.51641 2.97391
N 9.40281 0.64351 0.69567
F 7.85684 0.44601 -1.90088
F 5.23060 0.24666 -1.96089
C 10.17313 0.69826 -0.63855
C 9.72555 1.96134 1.43864
C 9.96519 -0.56560 1.47873
H 11.04661 -0.44038 1.54164
H 9.53382 -0.58919 2.47657
H 9.71712 -1.47316 0.92751
H 10.81029 2.03036 1.52723
H 9.33637 2.78930 0.84502
H 9.27200 1.94714 2.42661
H 11.22690 0.80303 -0.37958
H 10.01554 -0.22552 -1.19115
H 9.84286 1.55934 -1.21606
C 0.92063 -5.89090 -0.08048
C 1.01362 -7.23448 -0.46910
C 0.58387 -7.65913 -1.74101
C 0.06064 -6.64362 -2.57159
C -0.01908 -5.31298 -2.16391
F 1.34795 -5.57828 1.20204
F 1.53747 -8.10291 0.47667
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F -0.52918 -4.39435 -3.06861
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C 1.24995 -10.08310 -1.25699
C -0.78583 -9.56725 -2.56816
C 1.52561 -9.12829 -3.52070
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H 2.27577 -9.80055 -1.02813
H 0.64410 -10.11637 -0.35406
H 1.56929 -10.16867 -3.84423
H 1.08409 -8.51379 -4.30124
H 2.52151 -8.76798 -3.26040
H -0.70854 -10.59730 -2.91880
H -1.37390 -9.51907 -1.65096
H -1.22532 -8.94225 -3.34203
C -5.42653 -1.16830 2.16207
C -6.80328 -1.33272 2.31413
C -7.72404 -0.95196 1.31359
C -7.15906 -0.38822 0.15362
C -5.77173 -0.22863 0.02550
F -4.60928 -1.57259 3.20477
F -7.24785 -1.89324 3.50682
N -9.19391 -1.17331 1.54095
F -7.91934 0.03541 -0.92524
F -5.30703 0.32814 -1.15631
C -10.09539 -0.73232 0.37079
C -9.45912 -2.68284 1.75215
C -9.65336 -0.36808 2.77865
H -11.12017 -0.94156 0.67780
H -9.96989 0.33360 0.19300
H -9.84709 -1.30889 -0.51843
H -10.53464 -2.81284 1.87748
H -9.10966 -3.21579 0.86701
H -8.93609 -3.02539 2.64163
H -10.71780 -0.55959 2.91845
H -9.09906 -0.69464 3.65516
H -9.47874 0.69010 2.58058
C 0.18838 5.18205 3.02784
C 0.09304 6.52715 3.38036
C -0.50541 7.49118 2.53884
C -0.99638 6.99732 1.31492
C -0.88596 5.64123 0.98006
F 0.76563 4.32037 3.94782
F 0.60289 6.89558 4.62212
N -0.57998 8.92311 2.99005
F -1.59927 7.80792 0.36429
F -1.37507 5.26258 -0.26276
C -1.25419 9.87394 1.98183
C -1.40239 9.01291 4.29644
C 0.84840 9.46819 3.22074
H -1.44237 10.06306 4.58837
H -2.40469 8.63416 4.09436
H -0.91799 8.42874 5.07498
H -1.24414 10.86340 2.43882
H -0.68505 9.88522 1.05432
H -2.27962 9.55431 1.80645
H 0.75606 10.50925 3.53286
H 1.34053 8.88854 3.99809
H 1.39483 9.39755 2.27970
C 3.11083 2.25097 -3.77188
C 2.56064 3.12977 -4.73288
C 1.21579 3.00536 -5.11335
C 0.42784 2.00341 -4.52018
C 2.30253 1.26533 -3.18559
C 0.94260 1.13159 -3.53966
O -0.90111 1.91445 -4.97226
C -1.67106 0.79963 -4.59593
C 0.05421 0.11454 -2.85740
C -1.23494 -0.11638 -3.61599
C -2.89971 0.64726 -5.26270
C -3.70887 -0.45757 -4.95846
C -3.28506 -1.40432 -3.99816
C -2.06034 -1.22816 -3.33750
H -3.19499 1.38058 -6.00676
H -4.65866 -0.58589 -5.47041
H -3.90732 -2.26471 -3.76976
H -1.73934 -1.94786 -2.59112
H -0.88488 1.30788 -1.43697
H 0.58942 -0.82040 -2.67825
H 0.77394 3.65620 -5.86156
H 3.17953 3.89815 -5.18812
H 4.15491 2.33703 -3.48640
H 2.72083 0.59640 -2.43964

2

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(4/3)
Mn 0.07396 -0.49362 0.41180
N 0.32435 -0.86671 2.51227
O -0.11999 -0.16043 -1.36536
N 1.50531 0.94328 0.56916
N -1.35234 0.86943 0.93105
N -1.33946 -1.95590 0.39539
N 1.52218 -1.89796 0.09846
C 2.87300 0.78535 0.37915
C 3.54615 2.06932 0.52164
C 2.57853 3.00120 0.79535
C 1.30507 2.29485 0.82658
H 2.71941 4.05929 0.96263
H 4.60936 2.23869 0.43344
C 3.52572 -0.42692 0.09877
C -2.71618 0.64337 1.06891
C -3.40103 1.89364 1.37217
C -2.44389 2.87372 1.41183
C -1.16493 2.23089 1.13566
C 0.06693 2.90299 1.08875
H -2.59295 3.92539 1.60902
H -4.46355 2.00978 1.52964
C -1.13918 -3.31145 0.14556
C -2.40886 -4.01946 0.20353
C -3.37475 -3.09059 0.49604
C -2.70612 -1.80437 0.61974
C -3.35520 -0.59917 0.93236
H -4.43338 -3.26727 0.61985
H -2.54810 -5.08005 0.05198
C 2.88594 -1.66953 -0.03741
C 3.56965 -2.91586 -0.36090
C 2.61221 -3.89436 -0.41842
C 1.33382 -3.25518 -0.13170
C 0.09968 -3.92403 -0.10459
H 2.75936 -4.94074 -0.64312
H 4.63042 -3.02797 -0.53208
C 0.05724 4.38106 1.34101
C -4.83975 -0.64079 1.13670
C 0.10606 -5.40130 -0.35772
C 5.01538 -0.39118 -0.06086
C 5.88770 -0.78249 0.96336
C 7.27483 -0.74090 0.82366
C 7.90060 -0.30313 -0.36383
C 7.03029 0.08746 -1.39964
C 5.63834 0.03864 -1.23625
F 5.37121 -1.21862 2.17180
F 8.03341 -1.14795 1.91451
N 9.40189 -0.27745 -0.43945
F 7.47935 0.53576 -2.63063
F 4.85884 0.43595 -2.31061
C 9.96962 0.21282 -1.78667
C 9.95545 0.67875 0.64325
C 9.95464 -1.70642 -0.22622
H 11.04075 -1.65159 -0.30680
H 9.67296 -2.06560 0.76049
H 9.54437 -2.34940 -1.00579
H 11.04257 0.67309 0.55867
H 9.56145 1.67709 0.44971
H 9.65765 0.32962 1.62905
H 11.05491 0.17959 -1.69031
H 9.64623 -0.45241 -2.58467
H 9.64273 1.23381 -1.97223
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C 0.13307 -8.26321 -0.83667
C -0.16871 -7.32678 -1.84916
C -0.18265 -5.95195 -1.61286
F 0.69729 -5.88202 1.92009
F 0.73226 -8.49479 1.53172
F -0.46260 -7.75034 -3.13938
F -0.48675 -5.11446 -2.67258
N 0.12839 -9.73035 -1.16438
O 0.45767 -10.65481 0.02457
C -1.27650 -10.14651 -1.66196
C 1.19255 -10.01551 -2.25033
H 0.42252 -11.67353 -0.36225
H 1.45502 -10.43107 0.39661
H -0.28911 -10.52602 0.80567
H 1.17382 -11.08653 -2.45443
H 0.95324 -9.45948 -3.15365
H 2.16589 -9.71855 -1.85802
H -1.24429 -11.21565 -1.87354
H -1.99425 -9.93689 -0.86775
H -1.52565 -9.59652 -2.56610
C -5.41857 -0.84705 2.39541
C -6.79986 -0.88361 2.58745
C -7.71355 -0.71217 1.52501
C -7.13836 -0.50401 0.25648
C -5.74673 -0.47300 0.08668
F -4.60442 -1.02506 3.50096
F -7.25360 -1.09890 3.88305
N -9.18946 -0.76102 1.80615
F -7.89163 -0.31892 -0.89071
F -5.26717 -0.26141 -1.19558
C -10.08795 -0.55894 0.56878
C -9.55838 -2.14432 2.39236
C -9.56185 0.36130 2.80370
H -11.11599 -0.61807 0.92707
H -9.89983 0.42146 0.13557
H -9.89905 -1.34906 -0.15516
H -10.63438 -2.14596 2.56873
H -9.28958 -2.90806 1.66114
H -9.02838 -2.30038 3.32889
H -10.63622 0.29785 2.97923
H -9.02308 0.21729 3.73702
H -9.30403 1.31927 2.35036
C 0.20323 4.92564 2.62301
C 0.18232 6.30033 2.85985
C 0.01341 7.24217 1.82156
C -0.12977 6.70139 0.52908
C -0.10665 5.31567 0.31489
F 0.37067 4.08247 3.70835
F 0.32838 6.71803 4.17706
N -0.01387 8.70857 2.15416
F -0.30191 7.48346 -0.60078
F -0.25767 4.87155 -0.98851
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C -1.20101 8.99843 3.10363
C 1.31672 9.11772 2.82943
H -1.19182 10.06683 3.32230
H -2.12319 8.71996 2.59268
H -1.08153 8.43057 4.02332
H -0.19537 10.65489 1.32398
H 0.64630 9.50490 0.25010
H -1.13518 9.41953 0.44292
H 1.26535 10.18932 3.02456
H 1.43602 8.57462 3.76359
H 2.13427 8.89297 2.14394
H -0.82635 -0.69426 -1.78859
C 0.45268 -1.07502 3.65596
C 0.61289 -1.33444 5.08405
H 1.66346 -1.54129 5.31325
H 0.28913 -0.46348 5.66334
H 0.00963 -2.19941 5.37892

2 + xanthene cation

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(5/3) Intermediate
Mn 0.07028 -0.51004 0.43956
N 0.33726 -0.87767 2.52538
O -0.15380 -0.18432 -1.34524
N 1.49860 0.93357 0.58989
N -1.35119 0.85739 0.94948
N -1.33761 -1.97985 0.44214
N 1.51135 -1.90681 0.09906
C 2.86308 0.77931 0.37385
C 3.53895 2.06070 0.52670
C 2.57637 2.98752 0.83200
C 1.30293 2.28145 0.86867
H 2.71999 4.04238 1.01651
H 4.60074 2.23120 0.42498
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C -2.71713 0.63120 1.06965
C -3.40294 1.87772 1.38296
C -2.44477 2.85547 1.44908
C -1.16483 2.21575 1.17498
C 0.06730 2.88790 1.14348
H -2.59417 3.90349 1.66452
H -4.46618 1.99229 1.53569
C -1.13796 -3.33752 0.20894
C -2.41024 -4.04278 0.25994
C -3.37788 -3.10700 0.52150
C -2.70653 -1.82078 0.63928
C -3.35710 -0.60987 0.92375
H -4.43961 -3.27729 0.62611
H -2.54934 -5.10496 0.11966
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C 3.55772 -2.91836 -0.37727

C 2.60623 -3.90487 -0.39910
C 1.32925 -3.27144 -0.10150
C 0.10098 -3.94919 -0.04158
H 2.75756 -4.95437 -0.60546
H 4.61593 -3.02733 -0.56516
C 0.05731 4.36258 1.41284
C -4.84652 -0.63894 1.09156
C 0.11350 -5.42945 -0.27589
C 4.99726 -0.38456 -0.12444
C 5.89320 -0.77670 0.87877
C 7.27684 -0.72354 0.71090
C 7.87486 -0.27238 -0.48581
C 6.98079 0.11946 -1.50089
C 5.59316 0.05863 -1.30857
F 5.40457 -1.22445 2.09426
F 8.06021 -1.13216 1.78290
N 9.37399 -0.23459 -0.59147
F 7.40089 0.58154 -2.73680
F 4.78777 0.46144 -2.36397
C 9.91131 0.26867 -1.94644
C 9.94093 0.71983 0.48604
C 9.94221 -1.66062 -0.39873
H 11.02597 -1.59636 -0.50088
H 9.68335 -2.02828 0.59106
H 9.52122 -2.30162 -1.17419
H 11.02547 0.73036 0.37436
H 9.52830 1.71408 0.31107
H 9.67277 0.35782 1.47571
H 10.99850 0.24189 -1.87157
H 9.57671 -0.39319 -2.74270
H 9.57468 1.28885 -2.11804
C 0.40448 -6.34630 0.73825
C 0.42721 -7.73438 0.54073
C 0.15484 -8.29606 -0.72171
C -0.13874 -7.37238 -1.74830
C -0.15970 -5.99508 -1.52776
F 0.68320 -5.88091 2.01302
F 0.72902 -8.49879 1.65534
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F -0.45540 -5.17009 -2.59967
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C 0.47714 -10.67744 0.17010
C -1.23908 -10.19291 -1.54220
C 1.23677 -10.06041 -2.10248
H 0.44865 -11.70027 -0.20636
H 1.47007 -10.44756 0.55017
H -0.27810 -10.54244 0.94193
H 1.22282 -11.13350 -2.29565
H 1.00746 -9.51435 -3.01442
H 2.20444 -9.75700 -1.70111
H -1.20195 -11.26481 -1.73842
H -1.96761 -9.97360 -0.76041
H -1.47769 -9.65608 -2.45703
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C -6.84603 -0.92669 2.47869
C -7.72975 -0.66038 1.41026
C -7.11961 -0.37995 0.17223
C -5.72398 -0.37172 0.03710
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F -7.33519 -1.20075 3.74964
N -9.21226 -0.68022 1.65765
F -7.84054 -0.09627 -0.97552
F -5.20813 -0.07797 -1.21636
C -10.07636 -0.40523 0.41050
C -9.63626 -2.07339 2.18137
C -9.57221 0.41387 2.68999
H -11.11353 -0.46289 0.74146
H -9.86171 0.59077 0.02941
H -9.88200 -1.16341 -0.34560
H -10.71702 -2.05106 2.32427
H -9.36519 -2.81746 1.43135
H -9.14085 -2.27844 3.12697
H -10.65094 0.37453 2.84463
H -9.05374 0.22048 3.62620
H -9.28021 1.37996 2.27636
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C 0.18121 6.26559 2.95170
C 0.00763 7.21831 1.92407
C -0.13730 6.69115 0.62594
C -0.11151 5.30796 0.39757
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F 0.32937 6.66931 4.27273
N -0.02088 8.68091 2.27254
F -0.31399 7.48446 -0.49521
F -0.26596 4.87618 -0.91085
C -0.20083 9.62172 1.06366
C -1.20589 8.95913 3.22832
C 1.31121 9.08436 2.94860
H -1.19650 10.02489 3.45952
H -2.12920 8.68648 2.71624
H -1.08407 8.38064 4.14104
H -0.20973 10.63570 1.46362
H 0.63466 9.50029 0.37661
H -1.14646 9.40681 0.57026
H 1.25978 10.15402 3.15388
H 1.43283 8.53255 3.87735
H 2.12726 8.86649 2.25911
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C -4.24821 3.78505 -4.13189
C -3.10715 4.33356 -4.72743
C -1.85932 3.78956 -4.38839
C -2.91979 2.17127 -2.87151
C -1.72814 2.70494 -3.45962
O -0.73796 4.33222 -4.98499
C 0.52679 3.84921 -4.71056
C -0.43917 2.20315 -3.16645
C 0.69984 2.76585 -3.78707
C 1.61179 4.45342 -5.36288
C 2.89582 3.96841 -5.09177
C 3.10810 2.89101 -4.17974
C 2.02997 2.29811 -3.53661
H 1.44262 5.27081 -6.05481
H 3.74943 4.42152 -5.58704
H 4.11710 2.53911 -3.99374
H 2.17240 1.47617 -2.84190
H -0.30259 -0.99541 -1.87627
H -0.32422 1.36958 -2.45988
H -3.16810 5.15406 -5.43355
H -5.22387 4.19101 -4.38190
H -5.06353 2.30047 -2.76377
H -2.83175 1.34674 -2.17091
C 0.47872 -1.09442 3.66574
C 0.65404 -1.36614 5.08946
H 1.70952 -1.55841 5.30854
H 0.32076 -0.50663 5.68031
H 0.06684 -2.24377 5.37932

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(5/3) Reb Transition State
Mn -0.25458 0.17992 -0.24660
N 0.02647 -0.32898 1.75574
O -0.54551 0.57747 -2.05628
N 1.15088 1.62370 -0.03010
N -1.69216 1.48231 0.36851
N -1.64780 -1.29104 -0.37351
N 1.20427 -1.16666 -0.70308
C 2.53171 1.48061 -0.15949
C 3.19048 2.74355 0.13185
C 2.20819 3.65026 0.43671
C 0.93855 2.94814 0.34958
H 2.33802 4.68742 0.70915
H 4.25611 2.91816 0.11757
C 3.20453 0.29801 -0.50795
C -3.05159 1.22451 0.51264
C -3.75126 2.44337 0.89183
C -2.80997 3.43547 0.98027
C -1.52508 2.83295 0.65646
C -0.30434 3.52540 0.65065
H -2.97487 4.47191 1.23613
H -4.81468 2.53707 1.05707
C -1.43164 -2.62019 -0.73395
C -2.68105 -3.35947 -0.67081
C -3.65143 -2.47826 -0.26762
C -3.00888 -1.18734 -0.08716
C -3.67378 -0.01908 0.31830
H -4.69651 -2.69219 -0.09861
H -2.80335 -4.41094 -0.88573
C 2.57008 -0.92207 -0.79181
C 3.26258 -2.12220 -1.23985
C 2.31020 -3.09027 -1.42137
C 1.02752 -2.49613 -1.07281
C -0.19523 -3.18440 -1.08719
H 2.46414 -4.10252 -1.76505
H 4.32530 -2.20967 -1.41311
C -0.32911 4.97912 1.01618
C -5.14889 -0.10778 0.56024
C -0.18549 -4.62421 -1.50101
C 4.70256 0.32709 -0.53963
C 5.47328 -0.24342 0.48332
C 6.86772 -0.22002 0.47435
C 7.60633 0.38049 -0.56825
C 6.84016 0.95462 -1.60063
C 5.43877 0.92074 -1.56836
F 4.84338 -0.84754 1.55785
F 7.51722 -0.81518 1.54812
N 9.10856 0.36997 -0.50951
F 7.40318 1.57833 -2.70068
F 4.76864 1.50740 -2.63167
C 9.80059 1.05628 -1.70433
C 9.57984 1.11898 0.76019
C 9.61482 -1.09182 -0.49343
H 10.70395 -1.06031 -0.45349
H 9.22492 -1.60647 0.38138
H 9.28139 -1.57710 -1.41137
H 10.67025 1.12811 0.75007
H 9.18992 2.13689 0.71921
H 9.21999 0.60163 1.64625
H 10.87258 0.96898 -1.52700
H 9.53170 0.54358 -2.62550
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C 0.23293 -5.65257 -0.65158
C 0.23948 -7.00515 -1.02191
C -0.18487 -7.41338 -2.30102
C -0.60159 -6.37635 -3.16372
C -0.60206 -5.03734 -2.77335
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F -1.02365 -4.09307 -3.69399
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C 0.24087 -9.88207 -1.75173
C -1.66573 -9.21675 -3.17880
C 0.72260 -8.98390 -4.00903
H 0.15385 -10.85207 -2.24134
H 1.27599 -9.69632 -1.47298
H -0.40990 -9.84474 -0.88037
H 0.69231 -10.02850 -4.32096
H 0.37681 -8.34396 -4.81743
H 1.73128 -8.70733 -3.69960
H -1.65142 -10.25515 -3.51128
H -2.29745 -9.10680 -2.29663
H -2.01073 -8.57385 -3.98467
C -5.69919 -0.13001 1.84863
C -7.07247 -0.22138 2.07574
C -8.00846 -0.30523 1.02201
C -7.46290 -0.27727 -0.27600
C -6.07929 -0.17920 -0.48095
F -4.86274 -0.07212 2.95050
F -7.49483 -0.22923 3.39906
N -9.47342 -0.41325 1.34353
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C -10.39283 -0.52072 0.11002
C -9.72494 -1.68460 2.19009
C -9.92510 0.84481 2.12233
H -11.40913 -0.61104 0.49372
H -10.30187 0.37947 -0.49439
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H -10.79616 -1.74175 2.38473
H -9.39559 -2.54999 1.61431
H -9.18066 -1.61492 3.12858
H -10.99261 0.74216 2.32078
H -9.37608 0.91134 3.05860
H -9.73577 1.71835 1.49774
C -0.25966 5.42291 2.34255
C -0.29904 6.77566 2.68168
C -0.41297 7.79407 1.71029
C -0.47847 7.35476 0.37392
C -0.43522 5.98960 0.05683
F -0.15218 4.49828 3.36683
F -0.22862 7.09169 4.03236
N -0.46729 9.23017 2.15173
F -0.59212 8.22087 -0.69980
F -0.51299 5.64379 -1.28359
C -0.58337 10.25167 1.00186
C -1.70641 9.44115 3.05458
C 0.82526 9.58693 2.92401
H -1.73162 10.49467 3.33414
H -2.59591 9.17658 2.48158
H -1.62109 8.82238 3.94475
H -0.61104 11.23547 1.47078
H 0.28548 10.17339 0.35117
H -1.50270 10.07575 0.44738
H 0.75872 10.63928 3.20207
H 0.90153 8.96954 3.81546
H 1.67551 9.41979 2.26187
C -3.74952 3.50043 -3.41592
C -4.26377 2.94833 -4.62090
C -3.46667 2.13617 -5.43548
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C -2.44197 3.22329 -3.02407
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O -1.37500 1.09242 -5.88843
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C 0.56710 1.38152 -4.42516
C 0.71894 0.19777 -6.58991
C 2.08838 0.00726 -6.37057
C 2.71526 0.50518 -5.19569
C 1.96244 1.18056 -4.23746
H 0.22819 -0.16337 -7.48726
H 2.67940 -0.52120 -7.11287
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H 2.43110 1.55822 -3.33505
H -1.22885 -0.00348 -2.45564
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H -4.38038 4.13634 -2.80329
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C 0.37679 -1.00034 4.27217
H 1.42666 -1.25600 4.44932
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(5/3) Hydroxylated Product
Mn 0.02922 -0.08214 0.32736
N 0.26303 -0.52139 2.26747
O -0.31151 0.22339 -1.59438
N 1.40284 1.38639 0.49389
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C 1.19010 2.68862 0.95532
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H 4.48856 2.73653 0.53329
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C -2.79582 0.95984 0.94399
C -3.50110 2.15786 1.36651
C -2.55684 3.13037 1.57043
C -1.26554 2.54332 1.25744
C -0.04684 3.23442 1.32537
H -2.72507 4.14932 1.88648
H -4.57004 2.24913 1.49142
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C -2.73244 -1.44849 0.35300
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C 2.85548 -1.13990 -0.25304
C 3.56636 -2.35218 -0.62045
C 2.63657 -3.35618 -0.69902
C 1.34545 -2.76839 -0.38528
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H 2.81156 -4.39028 -0.95657
H 4.62815 -2.42797 -0.80234
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C 0.19013 -4.95125 -0.65609
C 4.95793 0.18604 -0.20151
C 5.82489 -0.21867 0.82191
C 7.21241 -0.14243 0.70103
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C 6.97697 0.75162 -1.49852
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C 9.87782 1.32316 0.58391
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H 9.63266 -1.42410 0.63202
H 9.50660 -1.66964 -1.14016
H 10.96549 1.33407 0.50638
H 9.47256 2.32130 0.41386
H 9.57784 0.94370 1.55780
H 11.00076 0.89711 -1.75252
H 9.60789 0.26934 -2.67485
H 9.57740 1.93950 -2.02094
C 0.52468 -5.88496 0.32875
C 0.57910 -7.26635 0.09486
C 0.29470 -7.80241 -1.17607
C -0.04310 -6.86111 -2.17260
C -0.09294 -5.49047 -1.91720
F 0.81395 -5.44388 1.60939
F 0.92350 -8.04944 1.18308
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H -1.02865 -10.77660 -2.22015
H -1.78812 -9.52517 -1.18789
H -1.35964 -9.15756 -2.89146
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H -9.12743 -2.09884 2.88864
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H -9.46306 1.49515 1.83791
C -0.09907 4.89601 3.23729
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H -0.97287 9.81822 1.91108
H 1.11587 9.87222 4.86630
H 1.15093 8.12524 5.22637
H 2.03692 8.76242 3.80240
C -2.44155 3.97692 -2.73071
C -3.21623 3.61510 -3.85739
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H 1.62006 -1.28418 5.03116
H 0.20210 -0.27955 5.42893
H -0.00849 -2.00936 5.05306