

Supporting Information

Computational Insight into the Alkane- Hydroxylation Mechanism by Non-Heme Fe(PyTACN) Iron Complexes. Effect of the Substrate and Solvent

Verònica Postils, Anna Company, Miquel Solà, Miquel Costas* and Josep M. Luis**

Institut de Química Computacional i Catàlisi (IQCC) and Departament de Química,
Universitat de Girona, Campus de Montilivi, 17071 Girona, Catalonia, Spain.

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Ionization Energies and Electron Affinities

		G_g (kcal/mol)	G_{g+corr} (kcal/mol)	G_{solv} (kcal/mol)
EA	Fe(IV) m1 $\rightarrow$ Fe(III) m2	-243.85	-159.79	-130.68
	Fe(IV) m3 $\rightarrow$ Fe(III) m4	-234.55	-115.17	-118.86
	Fe(IV) m5 $\rightarrow$ Fe(III) m6	-247.97	-134.15	-134.86
	Global Fe(IV) m3 $\rightarrow$ Fe(III) m6	-245.04	-130.18	-129.20
IE	Methyl	228.85	145.12	145.47
	Ethyl	190.35	116.20	116.04
	Cyclohexyl	162.24	103.79	103.25
	DMB	151.68	93.59	92.17

Table S1. Gibbs Energy values at gas-phase (G_g), at gas-phase including the dispersion and solvent corrections (G_{g+corr}), and at solvent (acetonitrile) (G_{solv}) for the ionization energies (IE) of the radical substrates and for the electron affinities (EA) of the $Fe^{IV}(OH)_2$ moiety at different multiplicities.

G_g (kcal/mol)				
Radical $\rightarrow$ Cation				
	Methyl	Ethyl	Cyclohexyl	DMB
m2	-15.01	-53.51	-81.61	-92.17
m4	-5.70	-44.20	-72.31	-82.87
m6	-19.12	-57.62	-85.73	-96.29
Global	-16.20	-54.70	-82.80	-93.36
G_{g+corr} (kcal/mol)				
m2	-14.67	-43.59	-56.00	-66.19
m4	29.95	1.02	-11.38	-21.58
m6	10.97	-17.95	-30.36	-40.55
Global	14.94	-13.98	-26.39	-36.58
G_{solv} (kcal/mol)				
m2	14.79	-14.64	-27.43	-38.51
m4	26.61	-2.83	-15.62	-26.70
m6	10.61	-18.82	-31.61	-42.70
Global	16.27	-13.16	-25.95	-37.03

Table S2. Energy differences between the IE of the deprotonated substrates and the EA of the $Fe^{IV}(OH)_2$ moiety at different catalyst multiplicities. Negative values account for a favorable substrate oxidation (cationic forms), while positive values indicate that deprotonated substrate oxidation is not favorable and they keep the radical form. Values in kcal/mol and for gas-phase (G_g), gas-phase including the dispersion and solvent corrections (G_{g+corr}), and solvent (G_{solv}) computational methodologies.

Mulliken Spin Populations

		Fe	O (oxo)	O (hydroxyl)	N (trans to pyridine)
Methane	A^{2 a}	1.899	-0.868	0.1845	NS
	A⁴	2.054	0.914	0.1771	NS
	A⁶	3.182	0.591	0.0983	0.800
Ethane	A^{2 a}	1.885	-0.862	0.188	NS
	A⁴	2.031	0.927	0.180	NS
	A⁶	3.168	0.603	0.097	0.799
Cyclohexane	A^{2 a}	1.880	-0.858	0.189	NS
	A⁴	2.026	0.927	0.181	NS
	A⁶	3.167	0.605	0.096	0.799
2,3-DMB	A^{2 a}	1.885	-0.860	0.187	NS
	A⁴	2.044	0.920	0.178	NS
	A⁶	3.187	0.592	0.096	0.801

NS=Not Significant value.

^a. S=1/2 monoradicaloid energies have been evaluated and they are always higher in energy than triradicaloid structures.

Table S3. Mulliken spin population analysis of **A** structures.

UOPBE Energy values

		ΔE_{elec} (UOPBE)	ΔE_{elec} (UB3LYP)
A	m2	19.45	9.16
	m4	0.00	0.00
	m6	23.27	14.02
TS_{abs}	m2	7.04	2.68
	m4	0.00	0.00

Table S4. Ethane relative electronic energies obtained with single point calculations at UOPBE/6-311G(d,p)~SDD + SMD level of theory for the corresponding UB3LYP geometries.

		Methyl		Ethyl		Cyclohexyl		DMB	
		ΔE_{elec} (UOPBE)	ΔE_{elec} (UB3LYP)	ΔE_{elec} (UOPBE)	ΔE_{elec} (UB3LYP)	ΔE_{elec} (UOPBE)	ΔE_{elec} (UB3LYP)	ΔE_{elec} (UOPBE)	ΔE_{elec} (UB3LYP)
I_{rad}	m2	0.00	0.00	0.21	0.00	0.00	0.32		
	m4	1.95	0.61	0.00	1.55	0.54	0.00	0.00	0.00
	m6	8.51	9.62						
I_{cat}	m2			10.90	5.17	8.61	3.76		
	m4			9.29	7.94	8.47	7.97	9.53	8.18
	m6			0.00	0.00	0.00	0.00	0.00	0.00

Table S5. I_{rad} and I_{cat} relative Electronic Energies obtained with **single point calculations** at UOPBE/6-311G(d,p)~SDD + SMD level of theory for the corresponding UB3LYP geometries.

Magnitude of the SPIN Contamination

	A^2		TS_{abs}^2		I_{rad}^2		$TS_{reb_NCH2}^2$		$TS_{reb_NCH3}^2$	
	$\langle \hat{S}_s^2 \rangle$	ΔE	$\langle \hat{S}_s^2 \rangle$	ΔE	$\langle \hat{S}_s^2 \rangle$	ΔE	$\langle \hat{S}_s^2 \rangle$	ΔE	$\langle \hat{S}_s^2 \rangle$	ΔE
Methane (solv.)	1.815	3.39	1.799	1.14	1.736	-1.01	1.576	-1.33	1.610	-0.37
Ethane (solv.)	1.813	3.43	1.796	1.42	1.688	-1.18	1.459	-1.12	1.769	0.06
Cyclohexane (solv.)	1.812	3.45	1.800	1.84	1.801	0.10			1.786	0.09
2,3-DMB (solv.)	1.814	3.43	1.770	1.71						
Methane (gas)	1.812	3.42	1.757	0.95	1.723	-0.95	1.768	0.04	1.758	-0.30

Table S6. Value of the square of the total spin angular momentum operator, $\langle \hat{S}_s^2 \rangle$, obtained for cases with spin contamination and the amount of energy corrected calculated as: $\Delta E = (E_{spin\ corr} - E_s)$ in kcal·mol⁻¹. E_s refers to the original electronic energy obtained for the calculation and $E_{spin\ corr}$ refers to the final reported energy value obtained applying eq. 1 of the manuscript.

Analysis of the electron transfer in the initial compound A

		G_{solv} (kcal/mol)
EA	Fe(V) m2 $\rightarrow$ Fe(IV) m1	-135.60
	Fe(V) m4 $\rightarrow$ Fe(IV) m3	-126.66
	Fe(V) m6 $\rightarrow$ Fe(IV) m5	-140.57
	Global Fe(V) m4 $\rightarrow$ Fe(III) m5	-132.17
IE	Methane	202.42
	Ethane	197.29
	Cyclohexane	159.84
	2,3-DMB	155.87

Table S7. Gibbs energy values at solvent (acetonitrile) (G_{solv}) for the ionization energies (IE) of the alkane substrates and for the electron affinities (EA) of the $\text{Fe}^{\text{V}}(\text{O})(\text{OH})$ catalyst at different multiplicities.

G_{golv} (kcal/mol)				
Alkane $\rightarrow$ Radical alkane				
	Methane	Ethane	Cyclohexane	2,3-DMB
m2	66.82	75.75	61.85	70.25
m4	61.70	70.63	56.72	65.13
m6	24.25	33.18	19.27	27.67
Global	20.28	29.21	15.30	23.70

Table S8. Energy differences between the IE of the substrates and the EA of the $\text{Fe}^{\text{V}}(\text{O})(\text{OH})$ catalyst at different catalyst multiplicities. Negative values account for a favorable substrate oxidation (radical forms), while positive values indicate that substrate oxidation is not favorable and they keep the neutral form. Values in kcal/mol and at solvent (G_{solv}).

Analysis of the Iron-bishydroxo intermediates' stability

At gas-phase

UB3LYP/6-311G(d,p)~SDD			Substrates / ΔG_g (kcal/mol)			
S	Catalyst Configuration	Substrate Configuration	Methyl	Ethyl	Cyclohexyl	2,3-DMB
$\frac{1}{2}$	Fe^{III} 		15.65 (0.00)	15.65 (0.00)	15.65 (0.00)	16.65 (0.00)
	Fe^{IV} 		30.66 (15.01)	69.16 (53.51)	97.26 (81.61)	107.82 (92.17)
	Fe^{IV} 		16.20 (0.54)	54.70 (39.05)	82.80 (67.15)	93.36 (77.71)
$\frac{3}{2}$	Fe^{III} 		10.49 (0.00)	10.49 (0.00)	10.49 (0.00)	10.49 (0.00)
	Fe^{IV} 		16.20 (5.70)	54.70 (44.20)	82.80 (72.31)	93.36 (82.87)
	Fe^{IV} 		19.12 (8.63)	57.62 (47.13)	85.73 (75.24)	96.29 (85.79)
$\frac{5}{2}$	Fe^{III} 		0.00 (0.00)	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)
	Fe^{IV} 		19.12 (19.12)	57.62 (57.62)	85.73 (85.73)	96.29 (96.29)

Table S9. Relative Gibbs energies (ΔG_g) in kcal/mol for radical and cation iron-bishydroxo catalysts electronic configurations evaluated considering catalyst and substrate separated at infinite distances. Values in parenthesis correspond to Gibbs energy differences within the same multiplicity species.

At gas-phase including single-point dispersion and acetonitrile solvent corrections

UB3LYP/6-311G(d,p)~SDD			Substrates / ΔG_{g+corr} (kcal/mol)			
S	Catalyst Configuration	Substrate Configuration	Methyl	Ethyl	Cyclohexyl	2,3-DMB
$1/2$	Fe^{III}		27.14 (27.14)	12.20 (0.00)	12.20 (0.00)	12.20 (0.00)
	Fe^{IV}		41.81 (41.81)	55.79 (43.59)	68.20 (56.00)	78.40 (66.19)
	Fe^{IV}		0.00 (0.00)	13.98 (1.78)	26.39 (14.18)	36.58 (24.38)
$3/2$	Fe^{III}		29.95 (29.95)	15.01 (1.02)	15.01 (0.00)	15.01 (0.00)
	Fe^{IV}		0.00 (0.00)	13.98 (0.00)	26.39 (11.38)	36.58 (21.58)
	Fe^{IV}		3.97 (3.97)	17.95 (3.97)	30.36 (15.35)	40.55 (25.55)
$5/2$	Fe^{III}		14.94 (10.97)	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)
	Fe^{IV}		3.97 (0.00)	17.95 (17.95)	30.36 (30.36)	40.55 (40.55)

Table S10. Relative Gibbs energies (ΔG_{g+corr}) in kcal/mol for radical and cation iron-bishydroxo catalysts electronic configurations evaluated considering catalyst and substrate separated at infinite distances. Values in parenthesis correspond to Gibbs energy differences within the same multiplicity species.

For the intermediates evaluated as an adduct

UB3LYP/6-311G(d,p)-SDD			Substrates / ΔG_g (kcal/mol)		Substrates / ΔG_{g+corr} (kcal/mol)	
S	Electronic Configuration	Iron Substrate	Methane	Cyclohexane	Methane	Cyclohexane
1/2	Fe ^{III}		- ^a	14.07	- ^a	10.22
	Fe ^{IV}		0.00	- ^a	0.00	- ^a
3/2	Fe ^{III}		- ^a	11.63	- ^a	9.55
	Fe ^{IV}		1.43	- ^a	1.08	- ^a
5/2	Fe ^{III}		- ^a	0.00	- ^a	0.00
	Fe ^{IV}		20.70^b	- ^a	- ^a	- ^a

^a We were unable to optimize the intermediate in this particular electronic structure. ^b ΔE_{elec} value.

Table S11. Relative Gibbs Energies at gas-phase (ΔG_g) and at gas-phase including single-point dispersion and acetonitrile solvent corrections (ΔG_{g+corr}) (kcal/mol) for radical and cation iron-bishydroxo intermediates for different spin multiplicities.

Radical stability against dissociation

It is widely accepted that when continuum solvation models are applied to calculate the solvation free energy of reactions that imply a change in the molecularity (i. e. association and dissociation reactions), the solvation entropy may be greatly overestimated.¹⁻³ There exist many published works where this overestimation of the solvation entropy has been reported and treated.⁴⁻⁹

The majority of approaches to compute the Gibbs energy of dissociation reactions in solution consider that most of the changes between gas-phase and solution free energies are due to the entropic term. Then, the Gibbs energy in solution can be computed through the following general expression:

$$\Delta G_{(sol)} = \Delta G_{(gas)} + \Delta G^{o/*} - \lambda T \Delta S_{(gas)}$$

The $\lambda T \Delta S_{(gas)}$ term determines the reduction of the gas-phase dissociation reaction entropy when the reaction takes place at solution. It has been proposed several approaches to compute $\lambda T \Delta S_{(gas)}$.¹⁰⁻¹² Here we have used the method proposed by Wertz based on the empirical correlation between solvent S_{gas} and S_{liq} .¹⁰ Wertz method was derived from the experimental evidence that different small molecules lose the same fraction of their entropy upon going from the gas phase into solution. Then, despite differences in the solute-solvent

interactions, the entropy of solution is a fairly constant fraction of the gaseous-phase entropy, which only depends on the solvent physical constants.^{10,13}

The fraction of entropy that is lost in going from gas to liquid is given by :

$$\alpha = \frac{S_{liq}^o - (S_{gas}^o + R \ln(\frac{V_{m,liq}}{V_{m,gas}}))}{(S_{gas}^o + R \ln(\frac{V_{m,liq}}{V_{m,gas}}))} \quad 13$$

Where S_{liq}^o and S_{gas}^o are the standard molar entropy of the solvent at liquid and gas phases, $V_{m,liq}$ is the molar volume of the solvent at liquid-phase and $V_{m,gas}$ is the ideal gas molar volume of the solvent. Then, using Wertz approach, the expression used to compute the $\lambda S_{(gas)}$ term is:

$$\lambda S_{(gas)} = \alpha \left(S_{(gas)} + R \ln \left(\frac{V_{m,liq}}{V_{m,gas}} \right) \right).$$

The right-hand term inside the parenthesis accounts for changes in molar volume.

For acetonitrile, which is the solvent considered in this paper, at 298.15K, S_{liq}^o is 149.62 J/molK and S_{gas}^o is 245.48 J/molK,¹⁴ $V_{m,liq}$ is 0.052 l. and $V_{m,gas}$ is 24.45 l. Then, the quantitative expression obtained for acetonitrile is: $S_{soln} = -0.23(S_{gas} - 12.22)$ (cal/molK).

$\Delta G_{(sol)} = \Delta G_{(gas)} - \lambda T \Delta S_{(gas)}$ (kcal/mol)	Methyl	Ethyl	Cyclohexyl	2,3-DMB
I_{rad}^4	0.00	0.00	0.00	0.00
I_{rad}^2	-1.42	-3.82	-2.09	---
Dissociated: $Fe^{IV}(OH)_2 \cdots \cdots R\cdot$	0.87	-2.81	3.92	1.67

Table S12. Gibbs energy ($\Delta G_{(sol)}$) stabilization of radical intermediates against dissociation in acetonitrile solution. Energies are given in kcal/mol. Dissociated intermediates have been evaluated considering the catalyst form ($Fe^{IV}(OH)_2$) and the radical deprotonated substrate at infinite distance.

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Correlations of:

TS Energy Barriers of the H-Abstraction

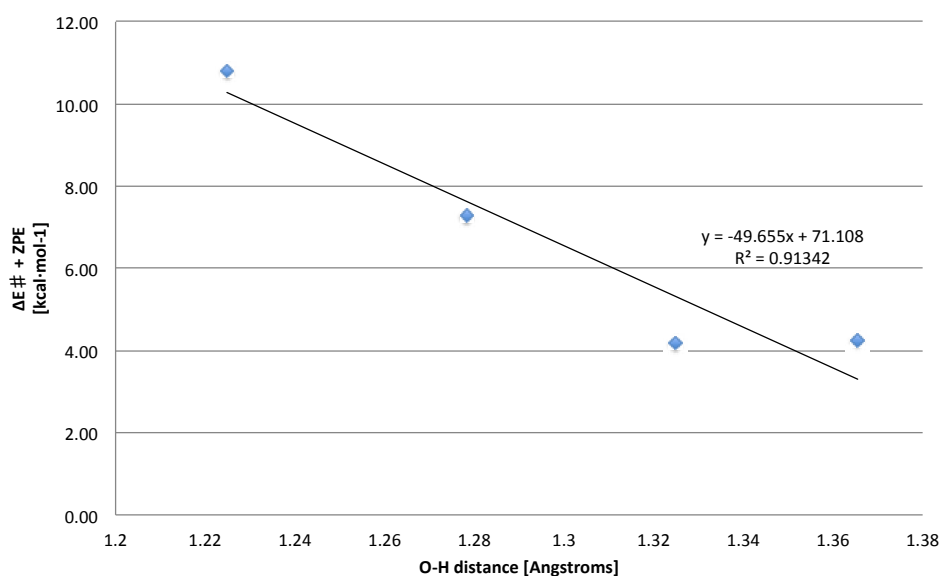


Figure S1. Correlation of the HAT energy barrier ($\Delta E^\ddagger + \text{ZPE}$) with respect to the transition state's O···H distance of the new formed bond.

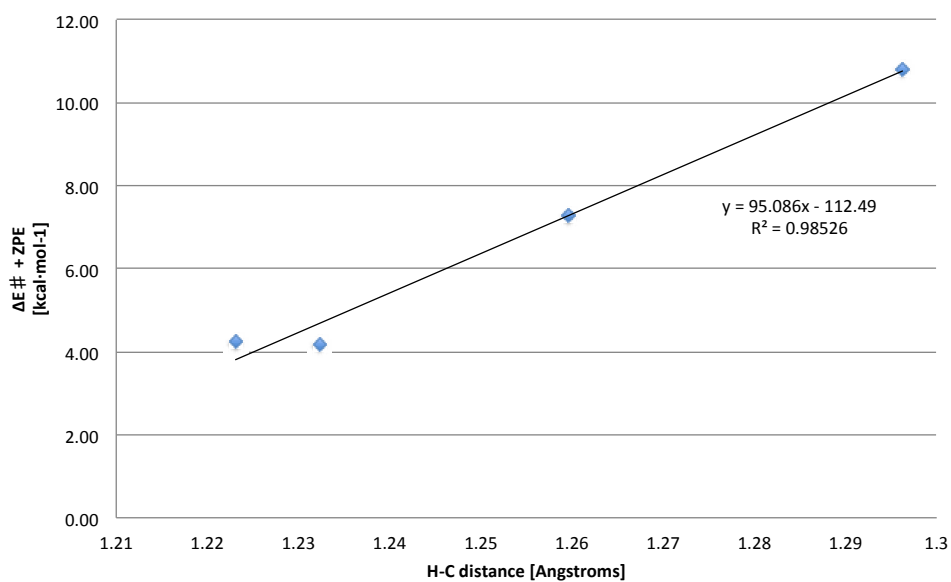


Figure S2. Correlation of the HAT energy barrier ($\Delta E^\ddagger + \text{ZPE}$) with respect to the transition state's C···H distance of the substrate cleaved bond.

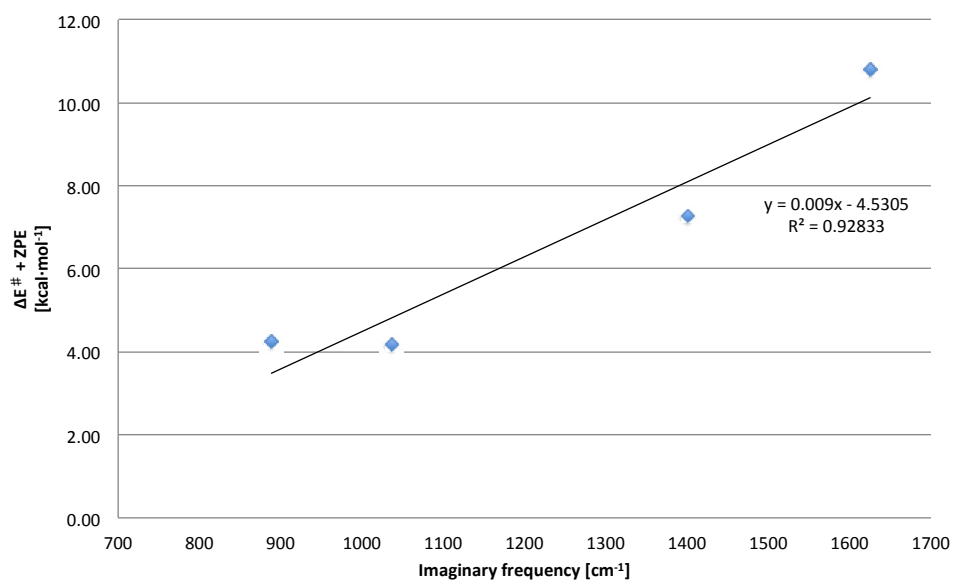


Figure S3. Correlation of the HAT energy barrier ($\Delta E^\ddagger + \text{ZPE}$) with respect to the transition state's imaginary frequency.

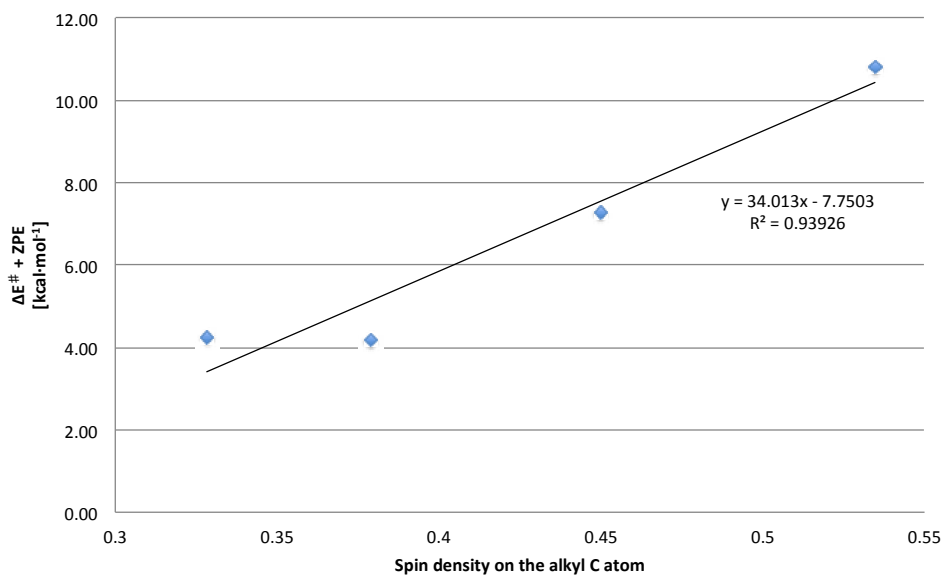


Figure S4. Correlation of the HAT energy barrier ($\Delta E^\ddagger + \text{ZPE}$) with respect to the spin density (radical character) of the C bonded to the abstracted hydrogen on the transition state.

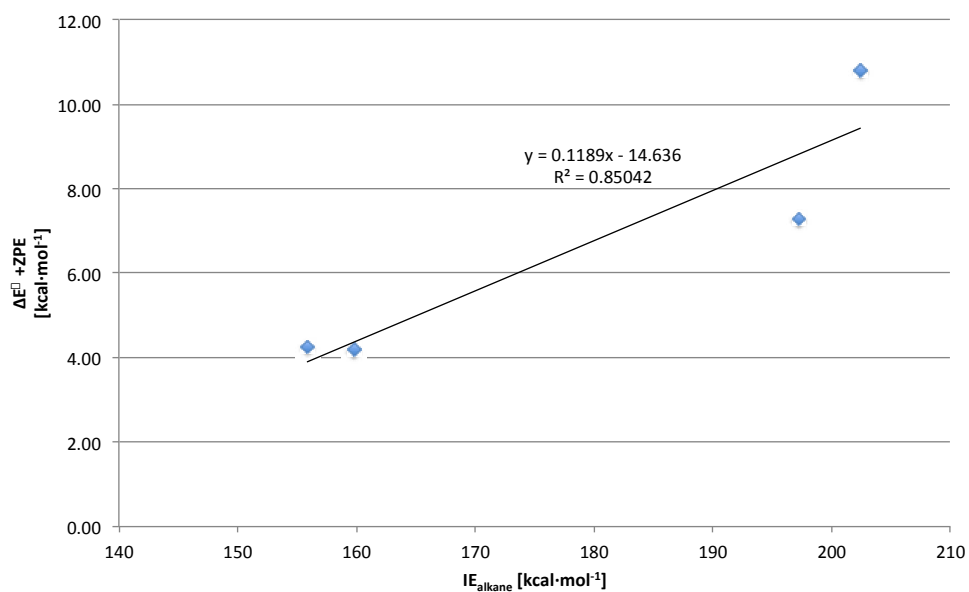


Figure S5. Correlation of the height of the HAT energy barrier ($\Delta E^{\ddagger} + \text{ZPE}$) with respect to the IE of the substrate.

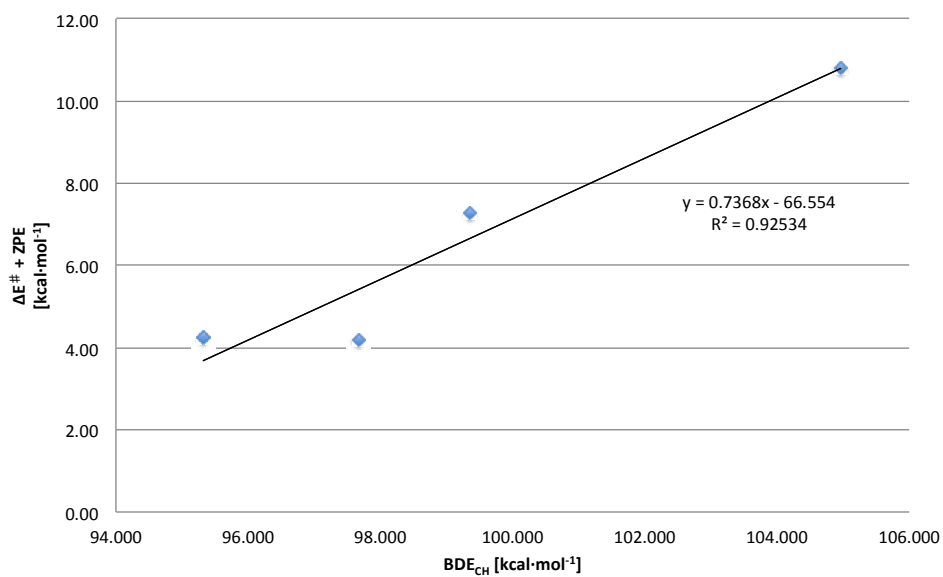


Figure S6. Correlation of the HAT energy barrier ($\Delta E^{\ddagger} + \text{ZPE}$) with the BDE_{CH} of substrates.

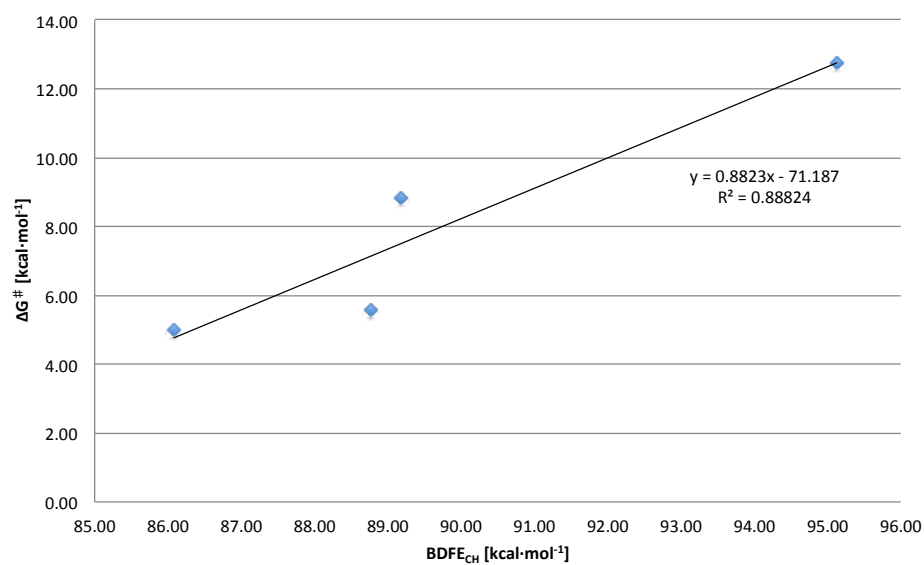


Figure S7. Correlation of the HAT free energy barrier ($\Delta G^\ddagger$) with the C-H bond dissociation free energy of substrates ($BDFE_{CH}$).

$I_{\text{cat}} - I_{\text{rad}}$ energy difference

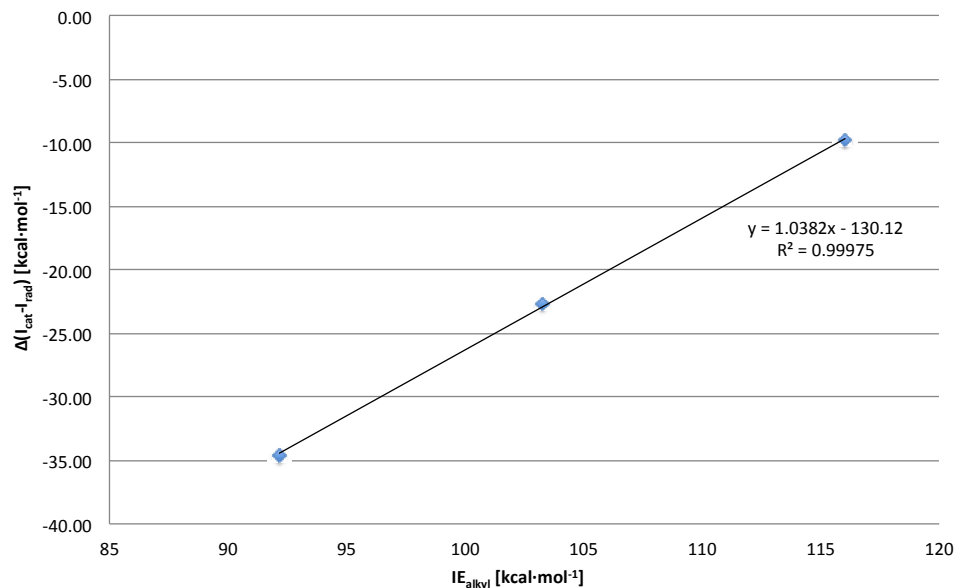


Figure S8. Correlation of the $I_{\text{cat}} - I_{\text{rad}}$ energy difference with the IE of the radical alkyl. [Only ethyl, cyclohexyl and 2,3-dimethanebutyl data are included because the I_{cat} is not optimized for the methyl substrate.]

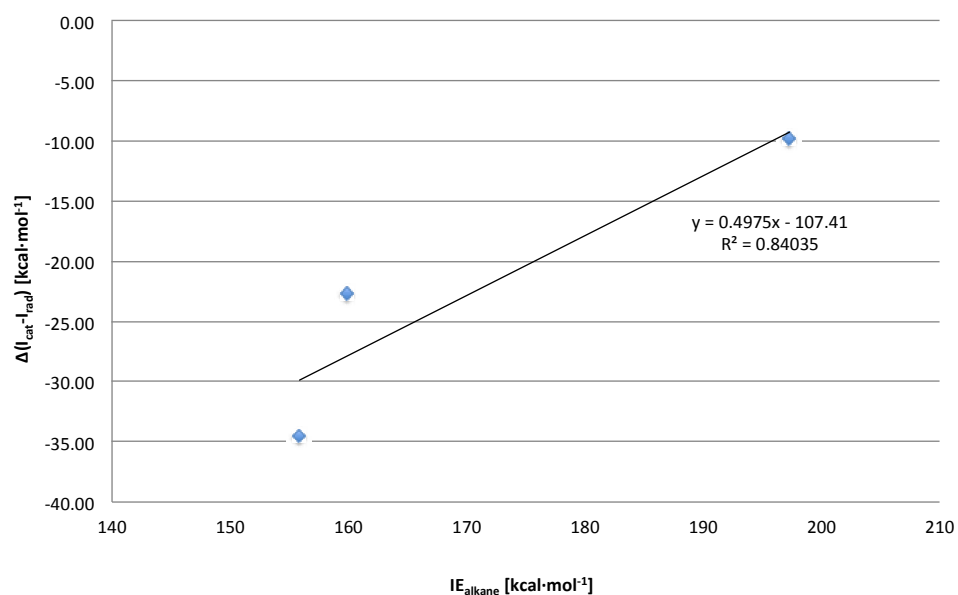


Figure S9. Correlation of the $I_{\text{cat}} - I_{\text{rad}}$ energy difference with the IE of the substrate. [Only ethyl, cyclohexyl and 2,3-dimethanebutyl correlations are evaluated because the I_{cat} is not detected for the methyl substrate.]

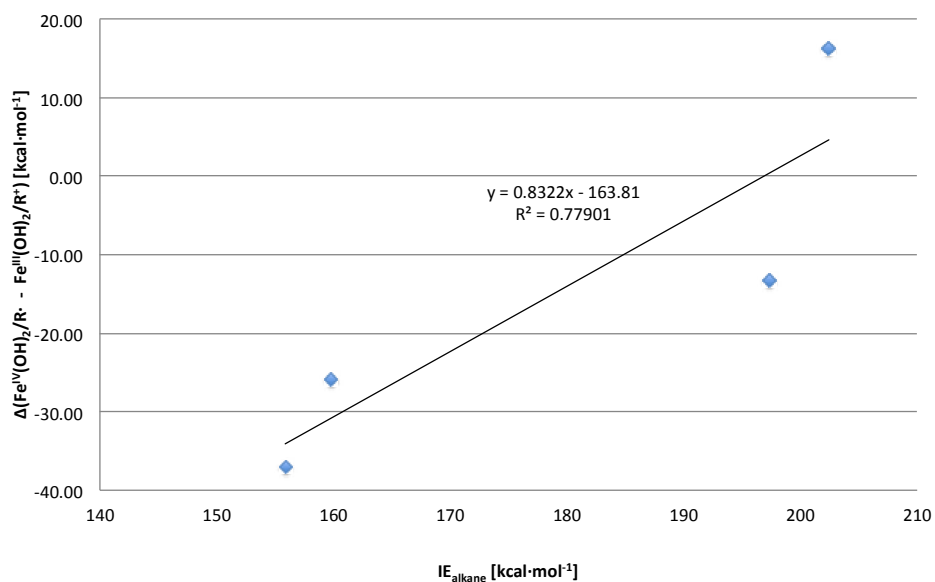


Figure S10. Stabilization of the cation intermediate ($\text{Fe}^{\text{IV}}(\text{OH})_2/\text{R}\cdot$) versus the radical intermediate ($\text{Fe}^{\text{III}}(\text{OH})_2/\text{R}^+$) with respect to the IE of the alkane substrate. The global cationic and radical intermediate energies have been calculated considering the catalyst and the alkyl substrate at infinite distance.

Self-Interaction Error (SIE) Analyses

Acetonitrile Solution

The self-interaction error (SIE) effect in the energy of the compounds is evaluated calculating the delocalization error at 60Å accordingly to:

$$\Delta E_{deloc(60\text{ Å})} = E(Fe_{complex} - Alkyl)_{60\text{ Å}} - E(Fe_{complex}) - E(Alkyl) - \frac{1}{4\pi\epsilon} \frac{Q_1 Q_2}{r},^1$$

Where $E(Fe_{complex} - Alkyl)_{60\text{ Å}}$ is the energy of the Fe complex and the alkyl separated by 60 Å, $E(Fe_{complex})$ is the energy of the isolated Fe complex, $E(Alkyl)$ is the energy of the isolated alkyl, and $\frac{1}{4\pi\epsilon} \frac{Q_1 Q_2}{r}$ is the Coulomb interaction in the localized state at $r=60\text{ Å}$. The Coulomb repulsion between two plus charges at gas-phase ($\epsilon_0 = 1$) at 60Å is 5.53 kcal/mol. The Coulomb repulsion considered between two plus charges at acetonitrile solution ($\epsilon_r = 37.5$) at 60Å is 0.15 kcal/mol.

Iron complex	Q _{tot}	S _{tot}	Mulliken Spin Densities			$\hat{S}^2$	E _{electronic} (a.u.)	E _{rel.}
			Fe	O (trans NCH ₂)	O (trans NCH ₃)			
[Fe ^{IV} (OH) ₂ (PyTACN)] ²⁺	+2	0	0.00	0.00	0.00	0.00	-1042.605618	22.60
[Fe ^{IV} (OH) ₂ (PyTACN)] ²⁺	+2	1	1.96	0.07	0.16	2.06	-1042.641636	0.00
[Fe ^{IV} (OH) ₂ (PyTACN)] ²⁺	+2	2	3.55	0.13	0.15	6.13	-1042.626859	9.27
[Fe ^{III} (OH) ₂ (PyTACN)] ⁺	+1	1/2	1.00	0.02	0.04	0.78	-1042.828693	-117.38
[Fe ^{III} (OH) ₂ (PyTACN)] ⁺	+1	3/2	2.83	0.02	0.04	3.81	-1042.824940	-115.03
[Fe ^{III} (OH) ₂ (PyTACN)] ⁺	+1	5/2	4.15	0.24	0.25	8.76	-1042.837298	-122.78

Table S13. Absolute (a.u.) and relative (kcal/mol) electronic energies of the [Fe^x(OH)₂(PyTACN)]⁺ⁿ catalysts ((x,n) being (IV,2) or (III,1)) obtained taking into account the effect of the acetonitrile solution and the D2 dispersion during the optimization ($E_{elec}^{solv} + E_{disp}^{solv}$). Mulliken spin densities of iron and oxygen atoms are also indicated. Q_{tot} and S_{tot} denote the total charge and total electronic spin angular momentum of the system.

Alkyl	Q _{tot}	S _{tot}	Mulliken Spin Densities		E _{electronic} (a.u.)
			C _{alkyl}	$\hat{S}^2$	
·CH ₃	0	2	1.14	0.75	-39.852819
·CH ₂ CH ₃	0	2	1.08	0.75	-79.187314
·C ₆ H ₁₁	0	2	1.02	0.75	-235.300359
·C(CH ₃) ₂ CH(CH ₃) ₂	0	2	0.95	0.75	-236.513442
CH ₃ ⁺	+1	1	0.00	0.00	-39.623821
CH ₂ CH ₃ ⁺	+1	1	0.00	0.00	-79.006025
C ₆ H ₁₁ ⁺	+1	1	0.00	0.00	-235.138494
C(CH ₃) ₂ CH(CH ₃) ₂ ⁺	+1	1	0.00	0.00	-236.369177

Table S14. Absolute electronic energies (a.u.) of the alkyl substrates studied in this project obtained taking into account the effect of the acetonitrile solution and the D2 dispersion during the optimization ($E_{elec}^{solv} + E_{disp}^{solv}$). Mulliken spin densities of alkyl

¹ Johansson, A. J.; Blomberg, M. R. A.; Siegbahn, P. E. M. *J. Chem. Phys.* **2008**, *129*, 154301.

carbons are also indicated. Q_{tot} and S_{tot} denote the total charge and total electronic spin angular momentum of the system.

System	IE+AE	S _{tot}	Mulliken Spin Densities					Ŝ ²	SIE (ΔE _{deloc} (60Å))	
			Fe	O (trans NCH ₂)	O (trans NCH ₃)	C _{alkyl}	Alkyl _{Global}			
Localized reference state [+2,0]										
Fe ^{IV} (OH) ₂ $\xrightarrow{60\text{\AA}}$ $\cdot\text{CH}_2\text{CH}_3$	-2.79	1/2	1.95	0.07	0.17	-1.08	-1.00	0.96	0.82	
	-2.83	3/2	1.95	0.08	0.16	1.08	1.00	3.75	0.25	
Fe ^{IV} (OH) ₂ $\xrightarrow{60\text{\AA}}$ $\cdot\text{C}_6\text{H}_{11}$	-15.58	1/2	1.95	0.08	0.16	-1.01	-1.00	0.96	0.77	
	-15.62	3/2	1.95	0.08	0.16	1.01	1.00	3.75	0.80	
Fe ^{IV} (OH) ₂ $\xrightarrow{60\text{\AA}}$ $\cdot\text{C}(\text{CH}_3)_2\text{CH}(\text{CH}_3)_2$	-26.70	3/2	1.97	0.07	0.15	0.95	1.00	3.75	0.83	
Localized reference state [+1,+1]										
Fe ^{III} (OH) ₂ $\xrightarrow{60\text{\AA}}$ CH_2CH_3^+	2.79	1/2	1.01	0.02	0.04	0.00	0.00	0.75	0.17	
	2.83	3/2	2.85	-0.03	0.11	0.00	0.00	3.75	0.95	
	18.82	5/2	4.16	0.24	0.25	0.00	0.00	8.75	0.52	
Fe ^{III} (OH) ₂ $\xrightarrow{60\text{\AA}}$ $\text{C}_6\text{H}_{11}^+$	15.58	1/2	0.97	0.05	0.05	0.00	0.00	0.75	1.17	
	15.62	3/2	2.85	-0.03	0.11	0.00	0.00	3.75	0.96	
	31.61	5/2	4.15	0.24	0.25	0.00	0.00	8.75	0.27	
Fe ^{III} (OH) ₂ $\xrightarrow{60\text{\AA}}$ $\text{C}(\text{CH}_3)_2\text{CH}(\text{CH}_3)_2^+$	26.70	3/2	2.85	-0.02	0.11	0.00	0.00	3.75	1.58	
	42.70	5/2	4.16	0.24	0.24	0.00	0.00	8.75	0.43	

Table S15. Evaluation of the SIE at 60Å of the $\text{Fe}^{\text{III}}(\text{OH})_2/\text{R}^+$ (I_{cat}) and $\text{Fe}^{\text{IV}}(\text{OH})_2/\text{R}\cdot$ (I_{rad}) intermediate species for ethane, cyclohexane and 2,3-dimethylbutane substrates taking into account the effect of the **acetonitrile solution** and the D2 dispersion during the optimization ($E_{\text{elec}}^{\text{solv}} + E_{\text{disp}}^{\text{solv}}$). Mulliken spin densities of iron, oxygens, the alkyl carbon atom and the whole alkyl substrate are also specified. The IE+AE term at G_{solv} energies is indicated for each system. Negative values of the IE+AE reflect that the reduction of the oxidized specie is favorable instead of the current situation. Positive values of the IE+AE term reflect the energy cost of the reduction of the current oxidized specie. All energies are given in kcal/mol.

No SIE is found neither for radical or cationic intermediates at acetonitrile solution. Slightly positive values of the delocalization error are found instead of negative or zero values. This is mainly due to two factors. First, the spin contamination of the independent $\text{Fe}_{\text{complex}}$ species has not been corrected (see Table S9), which cause an extra stabilization of the infinite distance separate species respect to the ones separated 60Å. Second, single-point calculations of the 60Å-separated species are done taking into account the $\text{Fe}_{\text{complex}}$ and alkyl geometries of the I_{rad} and I_{cat} minima, which are not the most stable geometries at 60Å.

Gas-phase

Iron complex	Q _{tot}	S _{tot}	Mulliken Spin Densities			$\hat{S}^2$	E _{electronic} (a.u.)	E _{rel.}
			Fe	O (trans NCH ₂)	O (trans NCH ₃)			
[Fe ^{IV} (OH) ₂ (PyTACN)] ²⁺	+2	0	0.04	-0.03	-0.03	1.04	-1042.249775	13.97
[Fe ^{IV} (OH) ₂ (PyTACN)] ²⁺	+2	1	1.43	0.08	0.17	2.06	-1042.272033	0.00
[Fe ^{IV} (OH) ₂ (PyTACN)] ²⁺	+2	2	3.52	0.14	0.14	6.13	-1042.261444	6.64
[Fe ^{III} (OH) ₂ (PyTACN)] ⁺	+1	1/2	1.00	0.02	0.04	0.79	-1042.635780	-228.26
[Fe ^{III} (OH) ₂ (PyTACN)] ⁺	+1	3/2	2.83	0.03	0.04	3.81	-1042.637386	-229.26
[Fe ^{III} (OH) ₂ (PyTACN)] ⁺	+1	5/2	4.13	0.27	0.28	8.76	-1042.653487	-239.37

Table S16. Absolute (a.u.) and relative (kcal/mol) electronic energies of the [Fe^X(OH)₂(PyTACN)]⁺ⁿ catalysts ((x,n) being (IV,2) or (III,1)) obtained at **gas-phase** (E_{elec}^g). Mulliken spin densities of iron and oxygen atoms are also indicated. Q_{tot} and S_{tot} denote the total charge and total electronic spin angular momentum of the system.

Alkyl	Q _{tot}	S _{tot}	Mulliken Spin Densities		E _{electronic} (a.u.)
			C _{alkyl}	S ²	
·C ₆ H ₁₁	0	2	1.02	0.75	-235.277295
C ₆ H ₁₁ ⁺	+1	1	0.00	0.00	-235.021145

Table S17. Absolute (a.u.) electronic energies of the cyclohexyl substrates studied at **gas-phase** (E_{elec}^g). Mulliken spin densities of the alkyl carbon are also indicated. Q_{tot} and S_{tot} denote the total charge and total electronic spin angular momentum of the system.

System	IE+AE	S _{tot}	Mulliken Spin Densities					$\hat{S}^2$	SIE ($\Delta E_{deloc(60\text{\AA})}$)
			Fe	O (trans NCH ₂)	O (trans NCH ₃)	C _{alkyl}	Alkyl _{Global}		
Fe ^{IV} (OH) ₂ $\xrightarrow{60\text{\AA}}$ ·C ₆ H ₁₁	-67.15	1/2	1.93	0.08	0.17	-1.02	-1.00	0.96	0.04
	-72.31	3/2	1.94	0.08	0.17	1.02	1.00	3.75	0.07
	-85.73	5/2	3.52	0.14	0.14	1.02	1.00	8.75	-0.02
Fe ^{III} (OH) ₂ $\xrightarrow{60\text{\AA}}$ C ₆ H ₁₁ ⁺	67.15	1/2	1.00	0.02	0.04	0.00	0.00	0.75	-0.28
	72.31	3/2	2.83	0.03	0.04	0.00	0.00	3.75	-0.40
	85.75	5/2	4.13	0.27	0.28	0.00	0.00	8.75	-0.15

Table S18. Evaluation of the SIE at 60Å of the Fe^{III}(OH)₂/R⁺ (I_{cat}) and Fe^{IV}(OH)₂/R· (I_{rad}) intermediate species for the cyclohexane substrate at **gas-phase** (E_{elec}^g). Mulliken spin densities of iron, the oxygens, the alkyl carbon atom and the whole cyclohexyl substrate are also specified. The IE+AE term at G_g energies is given for each system. Negative values reflect that the reduction of the oxidized specie is favorable instead of the current situation. Positive values of the IE+AE term reflect the energy cost of the reduction of the current oxidized specie. All energies are given in kcal/mol.

SIE is not found at the gas-phase case. In this study, the Fe_{complex} and alkyl geometries of the 60Å-separated species are the same as the separate species geometries. These geometries are more close to the optimized geometries and remove the positive values of the delocalization error.

XYZ Coordinates

METHANE_AT_SOLVENT

A_meta_2.log

51

H	-1.34199	-3.30626	-0.58837
H	-3.30032	-1.48560	-1.82642
H	-2.48083	-2.31772	0.30980
C	-1.47345	-2.34165	-0.09667
H	-3.56065	-0.64504	0.46812
H	-0.67807	-2.78815	1.86790
C	-2.64016	-0.67836	-1.49693
H	-2.30523	-1.16712	2.20698
H	-4.11873	0.61898	-0.62063
C	-0.58664	-1.74905	-2.29603
C	-3.24446	0.04831	-0.30711
N	-1.31129	-1.23834	-1.10638
C	-0.44458	-2.17409	0.99534
H	-2.46972	0.01032	-2.32259
H	0.53971	-2.45252	0.62396
C	-1.58272	-0.35631	2.26977
H	-1.27125	-0.26147	3.31054
H	-3.20922	1.06996	2.17135
N	-0.39206	-0.73212	1.42277
N	-2.23211	1.00059	0.28459
C	-2.19225	0.95360	1.78898
H	1.10009	-1.22745	2.85924
C	-2.53285	2.38823	-0.16566
C	0.92263	-0.47515	2.08790
H	-1.58937	1.80093	2.11139
Fe	-0.36672	0.44299	-0.25946
H	0.88765	0.51277	2.54786
C	1.97551	-0.52087	1.01327
N	1.53284	-0.20142	-0.22433
H	3.62054	-1.16512	2.21457
C	3.29297	-0.89624	1.21864
C	2.35555	-0.23083	-1.28227
H	1.92496	0.04983	-2.23349
C	4.15817	-0.93456	0.12751
C	3.68384	-0.60279	-1.13900
H	5.19234	-1.22664	0.26488
H	4.32713	-0.62366	-2.00863
H	-1.75377	3.06277	0.18826
H	-3.50068	2.68137	0.25064
H	-2.57361	2.40010	-1.25346
H	0.36382	-2.17357	-1.97271
H	-0.41372	-0.92937	-2.99022
H	-1.19074	-2.52574	-2.77516
O	0.26557	1.84960	0.57087
O	-0.35197	1.14788	-1.88329
H	-0.05487	2.07204	-1.85555
C	3.47529	2.81319	-0.26453
H	2.39702	2.71115	-0.11765
H	3.80228	3.78614	0.11511
H	3.70684	2.74344	-1.33077
H	3.99361	2.01669	0.27436

A_meta_4.log

51

H	-1.21932	-3.29853	-0.69405
H	-3.21666	-1.49948	-1.92363
H	-2.41134	-2.38002	0.20677
C	-1.39614	-2.35315	-0.17909
H	-3.53410	-0.76393	0.40695
H	-0.63950	-2.82834	1.79342
C	-2.58968	-0.68631	-1.54632
H	-2.28334	-1.27997	2.16264
H	-4.13199	0.51491	-0.64362
C	-0.50157	-1.66963	-2.34614
C	-3.23917	-0.03235	-0.34103
N	-1.25243	-1.21617	-1.15047
C	-0.39702	-2.18891	0.94188
H	-2.42773	0.04341	-2.33810
H	0.59997	-2.44323	0.58924
C	-1.59407	-0.44327	2.25396
H	-1.29587	-0.36142	3.29973
H	-3.28135	0.91077	2.16412
N	-0.38124	-0.75826	1.41106
N	-2.27335	0.93756	0.29585
C	-2.25340	0.85155	1.79804
H	1.10799	-1.24964	2.85500
C	-2.61825	2.32364	-0.12566
C	0.92466	-0.49171	2.09055
H	-1.69548	1.71664	2.15113
Fe	-0.35362	0.49119	-0.21944
H	0.87338	0.49159	2.56060
C	1.98133	-0.51446	1.01865
N	1.53567	-0.18759	-0.21597
H	3.63352	-1.15687	2.20970
C	3.30166	-0.88016	1.21734
C	2.35378	-0.19830	-1.27627
H	1.92005	0.09201	-2.22303
C	4.16515	-0.90011	0.12336
C	3.68605	-0.56084	-1.13860
H	5.20208	-1.18426	0.25629
H	4.32778	-0.56627	-2.00959
H	-1.87697	3.01637	0.26817
H	-3.60819	2.56124	0.27401
H	-2.63429	2.36197	-1.21371
H	0.45216	-2.08881	-2.02580
H	-0.33447	-0.82288	-3.00895
H	-1.08207	-2.44051	-2.86301
O	0.16142	1.81668	0.60663
O	-0.34518	1.23092	-1.84176
H	-0.06937	2.16047	-1.80218
C	3.39470	2.83763	-0.21927
H	2.32731	2.67928	-0.04730
H	3.68527	3.81862	0.16909
H	3.60361	2.79635	-1.29171
H	3.96444	2.05839	0.29251

A_meta_6.log

51

H	1.31962	-2.00189	2.70836
H	3.55410	0.07706	2.17414
H	2.43112	-2.07213	1.36209
C	1.47397	-1.66749	1.68185
H	3.72050	-1.16813	0.04151
H	0.42685	-3.25479	0.63372
C	2.87643	0.37298	1.36630
H	2.18341	-2.40831	-0.70879
H	4.51773	0.41300	0.03398
C	1.06254	0.37263	2.95215
C	3.54987	-0.09581	0.05982
N	1.51634	-0.16701	1.64130

C	0.33215	-2.18083	0.81776
H	2.79312	1.45991	1.35762
H	-0.61699	-1.99058	1.31884
C	1.49334	-1.83760	-1.32375
H	1.15725	-2.51159	-2.11330
H	3.04939	-1.15714	-2.59453
N	0.30650	-1.44535	-0.48796
N	2.84386	0.28801	-1.15539
C	2.22292	-0.69860	-2.02881
H	-1.04004	-2.83188	-1.37016
C	3.01790	1.64034	-1.62895
C	-0.94481	-1.74997	-1.24297
H	1.57696	-0.16742	-2.72261
Fe	0.09475	0.59917	0.11401
H	-0.84277	-1.28820	-2.22825
C	-2.16295	-1.18156	-0.56392
N	-1.96429	-0.07024	0.16190
H	-3.55660	-2.64721	-1.27747
C	-3.42728	-1.74249	-0.69671
C	-2.98969	0.53204	0.77825
H	-2.75136	1.42320	1.34415
C	-4.50213	-1.11855	-0.06822
C	-4.28285	0.03616	0.68207
H	-5.49949	-1.53317	-0.15659
H	-5.09422	0.54280	1.18850
H	2.25490	1.88143	-2.36332
H	4.02069	1.69805	-2.08019
H	2.99061	2.32822	-0.78060
H	0.04554	0.02297	3.13648
H	1.07065	1.45993	2.91573
H	1.72775	0.01158	3.74408
O	0.02378	1.14939	-1.42802
O	-0.06271	2.18212	0.96768
H	-0.27394	2.90625	0.36275
C	-2.65401	3.42495	-0.90395
H	-1.94095	2.69516	-1.29581
H	-2.54269	4.37335	-1.43841
H	-2.47021	3.58461	0.16186
H	-3.67218	3.04943	-1.03995

TSabs_meta_2.log

51

H	-1.04071	-3.43304	-0.18762
H	-3.14353	-1.91610	-1.57906
H	-2.24223	-2.43458	0.61163
C	-1.23930	-2.43043	0.19318
H	-3.44942	-0.81858	0.60255
H	-0.40151	-2.58695	2.18464
C	-2.54228	-1.02839	-1.36213
H	-2.14544	-1.05818	2.32692
H	-4.10430	0.25392	-0.62424
C	-0.42870	-2.03330	-2.07902
C	-3.18660	-0.20603	-0.25702
N	-1.17031	-1.44209	-0.93919
C	-0.21729	-2.06424	1.24296
H	-2.43339	-0.43402	-2.26807
H	0.78089	-2.31641	0.89175
C	-1.47897	-0.19844	2.30400
H	-1.17725	0.02384	3.32837
H	-3.19042	1.11053	2.08569
N	-0.26631	-0.58276	1.49510
N	-2.24217	0.88004	0.19496
C	-2.17588	1.00971	1.69135
H	1.27355	-0.78725	2.95371
C	-2.65617	2.17649	-0.40641
C	1.03073	-0.15262	2.09841

H	-1.61756	1.92088	1.89780
Fe	-0.33798	0.38963	-0.30883
H	0.92735	0.88170	2.42667
C	2.07207	-0.25742	1.01594
N	1.58959	-0.14709	-0.24261
H	3.78152	-0.57626	2.25743
C	3.42047	-0.47887	1.24165
C	2.40073	-0.25662	-1.30334
H	1.93622	-0.14874	-2.27362
C	4.27666	-0.58329	0.14719
C	3.76026	-0.48030	-1.14189
H	5.33544	-0.75418	0.30091
H	4.39388	-0.56510	-2.01481
H	-1.92145	2.93765	-0.15412
H	-3.63765	2.44419	-0.00426
H	-2.71724	2.05230	-1.48675
H	0.55315	-2.35532	-1.73232
H	-0.32150	-1.28615	-2.86295
H	-0.98442	-2.89733	-2.45690
O	0.14907	1.96788	0.39255
O	-0.38620	0.91537	-2.00170
H	-0.17450	1.86023	-2.06632
C	2.31628	2.87625	-0.52989
H	1.26650	2.41663	-0.03263
H	2.27555	3.93545	-0.26998
H	2.25191	2.68929	-1.60156
H	3.12345	2.33334	-0.03774

TSabs_meta_4.log

51			
H	-1.03120	-3.43131	0.10205
H	-3.14573	-2.04499	-1.40696
H	-2.23354	-2.37332	0.81767
C	-1.23182	-2.40068	0.39783
H	-3.44836	-0.77149	0.68107
H	-0.39013	-2.38618	2.39354
C	-2.54754	-1.14035	-1.26437
H	-2.12818	-0.86035	2.41475
H	-4.11081	0.19327	-0.62826
C	-0.43627	-2.19499	-1.90464
C	-3.19082	-0.23342	-0.22828
N	-1.17181	-1.51082	-0.81438
C	-0.20721	-1.94531	1.41084
H	-2.44486	-0.61985	-2.21527
H	0.79032	-2.22694	1.08068
C	-1.46783	-0.00181	2.31689
H	-1.16182	0.30664	3.31736
H	-3.18936	1.26816	1.99599
N	-0.25703	-0.44694	1.53637
N	-2.24614	0.88804	0.12873
C	-2.17478	1.14462	1.60832
H	1.29107	-0.51161	3.00070
C	-2.67197	2.12919	-0.57382
C	1.04184	0.03790	2.09000
H	-1.62329	2.07385	1.73455
Fe	-0.34070	0.36855	-0.34408
H	0.93932	1.09918	2.31957
C	2.07528	-0.17115	1.01525
N	1.58207	-0.17601	-0.24429
H	3.79341	-0.38259	2.26752
C	3.42467	-0.37566	1.25000
C	2.38495	-0.37835	-1.29793
H	1.91271	-0.35638	-2.27021
C	4.27179	-0.57967	0.16213
C	3.74563	-0.58749	-1.12729
H	5.33140	-0.73944	0.32186

H	4.37238	-0.74930	-1.99432
H	-1.94445	2.91505	-0.38502
H	-3.65499	2.41937	-0.19147
H	-2.73543	1.91970	-1.64072
H	0.54532	-2.49134	-1.53490
H	-0.32813	-1.51349	-2.74607
H	-0.99525	-3.08500	-2.21037
O	0.13718	1.99311	0.17354
O	-0.39830	0.74375	-2.08289
H	-0.22580	1.68654	-2.22929
C	2.37647	2.82335	-0.63172
H	1.23954	2.37828	-0.19634
H	2.32273	3.88562	-0.38953
H	2.36314	2.60923	-1.69986
H	3.13310	2.27474	-0.07224

TSabs_meta_6.log

51

H	1.07542	-3.19401	1.24671
H	3.26407	-1.33986	2.01515
H	2.22671	-2.53228	0.09775
C	1.25320	-2.37250	0.55224
H	3.49534	-1.07962	-0.43135
H	0.26511	-3.14054	-1.21248
C	2.67311	-0.56728	1.51431
H	2.04381	-1.80494	-1.91220
H	4.24791	0.29888	0.34932
C	0.60289	-1.25847	2.63892
C	3.29178	-0.19858	0.17356
N	1.27882	-1.07549	1.32754
C	0.15966	-2.32882	-0.48789
H	2.60409	0.30937	2.15812
H	-0.81141	-2.41130	-0.00601
C	1.40598	-0.95373	-2.13792
H	1.06318	-1.06200	-3.16803
H	3.15838	0.23589	-2.50018
N	0.21539	-1.01604	-1.21857
N	2.38123	0.71773	-0.57738
C	2.19018	0.34985	-2.00144
H	-1.29238	-1.62991	-2.57697
C	2.83731	2.11853	-0.43857
C	-1.06947	-0.77576	-1.93158
H	1.64803	1.17083	-2.47024
Fe	0.31131	0.48708	0.28038
H	-0.94747	0.11582	-2.54975
C	-2.16894	-0.55740	-0.92241
N	-1.76240	-0.11403	0.28129
H	-3.80708	-1.16296	-2.16414
C	-3.50877	-0.79921	-1.18886
C	-2.65094	0.09364	1.26358
H	-2.25158	0.45122	2.20413
C	-4.43985	-0.57684	-0.17648
C	-4.00650	-0.13207	1.07169
H	-5.49258	-0.75962	-0.35723
H	-4.70176	0.03978	1.88300
H	2.12185	2.78248	-0.92045
H	3.82329	2.22836	-0.90446
H	2.90894	2.36418	0.62184
H	-0.41671	-1.60374	2.46356
H	0.59586	-0.31298	3.17659
H	1.15484	-2.01154	3.20954
O	-0.07043	1.80169	-0.92530
O	0.37306	1.51334	1.74951
H	0.28260	2.46214	1.56849
C	-2.12283	3.07036	0.01727
H	-1.19242	2.50452	-0.46477

H	-2.05925	4.08345	-0.38567
H	-1.98951	3.03367	1.09867
H	-3.00439	2.52456	-0.32108

Irad_meta_2.log

51			
H	0.79497	-2.74069	2.18584
H	2.92102	-0.74789	2.53774
H	2.06823	-2.44241	1.01689
C	1.05533	-2.16636	1.29561
H	3.36468	-1.17573	0.15579
H	0.26312	-3.45615	-0.25367
C	2.38150	-0.14904	1.79845
H	2.08690	-2.37160	-1.19065
H	4.03822	0.39949	0.53825
C	0.18816	-0.47775	2.83542
C	3.10855	-0.16508	0.46363
N	1.00351	-0.69646	1.61559
C	0.08471	-2.46983	0.18062
H	2.27556	0.87072	2.16488
H	-0.93437	-2.43181	0.56013
C	1.47594	-1.63575	-1.70904
H	1.21147	-2.04511	-2.68479
H	3.26383	-0.51496	-2.18810
N	0.22206	-1.43059	-0.89625
N	2.23933	0.45942	-0.59937
C	2.23210	-0.32359	-1.88187
H	-1.29231	-2.41820	-2.02592
C	2.70255	1.84866	-0.86395
C	-1.03358	-1.40684	-1.70405
H	1.74478	0.30455	-2.62333
Fe	0.30395	0.41818	-0.01282
H	-0.86350	-0.77853	-2.57845
C	-2.10811	-0.81336	-0.82903
N	-1.65253	0.02140	0.13371
H	-3.79846	-1.77785	-1.71299
C	-3.46005	-1.09251	-0.94660
C	-2.49974	0.60729	0.99277
H	-2.05620	1.26715	1.72573
C	-4.35020	-0.48738	-0.06138
C	-3.86485	0.36963	0.92368
H	-5.41173	-0.69142	-0.13482
H	-4.52651	0.85170	1.63133
H	2.01122	2.32795	-1.55246
H	3.70587	1.80102	-1.29752
H	2.72962	2.39050	0.08035
H	-0.79739	-0.91808	2.68457
H	0.09699	0.59101	3.01739
H	0.67905	-0.96439	3.68401
O	-0.08709	1.32708	-1.54056
O	0.32750	1.83416	1.03110
H	0.05537	2.63116	0.52142
C	-1.16130	3.98167	-0.32702
H	-1.02304	1.56530	-1.59451
H	-0.55992	4.25368	-1.18597
H	-2.02462	3.33900	-0.45662
H	-1.04147	4.52410	0.60511

Irad_meta_4.log

51			
H	-1.17442	-3.39959	0.12032
H	-3.23230	-1.95986	-1.39587
H	-2.33547	-2.29368	0.83211
C	-1.33607	-2.36085	0.41145
H	-3.50425	-0.65328	0.67228
H	-0.47884	-2.36626	2.40127

C	-2.60727	-1.07205	-1.26466
H	-2.18542	-0.78103	2.40861
H	-4.12495	0.32238	-0.64910
C	-0.52438	-2.19723	-1.88783
C	-3.22258	-0.13249	-0.24029
N	-1.24459	-1.48091	-0.80708
C	-0.29191	-1.93484	1.41521
H	-2.48689	-0.56794	-2.22208
H	0.69419	-2.24496	1.07591
C	-1.49544	0.05362	2.30778
H	-1.18097	0.35706	3.30711
H	-3.17102	1.38009	1.97603
N	-0.29787	-0.43614	1.53279
N	-2.24001	0.95732	0.11259
C	-2.16072	1.22007	1.59069
H	1.24242	-0.54075	3.00151
C	-2.61708	2.21024	-0.59592
C	1.01375	0.01184	2.08734
H	-1.57625	2.12875	1.71095
Fe	-0.35837	0.36593	-0.35365
H	0.94122	1.07633	2.31189
C	2.04486	-0.23478	1.01755
N	1.55884	-0.20980	-0.24520
H	3.74281	-0.53790	2.27902
C	3.38162	-0.50535	1.25930
C	2.36058	-0.43666	-1.29531
H	1.89566	-0.38941	-2.27038
C	4.22524	-0.74183	0.17533
C	3.70906	-0.71022	-1.11771
H	5.27446	-0.95530	0.34068
H	4.33380	-0.89290	-1.98204
H	-1.85257	2.96239	-0.41862
H	-3.58302	2.54707	-0.20822
H	-2.70017	1.99593	-1.66066
H	0.44733	-2.51607	-1.51060
H	-0.39625	-1.52933	-2.73715
H	-1.10750	-3.07481	-2.18364
O	0.19210	2.01693	0.16282
O	-0.40407	0.72929	-2.09047
H	-0.22503	1.67143	-2.23491
C	3.01864	2.85573	-0.62043
H	1.13213	2.18102	-0.04402
H	2.80342	2.67704	-1.66741
H	2.81338	3.82958	-0.18975
H	3.58364	2.12560	-0.05396

Irad_meta_6.log

51

H	-1.23231	-3.36774	-0.34339
H	-3.35989	-1.72888	-1.57059
H	-2.34333	-2.37723	0.58769
C	-1.37083	-2.38325	0.10463
H	-3.54866	-0.80479	0.71535
H	-0.40063	-2.68972	2.00954
C	-2.74299	-0.86581	-1.30319
H	-2.09620	-1.13786	2.35448
H	-4.27226	0.33782	-0.40088
C	-0.70786	-1.90208	-2.20663
C	-3.32895	-0.12691	-0.10691
N	-1.35966	-1.34498	-0.99300
C	-0.26632	-2.10601	1.09494
H	-2.66060	-0.20004	-2.16203
H	0.69487	-2.36070	0.65511
C	-1.42403	-0.28303	2.32106
H	-1.06552	-0.10468	3.33623
H	-3.12495	1.03422	2.34449

N	-0.25820	-0.64653	1.44395
N	-2.37095	0.92070	0.35622
C	-2.16366	0.95970	1.82571
H	1.26848	-0.92832	2.88966
C	-2.77327	2.25047	-0.15699
C	1.05247	-0.27560	2.03921
H	-1.57763	1.85363	2.03267
Fe	-0.34971	0.43043	-0.40560
H	0.98024	0.75482	2.39219
C	2.12997	-0.38530	0.98766
N	1.70673	-0.26788	-0.28422
H	3.78027	-0.69378	2.31924
C	3.46878	-0.59341	1.28708
C	2.57727	-0.35171	-1.30000
H	2.16482	-0.24414	-2.29533
C	4.38123	-0.67615	0.23742
C	3.93113	-0.55932	-1.07682
H	5.43280	-0.83734	0.44356
H	4.61218	-0.62606	-1.91531
H	-2.00986	2.98106	0.10455
H	-3.73435	2.53512	0.28585
H	-2.87388	2.19422	-1.24142
H	0.29951	-2.22657	-1.94473
H	-0.67306	-1.13844	-2.98058
H	-1.29613	-2.75858	-2.55022
O	0.18308	1.97731	0.33527
O	-0.40294	0.98310	-2.12174
H	-0.23236	1.93253	-2.22277
C	2.92391	2.94834	-0.45695
H	1.05100	2.29640	0.00721
H	2.75869	3.92619	-0.01772
H	2.73483	2.79612	-1.51346
H	3.42867	2.17933	0.11588

Irad_MECP_dq_meta.log

51

H	-1.18392	-3.39727	0.13077
H	-3.23895	-1.95671	-1.38829
H	-2.34243	-2.28694	0.84027
C	-1.34335	-2.35744	0.41946
H	-3.50718	-0.64132	0.67421
H	-0.48434	-2.35781	2.40842
C	-2.61163	-1.07005	-1.26085
H	-2.18827	-0.76789	2.41036
H	-4.12589	0.33081	-0.65089
C	-0.53108	-2.20279	-1.88004
C	-3.22451	-0.12458	-0.24051
N	-1.25014	-1.48079	-0.80146
C	-0.29748	-1.93046	1.42052
H	-2.48973	-0.57035	-2.22045
H	0.68774	-2.24392	1.08142
C	-1.49606	0.06453	2.30612
H	-1.18011	0.37072	3.30414
H	-3.16944	1.39362	1.97097
N	-0.30019	-0.43154	1.53222
N	-2.23929	0.96391	0.10828
C	-2.15951	1.23047	1.58583
H	1.24046	-0.53882	2.99965
C	-2.61032	2.21621	-0.60412
C	1.01297	0.01403	2.08541
H	-1.57342	2.13814	1.70365
Fe	-0.35895	0.36540	-0.35742
H	0.94322	1.07839	2.31114
C	2.04423	-0.23645	1.01633
N	1.55992	-0.21012	-0.24705
H	3.73970	-0.54249	2.28054

C	3.37977	-0.51133	1.26034
C	2.36181	-0.44498	-1.29528
H	1.89866	-0.40001	-2.27142
C	4.22392	-0.75374	0.17797
C	3.70879	-0.72487	-1.11542
H	5.27238	-0.96955	0.34509
H	4.33363	-0.91406	-1.97852
H	-1.84151	2.96467	-0.42915
H	-3.57395	2.56026	-0.21708
H	-2.69447	1.99933	-1.66826
H	0.43980	-2.52281	-1.50158
H	-0.40162	-1.53883	-2.73208
H	-1.11669	-3.07996	-2.17220
O	0.18537	2.01770	0.17064
O	-0.40083	0.72042	-2.09356
H	-0.20940	1.66007	-2.23930
C	3.03861	2.85408	-0.64960
H	1.13676	2.17009	0.02945
H	2.81603	3.82144	-0.21330
H	2.84231	2.68021	-1.70076
H	3.57465	2.11292	-0.06897

TSreb_CH2_meta_2.log

51

H	0.74860	-1.91397	2.88769
H	2.87274	0.11294	2.66516
H	2.07188	-1.96960	1.73743
C	1.04643	-1.63687	1.87552
H	3.36478	-1.02596	0.53538
H	0.34186	-3.35415	0.75833
C	2.35191	0.44912	1.76380
H	2.17328	-2.56104	-0.41364
H	4.04554	0.59035	0.44164
C	0.13650	0.43563	2.79907
C	3.11193	0.03166	0.51664
N	0.97987	-0.14078	1.72442
C	0.12623	-2.28896	0.86877
H	2.23456	1.53141	1.79438
H	-0.90790	-2.17292	1.18670
C	1.56439	-2.03569	-1.14731
H	1.33544	-2.73091	-1.95588
H	3.34256	-1.07241	-1.91791
N	0.28567	-1.61810	-0.46771
N	2.26974	0.30563	-0.70101
C	2.30235	-0.82017	-1.69467
H	-1.17575	-2.93029	-1.30185
C	2.73926	1.55751	-1.35336
C	-0.94193	-1.86331	-1.28165
H	1.81540	-0.45089	-2.59409
Fe	0.30910	0.40076	-0.18458
H	-0.75042	-1.50976	-2.29495
C	-2.05241	-1.06659	-0.64604
N	-1.63842	0.02142	0.04539
H	-3.69677	-2.29302	-1.24689
C	-3.39376	-1.40837	-0.70154
C	-2.51980	0.79212	0.69812
H	-2.11333	1.64483	1.22252
C	-4.31899	-0.60679	-0.03513
C	-3.87694	0.50306	0.68056
H	-5.37325	-0.85511	-0.06462
H	-4.56580	1.14129	1.21820
H	2.05600	1.81414	-2.15973
H	3.74793	1.39202	-1.74320
H	2.76319	2.35200	-0.60740
H	-0.83850	-0.05099	2.78092
H	0.02344	1.50492	2.63011

H	0.61512	0.25680	3.76714
O	-0.05203	0.81043	-1.92934
O	0.29907	2.10125	0.35407
H	0.47478	2.68511	-0.40106
C	-1.60530	3.63129	-0.63237
H	-0.96632	1.10831	-2.03142
H	-0.88317	4.23726	-1.16850
H	-2.17403	2.88176	-1.16736
H	-1.89201	3.90580	0.37423

TSreb_CH2_meta_4.log

51

H	0.39296	-0.74792	3.37887
H	2.81986	0.61243	2.45718
H	1.62453	-1.51259	2.38860
C	0.68690	-0.96384	2.35103
H	3.06957	-1.35241	1.00252
H	-0.38988	-2.81198	2.01948
C	2.34365	0.64014	1.47274
H	1.53795	-2.92789	0.72395
H	3.99700	-0.04771	0.28176
C	0.18336	1.42780	2.31284
C	2.98876	-0.37160	0.54009
N	0.88861	0.32948	1.60783
C	-0.38283	-1.77890	1.66364
H	2.41968	1.64464	1.05985
H	-1.36097	-1.33959	1.84942
C	1.02233	-2.65150	-0.19398
H	0.65134	-3.56435	-0.66190
H	2.93809	-2.43253	-1.17664
N	-0.13869	-1.77167	0.18388
N	2.17564	-0.49998	-0.72403
C	1.96840	-1.92828	-1.14776
H	-1.85144	-3.00645	-0.11326
C	2.84681	0.25203	-1.81899
C	-1.41159	-2.09358	-0.52170
H	1.54859	-1.89200	-2.15010
Fe	0.29057	0.17144	-0.40042
H	-1.18586	-2.24009	-1.57854
C	-2.33039	-0.91141	-0.34142
N	-1.70061	0.27246	-0.16033
H	-4.19601	-1.94895	-0.46050
C	-3.71377	-0.98849	-0.33102
C	-2.39875	1.40211	0.02729
H	-1.81763	2.30519	0.15670
C	-4.45032	0.17944	-0.14176
C	-3.78609	1.38956	0.04493
H	-5.53315	0.14246	-0.13106
H	-4.32632	2.31406	0.20158
H	2.21492	0.23256	-2.70365
H	3.80871	-0.22635	-2.02628
H	3.00522	1.27763	-1.48794
H	-0.86621	1.15639	2.42697
H	0.27339	2.34186	1.72965
H	0.63436	1.56547	3.30067
O	-0.02522	-0.10936	-2.17702
O	0.60037	1.92430	-0.54653
H	0.60780	2.19239	-1.47855
C	0.97346	4.56747	-0.47001
H	-0.92057	0.15661	-2.42847
H	1.77296	4.50004	-1.19784
H	-0.04221	4.75107	-0.79784
H	1.20294	4.54352	0.58750

Prod_CH2_meta_2.log

51

H	0.53727	-1.75215	3.02045
H	2.81914	0.01349	2.68991
H	1.82211	-2.02328	1.85675
C	0.84024	-1.57610	1.98694
H	3.24311	-1.27287	0.64633
H	-0.06863	-3.28318	1.01037
C	2.34433	0.35113	1.76345
H	1.83772	-2.77720	-0.20473
H	4.05290	0.27156	0.45088
C	0.11564	0.62690	2.74205
C	3.07483	-0.20189	0.54953
N	0.92066	-0.09565	1.72616
C	-0.15835	-2.19465	1.03777
H	2.35945	1.44244	1.76157
H	-1.16826	-1.93328	1.34653
C	1.29978	-2.23395	-0.97999
H	1.01107	-2.94729	-1.75275
H	3.19469	-1.53855	-1.75410
N	0.05922	-1.64985	-0.34737
N	2.25785	0.05605	-0.68541
C	2.18834	-1.14439	-1.58386
H	-1.53950	-2.87961	-1.04943
C	2.83787	1.20030	-1.43270
C	-1.19410	-1.84620	-1.13340
H	1.76713	-0.79670	-2.52349
Fe	0.29063	0.31479	-0.22775
H	-0.97618	-1.62160	-2.17705
C	-2.21660	-0.87952	-0.58212
N	-1.69425	0.22526	0.00029
H	-3.97208	-1.99512	-1.08444
C	-3.58570	-1.09412	-0.62517
C	-2.50625	1.13593	0.55651
H	-2.02616	1.99169	1.01244
C	-4.43300	-0.14312	-0.05984
C	-3.88619	0.98592	0.54519
H	-5.50644	-0.28916	-0.08094
H	-4.51096	1.74080	1.00463
H	2.16824	1.46162	-2.24885
H	3.82396	0.92062	-1.81783
H	2.95399	2.04927	-0.75666
H	-0.90397	0.24243	2.71896
H	0.10913	1.69154	2.51325
H	0.54672	0.46351	3.73500
O	0.00745	0.65332	-2.01293
O	0.38506	2.28640	0.17317
H	1.24617	2.60587	0.48125
C	-0.14597	3.27240	-0.75831
H	-0.92559	0.70938	-2.25215
H	0.47158	3.30081	-1.65590
H	-1.15572	2.96099	-1.01023
H	-0.16103	4.23911	-0.25213

Prod_CH2_meta_4.log

51

H	0.33818	-0.86014	3.34951
H	2.81475	0.42867	2.50526
H	1.53420	-1.63946	2.33068
C	0.61873	-1.05430	2.31318
H	2.98753	-1.51172	0.98200
H	-0.51576	-2.85805	1.97854
C	2.35400	0.49975	1.51497
H	1.40740	-3.01726	0.61570
H	3.99412	-0.23194	0.32967
C	0.20277	1.34665	2.37032
C	2.96433	-0.51185	0.55571
N	0.88021	0.25975	1.62052

C	-0.48045	-1.82818	1.61008
H	2.50059	1.51026	1.13582
H	-1.44280	-1.35933	1.81034
C	0.88906	-2.67616	-0.28033
H	0.51727	-3.56138	-0.80149
H	2.78887	-2.48982	-1.30319
N	-0.24461	-1.80824	0.14345
N	2.15993	-0.54228	-0.71627
C	1.85584	-1.92661	-1.20540
H	-2.02720	-2.90905	-0.27763
C	2.88234	0.21120	-1.77475
C	-1.50640	-2.00129	-0.59849
H	1.40702	-1.80107	-2.18977
Fe	0.28460	0.25857	-0.38531
H	-1.26615	-2.08961	-1.66033
C	-2.38513	-0.78771	-0.37281
N	-1.74073	0.37553	-0.12635
H	-4.26210	-1.79393	-0.56634
C	-3.77129	-0.84558	-0.38682
C	-2.43650	1.50085	0.10111
H	-1.85484	2.39462	0.28786
C	-4.49978	0.31921	-0.15744
C	-3.82376	1.51103	0.09418
H	-5.58311	0.29405	-0.16509
H	-4.35461	2.43446	0.28583
H	2.25933	0.26288	-2.66507
H	3.82346	-0.30154	-1.99797
H	3.09589	1.21558	-1.40839
H	-0.83897	1.06487	2.52280
H	0.24197	2.27331	1.80204
H	0.69139	1.48537	3.33997
O	-0.01437	0.23880	-2.19758
O	0.68014	2.39851	-0.69480
H	0.59077	2.43501	-1.65926
C	1.57357	3.45781	-0.27557
H	-0.94535	0.35544	-2.42873
H	2.59061	3.25667	-0.62211
H	1.21799	4.40730	-0.68195
H	1.55626	3.50218	0.81138

TSreb_CH3_meta_2.log

51

H	-0.58693	-2.85567	2.10667
H	-2.88719	-2.76424	0.28261
H	-1.85632	-1.64774	2.17369
C	-0.87641	-1.86391	1.75660
H	-3.22566	-0.51539	1.23938
H	0.04985	-0.62447	3.27211
C	-2.38104	-1.91877	-0.19259
H	-1.83031	0.53779	2.56827
H	-4.04411	-0.55851	-0.31340
C	-0.19512	-3.01770	-0.28442
C	-3.06697	-0.61132	0.16765
N	-0.95677	-1.86469	0.25322
C	0.13915	-0.84095	2.20511
H	-2.37307	-2.05969	-1.27216
H	1.14363	-1.20914	2.00561
C	-1.26617	1.19379	1.90810
H	-0.94588	2.06157	2.48620
H	-3.12431	1.91456	1.06450
N	-0.05523	0.43194	1.43159
N	-2.22567	0.54934	-0.29775
C	-2.12073	1.64113	0.72744
H	1.55811	1.31768	2.50900
C	-2.80364	1.09942	-1.55412
C	1.21293	1.21693	1.47739

H	-1.66376	2.48967	0.22590
Fe	-0.30512	-0.03821	-0.54163
H	1.01571	2.20572	1.06633
C	2.21608	0.48598	0.62455
N	1.67156	-0.27584	-0.35198
H	3.99858	1.14609	1.60289
C	3.58889	0.54113	0.80414
C	2.45007	-0.99569	-1.17349
H	1.93606	-1.57292	-1.92982
C	4.40714	-0.19806	-0.04742
C	3.83147	-0.98091	-1.04580
H	5.48339	-0.16981	0.07412
H	4.43632	-1.57315	-1.71988
H	-2.15254	1.88241	-1.93432
H	-3.79603	1.50179	-1.33034
H	-2.88425	0.29099	-2.27946
H	0.83159	-2.95927	0.07749
H	-0.21008	-2.98083	-1.37152
H	-0.65455	-3.94679	0.06764
O	0.03543	1.60811	-1.25129
O	-0.48059	-0.79492	-2.15537
H	-0.39401	-0.12151	-2.84433
C	0.31477	4.04435	-0.50046
H	0.96571	1.72948	-1.49250
H	-0.36619	4.26539	-1.31114
H	-0.05000	4.03884	0.51889
H	1.38092	4.00727	-0.68842

TSreb_CH3_meta_4.log

51

H	-0.66385	-3.06888	1.82550
H	-2.97073	-2.72831	0.00674
H	-1.90578	-1.84323	2.01590
C	-0.93210	-2.04126	1.57492
H	-3.25290	-0.59142	1.18538
H	0.03155	-0.98466	3.20301
C	-2.43292	-1.85601	-0.37658
H	-1.84240	0.28169	2.61678
H	-4.06175	-0.44862	-0.36777
C	-0.27674	-2.99464	-0.57985
C	-3.08959	-0.57332	0.11005
N	-1.01409	-1.89359	0.08203
C	0.10964	-1.09039	2.11842
H	-2.41879	-1.88857	-1.46504
H	1.10444	-1.45501	1.87074
C	-1.25813	0.99357	2.03666
H	-0.92376	1.78340	2.71037
H	-3.09521	1.84314	1.27221
N	-0.05923	0.26338	1.48602
N	-2.22219	0.61415	-0.22739
C	-2.09527	1.58796	0.91099
H	1.56257	1.00832	2.65212
C	-2.77735	1.31201	-1.41789
C	1.22177	1.02149	1.61439
H	-1.61678	2.47608	0.50583
Fe	-0.30955	0.00936	-0.53920
H	1.03999	2.05022	1.30118
C	2.21694	0.36147	0.69594
N	1.66717	-0.27773	-0.36296
H	4.00369	0.86070	1.75753
C	3.58817	0.35801	0.89367
C	2.43568	-0.92497	-1.25083
H	1.91663	-1.40119	-2.07147
C	4.39768	-0.30801	-0.02465
C	3.81530	-0.96229	-1.10783
H	5.47250	-0.32332	0.11070

H	4.41300	-1.49423	-1.83636
H	-2.09714	2.10779	-1.71199
H	-3.75501	1.72422	-1.15103
H	-2.88856	0.58907	-2.22524
H	0.74637	-3.01085	-0.20402
H	-0.27594	-2.82649	-1.65526
H	-0.76572	-3.94690	-0.34943
O	0.08311	1.76714	-0.94420
O	-0.48900	-0.53295	-2.22123
H	-0.44171	0.22935	-2.81877
C	0.53503	4.30118	-0.51789
H	1.00531	1.87606	-1.22010
H	0.69176	4.49152	-1.57240
H	-0.44860	4.43213	-0.08618
H	1.38189	4.08871	0.12273

Prod_CH3_meta_2.log

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H	-0.58806	-3.20899	1.49083
H	-2.87002	-2.74720	-0.30261
H	-1.87236	-2.05771	1.80708
C	-0.88578	-2.16711	1.36476
H	-3.22742	-0.76764	1.13294
H	-0.00355	-1.28066	3.13110
C	-2.37259	-1.80988	-0.56884
H	-1.86315	0.00533	2.65960
H	-4.05099	-0.46716	-0.38813
C	-0.17992	-2.84656	-0.87284
C	-3.07125	-0.62042	0.06645
N	-0.95186	-1.83804	-0.10478
C	0.11160	-1.25613	2.04463
H	-2.34814	-1.69998	-1.65180
H	1.12245	-1.57216	1.79504
C	-1.29189	0.78700	2.16135
H	-0.99472	1.51785	2.91488
H	-3.15107	1.65319	1.46620
N	-0.07325	0.14941	1.55205
N	-2.22372	0.60670	-0.14290
C	-2.14299	1.46079	1.08732
H	1.54174	0.78303	2.80163
C	-2.79068	1.38242	-1.27639
C	1.19181	0.90181	1.77258
H	-1.70291	2.40925	0.79319
Fe	-0.31439	0.05061	-0.47060
H	1.00279	1.96042	1.59597
C	2.20600	0.37202	0.78799
N	1.67517	-0.18159	-0.32703
H	3.97457	0.85016	1.89285
C	3.57752	0.41400	0.98510
C	2.47440	-0.70047	-1.27214
H	1.97144	-1.11536	-2.13552
C	4.41336	-0.11910	0.00561
C	3.85555	-0.68770	-1.13742
H	5.48851	-0.09804	0.13854
H	4.47384	-1.11637	-1.91535
H	-2.13026	2.20501	-1.53461
H	-3.77385	1.76758	-0.98857
H	-2.88204	0.71758	-2.13330
H	0.84037	-2.87234	-0.49043
H	-0.17761	-2.56261	-1.92276
H	-0.64393	-3.82950	-0.74283
O	0.29866	2.02380	-0.98389
O	-0.45866	-0.24540	-2.25693
H	-0.19767	0.54154	-2.75313
C	0.10123	3.40434	-0.57565
H	1.20278	1.94653	-1.31485

H	-0.93235	3.68058	-0.77409
H	0.32267	3.53227	0.48557
H	0.76079	4.03682	-1.17171

Prod_CH3_meta_4.log

51			
H	-0.86646	-3.34446	1.37104
H	-3.19934	-2.55053	-0.43507
H	-2.03393	-2.08679	1.73123
C	-1.07970	-2.27971	1.24454
H	-3.29979	-0.63605	1.08610
H	0.00183	-1.55972	2.98754
C	-2.55394	-1.69084	-0.65157
H	-1.87289	-0.13532	2.64035
H	-4.08266	-0.19243	-0.41950
C	-0.48481	-2.93494	-1.03671
C	-3.12254	-0.45038	0.02969
N	-1.16577	-1.93315	-0.19898
C	0.03112	-1.47233	1.89829
H	-2.51399	-1.53698	-1.73050
H	0.99528	-1.83119	1.54174
C	-1.25127	0.64221	2.20260
H	-0.89906	1.28052	3.01436
H	-3.01908	1.73277	1.58524
N	-0.07545	-0.01707	1.53045
N	-2.19030	0.72648	-0.10327
C	-2.03231	1.47153	1.19182
H	1.53657	0.46791	2.84682
C	-2.69558	1.64567	-1.15608
C	1.22117	0.66893	1.82036
H	-1.49638	2.39091	0.96872
Fe	-0.28603	0.09488	-0.51156
H	1.06460	1.74361	1.70349
C	2.23487	0.18339	0.81874
N	1.70877	-0.19378	-0.36913
H	3.99142	0.40119	2.01987
C	3.59820	0.10698	1.05530
C	2.50123	-0.64977	-1.35104
H	2.00209	-0.92545	-2.27064
C	4.42959	-0.35901	0.03843
C	3.87519	-0.74553	-1.17999
H	5.49875	-0.42772	0.20021
H	4.49066	-1.11775	-1.98858
H	-1.97235	2.44172	-1.32415
H	-3.65073	2.07111	-0.83276
H	-2.83626	1.07601	-2.07394
H	0.54597	-3.04136	-0.69297
H	-0.48370	-2.58811	-2.07053
H	-0.99145	-3.90637	-0.96982
O	0.48133	2.29681	-0.81411
O	-0.42644	-0.03905	-2.29023
H	-0.48943	0.82259	-2.72602
C	0.37063	3.64802	-0.31387
H	1.38911	2.17017	-1.11744
H	0.88158	4.33552	-0.99236
H	-0.68714	3.90656	-0.28224
H	0.80262	3.72807	0.68846

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A_eta_2.log

54			
H	1.88223	-2.85292	1.61282
H	3.46584	-0.44400	2.23216
H	2.91874	-2.02483	0.46403
C	1.90118	-2.08220	0.84115
H	3.74662	-0.32419	-0.20700

H	1.30416	-3.24618	-0.88644
C	2.71438	0.10221	1.65495
H	2.70427	-1.56077	-1.68688
H	4.03307	1.28866	0.43303
C	0.79741	-0.98333	2.72517
C	3.27747	0.51311	0.30507
N	1.51194	-0.75934	1.44410
C	0.93031	-2.43266	-0.26070
H	2.39030	0.97653	2.21706
H	-0.02380	-2.72903	0.17042
C	1.87381	-0.94518	-2.02542
H	1.62973	-1.23931	-3.04670
H	3.25498	0.68697	-2.36473
N	0.69499	-1.22661	-1.12762
N	2.17303	1.05348	-0.57185
C	2.24308	0.53183	-1.98276
H	-0.61202	-2.38188	-2.34818
C	2.22509	2.54249	-0.57870
C	-0.59318	-1.40251	-1.86503
H	1.54319	1.12303	-2.57121
Fe	0.38461	0.39535	0.09253
H	-0.66317	-0.62413	-2.62554
C	-1.70468	-1.26065	-0.85899
N	-1.39009	-0.52626	0.23270
H	-3.18084	-2.43738	-1.85991
C	-2.95579	-1.84190	-0.98447
C	-2.27629	-0.34364	1.22206
H	-1.94865	0.26175	2.05540
C	-3.88942	-1.65225	0.03188
C	-3.54385	-0.90108	1.15263
H	-4.87510	-2.09477	-0.04705
H	-4.24089	-0.73961	1.96411
H	1.37836	2.93271	-1.14234
H	3.16311	2.85048	-1.04888
H	2.18434	2.89485	0.45062
H	-0.05999	-1.63048	2.54016
H	0.46559	-0.02653	3.12313
H	1.47707	-1.46894	3.43225
O	-0.39556	1.34401	-1.15380
O	0.15343	1.55871	1.40553
H	-2.96488	1.37991	-0.96426
C	-3.53517	2.25747	-0.64745
H	-4.48519	1.90871	-0.22991
H	-3.75800	2.84931	-1.54181
H	-0.31793	2.34649	1.08763
C	-2.75401	3.08666	0.37401
H	-2.54400	2.50464	1.27750
H	-1.80267	3.42672	-0.04950
H	-3.31839	3.97435	0.67873

A_eta_4.log

54

H	1.77049	-2.90507	1.58010
H	3.42414	-0.54769	2.25870
H	2.85549	-2.09467	0.46653
C	1.82948	-2.12115	0.82362
H	3.73172	-0.42232	-0.18656
H	1.24243	-3.23425	-0.93952
C	2.69711	0.02299	1.67341
H	2.66633	-1.59247	-1.70080
H	4.07264	1.16919	0.47791
C	0.74687	-1.01667	2.71473
C	3.29030	0.42357	0.33507
N	1.47303	-0.79825	1.44008
C	0.87030	-2.42885	-0.30221
H	2.39282	0.90530	2.23465

H	-0.09375	-2.72301	0.10650
C	1.86090	-0.94273	-2.03605
H	1.61522	-1.21026	-3.06436
H	3.30137	0.64585	-2.33106
N	0.66621	-1.20414	-1.15237
N	2.21554	1.01567	-0.54449
C	2.28013	0.51862	-1.96360
H	-0.65916	-2.30211	-2.40856
C	2.32196	2.50171	-0.52168
C	-0.62472	-1.34006	-1.89261
H	1.60738	1.14585	-2.54516
Fe	0.37049	0.42458	0.06878
H	-0.68611	-0.53469	-2.62636
C	-1.72735	-1.21650	-0.87465
N	-1.39466	-0.51760	0.23490
H	-3.22640	-2.34739	-1.89230
C	-2.98616	-1.77796	-1.00365
C	-2.26862	-0.34585	1.23540
H	-1.92722	0.23661	2.07940
C	-3.90905	-1.60213	0.02593
C	-3.54510	-0.88424	1.16165
H	-4.90146	-2.02862	-0.05662
H	-4.23392	-0.73179	1.98182
H	1.50289	2.93160	-1.09504
H	3.28145	2.77839	-0.96748
H	2.27678	2.83586	0.51353
H	-0.11627	-1.65434	2.52454
H	0.42291	-0.05709	3.11294
H	1.41446	-1.51202	3.42705
O	-0.30595	1.37301	-1.09220
O	0.16915	1.56304	1.42456
H	-2.92194	1.38311	-0.97571
C	-3.48626	2.26478	-0.66160
H	-4.44420	1.92623	-0.25388
H	-3.69448	2.86285	-1.55541
H	-0.27929	2.37412	1.13631
C	-2.70550	3.08167	0.37005
H	-2.50906	2.49354	1.27251
H	-1.74719	3.41491	-0.04401
H	-3.26301	3.97413	0.67361

A_eta_6.log

54

H	1.87314	-2.30591	2.34096
H	3.77122	0.12145	2.06738
H	2.89799	-2.02252	0.95467
C	1.91800	-1.80436	1.37357
H	3.97193	-0.76981	-0.23132
H	1.02248	-3.35038	0.14071
C	3.01948	0.43600	1.33551
H	2.58015	-2.07372	-1.12934
H	4.56989	0.88733	-0.03337
C	1.31575	-0.05843	2.96161
C	3.67460	0.25860	-0.04621
N	1.76065	-0.32192	1.56554
C	0.80165	-2.33742	0.48901
H	2.79223	1.49003	1.49671
H	-0.13190	-2.35161	1.05125
C	1.78288	-1.51835	-1.61502
H	1.49407	-2.10079	-2.49171
H	3.15752	-0.43956	-2.81444
N	0.60372	-1.43012	-0.68669
N	2.85214	0.72228	-1.15327
C	2.31298	-0.19269	-2.15142
H	-0.59575	-2.84978	-1.71835
C	2.80591	2.14262	-1.40279

C	-0.63667	-1.79474	-1.43426
H	1.56401	0.34625	-2.72502
Fe	0.14217	0.44409	0.23761
H	-0.65122	-1.18649	-2.34199
C	-1.87949	-1.50116	-0.63554
N	-1.77384	-0.51699	0.27067
H	-3.13575	-2.96635	-1.57045
C	-3.08047	-2.16937	-0.83943
C	-2.83318	-0.15028	1.00463
H	-2.66946	0.65413	1.70984
C	-4.18998	-1.79018	-0.08789
C	-4.06686	-0.76671	0.85129
H	-5.13989	-2.29211	-0.22993
H	-4.90726	-0.44964	1.45518
H	1.96201	2.38202	-2.04367
H	3.75267	2.41467	-1.89572
H	2.75299	2.67755	-0.45202
H	0.36304	-0.56523	3.12304
H	1.18282	1.01204	3.10083
H	2.06526	-0.44563	3.66041
O	-0.10649	1.20586	-1.19211
O	-0.18558	1.81925	1.36014
H	-2.50082	1.79629	-1.25132
C	-3.26586	2.55403	-1.06395
H	-4.21185	2.04257	-0.85789
H	-3.39452	3.13861	-1.98192
H	-0.51711	2.60575	0.90526
C	-2.86239	3.45832	0.10346
H	-2.74339	2.88391	1.02744
H	-1.91482	3.97015	-0.10418
H	-3.61641	4.23128	0.28770

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H	1.62510	-3.06247	1.42317
H	3.36981	-0.82373	2.20865
H	2.72424	-2.23261	0.33651
C	1.70304	-2.24288	0.70746
H	3.67960	-0.54977	-0.21908
H	1.04490	-3.23585	-1.10228
C	2.66353	-0.18643	1.66860
H	2.55462	-1.60126	-1.76750
H	4.07780	0.98062	0.54472
C	0.66910	-1.20044	2.66086
C	3.26688	0.27765	0.35319
N	1.40419	-0.94208	1.39955
C	0.71971	-2.44685	-0.42024
H	2.39888	0.66857	2.28856
H	-0.25468	-2.71217	-0.01539
C	1.77378	-0.90624	-2.06800
H	1.51946	-1.11285	-3.10833
H	3.26975	0.63970	-2.30341
N	0.57172	-1.16729	-1.19624
N	2.21494	0.96339	-0.48423
C	2.24983	0.53404	-1.92478
H	-0.81033	-2.13667	-2.49728
C	2.39332	2.43782	-0.39181
C	-0.72475	-1.20235	-1.93789
H	1.59295	1.21293	-2.46535
Fe	0.36753	0.38699	0.12580
H	-0.74495	-0.35908	-2.62833
C	-1.81946	-1.07003	-0.91182
N	-1.45512	-0.43441	0.22511
H	-3.36495	-2.08948	-1.97825
C	-3.10112	-1.57212	-1.06471
C	-2.32055	-0.28488	1.23710

H	-1.95176	0.23666	2.10923
C	-4.01552	-1.40861	-0.02596
C	-3.61875	-0.76536	1.14371
H	-5.02481	-1.78964	-0.12578
H	-4.29849	-0.62868	1.97427
H	1.58635	2.93092	-0.92970
H	3.35987	2.69626	-0.83402
H	2.37442	2.72290	0.65933
H	-0.22353	-1.78387	2.43484
H	0.39050	-0.25117	3.11439
H	1.31256	-1.76693	3.34159
O	-0.27362	1.49505	-1.11388
O	0.21876	1.48038	1.51658
H	-1.57314	1.86520	-0.94387
C	-2.66563	2.34101	-0.74982
H	-3.34833	1.48888	-0.74480
H	-2.80716	2.96047	-1.63962
H	-0.13020	2.34270	1.24124
C	-2.62744	3.12577	0.54152
H	-2.47315	2.47557	1.40710
H	-1.83618	3.88315	0.52317
H	-3.58186	3.64881	0.69000

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H	1.61023	-3.09591	1.35003
H	3.36652	-0.88753	2.18768
H	2.70947	-2.24752	0.27805
C	1.68985	-2.26061	0.65292
H	3.67956	-0.56480	-0.23446
H	1.02645	-3.20906	-1.17789
C	2.66506	-0.23423	1.66041
H	2.53644	-1.57539	-1.80938
H	4.08469	0.94786	0.55977
C	0.66844	-1.25708	2.63306
C	3.27063	0.25232	0.35482
N	1.40017	-0.97401	1.37562
C	0.70352	-2.43548	-0.47743
H	2.40631	0.61001	2.29744
H	-0.27041	-2.70909	-0.07755
C	1.76043	-0.86758	-2.09262
H	1.50122	-1.04904	-3.13645
H	3.26970	0.67002	-2.29359
N	0.55926	-1.13736	-1.22272
N	2.21986	0.95924	-0.46636
C	2.24897	0.56442	-1.91709
H	-0.83249	-2.06056	-2.54908
C	2.41054	2.43089	-0.34167
C	-0.74006	-1.14599	-1.95899
H	1.59647	1.26082	-2.43913
Fe	0.36704	0.38955	0.13338
H	-0.76152	-0.27970	-2.62108
C	-1.82699	-1.04341	-0.92173
N	-1.44948	-0.44375	0.23059
H	-3.38595	-2.02375	-2.00524
C	-3.11226	-1.53403	-1.07950
C	-2.30822	-0.31276	1.25109
H	-1.93064	0.18601	2.13262
C	-4.01870	-1.39183	-0.03045
C	-3.61048	-0.78111	1.15284
H	-5.03129	-1.76308	-0.13357
H	-4.28488	-0.66003	1.99015
H	1.61128	2.94277	-0.87289
H	3.38202	2.68842	-0.77347
H	2.38996	2.69401	0.71514
H	-0.22738	-1.83186	2.39783

H	0.39512	-0.31660	3.10785
H	1.31124	-1.84101	3.29969
O	-0.26831	1.54194	-1.03642
O	0.22295	1.45534	1.55313
H	-1.49888	1.86837	-0.91973
C	-2.65282	2.34294	-0.74687
H	-3.31443	1.47563	-0.76609
H	-2.76337	2.96490	-1.63844
H	-0.09259	2.33409	1.29238
C	-2.62654	3.10673	0.55347
H	-2.47870	2.44395	1.41036
H	-1.83744	3.86658	0.55317
H	-3.58364	3.62693	0.70073

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H	1.62060	-2.79395	1.90452
H	3.47837	-0.50062	2.25160
H	2.68547	-2.22578	0.62860
C	1.68950	-2.12247	1.04811
H	3.75484	-0.74320	-0.18546
H	0.85909	-3.39649	-0.49111
C	2.79329	0.04394	1.59493
H	2.45610	-2.00517	-1.48399
H	4.25920	0.87145	0.27514
C	0.82434	-0.70368	2.85159
C	3.39639	0.20516	0.20811
N	1.49908	-0.70140	1.52580
C	0.62522	-2.46675	0.03402
H	2.57185	1.01713	2.03261
H	-0.33630	-2.57282	0.53106
C	1.71269	-1.31800	-1.88149
H	1.41677	-1.69036	-2.86325
H	3.30555	-0.01098	-2.48381
N	0.51566	-1.35339	-0.96845
N	2.39359	0.78712	-0.73666
C	2.30967	0.08128	-2.03760
H	-0.83166	-2.46757	-2.16844
C	2.63667	2.23585	-0.90851
C	-0.76171	-1.47022	-1.72616
H	1.68649	0.69109	-2.69066
Fe	0.33241	0.42129	0.17564
H	-0.74440	-0.72671	-2.52539
C	-1.92162	-1.20343	-0.80187
N	-1.63588	-0.43556	0.26549
H	-3.39697	-2.32926	-1.87218
C	-3.19698	-1.70812	-1.00820
C	-2.58270	-0.15239	1.17190
H	-2.27969	0.46891	2.00449
C	-4.19032	-1.40805	-0.07848
C	-3.87891	-0.62689	1.03367
H	-5.19526	-1.78974	-0.21479
H	-4.62328	-0.38539	1.78107
H	1.86100	2.66607	-1.53895
H	3.62040	2.38549	-1.36802
H	2.62037	2.71361	0.07232
H	-0.12412	-1.23503	2.76114
H	0.65401	0.32189	3.17141
H	1.47138	-1.21977	3.56731
O	-0.12942	1.37686	-1.29223
O	0.16997	1.73314	1.38785
H	-1.58167	1.95042	-1.07331
C	-2.58846	2.47039	-0.90055
H	-3.32538	1.66564	-0.83574
H	-2.74257	3.05746	-1.81115
H	-0.05427	2.59622	1.00575

C	-2.51981	3.32767	0.34755
H	-2.36630	2.72446	1.24634
H	-1.71558	4.06913	0.27973
H	-3.46170	3.87723	0.47601

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H	1.45893	-2.14513	2.66405
H	2.97230	0.37251	2.64029
H	2.68808	-1.73533	1.48255
C	1.62098	-1.69606	1.68331
H	3.65138	-0.35153	0.38585
H	1.30642	-3.41212	0.39998
C	2.33987	0.65820	1.79468
H	2.83292	-2.05411	-0.70151
H	3.86819	1.38880	0.46709
C	0.24833	-0.04893	2.85475
C	3.12353	0.59281	0.49398
N	1.16606	-0.26189	1.70908
C	0.84215	-2.45105	0.63281
H	1.95107	1.66258	1.95572
H	-0.17330	-2.62874	0.98171
C	2.08024	-1.62990	-1.36313
H	2.00093	-2.27358	-2.24012
H	3.52581	-0.17077	-2.04442
N	0.76827	-1.62783	-0.62105
N	2.18755	0.75905	-0.67626
C	2.46464	-0.21667	-1.78508
H	-0.35543	-3.17956	-1.55969
C	2.28779	2.14967	-1.19523
C	-0.39326	-2.09511	-1.43359
H	1.86854	0.10686	-2.63462
Fe	0.29966	0.30285	-0.11265
H	-0.34017	-1.61455	-2.41095
C	-1.64240	-1.66387	-0.70774
N	-1.49011	-0.57173	0.07757
H	-2.95670	-3.19378	-1.41612
C	-2.86401	-2.31151	-0.79583
C	-2.52166	-0.08287	0.78176
H	-2.32089	0.79960	1.37352
C	-3.94345	-1.81103	-0.07027
C	-3.77051	-0.68520	0.73162
H	-4.90821	-2.30096	-0.12513
H	-4.58553	-0.27191	1.31114
H	1.54766	2.29116	-1.97909
H	3.29740	2.29967	-1.58919
H	2.10080	2.83831	-0.37237
H	-0.57407	-0.76078	2.78190
H	-0.13376	0.96910	2.82123
H	0.79558	-0.21683	3.78768
O	-0.22584	0.78565	-1.79092
O	-0.11640	1.83357	0.63362
H	-1.18571	0.73812	-1.89641
C	-1.98340	3.35224	-0.93507
H	-2.40833	2.56021	-1.54199
H	-1.23703	3.98966	-1.40022
H	-0.57717	2.41605	-0.02179
C	-2.69909	3.80109	0.28678
H	-3.12302	2.95735	0.84118
H	-2.05490	4.38506	0.95120
H	-3.54610	4.45274	0.00806

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H	1.72645	-3.01527	1.41715
H	3.41373	-0.73307	2.20065

H	2.80443	-2.15816	0.32979
C	1.78370	-2.19550	0.69993
H	3.71314	-0.45318	-0.23078
H	1.15665	-3.20405	-1.11174
C	2.69322	-0.11322	1.65943
H	2.61544	-1.52787	-1.77677
H	4.07448	1.08781	0.52959
C	0.72983	-1.17988	2.65724
C	3.28113	0.36388	0.34228
N	1.45185	-0.90089	1.39225
C	0.80711	-2.42656	-0.42866
H	2.40632	0.73568	2.27782
H	-0.15935	-2.72133	-0.02512
C	1.81521	-0.85420	-2.07535
H	1.56347	-1.06793	-3.11485
H	3.26368	0.73610	-2.31011
N	0.62304	-1.14950	-1.20068
N	2.20595	1.01936	-0.48803
C	2.24776	0.59925	-1.93068
H	-0.73323	-2.14466	-2.50890
C	2.33784	2.49855	-0.38943
C	-0.67289	-1.21414	-1.94005
H	1.56700	1.25861	-2.46276
Fe	0.38234	0.39100	0.12915
H	-0.71593	-0.36493	-2.62248
C	-1.76891	-1.12237	-0.91046
N	-1.41830	-0.48082	0.22812
H	-3.28552	-2.18741	-1.97441
C	-3.03440	-1.66482	-1.06030
C	-2.28614	-0.35822	1.24250
H	-1.93068	0.17400	2.11368
C	-3.94853	-1.53436	-0.01674
C	-3.56867	-0.87914	1.15213
H	-4.94497	-1.94868	-0.11277
H	-4.25019	-0.76468	1.98457
H	1.50912	2.96539	-0.91617
H	3.29113	2.78898	-0.84053
H	2.32273	2.77731	0.66349
H	-0.14526	-1.79076	2.43608
H	0.42512	-0.23915	3.11145
H	1.39462	-1.72581	3.33402
O	-0.31806	1.52511	-1.10064
O	0.19047	1.47948	1.51913
H	-1.29126	1.60600	-1.03532
C	-3.15882	2.32736	-0.71469
H	-3.66369	1.36811	-0.67414
H	-3.12467	2.84012	-1.67130
H	-0.17021	2.33179	1.22827
C	-2.83895	3.07087	0.53407
H	-2.66461	2.39847	1.37912
H	-1.96369	3.71968	0.40638
H	-3.67316	3.73426	0.82127

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H	-1.80586	-3.19669	0.67544
H	-3.85270	-1.74551	-0.90448
H	-2.76431	-1.86449	1.28492
C	-1.82300	-2.11283	0.80217
H	-3.77015	-0.18023	1.00792
H	-0.81443	-1.96755	2.70568
C	-3.12343	-0.92877	-0.92805
H	-2.30562	-0.17560	2.59447
H	-4.47661	0.64465	-0.36819
C	-1.29758	-2.43061	-1.55807
C	-3.55207	0.19803	0.01000

N	-1.77017	-1.45010	-0.55082
C	-0.65405	-1.67684	1.66138
H	-3.03254	-0.55032	-1.94664
H	0.25343	-2.16141	1.30589
C	-1.53899	0.54106	2.30026
H	-1.12715	0.96751	3.21820
H	-3.06570	2.02624	1.98196
N	-0.47298	-0.20063	1.55822
N	-2.47641	1.21945	0.09347
C	-2.16540	1.66576	1.46692
H	1.10131	-0.18249	2.99734
C	-2.77084	2.36101	-0.78901
C	0.89209	0.17575	1.98330
H	-1.45760	2.48822	1.36996
Fe	-0.59377	0.26437	-0.57690
H	0.95078	1.26639	1.97044
C	1.90605	-0.38866	1.01045
N	1.47070	-0.56807	-0.24621
H	3.51762	-0.58071	2.41861
C	3.20519	-0.72313	1.39100
C	2.30236	-1.06372	-1.17073
H	1.89072	-1.17423	-2.16754
C	4.06626	-1.25714	0.43484
C	3.61316	-1.42624	-0.87220
H	5.07925	-1.53116	0.70521
H	4.25359	-1.83295	-1.64509
H	-1.90973	3.02828	-0.79997
H	-3.66360	2.90086	-0.44513
H	-2.94385	1.98463	-1.79919
H	-0.31926	-2.80163	-1.24868
H	-1.21224	-1.93413	-2.52240
H	-2.00420	-3.26557	-1.61850
O	0.18611	1.91334	-0.40569
O	-0.64561	0.27724	-2.42462
H	1.14567	1.84213	-0.48784
C	4.11756	1.92618	0.20035
H	5.01532	1.72523	0.77738
H	3.24397	2.32622	0.70685
H	-0.37226	1.15598	-2.71314
C	4.10024	1.69896	-1.15808
H	4.97265	1.28571	-1.65483
H	3.20040	1.88414	-1.73771
H	4.46354	2.86277	-0.70906
Icat_eta_2.log			
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H	-1.84495	-3.22225	0.56429
H	-3.70517	-1.74559	-1.19166
H	-2.82844	-1.88395	1.12223
C	-1.85759	-2.13904	0.70511
H	-3.78152	-0.18267	0.73006
H	-0.96913	-2.02128	2.67951
C	-2.96750	-0.93683	-1.13663
H	-2.43718	-0.22434	2.50251
H	-4.32477	0.68065	-0.69782
C	-1.05071	-2.37655	-1.58086
C	-3.46190	0.19034	-0.24193
N	-1.67206	-1.44757	-0.61197
C	-0.74677	-1.72706	1.64946
H	-2.76818	-0.55482	-2.13773
H	0.18144	-2.20955	1.34563
C	-1.65525	0.49578	2.26302
H	-1.29495	0.91746	3.20369
H	-3.19460	1.93532	1.77218
N	-0.54519	-0.24609	1.57467
N	-2.35608	1.18121	-0.04330

C	-2.22169	1.61600	1.38296
H	1.02229	-0.36391	3.03031
C	-2.58396	2.35966	-0.90978
C	0.82118	0.08479	2.05294
H	-1.53609	2.45962	1.37576
Fe	-0.54074	0.31875	-0.39800
H	0.89383	1.17023	2.12162
C	1.79278	-0.42592	1.01246
N	1.31239	-0.45191	-0.25087
H	3.41781	-0.87174	2.33533
C	3.07098	-0.88713	1.30984
C	2.07975	-0.91772	-1.24623
H	1.62878	-0.90219	-2.23017
C	3.86417	-1.38911	0.27983
C	3.36462	-1.39948	-1.02019
H	4.85977	-1.76129	0.49030
H	3.95041	-1.77699	-1.84829
H	-1.73005	3.02680	-0.81413
H	-3.50984	2.86545	-0.61093
H	-2.65646	2.01604	-1.94078
H	-0.12065	-2.75830	-1.15670
H	-0.83396	-1.82535	-2.49379
H	-1.72755	-3.21498	-1.78387
O	0.23008	2.00345	-0.06133
O	-0.54970	0.49123	-2.24387
H	1.18949	1.97228	-0.14367
C	4.18667	1.81294	0.29589
H	5.09404	1.49536	0.80121
H	3.37692	2.23759	0.88208
H	0.25436	0.96177	-2.49304
C	4.07167	1.68470	-1.07017
H	4.88034	1.24631	-1.64706
H	3.15996	1.98564	-1.57862
H	4.55817	2.78204	-0.55290

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H	-1.77069	-3.18976	0.77032
H	-3.85000	-1.78884	-0.83300
H	-2.73728	-1.85219	1.35501
C	-1.79882	-2.10268	0.86720
H	-3.75843	-0.16727	1.03501
H	-0.76663	-1.90590	2.75361
C	-3.12258	-0.97095	-0.88226
H	-2.29124	-0.12585	2.60109
H	-4.47450	0.61545	-0.35992
C	-1.30025	-2.47970	-1.48988
C	-3.54718	0.18182	0.02531
N	-1.76698	-1.47807	-0.50238
C	-0.62369	-1.63341	1.70219
H	-3.04043	-0.62105	-1.91171
H	0.28404	-2.11648	1.34542
C	-1.52613	0.58716	2.29451
H	-1.11798	1.03208	3.20576
H	-3.05067	2.06913	1.94297
N	-0.45830	-0.16010	1.56610
N	-2.47397	1.21182	0.07422
C	-2.15332	1.69084	1.43690
H	1.12708	-0.07276	2.99107
C	-2.79532	2.34034	-0.81701
C	0.90511	0.24470	1.96639
H	-1.44243	2.50741	1.31322
Fe	-0.59361	0.26682	-0.59818
H	0.95372	1.33491	1.91292
C	1.91098	-0.34776	1.00301
N	1.46719	-0.54671	-0.24866

H	3.52343	-0.54403	2.40911
C	3.20497	-0.69891	1.38550
C	2.28654	-1.07563	-1.16542
H	1.86928	-1.19762	-2.15825
C	4.05137	-1.27335	0.43931
C	3.59057	-1.45862	-0.86215
H	5.05853	-1.56441	0.71369
H	4.21860	-1.89711	-1.62721
H	-1.94149	3.01625	-0.84986
H	-3.68709	2.87247	-0.45941
H	-2.98334	1.95368	-1.82021
H	-0.31496	-2.83611	-1.18475
H	-1.23120	-2.00536	-2.46662
H	-2.00056	-3.32203	-1.52181
O	0.17853	1.93269	-0.47581
O	-0.67369	0.21305	-2.45371
H	1.13320	1.87298	-0.60810
C	4.10158	1.91575	0.19750
H	4.98894	1.73738	0.79762
H	3.21383	2.31813	0.67661
H	-0.42074	1.08147	-2.78843
C	4.12092	1.67493	-1.15893
H	5.00772	1.25847	-1.62674
H	3.23059	1.83486	-1.76010
H	4.46150	2.84310	-0.73646

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H	1.41190	-1.93162	2.81238
H	2.93255	0.56113	2.65056
H	2.65461	-1.62061	1.61425
C	1.58630	-1.55716	1.80260
H	3.66141	-0.32481	0.47268
H	1.26297	-3.36548	0.65387
C	2.32472	0.79109	1.77027
H	2.83191	-2.11792	-0.52111
H	3.89207	1.41525	0.43054
C	0.20334	0.17870	2.82020
C	3.13941	0.62888	0.49733
N	1.14516	-0.12173	1.71453
C	0.81237	-2.38098	0.80019
H	1.94081	1.80732	1.85044
H	-0.21172	-2.51204	1.14446
C	2.10019	-1.72295	-1.22293
H	2.03095	-2.41822	-2.06075
H	3.58791	-0.33411	-1.96064
N	0.77316	-1.65544	-0.51340
N	2.22803	0.71265	-0.69891
C	2.51992	-0.34422	-1.72588
H	-0.34697	-3.25992	-1.36755
C	2.35363	2.05836	-1.31979
C	-0.37398	-2.16876	-1.31585
H	1.95086	-0.07471	-2.61234
Fe	0.32071	0.30441	-0.15598
H	-0.29415	-1.75431	-2.32139
C	-1.63350	-1.67763	-0.64705
N	-1.48408	-0.53452	0.06143
H	-2.94401	-3.24994	-1.26604
C	-2.85609	-2.32778	-0.70590
C	-2.52133	-0.00388	0.72506
H	-2.32259	0.91033	1.26638
C	-3.94247	-1.77738	-0.02853
C	-3.77265	-0.60316	0.70140
H	-4.90838	-2.26713	-0.06153
H	-4.59125	-0.15203	1.24670
H	1.62068	2.15012	-2.11787

H	3.36753	2.16901	-1.71599
H	2.17111	2.81222	-0.55433
H	-0.62192	-0.53271	2.78213
H	-0.17341	1.19288	2.70272
H	0.72611	0.07930	3.77694
O	-0.17067	0.68808	-1.88369
O	-0.10182	1.92002	0.45010
H	-1.12149	0.59062	-2.02176
C	-2.21630	2.98353	-0.95236
H	-2.63814	2.02122	-1.21648
H	-1.60404	3.48393	-1.69686
H	-0.32946	2.50117	-0.30196
C	-2.73122	3.72576	0.21221
H	-3.06574	3.06080	1.01245
H	-2.00531	4.44704	0.59979
H	-3.61322	4.31239	-0.10681

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H	0.93741	-0.59546	3.37002
H	2.32913	1.80337	2.43883
H	2.36983	-0.62622	2.35719
C	1.28348	-0.62922	2.33612
H	3.51493	0.24094	0.95442
H	1.28110	-2.76717	1.99378
C	1.88936	1.59354	1.45954
H	2.98469	-1.88753	0.67764
H	3.64620	1.84051	0.24219
C	-0.36390	1.17749	2.32701
C	2.94326	1.05056	0.50703
N	0.79182	0.59063	1.60498
C	0.76048	-1.86908	1.65219
H	1.44263	2.50242	1.06026
H	-0.30302	-1.98035	1.85308
C	2.38594	-1.90174	-0.23091
H	2.51947	-2.87472	-0.70599
H	3.91068	-0.74276	-1.23934
N	0.94406	-1.73246	0.16927
N	2.28514	0.53776	-0.74944
C	2.81994	-0.79711	-1.18854
H	0.09315	-3.66563	-0.12001
C	2.46249	1.53225	-1.84180
C	0.00076	-2.65520	-0.52522
H	2.41805	-0.97529	-2.18266
Fe	0.32652	0.15833	-0.39468
H	0.25497	-2.66437	-1.58571
C	-1.38736	-2.10259	-0.32260
N	-1.43906	-0.76392	-0.13141
H	-2.47343	-3.93996	-0.43891
C	-2.54159	-2.86845	-0.30082
C	-2.60919	-0.14307	0.07731
H	-2.56220	0.92851	0.21446
C	-3.76442	-2.23409	-0.08977
C	-3.79959	-0.85535	0.10656
H	-4.67997	-2.81310	-0.07036
H	-4.73044	-0.33123	0.27943
H	1.90709	1.20248	-2.71623
H	3.52985	1.60561	-2.07065
H	2.08843	2.49548	-1.49728
H	-1.12588	0.40826	2.45649
H	-0.76452	2.00666	1.74789
H	-0.03032	1.52838	3.30866
O	0.17162	-0.24388	-2.16818
O	-0.30025	1.81524	-0.52065
H	-0.73846	-0.46746	-2.40773
C	-2.42893	3.67510	-1.05149

H	-2.95480	2.86751	-1.55014
H	-1.88275	4.38298	-1.66606
H	-0.54674	2.03850	-1.43161
C	-2.62986	3.92318	0.39840
H	-2.73610	2.98859	0.95991
H	-1.80546	4.49981	0.82985
H	-3.55283	4.50226	0.57894

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H	0.60686	-1.94628	3.01198
H	2.83483	-0.11149	2.68551
H	1.89637	-2.17268	1.84396
C	0.90210	-1.75542	1.97886
H	3.29045	-1.37602	0.63492
H	0.03887	-3.48306	0.99645
C	2.34778	0.21627	1.76179
H	1.93365	-2.91467	-0.21871
H	4.05600	0.19156	0.44644
C	0.11448	0.42044	2.74784
C	3.09177	-0.30990	0.54380
N	0.93786	-0.27195	1.72611
C	-0.08039	-2.39750	1.02847
H	2.32951	1.30741	1.76517
H	-1.09657	-2.16449	1.33950
C	1.37704	-2.38579	-0.99087
H	1.10807	-3.10495	-1.76543
H	3.24777	-1.62996	-1.76750
N	0.12081	-1.84105	-0.35443
N	2.26624	-0.06978	-0.68863
C	2.23036	-1.26738	-1.59251
H	-1.44263	-3.11177	-1.06314
C	2.81333	1.09334	-1.43161
C	-1.12641	-2.06857	-1.14163
H	1.79615	-0.92875	-2.52949
Fe	0.29305	0.13053	-0.22514
H	-0.91435	-1.83111	-2.18362
C	-2.17647	-1.13416	-0.58647
N	-1.68758	-0.01924	0.00594
H	-3.89794	-2.29522	-1.10331
C	-3.53880	-1.38745	-0.63527
C	-2.52714	0.86128	0.56996
H	-2.07366	1.72486	1.03800
C	-4.41467	-0.46641	-0.06419
C	-3.90210	0.67168	0.55375
H	-5.48343	-0.64302	-0.09008
H	-4.54942	1.40341	1.01935
H	2.13091	1.34558	-2.23998
H	3.80240	0.83947	-1.82692
H	2.91733	1.93955	-0.75027
H	-0.89327	0.00577	2.72462
H	0.07594	1.48537	2.52436
H	0.55222	0.26370	3.73903
O	-0.00368	0.45947	-2.01049
O	0.32999	2.09632	0.18726
H	-0.93904	0.53794	-2.23415
C	-0.25855	3.07716	-0.73267
H	-1.26303	2.71204	-0.93268
H	0.31789	3.05211	-1.65749
H	1.19441	2.43917	0.46353
C	-0.26386	4.44348	-0.08471
H	-0.85243	4.44022	0.83706
H	0.75699	4.76866	0.14373
H	-0.70291	5.16434	-0.78140

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H	0.41657	-0.99380	3.35471
H	2.83194	0.39889	2.47787
H	1.64872	-1.72631	2.34450
C	0.70494	-1.18788	2.32049
H	3.08613	-1.55177	0.97922
H	-0.33592	-3.05126	2.01440
C	2.36189	0.43386	1.49012
H	1.58159	-3.13039	0.64542
H	4.02701	-0.23443	0.30433
C	0.18427	1.19330	2.35517
C	3.01290	-0.55986	0.53985
N	0.90123	0.12858	1.61019
C	-0.35628	-2.02576	1.63234
H	2.45823	1.44328	1.09296
H	-1.34123	-1.60630	1.83234
C	1.04266	-2.83070	-0.25296
H	0.71272	-3.74181	-0.75737
H	2.92478	-2.56737	-1.28951
N	-0.13006	-2.01321	0.16439
N	2.20410	-0.64518	-0.72621
C	1.96590	-2.04873	-1.19426
H	-1.85895	-3.20694	-0.22653
C	2.88480	0.12690	-1.79879
C	-1.38539	-2.28029	-0.56613
H	1.50611	-1.95942	-2.17742
Fe	0.29346	0.07501	-0.39032
H	-1.14733	-2.37524	-1.62789
C	-2.32161	-1.10789	-0.35486
N	-1.73515	0.08811	-0.12151
H	-4.14671	-2.20698	-0.53909
C	-3.70343	-1.23384	-0.36919
C	-2.48631	1.17914	0.09620
H	-1.95162	2.10217	0.27721
C	-4.48885	-0.10423	-0.15223
C	-3.87232	1.12131	0.08914
H	-5.56959	-0.18256	-0.16096
H	-4.44721	2.01972	0.27255
H	2.25956	0.12655	-2.68912
H	3.85250	-0.33825	-2.01283
H	3.03568	1.14912	-1.45184
H	-0.85070	0.88208	2.49582
H	0.20516	2.12340	1.79227
H	0.65882	1.34248	3.33038
O	-0.01531	0.00664	-2.20075
O	0.66816	2.18493	-0.74210
H	-0.95169	0.08579	-2.42568
C	1.08583	3.48595	-0.23628
H	1.81094	3.89806	-0.94201
H	1.59523	3.30232	0.70842
H	0.48086	2.26023	-1.68967
C	-0.10259	4.40723	-0.05177
H	-0.63747	4.54511	-0.99689
H	-0.79477	4.00591	0.69427
H	0.24885	5.38573	0.29213

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O	-0.32524	1.54354	-1.03119
O	0.23111	1.40203	1.58929
H	-1.31096	1.59344	-1.01780
C	-2.67574	2.48171	-0.71894
H	1.66025	-3.11713	1.29392
H	3.39988	-0.90867	2.13492
H	2.72718	-2.23920	0.21144
C	1.71545	-2.27284	0.60552

H	3.67766	-0.52993	-0.28001
H	1.02093	-3.20610	-1.22103
C	2.68444	-0.25092	1.63293
H	2.52326	-1.54160	-1.84674
H	4.07056	0.97463	0.53579
C	0.70515	-1.30991	2.61068
C	3.26415	0.27085	0.32845
N	1.42326	-0.99878	1.35064
C	0.70924	-2.44098	-0.50632
H	2.42565	0.57544	2.29265
H	-0.25662	-2.72048	-0.09037
C	1.73546	-0.83942	-2.11168
H	1.46665	-1.01032	-3.15484
H	3.22411	0.71875	-2.30905
N	0.54763	-1.13508	-1.23154
N	2.19175	0.97431	-0.46717
C	2.20869	0.59737	-1.92288
H	-0.85080	-2.06230	-2.54576
C	2.35525	2.44603	-0.32801
C	-0.75826	-1.14783	-1.95535
H	1.54083	1.29085	-2.42708
Fe	0.36291	0.36374	0.15440
H	-0.78809	-0.28284	-2.61826
C	-1.84174	-1.05199	-0.91219
N	-1.46275	-0.45692	0.24250
H	-3.40452	-2.01946	-2.00231
C	-3.12956	-1.53532	-1.07397
C	-2.32335	-0.32686	1.26193
H	-1.94364	0.16572	2.14643
C	-4.03740	-1.39159	-0.02662
C	-3.62801	-0.78732	1.15965
H	-5.05190	-1.75661	-0.13325
H	-4.30344	-0.66650	1.99623
H	1.52903	2.94390	-0.83004
H	3.30800	2.73215	-0.78326
H	2.35883	2.69564	0.73237
H	-0.19505	-1.87618	2.37131
H	0.44095	-0.38099	3.11199
H	1.35571	-1.91146	3.25338
H	-3.32791	1.61062	-0.75007
H	-2.57235	3.04524	-1.64277
H	-0.08522	2.28125	1.33147
C	-2.47029	3.18404	0.57851
H	-2.36570	2.48023	1.40983
H	-1.59627	3.84402	0.54824
H	-3.33948	3.82115	0.81227

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H	-2.20777	-3.15745	0.41737
H	-3.83529	-1.26862	-1.15676
H	-2.93752	-1.70302	1.07458
C	-2.03441	-2.09898	0.61800
H	-3.58324	0.18073	0.81009
H	-1.08875	-2.23261	2.56307
C	-2.96272	-0.60961	-1.11467
H	-2.25371	-0.21366	2.52862
H	-3.96791	1.21060	-0.55886
C	-1.34323	-2.34248	-1.71459
C	-3.21460	0.53767	-0.14825
N	-1.76508	-1.37853	-0.67201
C	-0.84869	-1.93550	1.53960
H	-2.74912	-0.22882	-2.11229
H	-0.02020	-2.54451	1.18362
C	-1.36111	0.37273	2.32031
H	-0.90726	0.64345	3.27464

H	-2.60964	2.09953	1.94486
N	-0.40760	-0.49861	1.54253
N	-1.94138	1.31209	0.08515
C	-1.70983	1.63222	1.53584
H	1.11391	-0.97551	2.95789
C	-1.97381	2.57303	-0.70365
C	1.00615	-0.42811	2.01865
H	-0.88660	2.34158	1.56595
Fe	-0.33439	0.16930	-0.39988
H	1.25958	0.62071	2.17630
C	1.86740	-1.01859	0.93231
N	1.34630	-0.92206	-0.31302
H	3.47319	-1.72216	2.15446
C	3.08565	-1.64232	1.14699
C	1.99825	-1.42482	-1.37158
H	1.51441	-1.30261	-2.33119
C	3.77543	-2.16301	0.05372
C	3.22355	-2.05830	-1.22110
H	4.72985	-2.65512	0.19804
H	3.72745	-2.45860	-2.09103
H	-1.01446	3.07596	-0.60754
H	-2.77793	3.20431	-0.31360
H	-2.16978	2.32508	-1.74601
H	-0.47896	-2.89876	-1.35086
H	-1.08126	-1.79775	-2.61996
H	-2.16461	-3.03709	-1.91995
O	0.71245	1.63514	-0.01043
O	-0.36278	0.42741	-2.15812
H	1.65271	1.47071	-0.16919
C	2.61824	3.53950	0.54453
H	3.23941	2.85739	1.11561
H	1.88423	4.12786	1.08246
H	0.08801	1.25877	-2.37236
C	2.92028	3.82429	-0.88039
H	3.32578	2.94605	-1.39508
H	2.03481	4.17603	-1.41968
H	3.68233	4.61888	-0.97082

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H	-0.30436	-3.72260	-0.31227
H	-2.67234	-2.58158	-1.60851
H	-1.65089	-3.00524	0.55251
C	-0.67598	-2.79403	0.12260
H	-3.07926	-1.66534	0.67028
H	0.20066	-2.88234	2.09971
C	-2.25421	-1.60670	-1.34131
H	-1.73855	-1.64769	2.36831
H	-4.01323	-0.71898	-0.47087
C	-0.01317	-2.15951	-2.14144
C	-2.99829	-0.98624	-0.17435
N	-0.81830	-1.75539	-0.96107
C	0.28147	-2.29616	1.18121
H	-2.28590	-0.94365	-2.20528
H	1.30149	-2.37170	0.80949
C	-1.22967	-0.68571	2.32754
H	-0.94848	-0.41379	3.34615
H	-3.14307	0.32032	2.19389
N	0.00238	-0.85233	1.48061
N	-2.25617	0.25177	0.25244
C	-2.14872	0.38663	1.74237
H	1.61996	-0.85625	2.87921
C	-2.96684	1.41745	-0.33047
C	1.23392	-0.24724	2.05756
H	-1.74095	1.37694	1.94177
Fe	-0.30900	0.09768	-0.30291

H	0.98597	0.74449	2.43725
C	2.23961	-0.14409	0.93502
N	1.69822	-0.05710	-0.30468
H	4.01725	-0.23513	2.12007
C	3.61369	-0.15025	1.11915
C	2.49267	0.02931	-1.38327
H	1.98626	0.10154	-2.33653
C	4.44225	-0.05703	0.00281
C	3.87516	0.03134	-1.26693
H	5.51903	-0.06071	0.12331
H	4.48773	0.10053	-2.15636
H	-2.44696	2.33532	-0.09150
H	-3.98145	1.45635	0.07836
H	-2.99759	1.29291	-1.41131
H	1.01765	-2.31784	-1.82501
H	-0.05765	-1.36569	-2.88350
H	-0.41671	-3.09166	-2.54934
O	0.24742	2.00183	0.45214
O	-0.50405	0.77401	-1.97950
H	1.17910	2.10706	0.21564
C	-0.28480	3.35856	0.57544
H	0.40965	3.90331	1.21925
H	-1.23199	3.27640	1.10403
H	-0.04384	1.61939	-2.06049
C	-0.42341	4.03054	-0.77535
H	0.54966	4.09065	-1.27385
H	-1.12006	3.48946	-1.42031
H	-0.79913	5.04910	-0.63428

Prod_CH3_eta_4.log
54

H	-0.74423	-3.82893	0.08311
H	-3.12795	-2.49444	-1.27998
H	-1.96162	-2.85108	0.87806
C	-1.00210	-2.80493	0.36624
H	-3.24844	-1.27543	0.85079
H	0.04040	-2.74574	2.27154
C	-2.51066	-1.59540	-1.16476
H	-1.86162	-1.32427	2.44248
H	-4.07885	-0.34563	-0.38182
C	-0.40762	-2.52999	-1.99348
C	-3.10099	-0.71428	-0.06867
N	-1.10994	-1.94204	-0.84010
C	0.07672	-2.26426	1.29075
H	-2.49556	-1.05101	-2.10984
H	1.05411	-2.44687	0.84691
C	-1.25081	-0.43027	2.33796
H	-0.91588	-0.13537	3.33371
H	-3.01987	0.81243	2.16536
N	-0.06168	-0.77769	1.48204
N	-2.20721	0.46401	0.22269
C	-2.03755	0.70571	1.69565
H	1.54233	-0.81216	2.89179
C	-2.77561	1.66984	-0.43140
C	1.22441	-0.23626	2.01940
H	-1.49292	1.64313	1.80042
Fe	-0.28379	0.08546	-0.37526
H	1.05646	0.80090	2.31461
C	2.24162	-0.29263	0.91085
N	1.71800	-0.20394	-0.33360
H	3.99910	-0.51012	2.11067
C	3.60761	-0.42854	1.10481
C	2.51499	-0.24335	-1.41267
H	2.01698	-0.15897	-2.36952
C	4.44257	-0.46583	-0.00997
C	3.89034	-0.37577	-1.28630

H	5.51337	-0.57220	0.11704
H	4.50918	-0.40688	-2.17351
H	-2.11137	2.51673	-0.28898
H	-3.75175	1.89000	0.01233
H	-2.88891	1.46544	-1.49534
H	0.62927	-2.72650	-1.71334
H	-0.42695	-1.81617	-2.81772
H	-0.88456	-3.46925	-2.30210
O	0.50139	2.19465	0.32369
O	-0.41348	0.63602	-2.07115
H	1.39469	2.20522	-0.04549
C	0.10592	3.57989	0.50860
H	0.84091	4.05894	1.16148
H	-0.84756	3.55538	1.03593
H	-0.46037	1.60004	-2.15569
C	-0.00178	4.30662	-0.81917
H	0.95912	4.28692	-1.34435
H	-0.76244	3.85065	-1.46076
H	-0.27658	5.35216	-0.64572

CYCLOHEXANE_AT_SOLVENT

A_ciclohex_2.log

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H	-4.08092	1.53491	1.24057
H	-4.09662	-1.30708	2.00372
H	-4.34559	0.21533	0.11641
C	-3.58143	0.85493	0.54946
H	-4.00656	-1.69522	-0.41991
H	-3.55389	2.07805	-1.23978
C	-3.11202	-1.35993	1.53048
H	-3.69090	-0.14232	-1.95422
H	-3.40098	-3.14742	0.36603
C	-2.25552	0.67286	2.59318
C	-3.20435	-2.08823	0.19976
N	-2.58476	0.01793	1.30296
C	-2.86009	1.64273	-0.51712
H	-2.41618	-1.86534	2.19817
H	-2.28162	2.44065	-0.05656
C	-2.62862	-0.20086	-2.18029
H	-2.48509	0.12898	-3.20966
H	-2.82062	-2.34139	-2.43983
N	-1.90551	0.73910	-1.24835
N	-1.90555	-1.94997	-0.55992
C	-2.11339	-1.62441	-2.01556
H	-1.34829	2.36921	-2.49972
C	-1.11772	-3.20794	-0.43052
C	-0.86689	1.57648	-1.92298
H	-1.14749	-1.74327	-2.50400
Fe	-0.87201	-0.36142	0.13960
H	-0.29322	0.93722	-2.59444
C	0.02121	2.13668	-0.84328
N	0.05311	1.40874	0.29664
H	0.69466	3.88553	-1.86858
C	0.74544	3.31242	-0.95185
C	0.77981	1.80507	1.35111
H	0.75640	1.16121	2.21901
C	1.51279	3.73099	0.13296
C	1.52349	2.97413	1.30212
H	2.09031	4.64523	0.06780
H	2.10201	3.27322	2.16608
H	-0.14855	-3.08160	-0.91178
H	-1.67591	-4.01355	-0.91548
H	-0.98457	-3.42695	0.62772
H	-1.91223	1.68808	2.39385
H	-1.47508	0.10451	3.09459
H	-3.15458	0.70717	3.21626

O	0.42449	-0.76297	-0.96298
O	-0.16504	-1.12396	1.57051
H	0.69996	-1.51248	1.36046
C	3.40049	0.26423	-0.19519
H	2.43737	0.62222	-0.56859
C	4.25834	-0.24171	-1.36264
H	3.71370	-1.04005	-1.88432
H	4.42541	0.56378	-2.08617
C	3.18948	-0.83508	0.85415
H	2.60853	-0.44501	1.69728
H	2.61192	-1.64950	0.39566
C	5.60030	-0.79806	-0.86435
H	6.18786	-1.18258	-1.70520
H	6.17789	0.01797	-0.40995
C	4.52953	-1.39612	1.35277
H	4.35776	-2.20225	2.07433
H	5.07494	-0.60035	1.87723
C	5.38666	-1.90086	0.18254
H	6.35130	-2.26739	0.55031
H	4.87653	-2.74909	-0.29322
H	3.90270	1.11747	0.27835

A_ciclohex_4.log

64

H	-4.02422	1.62694	1.18717
H	-4.10833	-1.19849	2.03039
H	-4.32298	0.28520	0.09917
C	-3.54189	0.91429	0.51683
H	-4.03845	-1.61281	-0.39552
H	-3.49379	2.07735	-1.30985
C	-3.12972	-1.28384	1.54895
H	-3.65826	-0.11795	-1.99697
H	-3.48755	-3.07529	0.40979
C	-2.22901	0.74504	2.56976
C	-3.25251	-2.02615	0.23084
N	-2.56818	0.07345	1.29196
C	-2.80595	1.65748	-0.57246
H	-2.44127	-1.79827	2.21781
H	-2.22301	2.46508	-0.13587
C	-2.59438	-0.21757	-2.20146
H	-2.41937	0.08125	-3.23545
H	-2.86684	-2.35605	-2.39884
N	-1.85904	0.72492	-1.27891
N	-1.94917	-1.94702	-0.52766
C	-2.13453	-1.65414	-1.99192
H	-1.25847	2.31882	-2.55965
C	-1.20352	-3.22582	-0.35904
C	-0.79890	1.53778	-1.95009
H	-1.17081	-1.82511	-2.46766
Fe	-0.83262	-0.37622	0.11973
H	-0.21152	0.87737	-2.58984
C	0.06207	2.11776	-0.85931
N	0.06062	1.41119	0.29440
H	0.76993	3.84601	-1.89481
C	0.79375	3.28797	-0.96777
C	0.76214	1.81863	1.36026
H	0.71666	1.18759	2.23640
C	1.53499	3.72128	0.13026
C	1.51294	2.98408	1.31079
H	2.11856	4.63161	0.06452
H	2.07233	3.29309	2.18378
H	-0.23281	-3.14621	-0.84481
H	-1.79297	-4.02384	-0.81903
H	-1.07973	-3.41737	0.70573
H	-1.87205	1.75215	2.35488
H	-1.45576	0.17488	3.08066

H	-3.12637	0.80300	3.19400
O	0.37380	-0.82931	-0.90205
O	-0.16719	-1.12477	1.59298
H	0.68557	-1.55304	1.41606
C	3.38794	0.27161	-0.18360
H	2.43192	0.64944	-0.55256
C	4.23619	-0.24058	-1.35567
H	3.67533	-1.02231	-1.88537
H	4.41990	0.56831	-2.07136
C	3.15535	-0.83345	0.85503
H	2.58134	-0.44097	1.70156
H	2.56157	-1.63131	0.38777
C	5.56646	-0.82926	-0.86343
H	6.14607	-1.21773	-1.70798
H	6.16076	-0.02964	-0.40141
C	4.48320	-1.42763	1.34786
H	4.29439	-2.23779	2.06061
H	5.04451	-0.64898	1.88118
C	5.33065	-1.93758	0.17285
H	6.28771	-2.32657	0.53737
H	4.80434	-2.77117	-0.31112
H	3.90762	1.10978	0.29806

A_ciclohex_6.log

64

H	-4.09930	1.70911	1.03374
H	-4.40768	-1.32110	1.64806
H	-4.36888	0.48094	-0.18075
C	-3.59339	0.99863	0.37914
H	-4.25161	-1.47696	-0.81371
H	-3.20922	2.29652	-1.31989
C	-3.40542	-1.35538	1.20782
H	-3.47251	0.04750	-2.03483
H	-3.99487	-3.01027	0.03270
C	-2.77329	0.49202	2.61999
C	-3.56909	-2.02329	-0.16933
N	-2.81837	0.01381	1.21019
C	-2.65355	1.76046	-0.54528
H	-2.76655	-1.97575	1.83713
H	-2.07265	2.47751	0.03488
C	-2.40073	-0.07284	-2.16480
H	-2.17380	0.27474	-3.17404
H	-2.63884	-2.04607	-2.90375
N	-1.68647	0.80818	-1.17946
N	-2.31987	-2.24451	-0.88824
C	-2.02540	-1.55005	-2.13477
H	-1.02309	2.24518	-2.59723
C	-1.54105	-3.40427	-0.52167
C	-0.59208	1.54136	-1.87993
H	-0.97626	-1.71174	-2.36581
Fe	-0.72770	-0.08788	0.52186
H	-0.00949	0.79595	-2.42777
C	0.32028	2.24856	-0.91318
N	0.40159	1.71135	0.31436
H	0.98709	3.77597	-2.26296
C	1.07858	3.35704	-1.26865
C	1.22527	2.23450	1.23318
H	1.23615	1.74229	2.19687
C	1.94575	3.90097	-0.32474
C	2.02131	3.33412	0.94726
H	2.55316	4.76228	-0.57702
H	2.68150	3.73454	1.70572
H	-0.55611	-3.35594	-0.97635
H	-2.09215	-4.28793	-0.87816
H	-1.47490	-3.46491	0.56789
H	-2.28796	1.46904	2.63847

H	-2.19544	-0.20934	3.21829
H	-3.79409	0.57605	3.00800
O	0.23303	-1.02448	-0.41626
O	-0.10837	-0.59332	2.14107
H	0.68310	-1.14480	2.06656
C	3.40054	-0.01883	-0.34640
H	2.45496	0.41941	-0.67049
C	3.93832	-0.96529	-1.42947
H	3.17921	-1.73099	-1.63746
H	4.10774	-0.41601	-2.36252
C	3.20157	-0.75984	0.98272
H	2.84362	-0.06831	1.75269
H	2.42322	-1.51941	0.83637
C	5.23287	-1.65660	-0.97719
H	5.58072	-2.35367	-1.74763
H	6.01657	-0.89806	-0.84889
C	4.49695	-1.44613	1.43911
H	4.32781	-1.99550	2.37201
H	5.25537	-0.67944	1.64707
C	5.03045	-2.39438	0.35457
H	5.96997	-2.85420	0.68030
H	4.30603	-3.20633	0.20535
H	4.11646	0.80063	-0.19801

TSabs_ciclohex_2.log

64

H	-3.82041	2.04123	1.03341
H	-4.20178	-0.67909	2.08091
H	-4.24181	0.65460	0.04423
C	-3.40657	1.23665	0.42416
H	-4.15441	-1.32142	-0.28870
H	-3.22087	2.24989	-1.48263
C	-3.23068	-0.90590	1.63112
H	-3.62722	0.00984	-1.96052
H	-3.74883	-2.75001	0.65016
C	-2.12143	1.09718	2.49686
C	-3.41092	-1.74946	0.37906
N	-2.52898	0.36250	1.27593
C	-2.58845	1.81291	-0.70652
H	-2.60796	-1.42566	2.35763
H	-1.92052	2.58130	-0.32326
C	-2.58062	-0.20481	-2.16601
H	-2.39278	-0.00258	-3.22117
H	-3.04895	-2.31759	-2.21770
N	-1.74856	0.72738	-1.32112
N	-2.10336	-1.86220	-0.36630
C	-2.25736	-1.66002	-1.84898
H	-0.97066	2.13386	-2.72148
C	-1.49672	-3.19427	-0.10011
C	-0.60356	1.35584	-2.04814
H	-1.31040	-1.95098	-2.30034
Fe	-0.86767	-0.35223	0.18163
H	-0.09882	0.58070	-2.62451
C	0.31948	1.92187	-1.00032
N	0.24621	1.31061	0.20402
H	1.19308	3.48700	-2.16321
C	1.16045	3.00483	-1.19479
C	0.97090	1.74538	1.24325
H	0.85347	1.20114	2.16946
C	1.93362	3.45585	-0.12634
C	1.83058	2.82635	1.11140
H	2.60077	4.29931	-0.25727
H	2.40710	3.15561	1.96569
H	-0.51716	-3.24200	-0.57098
H	-2.15565	-3.96273	-0.51429
H	-1.40262	-3.32311	0.97727

H	-1.64461	2.03173	2.20093
H	-1.42411	0.48592	3.06650
H	-3.00926	1.31456	3.09912
O	0.34332	-1.07465	-0.89330
O	-0.26892	-1.06359	1.69412
H	0.50798	-1.61927	1.52300
C	2.85133	-0.43917	-0.33948
H	1.73914	-0.65230	-0.60056
C	3.70574	-1.16281	-1.37018
H	3.46583	-2.23299	-1.35448
H	3.49680	-0.78629	-2.37625
C	3.11771	-0.91605	1.08115
H	2.50575	-0.36655	1.80123
H	2.85579	-1.97934	1.16043
C	5.20046	-0.98137	-1.03030
H	5.81086	-1.52948	-1.75566
H	5.45926	0.08119	-1.11878
C	4.61197	-0.73796	1.42108
H	4.80597	-1.11260	2.43154
H	4.84877	0.33340	1.41636
C	5.50058	-1.45686	0.39747
H	6.55691	-1.29018	0.63507
H	5.31759	-2.53719	0.46110
H	2.96174	0.64658	-0.42534

TSabs_ciclohex_4.log

64

H	3.84708	2.04258	-0.90846
H	4.23114	-0.65012	-2.02725
H	4.23211	0.62344	0.04790
C	3.41109	1.22393	-0.33424
H	4.12009	-1.35157	0.32731
H	3.19375	2.17863	1.59909
C	3.24840	-0.88027	-1.60503
H	3.55876	-0.07015	2.02360
H	3.72963	-2.75257	-0.65823
C	2.18088	1.15447	-2.44379
C	3.39176	-1.75644	-0.37125
N	2.54781	0.38344	-1.23275
C	2.57348	1.77539	0.79532
H	2.63772	-1.37680	-2.35758
H	1.92581	2.56537	0.42149
C	2.50472	-0.28059	2.19504
H	2.29089	-0.10688	3.25032
H	2.95301	-2.39799	2.19478
N	1.70467	0.68317	1.35568
N	2.06305	-1.87560	0.33437
C	2.17693	-1.72204	1.82601
H	0.90099	2.05032	2.78238
C	1.45427	-3.19451	0.01012
C	0.54753	1.30214	2.06921
H	1.21477	-2.01613	2.23978
Fe	0.84947	-0.34294	-0.19954
H	0.01459	0.51281	2.60039
C	-0.33552	1.91503	1.01346
N	-0.23087	1.34129	-0.20700
H	-1.23210	3.44811	2.20122
C	-1.17552	2.99636	1.21929
C	-0.93073	1.80798	-1.24962
H	-0.79484	1.28789	-2.18724
C	-1.92028	3.48230	0.14582
C	-1.79097	2.88720	-1.10659
H	-2.58750	4.32435	0.28528
H	-2.34722	3.24270	-1.96381
H	0.46238	-3.24874	0.45287
H	2.09714	-3.98040	0.41687

H	1.38951	-3.28849	-1.07305
H	1.70752	2.08697	-2.13599
H	1.49046	0.56667	-3.04577
H	3.08599	1.37678	-3.01818
O	-0.39649	-1.08841	0.78482
O	0.28054	-1.00379	-1.75425
H	-0.48863	-1.57734	-1.61672
C	-2.82045	-0.42921	0.32977
H	-1.63854	-0.67854	0.57366
C	-3.63666	-1.19595	1.35124
H	-3.37814	-2.26047	1.30136
H	-3.42488	-0.84185	2.36442
C	-3.08048	-0.86782	-1.09837
H	-2.48637	-0.28418	-1.80567
H	-2.80194	-1.92368	-1.21092
C	-5.14146	-1.03575	1.03041
H	-5.72961	-1.61787	1.74744
H	-5.42124	0.01785	1.15162
C	-4.58463	-0.71063	-1.41848
H	-4.77793	-1.06106	-2.43762
H	-4.84314	0.35469	-1.38086
C	-5.44518	-1.47826	-0.40694
H	-6.50730	-1.32826	-0.62889
H	-5.23881	-2.55184	-0.50295
H	-2.89948	0.65371	0.46056

Irad_ciclohex_2.log
64

H	-3.97208	1.85556	1.00348
H	-4.21730	-0.88213	2.02396
H	-4.29507	0.45718	-0.00688
C	-3.50241	1.08362	0.39271
H	-4.09785	-1.50840	-0.34963
H	-3.34321	2.12380	-1.50137
C	-3.22890	-1.05589	1.58883
H	-3.61410	-0.13509	-2.00370
H	-3.62781	-2.91738	0.58692
C	-2.24205	1.00165	2.48431
C	-3.34193	-1.89773	0.32783
N	-2.58970	0.25202	1.25306
C	-2.70002	1.71619	-0.71813
H	-2.59100	-1.54647	2.32234
H	-2.08239	2.51694	-0.31664
C	-2.55320	-0.28793	-2.18991
H	-2.35808	-0.06673	-3.24000
H	-2.89860	-2.42276	-2.26390
N	-1.79130	0.68356	-1.32410
N	-2.01688	-1.92876	-0.39293
C	-2.15195	-1.72457	-1.87634
H	-1.06821	2.13983	-2.70242
C	-1.33726	-3.22518	-0.12660
C	-0.67171	1.37896	-2.02618
H	-1.18069	-1.95448	-2.30662
Fe	-0.88398	-0.35652	0.18922
H	-0.11655	0.63551	-2.59833
C	0.20150	1.98714	-0.95929
N	0.14841	1.35716	0.23726
H	0.99921	3.61225	-2.09430
C	0.98418	3.11660	-1.13225
C	0.84786	1.81185	1.28616
H	0.75591	1.24557	2.20225
C	1.72374	3.59350	-0.05140
C	1.64979	2.93844	1.17542
H	2.34442	4.47411	-0.16531
H	2.20588	3.28353	2.03700
H	-0.34756	-3.20444	-0.57605

H	-1.94090	-4.02643	-0.56279
H	-1.26048	-3.36129	0.95138
H	-1.80737	1.95984	2.19922
H	-1.52599	0.42423	3.06549
H	-3.15217	1.17102	3.06807
O	0.42604	-1.02488	-0.86895
O	-0.27186	-1.04031	1.71039
H	0.53555	-1.55166	1.54230
C	3.16414	-0.08640	-0.29827
H	1.28964	-0.57873	-0.73127
C	3.88156	-0.78807	-1.40639
H	3.45405	-1.79037	-1.55259
H	3.79619	-0.24274	-2.35044
C	3.25622	-0.71925	1.05329
H	2.73759	-0.12933	1.81326
H	2.80051	-1.72077	1.02649
C	5.37624	-0.97449	-1.02051
H	5.88478	-1.55323	-1.79891
H	5.85619	0.01029	-0.97144
C	4.75027	-0.90605	1.43953
H	4.81633	-1.43703	2.39515
H	5.20740	0.08136	1.57492
C	5.50259	-1.67072	0.34156
H	6.55900	-1.77032	0.61330
H	5.08797	-2.68431	0.26472
H	3.01106	0.98610	-0.36824

Irad_ciclohex_4.log

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H	-3.97617	1.86209	0.98770
H	-4.22876	-0.87535	2.01495
H	-4.29793	0.46050	-0.01864
C	-3.50560	1.08702	0.38153
H	-4.10045	-1.50588	-0.35753
H	-3.33977	2.11877	-1.51666
C	-3.23883	-1.05001	1.58359
H	-3.60880	-0.14050	-2.01186
H	-3.63515	-2.91329	0.58381
C	-2.25425	1.00801	2.47900
C	-3.34761	-1.89431	0.32390
N	-2.59767	0.25672	1.24784
C	-2.69904	1.71482	-0.72952
H	-2.60367	-1.53968	2.32016
H	-2.08282	2.51751	-0.32983
C	-2.54727	-0.29355	-2.19461
H	-2.34885	-0.07468	-3.24456
H	-2.88949	-2.42902	-2.26517
N	-1.78821	0.67976	-1.32848
N	-2.01924	-1.92782	-0.39069
C	-2.14603	-1.72860	-1.87550
H	-1.05798	2.12923	-2.71022
C	-1.34219	-3.22436	-0.11662
C	-0.66507	1.37131	-2.02859
H	-1.17178	-1.95821	-2.29922
Fe	-0.88657	-0.35607	0.19222
H	-0.10776	0.62469	-2.59460
C	0.20391	1.98330	-0.96062
N	0.14242	1.35998	0.23897
H	1.01194	3.60007	-2.10023
C	0.99058	3.10964	-1.13562
C	0.83853	1.81791	1.28883
H	0.74088	1.25631	2.20723
C	1.72627	3.59004	-0.05367
C	1.64442	2.94154	1.17621
H	2.35016	4.46818	-0.16912
H	2.19742	3.28940	2.03865

H	-0.35028	-3.20628	-0.56115
H	-1.94491	-4.02607	-0.55323
H	-1.27136	-3.35723	0.96215
H	-1.81833	1.96575	2.19424
H	-1.54012	0.43123	3.06334
H	-3.16608	1.17853	3.05983
O	0.43278	-1.02843	-0.85150
O	-0.27572	-1.03605	1.71568
H	0.52482	-1.55806	1.54764
C	3.16243	-0.10698	-0.31530
H	1.29769	-0.58247	-0.71110
C	3.90199	-0.80554	-1.41081
H	3.49115	-1.81502	-1.55380
H	3.81822	-0.26811	-2.35950
C	3.24938	-0.72925	1.04187
H	2.71529	-0.14050	1.79190
H	2.80640	-1.73642	1.01808
C	5.39512	-0.96571	-1.00791
H	5.92112	-1.54068	-1.77745
H	5.85902	0.02679	-0.95935
C	4.74197	-0.89213	1.44448
H	4.80531	-1.41615	2.40409
H	5.18301	0.10272	1.57857
C	5.51760	-1.65202	0.35957
H	6.57242	-1.73342	0.64326
H	5.11963	-2.67237	0.28458
H	3.00136	0.96395	-0.39262

Irad_MECP_dq_ciclohex.log

64

H	-3.97862	1.86290	0.98529
H	-4.23127	-0.87596	2.01753
H	-4.29968	0.46250	-0.02243
C	-3.50713	1.08770	0.37956
H	-4.10602	-1.50499	-0.35798
H	-3.34212	2.12285	-1.51657
C	-3.24253	-1.04951	1.58232
H	-3.60954	-0.13689	-2.01357
H	-3.64303	-2.91281	0.58373
C	-2.25607	1.00660	2.47599
C	-3.35305	-1.89446	0.32305
N	-2.60114	0.25595	1.24545
C	-2.69985	1.71654	-0.73152
H	-2.60398	-1.53940	2.31588
H	-2.08414	2.51905	-0.33033
C	-2.54776	-0.29062	-2.19521
H	-2.34995	-0.07562	-3.24626
H	-2.89151	-2.42578	-2.26867
N	-1.78887	0.68322	-1.33122
N	-2.02491	-1.92809	-0.38972
C	-2.14926	-1.72673	-1.87372
H	-1.05109	2.13331	-2.71089
C	-1.34809	-3.22403	-0.11669
C	-0.66436	1.37298	-2.02802
H	-1.17361	-1.95506	-2.29503
Fe	-0.89036	-0.35531	0.19167
H	-0.10657	0.62528	-2.59226
C	0.20486	1.98327	-0.95824
N	0.14483	1.35848	0.24100
H	1.01250	3.60042	-2.09903
C	0.99164	3.11001	-1.13427
C	0.84083	1.81882	1.28970
H	0.74343	1.25664	2.20796
C	1.72848	3.59088	-0.05346
C	1.64701	2.94280	1.17712
H	2.35256	4.46879	-0.16957

H	2.19997	3.29156	2.03904
H	-0.35630	-3.20390	-0.56161
H	-1.94915	-4.02830	-0.55160
H	-1.27341	-3.35484	0.96198
H	-1.81898	1.96379	2.19092
H	-1.54050	0.42881	3.05754
H	-3.16633	1.17883	3.05923
O	0.44032	-1.03540	-0.85221
O	-0.27343	-1.04496	1.72313
H	0.55027	-1.52566	1.55059
C	3.18393	-0.10388	-0.31015
H	1.29499	-0.57284	-0.72708
C	3.89972	-0.80467	-1.40901
H	3.48921	-1.81559	-1.53914
H	3.81328	-0.26983	-2.35803
C	3.25019	-0.72717	1.03880
H	2.71375	-0.14145	1.78845
H	2.81409	-1.73649	1.00449
C	5.39846	-0.96815	-1.00630
H	5.91334	-1.54470	-1.78100
H	5.86398	0.02309	-0.96082
C	4.74749	-0.89342	1.44401
H	4.79870	-1.41883	2.40271
H	5.18917	0.10006	1.58125
C	5.51881	-1.65541	0.35938
H	6.57375	-1.73627	0.64234
H	5.12117	-2.67549	0.28531
H	2.97649	0.95748	-0.40169

Icat_ciclohex_2.log
64

H	-3.59861	1.66964	1.98608
H	-3.84091	-1.20944	2.36653
H	-4.20152	0.60047	0.73260
C	-3.30262	1.07350	1.11974
H	-4.26685	-1.20729	-0.05880
H	-3.40565	2.59977	-0.41834
C	-2.98598	-1.29353	1.68619
H	-3.98000	0.57729	-1.42246
H	-3.77223	-2.82914	0.39226
C	-1.65556	0.43092	2.78993
C	-3.43178	-1.79428	0.31976
N	-2.31466	0.02487	1.53000
C	-2.66816	1.95483	0.06831
H	-2.25563	-1.97602	2.12152
H	-1.91046	2.58196	0.53631
C	-2.98900	0.40833	-1.84197
H	-2.97396	0.85490	-2.83836
H	-3.60947	-1.60593	-2.32786
N	-1.99159	1.09895	-0.95605
N	-2.29119	-1.69517	-0.64983
C	-2.71278	-1.09652	-1.95852
H	-1.40885	2.87273	-2.00164
C	-1.72382	-3.04194	-0.89197
C	-0.97877	1.92462	-1.66464
H	-1.88814	-1.26564	-2.64542
Fe	-0.89636	-0.34048	-0.00084
H	-0.63046	1.36011	-2.52930
C	0.17095	2.16303	-0.70655
N	0.32065	1.22395	0.25592
H	0.86918	4.00273	-1.55389
C	1.01903	3.25976	-0.78043
C	1.29821	1.34343	1.16321
H	1.35862	0.54268	1.88813
C	2.04562	3.38111	0.15412
C	2.18591	2.41174	1.14494

H	2.72212	4.22684	0.11332
H	2.96837	2.47435	1.89031
H	-0.81568	-2.93480	-1.48201
H	-2.45638	-3.66559	-1.41743
H	-1.49026	-3.50902	0.06638
H	-1.20069	1.41240	2.64715
H	-0.88051	-0.29649	3.02290
H	-2.39474	0.48578	3.59767
O	0.07185	-0.75990	-1.53952
O	0.07690	-1.40878	1.17216
H	-0.31187	-2.28514	1.26725
C	3.42507	-0.59914	-0.93629
H	0.83197	-0.18048	-1.65755
C	4.73174	-0.70902	-1.52755
H	4.96175	-1.71535	-1.87815
H	4.95754	0.06622	-2.25793
C	2.89267	-1.63781	-0.12023
H	1.84195	-1.53161	0.17129
H	3.17756	-2.63856	-0.44640
C	5.64465	-0.44536	-0.21848
H	6.67107	-0.55651	-0.57258
H	5.49476	0.58357	0.11557
C	3.79185	-1.32869	1.21145
H	3.44265	-2.08412	1.91769
H	3.53940	-0.33985	1.59690
C	5.27162	-1.43399	0.87728
H	5.85604	-1.20668	1.77592
H	5.51263	-2.45364	0.56294
H	2.96696	0.38740	-0.88986

Icat_ciclohex_4.log
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H	-3.21602	1.55448	2.45729
H	-3.99047	-1.30029	2.27188
H	-4.10477	0.85664	1.11940
C	-3.10497	1.09644	1.47259
H	-4.55662	-0.68769	-0.05466
H	-3.11070	2.88344	0.26104
C	-3.20781	-1.36860	1.50827
H	-4.04711	1.16372	-1.02874
H	-4.35769	-2.42681	0.03203
C	-1.58060	-0.17779	2.89127
C	-3.82350	-1.47601	0.11378
N	-2.30917	-0.17594	1.60065
C	-2.42765	2.06900	0.52602
H	-2.58183	-2.23891	1.70652
H	-1.55549	2.49944	1.01366
C	-3.12432	0.98672	-1.58024
H	-3.14485	1.63861	-2.45731
H	-4.01409	-0.73664	-2.51972
N	-1.97710	1.35138	-0.69746
N	-2.75662	-1.38938	-0.92110
C	-3.06249	-0.47211	-2.04130
H	-1.27207	3.13434	-1.62875
C	-2.40808	-2.73035	-1.42422
C	-0.92889	2.11942	-1.39901
H	-2.25405	-0.59420	-2.76188
Fe	-0.97498	-0.47998	0.01346
H	-0.71025	1.60089	-2.33494
C	0.32547	2.17301	-0.55077
N	0.46239	1.19008	0.35610
H	1.13334	3.96190	-1.42076
C	1.27651	3.17977	-0.68488
C	1.52518	1.18156	1.16928
H	1.57745	0.36214	1.87618
C	2.39214	3.16326	0.14792

C	2.51765	2.15200	1.09990
H	3.14847	3.93508	0.06324
H	3.36530	2.10849	1.77199
H	-1.54482	-2.64516	-2.08356
H	-3.25495	-3.17106	-1.96700
H	-2.15127	-3.36977	-0.57782
H	-0.93407	0.70050	2.92697
H	-0.97624	-1.08088	2.95181
H	-2.29652	-0.14103	3.72002
O	-0.09251	-0.77309	-1.57690
O	-0.17961	-1.88928	0.94350
H	0.17630	-2.51310	0.29954
C	3.56094	-0.59964	-0.96336
H	0.76389	-0.32815	-1.58086
C	4.81997	-0.76920	-1.62674
H	5.00594	-1.79312	-1.95120
H	5.03011	-0.02222	-2.38970
C	3.05993	-1.59710	-0.06683
H	2.03984	-1.43336	0.27839
H	3.25084	-2.61631	-0.40430
C	5.81383	-0.50142	-0.36899
H	6.81146	-0.62317	-0.79431
H	5.69475	0.53009	-0.03114
C	4.05600	-1.34663	1.19500
H	3.74622	-2.10055	1.92054
H	3.86453	-0.35474	1.60585
C	5.50197	-1.48545	0.74749
H	6.15693	-1.27175	1.59978
H	5.69840	-2.50854	0.41446
H	3.11249	0.39195	-0.94503

TSreb_CH2_ciclohex_2.log

64

H	-2.78366	-1.02706	2.98672
H	-0.33459	-2.62888	2.82292
H	-2.56243	-2.37369	1.88209
C	-2.46840	-1.29523	1.97723
H	-1.36910	-3.50590	0.76904
H	-4.33281	-1.03265	0.91187
C	-0.14138	-2.10321	1.88291
H	-3.19274	-2.72175	-0.20990
H	0.35883	-3.80175	0.65867
C	-0.64298	0.11507	2.78922
C	-0.39954	-3.01912	0.69649
N	-1.02731	-0.90418	1.78326
C	-3.33388	-0.59123	0.95655
H	0.88619	-1.74293	1.87167
H	-3.42972	0.46135	1.21707
C	-2.81721	-2.05756	-0.98629
H	-3.55010	-2.04269	-1.79486
H	-1.50658	-3.63697	-1.67548
N	-2.69055	-0.68308	-0.39346
N	-0.35322	-2.22439	-0.58158
C	-1.47587	-2.55441	-1.52282
H	-4.29622	0.42239	-1.25896
C	0.95286	-2.44765	-1.25633
C	-3.20308	0.41150	-1.26086
H	-1.23854	-2.06283	-2.46325
Fe	-0.64992	-0.24802	-0.17290
H	-2.84470	0.23490	-2.27583
C	-2.64208	1.70847	-0.73125
N	-1.46770	1.59516	-0.06933
H	-4.20914	3.00291	-1.39468
C	-3.26166	2.94026	-0.87485
C	-0.87116	2.67430	0.45798
H	0.06953	2.49938	0.96286

C	-2.64874	4.06876	-0.33426
C	-1.44021	3.93495	0.34552
H	-3.11533	5.04138	-0.43600
H	-0.93957	4.78844	0.78369
H	1.02278	-1.79087	-2.11986
H	1.00960	-3.49569	-1.56596
H	1.75057	-2.22577	-0.54980
H	-1.32876	0.95916	2.71327
H	0.37559	0.44272	2.59187
H	-0.71223	-0.32278	3.79010
O	-0.37191	0.07705	-1.95212
O	1.00923	0.17781	0.34916
H	1.60169	0.35806	-0.40322
C	3.59557	0.78027	-0.62647
H	-0.38595	1.02447	-2.14431
C	4.12076	-0.60603	-0.73713
H	3.85488	-1.17593	0.16375
H	3.71350	-1.12818	-1.60553
C	4.09953	1.60859	0.49995
H	3.67584	2.61546	0.48610
H	3.83776	1.13307	1.45458
C	5.67776	-0.55180	-0.80630
H	6.06856	-1.57421	-0.80767
H	5.97600	-0.07816	-1.74849
C	5.65568	1.66502	0.42646
H	6.03388	2.21204	1.29585
H	5.95103	2.21927	-0.47178
C	6.24435	0.24952	0.37263
H	7.33547	0.30345	0.29427
H	6.00783	-0.27325	1.30818
H	3.17138	1.26555	-1.50232

TSreb_CH2_ciclohex_4.log

64

H	-2.78366	-1.02706	2.98672
H	-0.33459	-2.62888	2.82292
H	-2.56243	-2.37369	1.88209
C	-2.46840	-1.29523	1.97723
H	-1.36910	-3.50590	0.76904
H	-4.33281	-1.03265	0.91187
C	-0.14138	-2.10321	1.88291
H	-3.19274	-2.72175	-0.20990
H	0.35883	-3.80175	0.65867
C	-0.64298	0.11507	2.78922
C	-0.39954	-3.01912	0.69649
N	-1.02731	-0.90418	1.78326
C	-3.33388	-0.59123	0.95655
H	0.88619	-1.74293	1.87167
H	-3.42972	0.46135	1.21707
C	-2.81721	-2.05756	-0.98629
H	-3.55010	-2.04269	-1.79486
H	-1.50658	-3.63697	-1.67548
N	-2.69055	-0.68308	-0.39346
N	-0.35322	-2.22439	-0.58158
C	-1.47587	-2.55441	-1.52282
H	-4.29622	0.42239	-1.25896
C	0.95286	-2.44765	-1.25633
C	-3.20308	0.41150	-1.26086
H	-1.23854	-2.06283	-2.46325
Fe	-0.64992	-0.24802	-0.17290
H	-2.84470	0.23490	-2.27583
C	-2.64208	1.70847	-0.73125
N	-1.46770	1.59516	-0.06933
H	-4.20914	3.00291	-1.39468
C	-3.26166	2.94026	-0.87485
C	-0.87116	2.67430	0.45798

H	0.06953	2.49938	0.96286
C	-2.64874	4.06876	-0.33426
C	-1.44021	3.93495	0.34552
H	-3.11533	5.04138	-0.43600
H	-0.93957	4.78844	0.78369
H	1.02278	-1.79087	-2.11986
H	1.00960	-3.49569	-1.56596
H	1.75057	-2.22577	-0.54980
H	-1.32876	0.95916	2.71327
H	0.37559	0.44272	2.59187
H	-0.71223	-0.32278	3.79010
O	-0.37191	0.07705	-1.95212
O	1.00923	0.17781	0.34916
H	1.60169	0.35806	-0.40322
C	3.59557	0.78027	-0.62647
H	-0.38595	1.02447	-2.14431
C	4.12076	-0.60603	-0.73713
H	3.85488	-1.17593	0.16375
H	3.71350	-1.12818	-1.60553
C	4.09953	1.60859	0.49995
H	3.67584	2.61546	0.48610
H	3.83776	1.13307	1.45458
C	5.67776	-0.55180	-0.80630
H	6.06856	-1.57421	-0.80767
H	5.97600	-0.07816	-1.74849
C	5.65568	1.66502	0.42646
H	6.03388	2.21204	1.29585
H	5.95103	2.21927	-0.47178
C	6.24435	0.24952	0.37263
H	7.33547	0.30345	0.29427
H	6.00783	-0.27325	1.30818
H	3.17138	1.26555	-1.50232

Prod_CH2_ciclohex_2.log

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H	-3.23548	-0.78294	2.54834
H	-1.25706	-2.98643	2.51823
H	-3.16089	-2.02584	1.31334
C	-2.81094	-1.03070	1.57444
H	-2.12563	-3.31475	0.22754
H	-4.30893	-0.15521	0.27735
C	-0.78912	-2.43566	1.69633
H	-3.47392	-1.95764	-0.88362
H	-0.54534	-4.06768	0.31892
C	-0.89236	-0.30654	2.88614
C	-1.06618	-3.10978	0.36368
N	-1.30565	-1.03234	1.66186
C	-3.25908	-0.01723	0.54628
H	0.28558	-2.37672	1.86972
H	-3.13058	0.98765	0.94356
C	-2.80407	-1.35602	-1.49569
H	-3.35075	-1.04649	-2.38765
H	-1.84864	-3.16635	-2.19709
N	-2.41626	-0.14308	-0.69372
N	-0.59287	-2.22203	-0.75132
C	-1.56552	-2.15536	-1.88889
H	-3.52739	1.44600	-1.58529
C	0.70951	-2.72994	-1.24944
C	-2.48623	1.14443	-1.44400
H	-1.04372	-1.65998	-2.70447
Fe	-0.52215	-0.27662	-0.13057
H	-2.01089	0.99240	-2.41268
C	-1.72141	2.18016	-0.65382
N	-0.75947	1.69716	0.16991
H	-2.76652	3.88968	-1.40092
C	-1.98093	3.53935	-0.74336

C	-0.04037	2.54580	0.91938
H	0.71256	2.11364	1.56381
C	-1.22493	4.42200	0.02398
C	-0.24290	3.91774	0.87315
H	-1.40800	5.48851	-0.03270
H	0.35984	4.56911	1.49242
H	1.08208	-2.05200	-2.01310
H	0.56805	-3.73244	-1.66657
H	1.40899	-2.77901	-0.41555
H	-1.21374	0.73245	2.81384
H	0.18966	-0.35625	3.01141
H	-1.35454	-0.77195	3.76269
O	0.16231	0.12990	-1.78389
O	1.32723	-0.38096	0.68662
H	1.43319	0.05463	1.54647
C	2.60650	-0.25568	-0.02744
H	0.72033	0.91642	-1.73805
C	3.64564	-1.11545	0.67875
H	3.73932	-0.76886	1.71615
H	3.30883	-2.15566	0.69815
C	3.02767	1.20553	-0.10704
H	2.26743	1.79105	-0.63059
H	3.10441	1.60096	0.91420
C	5.00496	-0.99157	-0.02802
H	5.74930	-1.59169	0.50367
H	4.91831	-1.40142	-1.04201
C	4.38774	1.33006	-0.81176
H	4.69131	2.38080	-0.83482
H	4.28242	0.99745	-1.85187
C	5.45252	0.47372	-0.11386
H	6.40434	0.54623	-0.64955
H	5.61562	0.85949	0.90041
H	2.39677	-0.64373	-1.02065

Prod_CH2_ciclohex_4.log

64

H	-3.21932	-0.92391	2.55658
H	-1.17208	-3.04555	2.49131
H	-3.10739	-2.14590	1.30630
C	-2.80129	-1.13731	1.57163
H	-2.04257	-3.38949	0.20109
H	-4.39794	-0.33933	0.36464
C	-0.72906	-2.47334	1.67013
H	-3.45254	-2.10506	-0.88022
H	-0.43626	-4.08916	0.28366
C	-0.90701	-0.35519	2.88372
C	-0.98999	-3.15026	0.33420
N	-1.29377	-1.08578	1.65246
C	-3.33941	-0.14102	0.56193
H	0.34448	-2.38007	1.83905
H	-3.25008	0.86746	0.96346
C	-2.83236	-1.44646	-1.48687
H	-3.40200	-1.19800	-2.38557
H	-1.77554	-3.17121	-2.25673
N	-2.55152	-0.21712	-0.69367
N	-0.55120	-2.24526	-0.78344
C	-1.54158	-2.16216	-1.90353
H	-3.66885	1.34906	-1.62275
C	0.76170	-2.70704	-1.30445
C	-2.63038	1.05056	-1.44636
H	-1.04741	-1.60718	-2.69912
Fe	-0.43308	-0.28726	-0.11009
H	-2.13436	0.90388	-2.40801
C	-1.90396	2.12452	-0.66368
N	-0.90414	1.70211	0.14140
H	-3.06102	3.77543	-1.37670

C	-2.24276	3.46849	-0.73737
C	-0.21609	2.58413	0.88291
H	0.57228	2.18025	1.50466
C	-1.52641	4.38993	0.02229
C	-0.49916	3.94190	0.85018
H	-1.77422	5.44385	-0.02356
H	0.07421	4.62515	1.46303
H	1.10962	-2.00927	-2.06271
H	0.64449	-3.70754	-1.73325
H	1.47277	-2.74476	-0.47826
H	-1.27461	0.66902	2.82146
H	0.17544	-0.35570	3.00228
H	-1.34544	-0.85027	3.75621
O	0.28486	0.16076	-1.73245
O	1.48846	-0.31785	0.79865
H	1.64844	-0.02163	1.70602
C	2.73630	-0.16993	0.04092
H	0.49253	1.10303	-1.78735
C	3.82298	-1.01749	0.68598
H	3.96003	-0.68316	1.72295
H	3.50430	-2.06409	0.70520
C	3.11734	1.30037	-0.05285
H	2.31275	1.85512	-0.54419
H	3.23012	1.69800	0.96420
C	5.14467	-0.85752	-0.08259
H	5.92741	-1.44400	0.40767
H	5.01992	-1.26119	-1.09519
C	4.44056	1.45733	-0.81886
H	4.72342	2.51376	-0.85110
H	4.29415	1.12689	-1.85484
C	5.55430	0.61865	-0.17675
H	6.47942	0.71627	-0.75375
H	5.75500	1.00042	0.83235
H	2.48870	-0.55232	-0.94655

TSreb_CH3_ciclohex_2.log

64

H	-3.93583	1.76666	1.12671
H	-4.07774	-0.99234	2.10038
H	-4.25110	0.38101	0.09624
C	-3.46383	1.02051	0.48607
H	-4.02163	-1.57591	-0.28516
H	-3.38991	2.10758	-1.38753
C	-3.09951	-1.13262	1.63092
H	-3.62563	-0.15110	-1.92081
H	-3.48165	-2.98670	0.60958
C	-2.13561	0.93093	2.53431
C	-3.23221	-1.95524	0.35917
N	-2.50342	0.19630	1.30021
C	-2.71251	1.69704	-0.63505
H	-2.42595	-1.61986	2.33417
H	-2.10098	2.50271	-0.23417
C	-2.56886	-0.27325	-2.14905
H	-2.41920	-0.02727	-3.20123
H	-2.86430	-2.41439	-2.25739
N	-1.80042	0.69980	-1.29176
N	-1.93233	-1.93694	-0.40549
C	-2.12260	-1.70595	-1.87855
H	-1.15681	2.20131	-2.66283
C	-1.21412	-3.22167	-0.18999
C	-0.72206	1.43583	-2.01573
H	-1.16060	-1.90206	-2.34507
Fe	-0.81785	-0.34716	0.17022
H	-0.16935	0.71720	-2.62099
C	0.17386	2.04259	-0.96601
N	0.17465	1.38971	0.21936

H	0.89943	3.70470	-2.09669
C	0.92735	3.19130	-1.14421
C	0.90192	1.83966	1.25121
H	0.85520	1.25228	2.15749
C	1.69555	3.66310	-0.08118
C	1.67813	2.98381	1.13464
H	2.29486	4.55781	-0.20010
H	2.25868	3.32351	1.98219
H	-0.24083	-3.16673	-0.67125
H	-1.81190	-4.02985	-0.62210
H	-1.09684	-3.37697	0.88168
H	-1.73142	1.90400	2.25493
H	-1.38840	0.35928	3.08098
H	-3.03017	1.06897	3.14991
O	0.43505	-0.94498	-0.91166
O	-0.14492	-1.03880	1.64210
H	0.66961	-1.52370	1.43894
C	3.04896	-0.08607	-0.39124
H	1.26785	-0.49784	-0.80555
C	3.74090	-0.91021	-1.42311
H	3.26805	-1.90028	-1.48913
H	3.69583	-0.44231	-2.41014
C	3.07678	-0.60852	1.00543
H	2.57114	0.06609	1.70042
H	2.57647	-1.58771	1.04631
C	5.21975	-1.12997	-0.99054
H	5.70975	-1.79323	-1.71069
H	5.74373	-0.16722	-1.01330
C	4.55431	-0.83019	1.43948
H	4.57116	-1.28397	2.43570
H	5.05438	0.14296	1.50705
C	5.28900	-1.71643	0.42522
H	6.33474	-1.83926	0.72681
H	4.82928	-2.71316	0.42276
H	2.94244	0.98235	-0.55432

TSreb_CH3_ciclohex_4.log

64

H	-3.83609	2.19668	0.94701
H	-4.42312	-0.57272	1.88509
H	-4.25048	0.85663	-0.10599
C	-3.41697	1.38026	0.35556
H	-4.21798	-1.11854	-0.50090
H	-3.03167	2.44647	-1.49337
C	-3.42691	-0.80776	1.49595
H	-3.52688	0.22035	-2.06719
H	-3.95313	-2.59169	0.41473
C	-2.29860	1.11199	2.51289
C	-3.54533	-1.60254	0.20342
N	-2.66194	0.44356	1.24609
C	-2.48292	1.94121	-0.69474
H	-2.87324	-1.37763	2.24131
H	-1.80063	2.65202	-0.23278
C	-2.47821	-0.03093	-2.21706
H	-2.22353	0.19443	-3.25373
H	-3.01252	-2.12218	-2.37785
N	-1.66018	0.83650	-1.29642
N	-2.19422	-1.75871	-0.44692
C	-2.22857	-1.50662	-1.92775
H	-0.74286	2.23656	-2.61858
C	-1.67092	-3.12440	-0.18347
C	-0.45185	1.42645	-1.94541
H	-1.25829	-1.81150	-2.31209
Fe	-0.91540	-0.32749	0.22721
H	0.04171	0.63868	-2.51519
C	0.45740	1.91531	-0.84798

N	0.31596	1.26671	0.33051
H	1.46129	3.45562	-1.94076
C	1.37590	2.94322	-0.99113
C	1.06869	1.59822	1.38888
H	0.90061	1.02262	2.28918
C	2.16737	3.29189	0.10127
C	2.01006	2.61476	1.30858
H	2.89687	4.08792	0.01146
H	2.60461	2.86220	2.17823
H	-0.65778	-3.19535	-0.57231
H	-2.32408	-3.85027	-0.67772
H	-1.67436	-3.29424	0.89254
H	-1.73937	2.02054	2.28448
H	-1.67977	0.43918	3.10458
H	-3.20685	1.37238	3.06820
O	0.42830	-1.14691	-0.80502
O	-0.43366	-1.10684	1.76093
H	0.27924	-1.73785	1.57764
C	3.14811	-1.52067	-0.95683
H	1.26724	-0.67507	-0.70862
C	3.18819	-2.07112	0.42132
H	2.58747	-1.43649	1.08873
H	2.79300	-3.08787	0.46360
C	3.69394	-0.15244	-1.15726
H	3.65023	0.15477	-2.20409
H	3.12354	0.57109	-0.55793
C	4.65389	-2.02067	0.95037
H	4.66266	-2.35445	1.99251
H	5.26703	-2.71860	0.36956
C	5.16014	-0.10558	-0.62566
H	5.52628	0.92261	-0.70420
H	5.79044	-0.73664	-1.26182
C	5.22645	-0.60462	0.82194
H	6.26401	-0.59062	1.17173
H	4.65291	0.07543	1.46401
H	3.01017	-2.18211	-1.80429

Prod_CH3_ciclohex_2.log
64

H	3.85612	2.09321	-0.28812
H	4.33652	-0.42675	-1.72274
H	4.11256	0.54109	0.48813
C	3.34726	1.21408	0.10992
H	3.91930	-1.45417	0.47384
H	2.93531	1.87476	2.13026
C	3.30611	-0.68521	-1.46051
H	3.17463	-0.41056	2.28082
H	3.63601	-2.69039	-0.74080
C	2.38075	1.47953	-2.11914
C	3.27776	-1.73346	-0.35938
N	2.57864	0.53444	-0.99315
C	2.39677	1.61811	1.21462
H	2.78092	-1.04624	-2.34295
H	1.81876	2.48352	0.89687
C	2.10404	-0.60594	2.27442
H	1.75593	-0.59149	3.30849
H	2.55739	-2.70285	1.99630
N	1.44111	0.49382	1.49153
N	1.86721	-1.89340	0.15038
C	1.82446	-1.96995	1.64670
H	0.48743	1.68471	2.98953
C	1.28020	-3.12924	-0.43235
C	0.22279	1.05492	2.13585
H	0.84023	-2.34202	1.93056
Fe	0.81975	-0.21893	-0.32341
H	-0.39661	0.23312	2.50116

C	-0.51411	1.84354	1.08201
N	-0.27179	1.45367	-0.19016
H	-1.54079	3.18797	2.39007
C	-1.37592	2.89219	1.36182
C	-0.86771	2.08263	-1.21291
H	-0.62976	1.70700	-2.19872
C	-2.00711	3.54265	0.30383
C	-1.74654	3.13592	-1.00280
H	-2.68796	4.36297	0.49759
H	-2.21318	3.62091	-1.85017
H	0.23946	-3.21687	-0.12857
H	1.84885	-3.99505	-0.07935
H	1.33858	-3.05795	-1.51715
H	1.88746	2.37499	-1.74086
H	1.75705	1.00212	-2.87184
H	3.35371	1.74930	-2.54219
O	-0.90576	-1.16900	0.36383
O	0.38806	-0.70947	-2.01655
H	-0.38715	-1.28389	-2.02350
C	-2.31902	-0.76961	0.24509
H	-0.80176	-1.54672	1.24964
C	-3.16218	-1.71196	1.09547
H	-3.01446	-2.73640	0.73405
H	-2.82733	-1.66384	2.13830
C	-2.73748	-0.80687	-1.21586
H	-2.12783	-0.12029	-1.80428
H	-2.57931	-1.82327	-1.59747
C	-4.64593	-1.32962	0.98691
H	-5.24603	-2.02090	1.58549
H	-4.78774	-0.32548	1.40472
C	-4.22202	-0.42589	-1.33592
H	-4.52391	-0.47320	-2.38612
H	-4.34790	0.61298	-1.00671
C	-5.10665	-1.33916	-0.47715
H	-6.15224	-1.02244	-0.54441
H	-5.04747	-2.36382	-0.86496
H	-2.41589	0.24632	0.63167

Prod_CH3_ciclohex_4.log

64

H	3.82419	2.25534	-0.74134
H	4.45114	-0.56131	-1.73658
H	4.15859	0.87523	0.28466
C	3.36012	1.41065	-0.22505
H	4.06996	-1.12033	0.61553
H	2.82768	2.45112	1.60701
C	3.41920	-0.75123	-1.41746
H	3.32165	0.19634	2.16933
H	3.84585	-2.56953	-0.34707
C	2.39341	1.20783	-2.46132
C	3.43487	-1.58084	-0.13820
N	2.68354	0.51260	-1.19641
C	2.34280	1.94155	0.77032
H	2.89402	-1.29104	-2.20602
H	1.67957	2.64281	0.26647
C	2.26719	-0.05711	2.26088
H	1.96481	0.14094	3.29012
H	2.80124	-2.15066	2.38690
N	1.48799	0.82915	1.32279
N	2.04862	-1.74115	0.43530
C	2.03401	-1.52477	1.92148
H	0.55652	2.22636	2.64157
C	1.53614	-3.10122	0.12366
C	0.27076	1.42797	1.95235
H	1.06520	-1.86006	2.28829
Fe	0.79868	-0.27120	-0.27553

H	-0.24213	0.65161	2.52297
C	-0.61454	1.93851	0.84757
N	-0.47721	1.28935	-0.32951
H	-1.58784	3.49930	1.94013
C	-1.50614	2.99067	0.98820
C	-1.20663	1.65226	-1.39438
H	-1.04173	1.07951	-2.29726
C	-2.27369	3.36945	-0.11085
C	-2.12072	2.69401	-1.32001
H	-2.97962	4.18692	-0.02546
H	-2.69696	2.96352	-2.19540
H	0.50524	-3.18107	0.46375
H	2.16090	-3.84385	0.63007
H	1.58625	-3.25248	-0.95406
H	1.80092	2.09954	-2.24636
H	1.81787	0.54186	-3.10463
H	3.32295	1.50275	-2.96519
O	-0.98386	-1.32199	0.90478
O	0.34202	-1.04672	-1.81736
H	-0.21530	-1.83052	-1.72132
C	-2.40828	-1.52174	0.64916
H	-0.87547	-1.32635	1.86476
C	-2.61761	-1.76523	-0.83715
H	-2.25311	-0.89827	-1.39574
H	-2.04710	-2.64683	-1.14978
C	-3.22366	-0.33332	1.14790
H	-3.04631	-0.18786	2.21905
H	-2.88789	0.56349	0.62316
C	-4.11158	-1.97773	-1.13266
H	-4.25234	-2.12355	-2.20777
H	-4.44833	-2.89381	-0.63174
C	-4.71726	-0.55246	0.86387
H	-5.28854	0.31517	1.20775
H	-5.07117	-1.42286	1.43040
C	-4.95232	-0.79485	-0.63330
H	-6.01390	-0.98024	-0.82576
H	-4.66896	0.10702	-1.19029
H	-2.70587	-2.42126	1.19914

2,3-DMB_AT_SOLVENT

A_DMB_2.log

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H	-3.51575	2.01417	1.60679
H	-3.97085	-0.83594	2.19723
H	-4.12043	0.83823	0.45492
C	-3.21581	1.30842	0.83112
H	-4.16136	-1.07166	-0.24615
H	-3.15266	2.62375	-0.88928
C	-3.05555	-1.02151	1.62813
H	-3.72706	0.50631	-1.69715
H	-3.74354	-2.65086	0.40215
C	-1.75860	0.75311	2.71277
C	-3.38663	-1.62884	0.27457
N	-2.31517	0.26062	1.42818
C	-2.47612	2.03447	-0.26630
H	-2.40467	-1.68524	2.19477
H	-1.73088	2.69669	0.16914
C	-2.71551	0.29652	-2.03842
H	-2.61955	0.67152	-3.05801
H	-3.27872	-1.76281	-2.39842
N	-1.76127	1.03865	-1.13759
N	-2.15336	-1.65410	-0.59751
C	-2.42915	-1.19852	-2.00593
H	-1.05065	2.62854	-2.36369
C	-1.58426	-3.03137	-0.61445
C	-0.65956	1.73613	-1.87033

H	-1.54225	-1.43480	-2.59176
Fe	-0.80488	-0.31307	0.07854
H	-0.26024	1.05298	-2.62061
C	0.39548	2.08151	-0.85318
N	0.42151	1.26993	0.22912
H	1.21283	3.80452	-1.81762
C	1.26106	3.15852	-0.95065
C	1.28545	1.48171	1.23182
H	1.25224	0.77741	2.05088
C	2.16384	3.39014	0.08493
C	2.17250	2.54673	1.19245
H	2.85077	4.22598	0.02884
H	2.85929	2.69652	2.01445
H	-0.64890	-3.03248	-1.17267
H	-2.30841	-3.69520	-1.09459
H	-1.40931	-3.34758	0.41269
H	-1.25208	1.70215	2.53482
H	-1.05538	0.02120	3.10501
H	-2.57807	0.90325	3.42240
O	0.30239	-0.84452	-1.16697
O	-0.12243	-1.29119	1.38559
H	2.29497	-0.77035	0.36842
C	3.23866	-1.27900	0.59249
H	0.57150	-1.88363	1.05520
C	4.15733	-1.02327	-0.62259
H	5.14857	-1.43100	-0.37959
C	4.29749	0.47983	-0.90212
H	4.91851	0.64800	-1.78859
H	3.31008	0.91728	-1.08968
H	4.75082	1.01857	-0.06646
C	3.81258	-0.69011	1.88617
H	3.98579	0.38547	1.81204
H	3.12581	-0.86331	2.72165
H	4.76686	-1.17386	2.12832
C	2.93797	-2.76855	0.80723
H	2.36235	-2.91444	1.72960
H	2.37073	-3.19937	-0.02199
H	3.86906	-3.33798	0.91293
C	3.64199	-1.71909	-1.88958
H	3.63757	-2.80768	-1.78831
H	2.61759	-1.39354	-2.10505
H	4.27192	-1.46206	-2.74794

A_DMB_4.log

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H	-3.42925	2.09274	1.59783
H	-3.94479	-0.74627	2.25057
H	-4.08793	0.91306	0.48150
C	-3.16283	1.36200	0.83299
H	-4.18428	-0.97650	-0.19296
H	-3.10755	2.63123	-0.92077
C	-3.04727	-0.95624	1.66132
H	-3.71327	0.55119	-1.70670
H	-3.81822	-2.56655	0.46057
C	-1.70387	0.79591	2.70851
C	-3.42437	-1.55973	0.32070
N	-2.28093	0.30344	1.43406
C	-2.42821	2.05111	-0.29225
H	-2.40036	-1.63395	2.21617
H	-1.67487	2.71939	0.11806
C	-2.70961	0.29981	-2.04253
H	-2.59913	0.65047	-3.06928
H	-3.35399	-1.74372	-2.34929
N	-1.73281	1.03284	-1.15515
N	-2.20559	-1.63962	-0.56629
C	-2.47840	-1.20349	-1.98019

H	-0.99783	2.59238	-2.40909
C	-1.67934	-3.03345	-0.55923
C	-0.61933	1.70788	-1.89218
H	-1.60739	-1.48636	-2.56783
Fe	-0.77394	-0.33022	0.04988
H	-0.21495	1.00608	-2.62347
C	0.42332	2.06606	-0.86676
N	0.43065	1.26948	0.22690
H	1.26079	3.77464	-1.83797
C	1.29420	3.13784	-0.96353
C	1.28273	1.48425	1.23767
H	1.23829	0.78671	2.06185
C	2.18432	3.37684	0.08244
C	2.17610	2.54506	1.19775
H	2.87548	4.20915	0.02623
H	2.85439	2.69861	2.02607
H	-0.75485	-3.07432	-1.13197
H	-2.43394	-3.68171	-1.01351
H	-1.50049	-3.33238	0.47245
H	-1.18864	1.73855	2.52274
H	-1.00502	0.05774	3.09718
H	-2.51233	0.96035	3.42809
O	0.22756	-0.89700	-1.12399
O	-0.11334	-1.30173	1.38951
H	2.28376	-0.77846	0.38572
C	3.23014	-1.28912	0.59171
H	0.58084	-1.90570	1.08387
C	4.11995	-1.05057	-0.64809
H	5.11289	-1.46726	-0.42856
C	4.26792	0.44895	-0.94159
H	4.86590	0.60469	-1.84598
H	3.28048	0.89568	-1.10479
H	4.75024	0.98749	-0.12217
C	3.83672	-0.68954	1.86538
H	4.00432	0.38602	1.77855
H	3.17234	-0.85854	2.71964
H	4.79858	-1.16845	2.08635
C	2.93078	-2.77614	0.82752
H	2.37953	-2.91229	1.76606
H	2.34023	-3.21204	0.01713
H	3.86254	-3.34778	0.91296
C	3.56340	-1.74977	-1.89588
H	3.55175	-2.83752	-1.78723
H	2.53658	-1.41553	-2.08496
H	4.17158	-1.50424	-2.77311

A_DMB_6.log

66

H	-3.31172	2.17753	1.81572
H	-4.32650	-0.73382	1.95318
H	-4.05614	1.32974	0.48075
C	-3.10314	1.52456	0.96735
H	-4.56389	-0.42131	-0.48348
H	-2.62454	3.02832	-0.52326
C	-3.43909	-0.91944	1.33862
H	-3.57296	1.10886	-1.54567
H	-4.60173	-2.11460	0.03528
C	-2.12765	0.38201	2.88871
C	-3.96546	-1.23193	-0.07790
N	-2.50682	0.23592	1.45708
C	-2.13020	2.22503	0.03070
H	-2.91643	-1.79261	1.73001
H	-1.30984	2.64735	0.60903
C	-2.60114	0.77083	-1.89326
H	-2.43398	1.25905	-2.85508
H	-3.44227	-0.89099	-2.90722

N	-1.54742	1.23416	-0.92841
N	-2.93356	-1.58178	-1.04584
C	-2.62800	-0.72587	-2.18398
H	-0.74996	2.72849	-2.21225
C	-2.42139	-2.93181	-1.02140
C	-0.41051	1.82845	-1.69267
H	-1.69583	-1.07452	-2.61963
Fe	-0.62411	-0.19968	0.36735
H	-0.10414	1.08575	-2.43358
C	0.75424	2.13684	-0.79046
N	0.86512	1.35994	0.29886
H	1.55214	3.76152	-1.93853
C	1.67046	3.14665	-1.05515
C	1.86357	1.55228	1.17081
H	1.89085	0.88763	2.02405
C	2.71786	3.34745	-0.15930
C	2.81461	2.54336	0.97471
H	3.44647	4.12876	-0.34071
H	3.61125	2.67488	1.69495
H	-1.49506	-2.99098	-1.58553
H	-3.19097	-3.57615	-1.47485
H	-2.28294	-3.24959	0.01454
H	-1.41240	1.20190	2.97326
H	-1.66474	-0.54048	3.23257
H	-3.02102	0.60747	3.48120
O	-0.02955	-1.06600	-0.88876
O	0.01015	-1.24595	1.70213
H	2.33925	-0.95728	0.50250
C	3.27065	-1.52656	0.58039
H	0.56013	-1.97154	1.37704
C	3.92792	-1.48554	-0.81751
H	4.91920	-1.95285	-0.73146
C	4.10901	-0.03925	-1.30161
H	4.54154	-0.02398	-2.30788
H	3.13850	0.46784	-1.34259
H	4.76314	0.54017	-0.64566
C	4.15734	-0.87358	1.64729
H	4.39934	0.16396	1.40794
H	3.65607	-0.88504	2.62109
H	5.09836	-1.42921	1.74562
C	2.91296	-2.95005	1.02812
H	2.52163	-2.93927	2.05218
H	2.15947	-3.40715	0.38026
H	3.80030	-3.59481	1.02061
C	3.11242	-2.26362	-1.85970
H	3.07585	-3.33319	-1.63451
H	2.08414	-1.88529	-1.88666
H	3.55336	-2.14379	-2.85547

TSabs_DMB_2.log

66

H	3.71847	2.24704	-0.50477
H	4.29945	-0.38527	-1.68775
H	4.04584	0.79374	0.42072
C	3.25044	1.38998	-0.01822
H	3.95376	-1.18572	0.60997
H	2.79878	2.24190	1.92207
C	3.28389	-0.65755	-1.38580
H	3.16603	-0.01301	2.30330
H	3.72532	-2.55408	-0.46756
C	2.25433	1.38732	-2.25156
C	3.32123	-1.58317	-0.18035
N	2.51152	0.57274	-1.04076
C	2.28077	1.86478	1.03751
H	2.77325	-1.13503	-2.22032
H	1.65726	2.65847	0.63141

C	2.10596	-0.25580	2.33443
H	1.76340	-0.13952	3.36318
H	2.60658	-2.36221	2.29686
N	1.38317	0.73066	1.45144
N	1.92830	-1.77613	0.36604
C	1.86436	-1.68577	1.86498
H	0.40453	2.02878	2.83124
C	1.39741	-3.09259	-0.08114
C	0.14275	1.30191	2.05926
H	0.86754	-2.01999	2.15002
Fe	0.73759	-0.24724	-0.22880
H	-0.42893	0.48546	2.50132
C	-0.63528	1.93711	0.93808
N	-0.42416	1.38420	-0.27851
H	-1.61780	3.46163	2.06645
C	-1.47984	3.02454	1.08595
C	-1.03398	1.86697	-1.36855
H	-0.81568	1.36391	-2.29996
C	-2.12392	3.53388	-0.04002
C	-1.89745	2.95029	-1.28302
H	-2.79111	4.38230	0.05322
H	-2.37770	3.32013	-2.17929
H	0.36064	-3.18481	0.23425
H	2.00687	-3.88113	0.36970
H	1.46670	-3.14266	-1.16692
H	1.72277	2.29345	-1.96030
H	1.65074	0.80949	-2.94886
H	3.20881	1.65700	-2.71479
O	-0.58406	-1.04945	0.62425
O	0.37732	-0.85760	-1.85773
H	-1.89166	-1.03968	-0.16990
C	-2.87739	-1.44758	-0.63824
H	-0.37082	-1.47425	-1.84674
C	-3.95612	-1.07705	0.39461
H	-4.90171	-1.47559	-0.00345
C	-4.09918	0.43979	0.56263
H	-4.85492	0.66404	1.32231
H	-3.15000	0.87143	0.89301
H	-4.39494	0.93553	-0.36459
C	-3.08144	-0.79138	-1.99880
H	-3.09614	0.29712	-1.94148
H	-2.30192	-1.09045	-2.70609
H	-4.04429	-1.12230	-2.41092
C	-2.65110	-2.94950	-0.77881
H	-1.91267	-3.15920	-1.55976
H	-2.30299	-3.39879	0.15272
H	-3.59103	-3.43850	-1.06646
C	-3.69553	-1.72026	1.76247
H	-3.70872	-2.81197	1.71440
H	-2.71751	-1.40541	2.14225
H	-4.46086	-1.40331	2.47815

TSabs_DMB_4.log

66

H	3.75105	2.17624	-0.28184
H	4.32651	-0.41205	-1.57945
H	4.02492	0.66742	0.56952
C	3.25379	1.30189	0.14080
H	3.86744	-1.30595	0.67263
H	2.76858	2.03492	2.11959
C	3.29506	-0.67415	-1.32552
H	3.02723	-0.21596	2.40403
H	3.66139	-2.61942	-0.47644
C	2.35280	1.43311	-2.12949
C	3.26528	-1.65304	-0.16375
N	2.53672	0.55604	-0.95019

C	2.26398	1.73850	1.19727
H	2.80360	-1.10107	-2.19856
H	1.68689	2.58477	0.83060
C	1.96195	-0.43525	2.36903
H	1.56924	-0.36729	3.38423
H	2.43125	-2.54431	2.22860
N	1.31034	0.61633	1.50608
N	1.84576	-1.83522	0.31076
C	1.71734	-1.83099	1.80815
H	0.29321	1.86355	2.90987
C	1.30865	-3.11292	-0.23459
C	0.05834	1.19783	2.07645
H	0.70454	-2.16225	2.02847
Fe	0.70967	-0.25082	-0.25142
H	-0.57102	0.37851	2.42679
C	-0.62291	1.93197	0.95300
N	-0.35414	1.44361	-0.27978
H	-1.62539	3.42028	2.11072
C	-1.43702	3.03948	1.11530
C	-0.87132	2.01548	-1.37492
H	-0.61677	1.55542	-2.31901
C	-1.98537	3.64126	-0.01556
C	-1.69584	3.12726	-1.27653
H	-2.62645	4.50848	0.08787
H	-2.10189	3.57018	-2.17634
H	0.25772	-3.20133	0.03086
H	1.88390	-3.93773	0.19553
H	1.42411	-3.10294	-1.31752
H	1.84536	2.34495	-1.81453
H	1.75212	0.91089	-2.87216
H	3.33171	1.68748	-2.54845
O	-0.65105	-1.06888	0.46739
O	0.37468	-0.77921	-1.92495
H	-1.83690	-1.03043	-0.20846
C	-2.90993	-1.29696	-0.73152
H	-0.35979	-1.41034	-1.95570
C	-3.91324	-1.04019	0.40146
H	-4.90951	-1.15032	-0.05483
C	-3.79379	0.37869	0.97128
H	-4.58366	0.55491	1.70820
H	-2.83020	0.49203	1.47660
H	-3.86962	1.14997	0.20251
C	-3.08582	-0.39755	-1.94274
H	-3.13650	0.65936	-1.68308
H	-2.27440	-0.53874	-2.66230
H	-4.02422	-0.66891	-2.44691
C	-2.74729	-2.75517	-1.13237
H	-2.04759	-2.85229	-1.96900
H	-2.38896	-3.37087	-0.30564
H	-3.71577	-3.15597	-1.46143
C	-3.78802	-2.05377	1.54586
H	-4.00118	-3.07436	1.21848
H	-2.77339	-2.02874	1.95832
H	-4.48871	-1.80041	2.34776
Irad_DMB_4.log			
66			
H	3.84641	2.10907	-0.36764
H	4.37579	-0.50515	-1.60678
H	4.10640	0.61852	0.52113
C	3.34124	1.25419	0.08417
H	3.93759	-1.34794	0.66425
H	2.88077	2.04816	2.04501
C	3.34523	-0.75497	-1.33828
H	3.13009	-0.20708	2.38212
H	3.70352	-2.68470	-0.45154

C	2.40139	1.34668	-2.17335
C	3.31949	-1.70858	-0.15455
N	2.60174	0.49054	-0.98091
C	2.36640	1.72948	1.13564
H	2.84224	-1.19483	-2.19797
H	1.79007	2.56766	0.74944
C	2.06259	-0.41676	2.36314
H	1.68168	-0.31890	3.38029
H	2.50486	-2.53383	2.27106
N	1.41059	0.62083	1.48321
N	1.90516	-1.86747	0.34263
C	1.79423	-1.82350	1.84025
H	0.42474	1.90373	2.87362
C	1.34597	-3.15146	-0.16232
C	0.16993	1.22128	2.05996
H	0.77986	-2.13355	2.07878
Fe	0.78863	-0.28414	-0.24501
H	-0.45544	0.41135	2.43717
C	-0.52813	1.93216	0.93297
N	-0.30356	1.39671	-0.28915
H	-1.46247	3.48207	2.06713
C	-1.31518	3.06115	1.08099
C	-0.85570	1.93322	-1.38559
H	-0.63852	1.43688	-2.32088
C	-1.89226	3.63035	-0.05228
C	-1.66227	3.05927	-1.30093
H	-2.51326	4.51331	0.03984
H	-2.09620	3.47238	-2.20190
H	0.29585	-3.21171	0.11263
H	1.91082	-3.97289	0.28800
H	1.45563	-3.17500	-1.24577
H	1.89350	2.26150	-1.86764
H	1.79561	0.81007	-2.90114
H	3.37553	1.59628	-2.60548
O	-0.63422	-1.10302	0.52859
O	0.43288	-0.84724	-1.89600
H	-1.49322	-0.83019	0.14716
C	-3.31537	-1.26592	-0.75371
H	-0.31032	-1.47079	-1.89069
C	-4.21242	-0.77681	0.35929
H	-5.18357	-0.53134	-0.10583
C	-3.67927	0.52590	0.98691
H	-4.42474	0.95409	1.66534
H	-2.77306	0.32125	1.56639
H	-3.43675	1.27210	0.22869
C	-3.21818	-0.42388	-1.98762
H	-3.37388	0.63817	-1.78770
H	-2.25072	-0.54501	-2.48922
H	-3.98596	-0.73989	-2.71599
C	-3.01444	-2.72098	-0.92771
H	-2.16193	-2.86674	-1.60059
H	-2.80655	-3.22483	0.01865
H	-3.87346	-3.24007	-1.38981
C	-4.46796	-1.81255	1.45926
H	-4.92573	-2.72311	1.06219
H	-3.52981	-2.08959	1.95295
H	-5.13817	-1.39372	2.21656
Icat_DMB_4.log			
66			
H	-3.85135	1.94966	1.11561
H	-4.33464	-0.88257	1.78259
H	-4.21011	0.71984	-0.07998
C	-3.39784	1.22859	0.43266
H	-4.19349	-1.20663	-0.66186
H	-3.11525	2.51892	-1.27644

C	-3.34923	-1.06544	1.34026
H	-3.51246	0.33686	-2.07086
H	-3.88801	-2.74648	0.11424
C	-2.30692	0.77628	2.56608
C	-3.48742	-1.73860	-0.02561
N	-2.60234	0.22438	1.22237
C	-2.51084	1.94679	-0.56400
H	-2.76289	-1.69731	2.00725
H	-1.85825	2.63776	-0.03352
C	-2.45562	0.14075	-2.24711
H	-2.23893	0.45326	-3.27189
H	-2.90981	-1.91795	-2.69688
N	-1.66212	0.95782	-1.28293
N	-2.16032	-1.79990	-0.70016
C	-2.16785	-1.35814	-2.11380
H	-0.82862	2.45046	-2.55448
C	-1.57920	-3.15003	-0.58153
C	-0.50495	1.62847	-1.90585
H	-1.17202	-1.57308	-2.50040
Fe	-0.81801	-0.35419	0.28263
H	0.01835	0.89029	-2.51758
C	0.42650	2.15090	-0.83142
N	0.35532	1.53108	0.35959
H	1.32167	3.69629	-2.02032
C	1.29713	3.21308	-1.05115
C	1.13241	1.94368	1.36875
H	1.02938	1.40175	2.30090
C	2.11233	3.63853	-0.00571
C	2.02670	2.99821	1.22977
H	2.80038	4.46330	-0.15064
H	2.63774	3.30478	2.06926
H	-0.56300	-3.13160	-0.97425
H	-2.18481	-3.88007	-1.13469
H	-1.55208	-3.43158	0.47273
H	-1.77183	1.71934	2.44354
H	-1.68332	0.06762	3.10752
H	-3.24309	0.95263	3.10752
O	0.53256	-1.00999	-0.78892
O	-0.28690	-1.24268	1.84299
H	1.25349	-0.37323	-0.85207
C	3.55337	-1.44508	0.66313
H	0.22099	-2.02372	1.59097
C	4.58255	-0.75636	-0.12072
H	5.19956	-0.17649	0.57280
C	3.76859	0.29839	-0.95741
H	4.50746	0.92771	-1.45766
H	3.17052	-0.21390	-1.71446
H	3.13807	0.92556	-0.32743
C	3.03790	-0.82394	1.87382
H	3.45851	0.16043	2.07229
H	1.93652	-0.81919	1.86093
H	3.29147	-1.52149	2.69192
C	3.03391	-2.73667	0.23086
H	2.17485	-3.07486	0.80580
H	2.82174	-2.70800	-0.84418
H	3.87108	-3.44840	0.33223
C	5.43273	-1.62551	-1.04313
H	5.95298	-2.40442	-0.47911
H	4.81827	-2.09906	-1.81326
H	6.17457	-0.99312	-1.53660
TSreb_CH2_DMB_4.log			
66			
H	-3.66198	-0.40984	2.24522
H	-2.00278	-2.80134	2.47947
H	-3.57633	-1.65670	1.01400

C	-3.15112	-0.70763	1.32862
H	-2.53205	-3.11517	0.10013
H	-4.34795	0.34238	-0.13654
C	-1.34343	-2.33434	1.74206
H	-3.56616	-1.61172	-1.14999
H	-1.06057	-4.01429	0.42668
C	-1.32436	-0.14704	2.84626
C	-1.48880	-3.01224	0.38903
N	-1.68240	-0.88522	1.61042
C	-3.33139	0.34649	0.26401
H	-0.31233	-2.38938	2.08783
H	-3.12287	1.33007	0.68046
C	-2.76897	-1.09514	-1.68213
H	-3.16859	-0.75214	-2.63768
H	-1.94667	-3.01061	-2.25510
N	-2.36203	0.09208	-0.85118
N	-0.77448	-2.21093	-0.66970
C	-1.58840	-2.03302	-1.92137
H	-3.13015	1.78238	-1.90152
C	0.52461	-2.86013	-0.99853
C	-2.16548	1.35305	-1.61990
H	-0.91615	-1.61798	-2.66787
Fe	-0.50065	-0.30544	-0.02271
H	-1.59616	1.11811	-2.52022
C	-1.38066	2.29589	-0.74034
N	-0.58739	1.69455	0.17698
H	-2.10578	4.13513	-1.55178
C	-1.44890	3.67738	-0.82321
C	0.16272	2.42074	1.01832
H	0.77498	1.86177	1.71290
C	-0.66928	4.44258	0.04194
C	0.14493	3.80781	0.97706
H	-0.70296	5.52433	-0.00924
H	0.76092	4.37043	1.66623
H	1.06944	-2.22917	-1.69608
H	0.31855	-3.83859	-1.44264
H	1.09428	-2.97845	-0.07787
H	-1.59920	0.90004	2.71947
H	-0.25368	-0.23533	3.01861
H	-1.87810	-0.57248	3.68889
O	0.40199	-0.00707	-1.57814
O	0.91758	-0.57798	1.00577
H	0.82700	0.86382	-1.59664
C	3.97171	-0.51088	0.53623
H	1.77180	-0.50929	0.53271
C	4.22707	0.31175	-0.70141
H	5.32457	0.44180	-0.75897
C	3.61955	1.72298	-0.62515
H	3.83307	2.26936	-1.54883
H	2.53205	1.67310	-0.50264
H	4.02344	2.29778	0.21199
C	4.12696	0.13319	1.87557
H	3.55599	1.06324	1.96338
H	3.81860	-0.54448	2.67592
H	5.18391	0.40260	2.05401
C	4.04126	-2.00247	0.45526
H	3.74185	-2.46407	1.40016
H	3.41456	-2.40207	-0.34855
H	5.07002	-2.33841	0.23167
C	3.78443	-0.38353	-1.99921
H	4.29014	-1.34203	-2.14039
H	2.70447	-0.56078	-1.98506
H	4.02040	0.25386	-2.85720

Prod_CH2_DMB_4.log
66

H	4.01033	2.23442	0.46388
H	4.93898	0.00484	-1.26536
H	4.25321	0.58508	1.01257
C	3.51263	1.27473	0.61540
H	4.19617	-1.37391	0.67217
H	2.75078	1.56533	2.61632
C	3.90087	-0.33835	-1.21473
H	3.07563	-0.76317	2.40338
H	4.27731	-2.40731	-0.74420
C	2.92063	1.85273	-1.70016
C	3.76176	-1.55007	-0.30891
N	3.01986	0.75728	-0.70654
C	2.36379	1.43860	1.60075
H	3.55486	-0.58512	-2.22090
H	1.78904	2.32604	1.34031
C	2.02773	-0.95766	2.17816
H	1.51963	-1.16465	3.12315
H	2.50554	-3.00241	1.64254
N	1.45922	0.25967	1.53479
N	2.29982	-1.86807	-0.14835
C	1.89560	-2.17766	1.26115
H	0.06711	1.07637	2.93903
C	1.94819	-3.00608	-1.03759
C	0.08517	0.61518	1.94650
H	0.85405	-2.49608	1.20889
Fe	1.16484	-0.20344	-0.58382
H	-0.51270	-0.29918	1.97542
C	-0.49045	1.56212	0.91634
N	-0.00345	1.43988	-0.33803
H	-1.80693	2.60716	2.23546
C	-1.44587	2.52024	1.21910
C	-0.44621	2.23885	-1.32119
H	-0.01066	2.08337	-2.29985
C	-1.92153	3.34517	0.20389
C	-1.41257	3.20706	-1.08694
H	-2.67621	4.09223	0.41798
H	-1.75150	3.83512	-1.90026
H	0.87880	-3.19045	-0.97394
H	2.51334	-3.88932	-0.72319
H	2.21735	-2.74183	-2.06172
H	2.33395	2.66524	-1.27278
H	2.42671	1.47405	-2.59711
H	3.92210	2.21711	-1.95325
O	-0.30390	-1.21852	-0.80181
O	-2.75404	0.04043	-0.77516
H	-1.16448	-0.74875	-0.80197
C	-4.02037	-0.34410	-0.17165
H	-2.81818	0.96588	-1.04279
C	-3.88573	-1.82574	0.25402
H	-4.87320	-2.10007	0.64275
C	-2.85516	-2.04214	1.37256
H	-2.82443	-3.10376	1.63911
H	-1.85706	-1.75272	1.03472
H	-3.09980	-1.47714	2.27504
C	-4.29485	0.56819	1.02635
H	-3.46327	0.55969	1.73181
H	-4.44159	1.59682	0.68183
H	-5.20312	0.24393	1.54393
C	-5.12739	-0.15408	-1.21247
H	-5.20653	0.90717	-1.47229
H	-4.91631	-0.71788	-2.12298
H	-6.09038	-0.48090	-0.80814
C	-3.55427	-2.75406	-0.92378
H	-4.30318	-2.70150	-1.71761
H	-2.57884	-2.49834	-1.34779
H	-3.50895	-3.79011	-0.57302

TSreb_CH3_DMB_4.log

66

H	4.03866	1.93081	0.04333
H	4.52477	-0.65436	-1.33530
H	4.10919	0.37109	0.84251
C	3.43588	1.08245	0.37191
H	3.79961	-1.62133	0.80357
H	2.81037	1.79731	2.32087
C	3.45449	-0.83000	-1.18758
H	2.93579	-0.52666	2.48182
H	3.57893	-2.84332	-0.43807
C	2.75182	1.38414	-1.95578
C	3.23742	-1.86621	-0.09480
N	2.77536	0.44339	-0.81403
C	2.37914	1.55249	1.34723
H	3.01061	-1.16649	-2.12348
H	1.88315	2.43670	0.95183
C	1.85987	-0.65288	2.37895
H	1.41791	-0.59524	3.37463
H	2.14203	-2.78953	2.17990
N	1.34190	0.48071	1.53228
N	1.77490	-1.95481	0.25773
C	1.53088	-1.99665	1.73968
H	0.31150	1.71357	2.93496
C	1.18009	-3.15706	-0.38297
C	0.08892	1.10123	2.05794
H	0.47763	-2.23289	1.86895
Fe	0.81794	-0.25258	-0.31219
H	-0.59287	0.29675	2.33515
C	-0.50394	1.91964	0.94222
N	-0.18145	1.49402	-0.30037
H	-1.54061	3.36032	2.13270
C	-1.30601	3.03337	1.12796
C	-0.63420	2.13775	-1.38454
H	-0.33890	1.72608	-2.33993
C	-1.78826	3.70685	0.00763
C	-1.44483	3.25768	-1.26507
H	-2.42125	4.57783	0.12838
H	-1.79835	3.75844	-2.15680
H	0.10625	-3.15357	-0.21123
H	1.63817	-4.04821	0.05705
H	1.39207	-3.11985	-1.45077
H	2.26429	2.30726	-1.64135
H	2.19719	0.93308	-2.77665
H	3.77815	1.60231	-2.27042
O	-0.75245	-1.03773	0.25771
O	0.58981	-0.65608	-2.03533
H	-1.54728	-0.56579	-0.04423
C	-3.43712	-1.07647	-0.82386
H	-0.20818	-1.19793	-2.13785
C	-4.29196	-0.79612	0.38214
H	-5.25154	-0.41639	-0.01099
C	-3.70397	0.33309	1.25519
H	-4.42043	0.61221	2.03429
H	-2.78461	-0.01020	1.73954
H	-3.47148	1.22299	0.66737
C	-3.29907	-0.00528	-1.85438
H	-3.42427	0.99858	-1.44471
H	-2.33334	-0.06385	-2.36958
H	-4.07073	-0.14731	-2.63147
C	-3.10460	-2.46095	-1.26248
H	-2.21393	-2.46054	-1.90000
H	-2.94642	-3.14361	-0.42641
H	-3.93051	-2.87141	-1.87087
C	-4.58558	-2.02521	1.24659

H	-5.06199	-2.82217	0.66865
H	-3.66057	-2.42208	1.67888
H	-5.25304	-1.74938	2.06853

Prod_CH3_DMB_4.log
66

H	4.61029	1.00265	0.13821
H	4.38207	-1.69505	-1.24272
H	4.14992	-0.48919	0.93862
C	3.75827	0.37378	0.40531
H	3.25131	-2.38181	0.80671
H	3.24499	1.37129	2.26647
C	3.30623	-1.50395	-1.17095
H	2.75002	-1.06872	2.37679
H	2.72573	-3.45323	-0.47730
C	3.35331	0.81330	-1.97194
C	2.68669	-2.42297	-0.12163
N	3.05103	-0.08177	-0.83380
C	2.80240	1.16564	1.28814
H	2.85217	-1.68617	-2.14685
H	2.54813	2.10988	0.80410
C	1.68995	-0.84686	2.28509
H	1.30170	-0.68758	3.29239
H	1.17819	-2.94287	2.08816
N	1.52157	0.40783	1.47193
N	1.25287	-2.05143	0.14898
C	0.93659	-1.98637	1.61462
H	0.85243	1.86349	2.88343
C	0.33950	-3.02661	-0.50136
C	0.45527	1.28690	2.04455
H	-0.13828	-1.81447	1.68817
Fe	0.93100	-0.07577	-0.42000
H	-0.34303	0.63840	2.41365
C	-0.11186	2.17577	0.97424
N	-0.03614	1.68488	-0.28234
H	-0.77779	3.76462	2.24457
C	-0.72703	3.39253	1.22935
C	-0.53918	2.37532	-1.31878
H	-0.43850	1.90941	-2.29006
C	-1.26022	4.11056	0.16150
C	-1.16002	3.59971	-1.13156
H	-1.74568	5.06338	0.33693
H	-1.56072	4.13387	-1.98298
H	-0.68477	-2.66376	-0.42498
H	0.44678	-3.99943	-0.00969
H	0.61995	-3.13359	-1.55054
H	3.09945	1.83640	-1.68795
H	2.74591	0.51530	-2.82633
H	4.41838	0.75545	-2.22378
O	0.35241	-0.35951	-2.11769
C	-3.50638	-0.59716	-0.59947
H	0.50248	-1.25440	-2.45010
C	-3.85211	-1.08272	0.83197
H	-4.89035	-0.77950	1.01055
C	-2.95832	-0.42581	1.89339
H	-3.14436	-0.87341	2.87500
H	-1.90787	-0.58468	1.63672
H	-3.13368	0.64966	1.97356
C	-3.53502	0.93026	-0.69335
H	-2.80575	1.38685	-0.02393
H	-3.30652	1.23988	-1.71832
H	-4.53052	1.30506	-0.43504
C	-4.47081	-1.17958	-1.63835
H	-4.22491	-0.78330	-2.62919
H	-4.39503	-2.26831	-1.67551
H	-5.50469	-0.90593	-1.40233

C	-3.76180	-2.60936	0.96931
H	-4.43290	-3.12801	0.27996
H	-2.73935	-2.94863	0.77452
H	-4.03071	-2.90623	1.98830
O	-2.17710	-1.08330	-0.87804
H	-1.75109	-0.55567	-1.56722

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H	0.68589	-2.70354	2.39489
H	2.98272	-0.79472	2.48581
H	1.92518	-2.56185	1.17438
C	0.93946	-2.19873	1.46066
H	3.28071	-1.41689	0.13028
H	-0.00130	-3.56615	0.06279
C	2.41663	-0.23256	1.73548
H	1.85625	-2.67840	-1.06199
H	4.03539	0.14293	0.36519
C	0.28458	-0.34132	2.93297
C	3.07476	-0.37465	0.36960
N	0.99937	-0.71199	1.67711
C	-0.09207	-2.52842	0.39810
H	2.38887	0.81128	2.04465
H	-1.09763	-2.39757	0.79497
C	1.26843	-1.94418	-1.61103
H	0.95673	-2.42490	-2.54056
H	3.09897	-0.98078	-2.25922
N	0.05879	-1.60056	-0.77622
N	2.19841	0.20307	-0.71973
C	2.09580	-0.69931	-1.92431
H	-1.55313	-2.58812	-1.77845
C	2.72334	1.54159	-1.14194
C	-1.22101	-1.57017	-1.55545
H	1.62917	-0.11360	-2.71503
Fe	0.27510	0.32439	-0.04923
H	-1.03820	-1.04947	-2.49700
C	-2.24389	-0.81046	-0.74648
N	-1.72781	0.09514	0.11914
H	-4.01254	-1.71850	-1.55028
C	-3.61456	-0.98257	-0.86237
C	-2.53820	0.86471	0.86731
H	-2.05788	1.58018	1.52123
C	-4.46328	-0.19134	-0.08903
C	-3.91780	0.74126	0.78917
H	-5.53770	-0.30412	-0.17218
H	-4.54575	1.37213	1.40493
H	2.03856	1.99785	-1.85493
H	3.70376	1.41191	-1.60759
H	2.81631	2.18162	-0.26704
H	-0.73621	-0.72080	2.89667
H	0.26672	0.74135	3.03017
H	0.79429	-0.77789	3.79643
O	-0.13982	1.06564	-1.55957
O	0.43030	1.78707	0.90424
H	0.25400	2.60912	0.41126
C	-0.05642	4.91099	-0.35102
H	-0.26160	4.01993	-0.95418
H	0.86113	5.38219	-0.70278
H	0.04364	4.67865	0.71303
H	-0.88863	5.60349	-0.47488

A_meta_g_4.log

51

H	0.53241	-2.80808	2.27127
H	2.87528	-0.96167	2.54309

H	1.82772	-2.64621	1.11489
C	0.84054	-2.26716	1.37416
H	3.22322	-1.51798	0.17086
H	-0.05618	-3.54557	-0.13179
C	2.35290	-0.35979	1.79157
H	1.80435	-2.66842	-1.17864
H	4.03485	-0.00290	0.49353
C	0.18493	-0.46336	2.91099
C	3.05389	-0.47837	0.44701
N	0.92877	-0.79555	1.66220
C	-0.15295	-2.52677	0.25557
H	2.34388	0.67432	2.13412
H	-1.17092	-2.41241	0.62349
C	1.26341	-1.87430	-1.69156
H	0.95963	-2.27763	-2.65970
H	3.15440	-0.94825	-2.21072
N	0.04220	-1.54197	-0.86609
N	2.23859	0.18049	-0.64236
C	2.14954	-0.64712	-1.89841
H	-1.56610	-2.43617	-1.96222
C	2.82506	1.51984	-0.97034
C	-1.22549	-1.44162	-1.66015
H	1.73681	0.00175	-2.66895
Fe	0.27377	0.35196	-0.06359
H	-1.02511	-0.85333	-2.55806
C	-2.24657	-0.73320	-0.80400
N	-1.72369	0.10046	0.12682
H	-4.02388	-1.56109	-1.67137
C	-3.61842	-0.88157	-0.93174
C	-2.52358	0.82303	0.92910
H	-2.03570	1.48981	1.62743
C	-4.45932	-0.14063	-0.10084
C	-3.90503	0.71879	0.84307
H	-5.53481	-0.23581	-0.19182
H	-4.52627	1.31080	1.50268
H	2.18960	2.03295	-1.68870
H	3.82086	1.37516	-1.39769
H	2.90155	2.11020	-0.05962
H	-0.84176	-0.81878	2.83002
H	0.18728	0.61457	3.05479
H	0.65841	-0.94646	3.77056
O	-0.02569	1.13800	-1.46768
O	0.43400	1.76881	0.97573
H	0.29363	2.61436	0.51316
C	0.02361	4.88805	-0.35973
H	-0.19378	3.97928	-0.93121
H	0.94018	5.34117	-0.73693
H	0.13502	4.68994	0.71026
H	-0.80540	5.58212	-0.49575

A_meta_g_6.log

51

H	0.49073	-1.75424	3.04576
H	3.18374	-0.18905	2.38694
H	1.67338	-2.26738	1.88196
C	0.79862	-1.63020	2.00618
H	3.18815	-1.91926	0.59312
H	-0.44228	-3.17256	1.11758
C	2.61325	0.00993	1.47066
H	1.49402	-2.92550	-0.17101
H	4.35346	-0.61685	0.43930
C	0.80379	0.64102	2.93452
C	3.28810	-0.85560	0.38151
N	1.15922	-0.19922	1.74534
C	-0.34845	-2.08104	1.10031
H	2.74751	1.06409	1.22564

H	-1.28984	-1.67015	1.46370
C	0.99441	-2.34153	-0.94219
H	0.58363	-3.08007	-1.63557
H	2.68968	-2.27631	-2.22123
N	-0.15123	-1.59471	-0.30640
N	2.88018	-0.61811	-1.00437
C	2.01793	-1.54318	-1.74567
H	-1.68881	-2.86405	-1.08601
C	3.65068	0.34221	-1.78024
C	-1.39405	-1.80967	-1.11636
H	1.55260	-0.96770	-2.54424
Fe	-0.07510	0.57637	0.01167
H	-1.15598	-1.56186	-2.15535
C	-2.51944	-0.92297	-0.64469
N	-2.13728	0.22765	-0.05191
H	-4.14440	-2.16092	-1.31052
C	-3.85764	-1.22884	-0.83925
C	-3.06602	1.11584	0.35470
H	-2.68551	2.01931	0.81358
C	-4.82246	-0.31201	-0.42179
C	-4.42103	0.87602	0.18374
H	-5.87463	-0.52691	-0.56599
H	-5.14287	1.60845	0.52085
H	3.07766	0.67632	-2.64099
H	4.57502	-0.15086	-2.11648
H	3.91883	1.19291	-1.15470
H	-0.26225	0.54515	3.13903
H	1.01356	1.68543	2.71975
H	1.36918	0.31471	3.81298
O	0.98266	0.94037	-1.18691
O	-0.30945	2.20599	0.65115
H	0.10244	2.93600	0.16059
C	0.85353	4.96035	-1.00456
H	1.07550	3.94818	-1.35762
H	1.67670	5.61415	-1.29250
H	0.75070	4.99666	0.08328
H	-0.06658	5.31449	-1.46891

TSabs_meta_g_2.log

51

H	-1.13021	-3.46625	0.01509
H	-3.24657	-1.94753	-1.44042
H	-2.29240	-2.39381	0.75236
C	-1.29252	-2.43161	0.32381
H	-3.47171	-0.72352	0.67817
H	-0.42281	-2.51596	2.30975
C	-2.59840	-1.07947	-1.27996
H	-2.10485	-0.90790	2.44863
H	-4.11337	0.28614	-0.59389
C	-0.55662	-2.20586	-2.01223
C	-3.19581	-0.16812	-0.21691
N	-1.22760	-1.52142	-0.87079
C	-0.24664	-2.02864	1.34595
H	-2.49573	-0.55267	-2.22739
H	0.74416	-2.32437	1.00463
C	-1.42756	-0.06297	2.33261
H	-1.10614	0.22176	3.33652
H	-3.12838	1.25668	2.08144
N	-0.24004	-0.53546	1.52639
N	-2.22465	0.92176	0.16977
C	-2.12808	1.11694	1.65931
H	1.33316	-0.70589	2.96907
C	-2.62380	2.20920	-0.47675
C	1.08621	-0.11532	2.08211
H	-1.56356	2.03499	1.81150
Fe	-0.31647	0.35185	-0.33449

H	1.01946	0.93625	2.36404
C	2.11566	-0.28757	0.99032
N	1.63098	-0.17762	-0.26970
H	3.83201	-0.63652	2.22891
C	3.46085	-0.53874	1.21599
C	2.44948	-0.30036	-1.32805
H	1.99310	-0.19067	-2.30308
C	4.31885	-0.66474	0.12336
C	3.80572	-0.54812	-1.16541
H	5.37350	-0.85837	0.27926
H	4.44006	-0.64518	-2.03704
H	-1.86386	2.96032	-0.27903
H	-3.58356	2.53622	-0.06762
H	-2.72206	2.05445	-1.54954
H	0.42745	-2.55545	-1.70181
H	-0.45187	-1.50675	-2.83845
H	-1.15174	-3.06506	-2.33473
O	0.17028	1.92639	0.30965
O	-0.39574	0.72896	-2.05951
H	-0.16404	1.64525	-2.26879
C	2.16028	3.26901	-0.55484
H	1.23964	2.55402	-0.14737
H	1.85925	4.26272	-0.22913
H	2.19269	3.16159	-1.63714
H	3.05368	2.90200	-0.05384

TSabs_meta_g_4.log

51

H	-1.09456	-3.44363	0.33836
H	-3.24105	-2.08796	-1.24360
H	-2.27212	-2.32568	0.97393
C	-1.27213	-2.38716	0.54895
H	-3.44791	-0.68698	0.77038
H	-0.41056	-2.26949	2.53657
C	-2.60063	-1.20310	-1.16258
H	-2.07752	-0.66357	2.55084
H	-4.12726	0.19701	-0.57495
C	-0.55662	-2.37472	-1.80511
C	-3.19714	-0.21089	-0.17622
N	-1.22251	-1.59196	-0.72619
C	-0.23175	-1.87825	1.53053
H	-2.51031	-0.75811	-2.15260
H	0.76099	-2.20358	1.22453
C	-1.40995	0.17008	2.33577
H	-1.07661	0.56007	3.29957
H	-3.13134	1.43249	1.96735
N	-0.22914	-0.37370	1.56515
N	-2.23382	0.92003	0.09374
C	-2.13094	1.26712	1.55491
H	1.35390	-0.38759	3.00880
C	-2.65907	2.13303	-0.67376
C	1.10000	0.10279	2.06463
H	-1.57933	2.20313	1.60898
Fe	-0.32362	0.32940	-0.37478
H	1.03415	1.17918	2.23312
C	2.11843	-0.18904	0.98847
N	1.61556	-0.21594	-0.26884
H	3.85054	-0.40732	2.23507
C	3.46595	-0.41813	1.22251
C	2.41978	-0.45201	-1.31957
H	1.95093	-0.44300	-2.29472
C	4.30835	-0.66471	0.13799
C	3.77763	-0.68473	-1.14888
H	5.36465	-0.84449	0.29932
H	4.40012	-0.87560	-2.01357
H	-1.91182	2.91302	-0.55688

H	-3.62195	2.48029	-0.28947
H	-2.76344	1.87263	-1.72536
H	0.42756	-2.69858	-1.46818
H	-0.45350	-1.74980	-2.68925
H	-1.15282	-3.25828	-2.05108
O	0.14432	1.97092	0.04010
O	-0.40763	0.55538	-2.12663
H	-0.22939	1.46531	-2.40344
C	2.25879	3.18268	-0.65163
H	1.22004	2.49194	-0.31717
H	1.95081	4.19266	-0.39133
H	2.38162	3.01806	-1.71971
H	3.07202	2.79628	-0.04204

TSabs_meta_g_6.log

51			
H	-1.16490	-3.41701	-0.51063
H	-3.37243	-1.70321	-1.62176
H	-2.27465	-2.48690	0.46637
C	-1.30644	-2.44838	-0.02773
H	-3.51883	-0.90649	0.71184
H	-0.29310	-2.84810	1.84285
C	-2.73497	-0.86577	-1.31770
H	-2.00692	-1.33258	2.31511
H	-4.26809	0.26627	-0.33826
C	-0.74214	-1.85824	-2.35442
C	-3.30798	-0.18599	-0.07824
N	-1.33894	-1.36335	-1.07732
C	-0.18995	-2.19743	0.96832
H	-2.67909	-0.16557	-2.15150
H	0.77569	-2.40980	0.51304
C	-1.35781	-0.45808	2.30960
H	-0.99497	-0.33934	3.33270
H	-3.09142	0.80614	2.46126
N	-0.19234	-0.75699	1.39826
N	-2.37891	0.86479	0.44488
C	-2.14362	0.79497	1.90999
H	1.34432	-1.08556	2.84025
C	-2.84280	2.22004	0.04088
C	1.11997	-0.40042	2.01641
H	-1.59197	1.69418	2.18205
Fe	-0.29452	0.38487	-0.40919
H	1.03148	0.60941	2.42406
C	2.21059	-0.43001	0.96954
N	1.79979	-0.19576	-0.29307
H	3.85579	-0.85488	2.28658
C	3.54691	-0.65881	1.26693
C	2.69580	-0.17068	-1.29665
H	2.30457	0.03007	-2.28661
C	4.47903	-0.63305	0.22982
C	4.04754	-0.38866	-1.07238
H	5.52823	-0.80758	0.43678
H	4.74272	-0.36784	-1.90174
H	-2.11248	2.96483	0.34737
H	-3.80852	2.43948	0.50761
H	-2.95734	2.25544	-1.04220
H	0.26084	-2.23926	-2.16241
H	-0.69281	-1.04287	-3.07192
H	-1.35995	-2.66688	-2.75527
O	0.04883	1.92690	0.44818
O	-0.34452	1.00553	-2.08109
H	-0.23823	1.95722	-2.21762
C	2.07361	3.45701	-0.37000
H	1.21407	2.73545	-0.03097
H	1.69254	4.45495	-0.15702
H	2.24538	3.29199	-1.43271

H	2.93935	3.20272	0.23950
Irad_meta_g_2.log			
51			
H	0.51499	-2.65376	2.41484
H	2.87611	-0.83913	2.55993
H	1.80526	-2.57088	1.24384
C	0.82195	-2.17137	1.48493
H	3.20748	-1.50201	0.21325
H	-0.08923	-3.52318	0.05509
C	2.36068	-0.26232	1.78477
H	1.79207	-2.69344	-1.03487
H	4.03595	0.01529	0.46152
C	0.19548	-0.27761	2.92259
C	3.04865	-0.44869	0.44042
N	0.92623	-0.68400	1.68846
C	-0.17657	-2.48388	0.38637
H	2.36626	0.78577	2.08019
H	-1.19270	-2.34161	0.75088
C	1.24222	-1.93515	-1.59124
H	0.93447	-2.39944	-2.53044
H	3.11409	-1.03017	-2.20179
N	0.02669	-1.55765	-0.77951
N	2.22952	0.16967	-0.66671
C	2.11651	-0.71635	-1.87867
H	-1.59293	-2.49205	-1.82229
C	2.83223	1.47825	-1.06899
C	-1.23653	-1.48711	-1.57776
H	1.67671	-0.10483	-2.66296
Fe	0.28843	0.36445	-0.05083
H	-1.02219	-0.95761	-2.50754
C	-2.25149	-0.71747	-0.76588
N	-1.72014	0.17652	0.10413
H	-4.03205	-1.60382	-1.56949
C	-3.62459	-0.87748	-0.87687
C	-2.52351	0.93488	0.87184
H	-2.03200	1.63511	1.53441
C	-4.46345	-0.09220	-0.08632
C	-3.90531	0.82291	0.80208
H	-5.53906	-0.19918	-0.16154
H	-4.52535	1.44613	1.43349
H	2.18016	1.96548	-1.78793
H	3.81327	1.29734	-1.51646
H	2.94614	2.10450	-0.18634
H	-0.83686	-0.62128	2.86514
H	0.21545	0.80592	3.00994
H	0.66859	-0.72487	3.80133
O	0.00316	1.16574	-1.64870
O	0.46191	1.82290	0.89091
H	0.37508	2.66539	0.37629
C	0.12933	4.54670	-0.34686
H	-0.87280	1.56266	-1.74066
H	0.45367	4.42895	-1.37269
H	-0.92861	4.65156	-0.14096
H	0.83840	4.89803	0.39293
Irad_meta_g_4.log			
51			
H	0.43258	-2.42690	2.65367
H	2.84306	-0.67507	2.61726
H	1.71659	-2.49937	1.47470
C	0.74716	-2.04928	1.67889
H	3.14721	-1.58870	0.35233
H	-0.21580	-3.51115	0.39943
C	2.34414	-0.16639	1.78561
H	1.69064	-2.86102	-0.77288

H	4.02523	-0.08114	0.44303
C	0.18092	-0.00021	2.91709
C	3.02358	-0.51300	0.46878
N	0.89679	-0.55259	1.73231
C	-0.26634	-2.44061	0.62051
H	2.38141	0.90600	1.97035
H	-1.27552	-2.22604	0.96885
C	1.16532	-2.14543	-1.40437
H	0.84007	-2.69114	-2.29243
H	3.06699	-1.37075	-2.09582
N	-0.03732	-1.64937	-0.63640
N	2.22350	0.01172	-0.69862
C	2.08026	-0.99161	-1.81200
H	-1.69095	-2.63443	-1.57319
C	2.86466	1.25324	-1.23543
C	-1.30133	-1.62147	-1.43636
H	1.66336	-0.45075	-2.65804
Fe	0.29007	0.33082	-0.11220
H	-1.07443	-1.19892	-2.41638
C	-2.28649	-0.73739	-0.70821
N	-1.72259	0.22322	0.06499
H	-4.09878	-1.63972	-1.41666
C	-3.66452	-0.86017	-0.80262
C	-2.49668	1.08480	0.74944
H	-1.97921	1.83252	1.33579
C	-4.47358	0.03175	-0.09876
C	-3.88165	1.01426	0.69021
H	-5.55245	-0.04472	-0.16369
H	-4.47763	1.72145	1.25255
H	2.22369	1.68420	-1.99912
H	3.83680	0.99584	-1.66458
H	3.00433	1.96314	-0.42277
H	-0.86065	-0.31901	2.89594
H	0.23218	1.08559	2.89215
H	0.64427	-0.36765	3.83708
O	0.02221	0.95102	-1.78844
O	0.51155	1.87961	0.68434
H	0.49086	2.67953	0.11654
C	0.47185	4.81539	-0.41376
H	-0.81515	1.41811	-1.90927
H	0.80003	4.71560	-1.44089
H	-0.57561	5.00331	-0.21458
H	1.19842	5.06060	0.35050

TSreb_CH2_meta_g_2.log

51

H	0.38431	-1.59109	3.17746
H	2.87053	-0.04918	2.59739
H	1.63292	-2.06958	2.05727
C	0.69075	-1.53012	2.13145
H	3.07505	-1.59339	0.69182
H	-0.37635	-3.24713	1.34464
C	2.37041	0.21966	1.66094
H	1.53100	-3.06135	0.00994
H	4.01615	-0.16782	0.32801
C	0.25023	0.81433	2.72478
C	2.99845	-0.52533	0.49226
N	0.90801	-0.09322	1.74270
C	-0.36827	-2.15745	1.24554
H	2.45879	1.29606	1.52414
H	-1.35502	-1.79414	1.52843
C	1.02100	-2.53455	-0.79564
H	0.64767	-3.29871	-1.48042
H	2.93322	-2.09043	-1.71235
N	-0.13717	-1.77723	-0.18963
N	2.18923	-0.32177	-0.76558

C	1.97248	-1.59645	-1.53613
H	-1.85289	-2.91478	-0.77700
C	2.86720	0.67871	-1.64824
C	-1.41877	-1.92532	-0.94798
H	1.55462	-1.30526	-2.49682
Fe	0.28572	0.24649	-0.27161
H	-1.19873	-1.81976	-2.01143
C	-2.34843	-0.82193	-0.50114
N	-1.72511	0.29548	-0.05291
H	-4.21418	-1.80630	-0.89007
C	-3.73236	-0.90186	-0.53913
C	-2.44512	1.35638	0.35438
H	-1.88220	2.21847	0.68676
C	-4.48530	0.19537	-0.12113
C	-3.83282	1.33762	0.33469
H	-5.56771	0.15460	-0.14779
H	-4.38428	2.20689	0.66898
H	2.22157	0.90792	-2.49134
H	3.81216	0.25922	-2.00398
H	3.06590	1.58230	-1.07520
H	-0.80553	0.55842	2.80800
H	0.35100	1.84186	2.38435
H	0.71913	0.70553	3.70692
O	0.00572	0.37487	-2.05297
O	0.59797	1.94339	0.03787
H	0.61422	2.57750	-0.70579
C	0.93189	4.89805	-0.50716
H	-0.82626	0.80223	-2.29583
H	1.77083	4.98196	-1.18598
H	-0.04382	5.23062	-0.83700
H	1.11682	4.76498	0.55254

TSreb_CH2_meta_g_4.log

51

H	0.38331	-1.47598	3.22178
H	2.88061	0.01581	2.57945
H	1.61979	-2.00755	2.11180
C	0.68298	-1.45735	2.17218
H	3.06446	-1.60113	0.73269
H	-0.40444	-3.19581	1.47023
C	2.38120	0.25502	1.63452
H	1.50765	-3.07533	0.11599
H	4.02101	-0.20065	0.31617
C	0.27157	0.91186	2.68453
C	2.99934	-0.54060	0.49329
N	0.91500	-0.03660	1.73189
C	-0.38683	-2.11201	1.31791
H	2.48205	1.32449	1.45701
H	-1.36861	-1.72696	1.58933
C	0.99487	-2.57976	-0.70761
H	0.62163	-3.37085	-1.36169
H	2.89972	-2.18629	-1.66178
N	-0.15832	-1.79957	-0.13058
N	2.19138	-0.37562	-0.77003
C	1.94708	-1.67513	-1.48944
H	-1.88780	-2.93158	-0.68758
C	2.88038	0.57675	-1.69444
C	-1.43777	-1.95366	-0.88423
H	1.51923	-1.41216	-2.45405
Fe	0.28998	0.24934	-0.28923
H	-1.21520	-1.88227	-1.95034
C	-2.35902	-0.82710	-0.47512
N	-1.73251	0.30327	-0.06648
H	-4.22820	-1.81910	-0.82661
C	-3.74367	-0.90411	-0.50822
C	-2.44984	1.37867	0.30562

H	-1.88351	2.25001	0.60670
C	-4.49356	0.20798	-0.12632
C	-3.83762	1.36337	0.28961
H	-5.57611	0.16860	-0.14934
H	-4.38644	2.24456	0.59587
H	2.23400	0.78156	-2.54339
H	3.81729	0.12945	-2.03787
H	3.09651	1.49899	-1.15859
H	-0.78724	0.67263	2.77752
H	0.38465	1.92639	2.31050
H	0.74076	0.82919	3.66915
O	0.00988	0.33387	-2.07729
O	0.61320	1.98727	-0.03675
H	0.64026	2.51044	-0.85359
C	0.98842	4.88995	-0.50305
H	-0.83201	0.73327	-2.33245
H	1.85697	4.84218	-1.14697
H	0.01862	5.10264	-0.93363
H	1.12304	4.95974	0.56691

Prod_CH2_meta_g_2.log

51

H	0.47071	-1.06264	3.33964
H	2.90360	0.39276	2.52227
H	1.68700	-1.69225	2.25674
C	0.74359	-1.15122	2.28606
H	3.11615	-1.39893	0.84521
H	-0.32936	-2.96473	1.77147
C	2.39995	0.52179	1.55810
H	1.53831	-2.95848	0.39832
H	4.04383	-0.03536	0.27884
C	0.26108	1.23727	2.52868
C	3.02823	-0.37079	0.49635
N	0.93869	0.21420	1.68121
C	-0.33462	-1.89868	1.52550
H	2.49432	1.57161	1.27959
H	-1.31821	-1.50701	1.78073
C	1.02022	-2.54466	-0.46630
H	0.64425	-3.39391	-1.04004
H	2.92181	-2.24129	-1.45005
N	-0.13950	-1.71585	0.04425
N	2.19599	-0.34372	-0.75691
C	1.96904	-1.71465	-1.33321
H	-1.85569	-2.94511	-0.30856
C	2.86444	0.49584	-1.79441
C	-1.43616	-1.99302	-0.64688
H	1.53912	-1.55710	-2.31980
Fe	0.25833	0.20838	-0.30354
H	-1.24211	-2.07304	-1.71788
C	-2.36946	-0.83857	-0.35728
N	-1.74959	0.33394	-0.07723
H	-4.22372	-1.89061	-0.60668
C	-3.75244	-0.94031	-0.38709
C	-2.48933	1.43014	0.16620
H	-1.94340	2.34359	0.35951
C	-4.51902	0.19649	-0.13263
C	-3.87715	1.39829	0.15047
H	-5.60082	0.14120	-0.15397
H	-4.43702	2.30231	0.35212
H	2.19202	0.61980	-2.63933
H	3.78847	0.01192	-2.12335
H	3.11497	1.46650	-1.37086
H	-0.78307	0.96208	2.67053
H	0.30489	2.21058	2.04489
H	0.74578	1.30368	3.50691
O	-0.03203	0.24838	-2.11957

O	0.41447	2.27441	-0.64814
H	0.22174	2.18061	-1.59777
C	1.20392	3.46917	-0.40107
H	-0.92589	0.09588	-2.44537
H	2.18771	3.39709	-0.86658
H	0.66882	4.33021	-0.80171
H	1.30692	3.58800	0.67484

Prod_CH2_meta_g_4.log

51

H	0.42169	-1.02833	3.33991
H	2.91575	0.34146	2.48753
H	1.63683	-1.70928	2.29122
C	0.70073	-1.15502	2.29198
H	3.04587	-1.52602	0.87413
H	-0.38028	-2.98143	1.89124
C	2.41109	0.44845	1.52098
H	1.48409	-3.06745	0.44608
H	4.03578	-0.22027	0.27420
C	0.30958	1.25404	2.51039
C	3.00569	-0.50653	0.49409
N	0.93779	0.19922	1.66640
C	-0.38259	-1.93704	1.56028
H	2.53796	1.48247	1.19675
H	-1.36345	-1.52724	1.79986
C	0.94929	-2.66635	-0.41534
H	0.58454	-3.53164	-0.97470
H	2.82458	-2.40641	-1.46613
N	-0.19222	-1.84205	0.08726
N	2.18700	-0.48602	-0.76938
C	1.89054	-1.85485	-1.31591
H	-1.96688	-2.96852	-0.32670
C	2.89315	0.31001	-1.81981
C	-1.47569	-2.03669	-0.62740
H	1.43401	-1.69210	-2.29140
Fe	0.28031	0.26815	-0.35626
H	-1.26618	-2.10172	-1.69813
C	-2.38202	-0.84943	-0.35798
N	-1.76560	0.32945	-0.10024
H	-4.24063	-1.89841	-0.57177
C	-3.76743	-0.94374	-0.37630
C	-2.50352	1.43213	0.13127
H	-1.95646	2.34763	0.31667
C	-4.53257	0.19686	-0.14105
C	-3.89005	1.40420	0.11997
H	-5.61452	0.14100	-0.15626
H	-4.44823	2.31147	0.31142
H	2.24967	0.40695	-2.69038
H	3.82249	-0.19456	-2.09826
H	3.12999	1.29779	-1.42677
H	-0.74356	1.02009	2.66091
H	0.38915	2.22051	2.01774
H	0.80253	1.30953	3.48549
O	0.01662	0.37059	-2.15332
O	0.65828	2.49154	-0.63104
H	0.55142	2.47013	-1.59269
C	1.15871	3.79886	-0.23149
H	-0.89295	0.50141	-2.44917
H	2.13249	3.98682	-0.68633
H	0.45104	4.57346	-0.52872
H	1.25757	3.80010	0.85159

Prod_CH2_meta_g_6.log

51

H	0.52485	-0.93202	3.38015
H	3.09836	0.32402	2.41325

H	1.67980	-1.67598	2.31162
C	0.77978	-1.06461	2.32635
H	3.06847	-1.59062	0.86757
H	-0.43378	-2.81615	1.97212
C	2.54637	0.42913	1.47195
H	1.42230	-3.02683	0.54203
H	4.10672	-0.35259	0.21644
C	0.55726	1.35618	2.57331
C	3.06569	-0.58430	0.45178
N	1.07702	0.26939	1.69982
C	-0.36658	-1.77998	1.62284
H	2.71388	1.44581	1.11025
H	-1.31023	-1.29447	1.86720
C	0.89894	-2.64732	-0.33527
H	0.48123	-3.52132	-0.84065
H	2.76207	-2.55579	-1.42230
N	-0.20659	-1.74518	0.13684
N	2.24431	-0.57181	-0.80107
C	1.86848	-1.93646	-1.28437
H	-1.94597	-2.95234	-0.16309
C	2.96889	0.15633	-1.88431
C	-1.51179	-2.01389	-0.52421
H	1.40651	-1.79643	-2.26143
Fe	0.25843	0.33438	-0.41736
H	-1.33274	-2.12283	-1.59708
C	-2.46262	-0.85897	-0.28176
N	-1.89006	0.34468	-0.05805
H	-4.27915	-1.98847	-0.47572
C	-3.84295	-1.01181	-0.30417
C	-2.67249	1.42248	0.14146
H	-2.16632	2.36509	0.31151
C	-4.65158	0.10453	-0.10111
C	-4.05677	1.34286	0.12874
H	-5.73055	0.00673	-0.11592
H	-4.65108	2.23162	0.29663
H	2.32324	0.24219	-2.75491
H	3.88383	-0.38105	-2.15178
H	3.23690	1.15349	-1.53518
H	-0.51120	1.21351	2.73641
H	0.71067	2.32470	2.10191
H	1.06374	1.35589	3.54368
O	-0.01399	0.37373	-2.24361
O	0.70722	2.43447	-0.71726
H	0.53239	2.44409	-1.67037
C	1.14107	3.75966	-0.28390
H	-0.81783	0.38454	-2.77329
H	1.91979	4.12212	-0.95477
H	0.29193	4.44323	-0.28350
H	1.54400	3.66772	0.72074

TSreb_CH3_meta_g_2.log

51

H	1.18191	-3.33613	0.95435
H	3.21928	-1.41700	1.98506
H	2.35316	-2.48566	-0.01972
C	1.33859	-2.42759	0.36985
H	3.48708	-0.84252	-0.39446
H	0.55211	-3.08712	-1.54160
C	2.56591	-0.64573	1.56398
H	2.18865	-1.53276	-2.09597
H	4.08151	0.50087	0.55160
C	0.51945	-1.57415	2.52742
C	3.18102	-0.06196	0.30079
N	1.21512	-1.21866	1.25748
C	0.32520	-2.35831	-0.75769
H	2.42151	0.12691	2.31788

H	-0.67139	-2.58223	-0.38058
C	1.49030	-0.70662	-2.22448
H	1.18860	-0.71382	-3.27378
H	3.15333	0.68043	-2.30338
N	0.29187	-0.97364	-1.34431
N	2.19977	0.84963	-0.39517
C	2.14362	0.63188	-1.88369
H	-1.23063	-1.57276	-2.72593
C	2.55251	2.27725	-0.11833
C	-1.02310	-0.75731	-2.02709
H	1.56246	1.45641	-2.28987
Fe	0.29927	0.38693	0.20487
H	-0.96533	0.17935	-2.58385
C	-2.08279	-0.65309	-0.95668
N	-1.63458	-0.20136	0.23968
H	-3.75800	-1.34663	-2.10274
C	-3.41835	-0.97627	-1.14316
C	-2.48515	-0.04859	1.27017
H	-2.06115	0.32759	2.19190
C	-4.30761	-0.81754	-0.08042
C	-3.83377	-0.35137	1.14280
H	-5.35583	-1.06094	-0.20693
H	-4.49358	-0.21959	1.99064
H	1.78259	2.92172	-0.53284
H	3.51691	2.50268	-0.58133
H	2.62461	2.42567	0.95759
H	-0.43976	-2.03867	2.30157
H	0.36179	-0.67227	3.11406
H	1.12708	-2.28053	3.10007
O	-0.22775	1.76223	-0.83290
O	0.29624	1.25182	1.74206
H	0.05693	2.18688	1.65209
C	-2.13887	4.10078	0.18909
H	-1.09544	2.14376	-0.61092
H	-1.26957	4.74411	0.22281
H	-2.67381	3.99878	-0.74713
H	-2.64079	3.84090	1.11227

TSreb_CH3_meta_g_4.log

51

H	-1.11091	-3.40567	0.94500
H	-3.30982	-2.28273	-0.76034
H	-2.23019	-2.15700	1.42650
C	-1.25594	-2.32356	0.96989
H	-3.39640	-0.54444	0.97729
H	-0.27623	-1.89109	2.85674
C	-2.64341	-1.41932	-0.86384
H	-1.94599	-0.27219	2.65136
H	-4.11212	0.10595	-0.47693
C	-0.65035	-2.73854	-1.37836
C	-3.17391	-0.24862	-0.04716
N	-1.25849	-1.77018	-0.42526
C	-0.15357	-1.67839	1.79021
H	-2.58760	-1.15871	-1.91979
H	0.81589	-2.07062	1.48726
C	-1.27165	0.49921	2.28191
H	-0.89562	1.03176	3.15778
H	-2.97248	1.74285	1.77561
N	-0.13140	-0.19021	1.57075
N	-2.17956	0.88728	-0.01848
C	-1.99812	1.47346	1.35554
H	1.50881	-0.00013	2.93433
C	-2.61483	1.96332	-0.96188
C	1.22050	0.33969	1.93528
H	-1.41616	2.38231	1.22284
Fe	-0.30323	0.17772	-0.45654

H	1.16666	1.42932	1.93735
C	2.19828	-0.12629	0.88218
N	1.65196	-0.33991	-0.33953
H	3.97200	-0.16165	2.08867
C	3.55290	-0.32479	1.10325
C	2.42080	-0.74040	-1.36749
H	1.91853	-0.88024	-2.31590
C	4.35809	-0.73708	0.04111
C	3.78398	-0.95067	-1.20904
H	5.41939	-0.89466	0.19228
H	4.37702	-1.27404	-2.05478
H	-1.84296	2.72592	-1.01573
H	-3.54870	2.40166	-0.59939
H	-2.77951	1.52981	-1.94659
H	0.34684	-3.01296	-1.03486
H	-0.58331	-2.27922	-2.36204
H	-1.26356	-3.64265	-1.43949
O	0.24712	1.92835	-0.35185
O	-0.46245	0.09600	-2.21318
H	-0.29752	0.94201	-2.65349
C	1.57815	4.49407	-0.52452
H	1.15297	2.09550	-0.65127
H	1.25489	4.63349	-1.54705
H	0.94524	4.83569	0.28190
H	2.61433	4.25504	-0.32176

Prod_CH3_meta_g_2.log

51

H	-0.52277	-3.48290	0.76424
H	-2.86559	-2.65555	-0.85610
H	-1.82695	-2.46931	1.32672
C	-0.83931	-2.44380	0.87101
H	-3.20331	-1.05833	1.00842
H	0.03353	-1.97799	2.79950
C	-2.37420	-1.67841	-0.90303
H	-1.81305	-0.58701	2.69787
H	-4.07031	-0.45523	-0.38190
C	-0.19808	-2.60988	-1.49848
C	-3.07131	-0.67436	-0.00188
N	-0.93830	-1.79682	-0.48765
C	0.14236	-1.68952	1.74956
H	-2.37683	-1.33746	-1.93748
H	1.16309	-1.92441	1.45191
C	-1.26381	0.28212	2.33740
H	-0.96560	0.84545	3.22437
H	-3.14394	1.26642	1.89112
N	-0.04908	-0.20745	1.59285
N	-2.25793	0.59487	0.05459
C	-2.15057	1.15437	1.44391
H	1.57431	0.15932	2.94760
C	-2.89537	1.59134	-0.85707
C	1.21921	0.48448	1.96481
H	-1.72323	2.15246	1.35065
Fe	-0.31359	0.15070	-0.41727
H	1.02692	1.55800	2.01049
C	2.23692	0.18801	0.88428
N	1.70690	-0.06827	-0.33905
H	4.01079	0.37288	2.07876
C	3.60876	0.17568	1.09238
C	2.52267	-0.34215	-1.37608
H	2.03685	-0.53645	-2.32388
C	4.45439	-0.09965	0.01779
C	3.90326	-0.36499	-1.23323
H	5.52853	-0.11359	0.15960
H	4.52771	-0.58834	-2.08866
H	-2.31343	2.50558	-0.88498

H	-3.90416	1.82275	-0.50397
H	-2.94055	1.17392	-1.86030
H	0.83020	-2.75342	-1.16938
H	-0.21216	-2.08537	-2.44993
H	-0.67439	-3.58845	-1.60402
O	0.37232	2.23541	-0.36063
O	-0.50222	0.22880	-2.20319
H	-0.17043	1.03032	-2.62566
C	-0.08452	3.60146	-0.61273
H	1.26986	2.16931	-0.70412
H	-0.45862	3.70350	-1.63203
H	-0.86706	3.83371	0.10505
H	0.74960	4.28393	-0.45130

Prod_CH3_meta_g_4.log

51

H	-0.94877	-3.48751	1.03882
H	-3.29911	-2.43701	-0.65560
H	-2.10660	-2.27667	1.51310
C	-1.14709	-2.41277	1.01441
H	-3.33428	-0.67009	1.04312
H	-0.08941	-1.89981	2.84307
C	-2.62160	-1.58524	-0.79220
H	-1.88730	-0.35343	2.64093
H	-4.10691	-0.07512	-0.40387
C	-0.63036	-2.88727	-1.34607
C	-3.14719	-0.39465	0.00613
N	-1.23263	-1.92320	-0.39091
C	-0.03436	-1.69170	1.76976
H	-2.59663	-1.34679	-1.85598
H	0.93592	-2.03874	1.41664
C	-1.23978	0.44023	2.27222
H	-0.88350	0.98480	3.14922
H	-2.96559	1.65688	1.77569
N	-0.07968	-0.19953	1.55004
N	-2.18664	0.77181	-0.01792
C	-1.99761	1.38431	1.34172
H	1.55084	0.07861	2.91604
C	-2.68862	1.80679	-0.97086
C	1.24558	0.40104	1.91641
H	-1.43113	2.30366	1.19598
Fe	-0.27847	0.11911	-0.48114
H	1.13471	1.48774	1.92282
C	2.25335	0.00847	0.86381
N	1.72547	-0.18766	-0.36848
H	4.01767	0.01997	2.08692
C	3.61396	-0.13169	1.09333
C	2.52189	-0.52743	-1.39928
H	2.02924	-0.66977	-2.35292
C	4.44570	-0.47469	0.02699
C	3.89200	-0.67790	-1.23455
H	5.51166	-0.58946	0.18382
H	4.50653	-0.95232	-2.08223
H	-1.95437	2.60247	-1.07398
H	-3.62912	2.22660	-0.60277
H	-2.85799	1.34621	-1.94217
H	0.39001	-3.11911	-1.03863
H	-0.60677	-2.44085	-2.33922
H	-1.20589	-3.81847	-1.38023
O	0.64158	2.51916	-0.43690
O	-0.38699	0.17083	-2.24447
H	-0.40548	1.02137	-2.70127
C	0.42062	3.95515	-0.36617
H	1.46963	2.38244	-0.91048
H	0.25562	4.37291	-1.36122
H	-0.46501	4.12026	0.24492

H	1.27108	4.44863	0.10700
Prod_CH3_meta_g_6.log			
51			
H	-1.16021	-3.44344	0.81161
H	-3.48726	-2.15968	-0.68394
H	-2.22055	-2.20641	1.42754
C	-1.28594	-2.36146	0.89102
H	-3.38621	-0.53512	1.15591
H	-0.15534	-2.10043	2.71464
C	-2.79176	-1.31784	-0.77860
H	-1.87370	-0.42419	2.68382
H	-4.20050	0.19252	-0.20051
C	-0.92414	-2.72627	-1.50928
C	-3.23150	-0.17957	0.13836
N	-1.39498	-1.75855	-0.47887
C	-0.11095	-1.77901	1.66805
H	-2.80927	-0.99143	-1.81936
H	0.82522	-2.15416	1.25360
C	-1.18585	0.35511	2.35903
H	-0.79768	0.81118	3.27322
H	-2.83262	1.72153	2.06211
N	-0.07668	-0.28687	1.58020
N	-2.23577	0.94823	0.15524
C	-1.91957	1.41805	1.53712
H	1.57596	-0.21804	2.93827
C	-2.75789	2.08504	-0.66028
C	1.26739	0.20629	1.97659
H	-1.30043	2.30990	1.42674
Fe	-0.29655	0.18168	-0.60483
H	1.21060	1.29024	2.11035
C	2.28268	-0.11604	0.90032
N	1.79492	-0.21821	-0.35438
H	4.00542	-0.19673	2.18149
C	3.63697	-0.27174	1.16551
C	2.63570	-0.46461	-1.37910
H	2.18467	-0.52362	-2.36163
C	4.50766	-0.52787	0.10756
C	3.99913	-0.62576	-1.18605
H	5.56789	-0.65384	0.29250
H	4.64414	-0.82628	-2.03171
H	-2.02205	2.88420	-0.68693
H	-3.68914	2.46301	-0.22764
H	-2.94729	1.74371	-1.67702
H	0.10051	-3.02739	-1.28968
H	-0.95083	-2.26079	-2.49223
H	-1.55950	-3.61721	-1.51817
O	0.33221	2.33861	-0.72357
O	-0.41024	0.37727	-2.40081
H	-0.69494	0.10629	-3.27708
C	1.32697	3.25727	-0.19691
H	0.31678	2.39446	-1.69020
H	1.19564	4.23656	-0.65714
H	1.15400	3.34700	0.87372
H	2.33512	2.88568	-0.38698

CYCLOHEXANE AT GAS-PHASE

A_ciclohex_g_2.log

64

H	4.21386	1.01536	1.71488
H	4.94493	-1.26498	-0.08031
H	3.73668	-0.64552	1.95641
C	3.42588	0.29144	1.49781
H	3.23553	-2.47901	1.19934
H	2.10735	0.70284	3.17161
C	3.90632	-1.19491	-0.42096

H	1.81407	-1.56458	2.70560
H	3.43433	-3.29485	-0.33423
C	3.93552	1.23336	-0.71669
C	3.09770	-2.36407	0.12517
N	3.29526	0.10058	0.01200
C	2.10937	0.77166	2.07950
H	3.90632	-1.20112	-1.51014
H	1.93923	1.81422	1.81528
C	0.90621	-1.41543	2.12290
H	0.07064	-1.47820	2.82280
H	1.02827	-3.47222	1.44826
N	0.96741	-0.03200	1.51922
N	1.62308	-2.18198	-0.15251
C	0.76132	-2.49021	1.04574
H	-0.41876	1.09996	2.69434
C	1.20785	-3.05136	-1.29976
C	-0.30566	0.74872	1.66485
H	-0.26537	-2.53953	0.68687
Fe	1.23611	-0.20662	-0.51740
H	-1.14572	0.09410	1.42559
C	-0.26250	1.89187	0.68091
N	0.49884	1.66657	-0.41586
H	-1.54133	3.25960	1.72522
C	-0.94618	3.08801	0.83703
C	0.58754	2.58927	-1.38989
H	1.19846	2.33283	-2.24515
C	-0.85851	4.05315	-0.16555
C	-0.07963	3.80140	-1.29160
H	-1.39185	4.99098	-0.06597
H	0.01182	4.52680	-2.08966
H	0.16907	-2.84916	-1.55628
H	1.31620	-4.10073	-1.01303
H	1.84398	-2.84177	-2.15740
H	3.49952	2.17457	-0.38278
H	3.76892	1.11416	-1.78474
H	5.01038	1.24888	-0.51495
O	-0.40168	-0.67402	-0.81765
O	1.77527	-0.14582	-2.19116
H	1.06973	-0.35902	-2.82138
C	-3.73529	0.03240	-0.71439
H	-2.64512	0.08794	-0.87520
C	-4.07469	0.25807	0.76544
H	-3.54489	-0.48636	1.37993
H	-3.73775	1.24950	1.09453
C	-4.25836	-1.31955	-1.21713
H	-4.04703	-1.43588	-2.28435
H	-3.72874	-2.13089	-0.69896
C	-5.58632	0.11387	1.02341
H	-5.79742	0.23493	2.08991
H	-6.11326	0.92459	0.50646
C	-5.76995	-1.46395	-0.95794
H	-6.10772	-2.45242	-1.28127
H	-6.30939	-0.73372	-1.57261
C	-6.11056	-1.23762	0.52038
H	-7.19292	-1.29322	0.66812
H	-5.67539	-2.04507	1.12361
H	-4.17668	0.83870	-1.31285
A_ciclohex_g_4.log			
64			
H	-3.64504	-0.44935	2.55361
H	-1.92633	-2.90608	2.51946
H	-3.69865	-1.69961	1.34031
C	-3.23083	-0.74869	1.58862
H	-2.77268	-3.11999	0.21742
H	-4.61654	0.28798	0.27980

C	-1.38535	-2.38553	1.72165
H	-3.97894	-1.58575	-0.92541
H	-1.28213	-4.02714	0.33113
C	-1.22358	-0.26715	2.92455
C	-1.69982	-3.02011	0.37547
N	-1.74506	-0.93440	1.69779
C	-3.55510	0.30561	0.54520
H	-0.31978	-2.44904	1.93855
H	-3.33158	1.29783	0.93295
C	-3.22305	-1.06586	-1.51264
H	-3.72183	-0.70101	-2.41276
H	-2.47774	-2.97832	-2.21087
N	-2.72370	0.10037	-0.69187
N	-1.12198	-2.19749	-0.75324
C	-2.08300	-2.00672	-1.89770
H	-3.63787	1.80136	-1.61903
C	0.13198	-2.84375	-1.25921
C	-2.63840	1.39072	-1.44930
H	-1.50455	-1.59497	-2.72270
Fe	-0.76425	-0.27306	-0.13124
H	-2.17320	1.19253	-2.41719
C	-1.77049	2.33311	-0.65114
N	-0.86685	1.72550	0.15426
H	-2.58278	4.18862	-1.35340
C	-1.84721	3.71523	-0.71463
C	-0.00658	2.44922	0.88983
H	0.70596	1.89571	1.48644
C	-0.96224	4.47777	0.04814
C	-0.03364	3.83680	0.86258
H	-1.00032	5.55972	0.00476
H	0.66979	4.39534	1.46638
H	0.59623	-2.20576	-2.00785
H	-0.12189	-3.80987	-1.70346
H	0.81884	-2.99273	-0.42888
H	-1.51636	0.78229	2.92273
H	-0.13872	-0.34254	2.94043
H	-1.63554	-0.74662	3.81725
O	-0.13284	0.04009	-1.60824
O	0.74585	-0.55523	0.73184
H	1.54769	-0.45893	0.18571
C	3.83368	-0.13534	-0.95580
H	2.75547	0.05099	-1.11620
C	4.08184	-1.21499	0.11188
H	3.62339	-0.91048	1.06532
H	3.61369	-2.16320	-0.18055
C	4.54039	1.18375	-0.60839
H	4.38418	1.91697	-1.40542
H	4.09549	1.60635	0.30390
C	5.58666	-1.43043	0.34337
H	5.74072	-2.16810	1.13583
H	6.02807	-1.85391	-0.56674
C	6.04292	0.96244	-0.37445
H	6.51674	1.90396	-0.08372
H	6.51111	0.65919	-1.31865
C	6.29713	-0.11437	0.68952
H	7.37055	-0.28869	0.79906
H	5.94196	0.24522	1.66422
H	4.20022	-0.49923	-1.92288
TSabs_ciclohex_g_4.log			
64			
H	4.27615	1.62980	-0.41513
H	4.41945	-1.08807	-1.68581
H	4.34292	0.10955	0.43517
C	3.65506	0.84214	0.01644
H	3.86734	-1.86262	0.58537

H	3.34156	1.68792	1.99014
C	3.36244	-1.15481	-1.40554
H	3.26040	-0.60394	2.33474
H	3.43369	-3.12562	-0.54126
C	2.78018	1.05043	-2.27214
C	3.19073	-2.10776	-0.23203
N	2.82393	0.19493	-1.05425
C	2.76414	1.43070	1.09678
H	2.80290	-1.50629	-2.27142
H	2.29723	2.34497	0.73505
C	2.17283	-0.66274	2.31769
H	1.83702	-0.53107	3.34831
H	2.30615	-2.82348	2.21800
N	1.66476	0.47146	1.46135
N	1.77384	-2.07028	0.28659
C	1.70259	-2.01727	1.78882
H	0.88185	1.86662	2.88719
C	1.02913	-3.27167	-0.20269
C	0.52833	1.23377	2.06788
H	0.66130	-2.19056	2.05174
Fe	0.86986	-0.31434	-0.27674
H	-0.19139	0.51421	2.46214
C	-0.11090	2.04631	0.96757
N	0.01949	1.51613	-0.27089
H	-0.86250	3.66322	2.16020
C	-0.77961	3.24510	1.16447
C	-0.51019	2.13880	-1.33665
H	-0.37923	1.64905	-2.29249
C	-1.33155	3.89982	0.06350
C	-1.19193	3.34095	-1.20364
H	-1.85737	4.83796	0.19543
H	-1.60256	3.82271	-2.08157
H	-0.01346	-3.19317	0.09377
H	1.47296	-4.17169	0.23142
H	1.10137	-3.31858	-1.28761
H	2.42676	2.04678	-2.00766
H	2.10320	0.60485	-2.99760
H	3.77908	1.13642	-2.71010
O	-0.55360	-0.93663	0.48075
O	0.45730	-0.75910	-1.94093
H	-0.40248	-1.19825	-2.00501
C	-3.09513	-0.28282	0.07551
H	-1.92295	-0.49166	0.22949
C	-3.80238	-0.82791	1.30138
H	-3.55918	-1.88753	1.43508
H	-3.49383	-0.30112	2.20871
C	-3.51501	-0.94962	-1.22176
H	-3.00833	-0.50569	-2.08534
H	-3.26237	-2.01589	-1.19462
C	-5.34085	-0.68998	1.11336
H	-5.83624	-1.13062	1.98265
H	-5.60810	0.37254	1.10030
C	-5.05406	-0.81238	-1.40155
H	-5.34674	-1.33875	-2.31401
H	-5.30466	0.24393	-1.54959
C	-5.80223	-1.35995	-0.18331
H	-6.87779	-1.20633	-0.31419
H	-5.65073	-2.44342	-0.11354
H	-3.16125	0.81029	0.01444
Prod_CH2_ciclohex_g_2.log			
64			
H	-3.18743	-0.86653	2.61636
H	-1.14431	-3.07041	2.50836
H	-3.09735	-2.11966	1.40815
C	-2.76607	-1.10930	1.63889

H	-2.06219	-3.36997	0.23875
H	-4.33014	-0.29974	0.37666
C	-0.71573	-2.48269	1.68904
H	-3.48741	-2.04431	-0.86285
H	-0.47845	-4.09709	0.28746
C	-0.83105	-0.39416	2.95020
C	-1.00321	-3.14174	0.34929
N	-1.25854	-1.08445	1.70407
C	-3.27508	-0.12101	0.60452
H	0.36003	-2.41393	1.85380
H	-3.19195	0.89454	0.98748
C	-2.82686	-1.42396	-1.46846
H	-3.39848	-1.12635	-2.34969
H	-1.84325	-3.20290	-2.21275
N	-2.46010	-0.20667	-0.65724
N	-0.57300	-2.24250	-0.77517
C	-1.57709	-2.19094	-1.89043
H	-3.64687	1.33701	-1.54713
C	0.72138	-2.73288	-1.33109
C	-2.59215	1.08203	-1.40615
H	-1.08535	-1.68236	-2.71655
Fe	-0.53173	-0.27421	-0.13699
H	-2.12027	0.95235	-2.38076
C	-1.86585	2.15661	-0.63014
N	-0.85145	1.72294	0.16001
H	-3.01651	3.81786	-1.35008
C	-2.19730	3.50195	-0.71574
C	-0.15495	2.62270	0.87683
H	0.65009	2.24118	1.48990
C	-1.46594	4.43023	0.02128
C	-0.43048	3.98143	0.83633
H	-1.70603	5.48520	-0.03492
H	0.15787	4.66833	1.43070
H	1.06753	-2.03332	-2.08643
H	0.58013	-3.72068	-1.77913
H	1.45415	-2.80942	-0.53027
H	-1.19203	0.63373	2.94954
H	0.25629	-0.39801	3.03097
H	-1.22614	-0.90723	3.83205
O	0.04715	0.12048	-1.80911
O	1.39648	-0.26750	0.60666
H	1.51057	0.06291	1.50537
C	2.73010	-0.15428	-0.07047
H	0.63655	0.88363	-1.84266
C	3.73476	-1.03609	0.66081
H	3.80637	-0.70847	1.70715
H	3.39333	-2.07515	0.67056
C	3.18015	1.30008	-0.13853
H	2.45146	1.90449	-0.68835
H	3.23900	1.70654	0.88090
C	5.12564	-0.93067	0.00369
H	5.83510	-1.53570	0.57214
H	5.08363	-1.36545	-1.00180
C	4.56983	1.40619	-0.79899
H	4.88705	2.45135	-0.79859
H	4.49394	1.10609	-1.85067
C	5.59997	0.52507	-0.08214
H	6.55823	0.57418	-0.60391
H	5.77702	0.91407	0.92762
H	2.53294	-0.53789	-1.07004

Prod_CH2_ciclohex_g_4.log

64

H	-3.11636	-0.97433	2.69412
H	-1.03030	-3.10903	2.49443
H	-3.03692	-2.20527	1.46396

C	-2.73393	-1.18585	1.69370
H	-2.01071	-3.43831	0.25440
H	-4.41297	-0.42850	0.57164
C	-0.64617	-2.50670	1.66353
H	-3.52438	-2.16447	-0.76263
H	-0.40260	-4.11153	0.25421
C	-0.78226	-0.42551	2.94824
C	-0.95713	-3.17418	0.33093
N	-1.22257	-1.12083	1.70797
C	-3.34640	-0.21004	0.69858
H	0.43304	-2.41358	1.79439
H	-3.27209	0.80663	1.08316
C	-2.92833	-1.49844	-1.38699
H	-3.55105	-1.26206	-2.25368
H	-1.89383	-3.20475	-2.22508
N	-2.62832	-0.26434	-0.60123
N	-0.59191	-2.26752	-0.81221
C	-1.65148	-2.19673	-1.87186
H	-3.85166	1.25894	-1.47714
C	0.68611	-2.72440	-1.43481
C	-2.79418	0.99992	-1.35405
H	-1.21048	-1.64404	-2.69975
Fe	-0.45801	-0.27573	-0.12800
H	-2.36165	0.86370	-2.34803
C	-2.05875	2.11255	-0.63409
N	-0.98408	1.74293	0.10103
H	-3.32160	3.71204	-1.30396
C	-2.45191	3.44265	-0.71699
C	-0.28035	2.68190	0.76105
H	0.57699	2.33623	1.32320
C	-1.72010	4.41435	-0.03892
C	-0.61775	4.02640	0.71789
H	-2.01088	5.45652	-0.09568
H	-0.02607	4.74842	1.26554
H	0.99022	-2.00705	-2.19232
H	0.54388	-3.70891	-1.88982
H	1.45591	-2.79519	-0.66776
H	-1.17259	0.59144	2.95991
H	0.30507	-0.39238	3.00205
H	-1.14258	-0.95475	3.83534
O	0.16093	0.12599	-1.78073
O	1.56100	-0.15964	0.68434
H	1.75966	-0.09777	1.62671
C	2.86754	-0.02435	-0.03974
H	0.36870	1.05890	-1.91772
C	3.86265	-1.03586	0.51490
H	3.99707	-0.85432	1.59073
H	3.47649	-2.05360	0.40378
C	3.37924	1.40700	0.06091
H	2.65228	2.09940	-0.37487
H	3.49566	1.67393	1.12021
C	5.22699	-0.89801	-0.18998
H	5.93282	-1.60141	0.25695
H	5.12093	-1.19061	-1.24117
C	4.74228	1.54528	-0.64695
H	5.10733	2.56752	-0.52555
H	4.60753	1.38999	-1.72389
C	5.76202	0.53657	-0.10440
H	6.69838	0.61780	-0.66090
H	5.99936	0.77836	0.93846
H	2.59985	-0.26077	-1.06895

Prod_CH2_ciclohex_g_6.log

64

H	-2.98097	-1.10487	2.78592
H	-0.90136	-3.28951	2.42635

H	-2.95305	-2.29732	1.52001
C	-2.61399	-1.29492	1.77465
H	-1.98380	-3.51720	0.23469
H	-4.30116	-0.44368	0.73255
C	-0.55373	-2.64109	1.61299
H	-3.50362	-2.18037	-0.64512
H	-0.38807	-4.20668	0.15434
C	-0.61993	-0.64800	3.01937
C	-0.92531	-3.26235	0.26832
N	-1.11133	-1.26301	1.75893
C	-3.22416	-0.26656	0.83054
H	0.53208	-2.56468	1.70136
H	-3.09869	0.73276	1.24516
C	-2.93455	-1.51770	-1.29652
H	-3.60595	-1.25274	-2.11672
H	-2.00298	-3.22527	-2.23275
N	-2.57052	-0.29004	-0.51095
N	-0.59938	-2.34985	-0.87352
C	-1.70802	-2.23408	-1.86934
H	-3.93644	1.15053	-1.30655
C	0.63948	-2.81446	-1.56141
C	-2.85764	0.97112	-1.24416
H	-1.30479	-1.67365	-2.71154
Fe	-0.38170	-0.22875	-0.20198
H	-2.47499	0.86382	-2.26210
C	-2.16378	2.13447	-0.56851
N	-1.03682	1.83691	0.11429
H	-3.55069	3.64787	-1.19937
C	-2.63982	3.43709	-0.65231
C	-0.35812	2.82528	0.72668
H	0.54166	2.53849	1.25597
C	-1.93364	4.45892	-0.02215
C	-0.77420	4.14735	0.68393
H	-2.28787	5.48145	-0.07563
H	-0.20170	4.91136	1.19366
H	0.91732	-2.09425	-2.32684
H	0.47322	-3.79525	-2.01803
H	1.44760	-2.89990	-0.83473
H	-0.96374	0.38436	3.09119
H	0.47026	-0.66673	3.05336
H	-0.97963	-1.19919	3.89446
O	0.17077	0.13818	-1.91631
O	1.53577	-0.08668	0.63995
H	1.70119	-0.05753	1.59074
C	2.86478	0.06047	-0.05944
H	0.42825	0.98075	-2.30488
C	3.83910	-0.96941	0.49354
H	3.95680	-0.81123	1.57475
H	3.44853	-1.98127	0.35082
C	3.37413	1.48699	0.08613
H	2.65654	2.19057	-0.34639
H	3.47431	1.72764	1.15299
C	5.21592	-0.82190	-0.18668
H	5.91018	-1.53910	0.25620
H	5.12507	-1.09072	-1.24551
C	4.75019	1.63386	-0.59600
H	5.11675	2.65137	-0.44416
H	4.63264	1.50469	-1.67832
C	5.75589	0.60784	-0.05976
H	6.70139	0.69675	-0.59930
H	5.97762	0.82485	0.99187
H	2.61038	-0.15592	-1.09661

Prod_CH3_ciclohex_g_2.log

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H	4.51644	-0.18191	0.16844
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H	3.62248	-2.67441	-1.17161
H	3.73688	-1.52719	0.95819
C	3.54386	-0.57282	0.47303
H	2.41277	-3.02073	0.96323
H	3.35159	0.36633	2.41659
C	2.61402	-2.26191	-1.06387
H	2.12591	-1.58140	2.63835
H	1.65329	-4.01313	-0.25484
C	3.23669	-0.06065	-1.91298
C	1.84750	-2.97885	0.03352
N	2.67988	-0.79977	-0.74158
C	2.87449	0.39503	1.43210
H	2.09777	-2.35270	-2.01869
H	2.96722	1.41245	1.05584
C	1.16304	-1.11979	2.42157
H	0.74304	-0.81758	3.38354
H	0.27601	-3.09000	2.24133
N	1.40989	0.08534	1.55262
N	0.54245	-2.26452	0.27764
C	0.22462	-2.11872	1.73771
H	1.15307	1.75307	2.87920
C	-0.53597	-3.03046	-0.41472
C	0.69243	1.31847	1.98641
H	-0.80587	-1.77167	1.80290
Fe	0.72228	-0.32183	-0.34935
H	-0.33826	1.05282	2.22792
C	0.71263	2.29085	0.82635
N	0.79075	1.71013	-0.39728
H	0.60331	4.11454	1.95316
C	0.65337	3.67012	0.96659
C	0.80627	2.47922	-1.50260
H	0.86296	1.95077	-2.44569
C	0.66508	4.46810	-0.17733
C	0.74365	3.86413	-1.42955
H	0.62024	5.54710	-0.08922
H	0.75929	4.45103	-2.33885
H	-1.48399	-2.51309	-0.32308
H	-0.62445	-4.02674	0.02780
H	-0.28535	-3.11476	-1.46962
H	3.34145	0.99411	-1.66213
H	2.55969	-0.17409	-2.75555
H	4.22152	-0.46153	-2.16866
O	-1.35858	0.18985	0.04193
O	0.35068	-0.60965	-2.08333
H	-0.55411	-0.38462	-2.33301
C	-2.76198	-0.31203	0.14729
H	-1.43432	1.08967	-0.29818
C	-3.36877	-0.53247	-1.23397
H	-3.34694	0.41730	-1.78500
H	-2.77624	-1.25373	-1.80531
C	-3.57908	0.66394	0.98805
H	-3.13115	0.77529	1.98030
H	-3.56195	1.65152	0.50631
C	-4.82890	-1.01323	-1.11533
H	-5.25186	-1.12346	-2.11607
H	-4.84563	-2.01130	-0.66128
C	-5.04062	0.18765	1.10603
H	-5.61172	0.92693	1.67174
H	-5.07203	-0.73951	1.69040
C	-5.67121	-0.04812	-0.27216
H	-6.68301	-0.44244	-0.15487
H	-5.77121	0.90798	-0.79965
H	-2.67042	-1.25802	0.68345

Prod_CH3_ciclohex_g_4.log
64

H	4.67900	-0.10874	0.53082
H	3.89822	-2.74180	-0.87730
H	3.83286	-1.45662	1.23470
C	3.68089	-0.52608	0.68819
H	2.44867	-2.98584	1.08826
H	3.23179	0.51653	2.54253
C	2.91433	-2.25702	-0.90140
H	2.06508	-1.54858	2.65451
H	1.82857	-3.98142	-0.20446
C	3.67915	-0.09302	-1.73491
C	1.99216	-2.94615	0.10043
N	3.01422	-0.80407	-0.61487
C	2.86266	0.46372	1.51330
H	2.51872	-2.35788	-1.91267
H	2.94960	1.46012	1.08188
C	1.11216	-1.09603	2.38560
H	0.63641	-0.79323	3.32082
H	0.21510	-3.05671	2.15201
N	1.39501	0.11443	1.52998
N	0.65853	-2.24767	0.21455
C	0.21867	-2.08727	1.64208
H	0.99690	1.74539	2.86514
C	-0.36645	-3.01602	-0.55058
C	0.60241	1.32096	1.93742
H	-0.80760	-1.72210	1.61508
Fe	0.81775	-0.27815	-0.41750
H	-0.42898	1.00532	2.11027
C	0.63701	2.31609	0.80264
N	0.75382	1.75706	-0.42598
H	0.46217	4.12126	1.95147
C	0.54518	3.69098	0.96095
C	0.78466	2.53656	-1.52272
H	0.88309	2.02059	-2.46951
C	0.56719	4.50321	-0.17301
C	0.69094	3.91867	-1.43077
H	0.49731	5.57977	-0.07231
H	0.71941	4.51883	-2.33102
H	-1.30654	-2.47097	-0.55633
H	-0.51650	-3.99726	-0.09085
H	-0.02263	-3.14625	-1.57473
H	3.73962	0.97197	-1.50790
H	3.09240	-0.22661	-2.64261
H	4.69301	-0.47437	-1.89766
O	-1.60686	0.14786	-0.04693
O	0.55584	-0.52332	-2.14974
H	-0.35294	-0.63704	-2.45782
C	-2.98549	-0.36976	0.10762
H	-1.69849	1.01583	-0.45957
C	-3.63174	-0.60056	-1.25583
H	-3.64435	0.35093	-1.80481
H	-3.03529	-1.30473	-1.84636
C	-3.81086	0.56989	0.98253
H	-3.33815	0.68323	1.96345
H	-3.82972	1.56347	0.51340
C	-5.07542	-1.11601	-1.10449
H	-5.52433	-1.22694	-2.09398
H	-5.05747	-2.11799	-0.65904
C	-5.25546	0.05696	1.13478
H	-5.83153	0.77365	1.72426
H	-5.24882	-0.87843	1.70708
C	-5.91672	-0.17853	-0.22923
H	-6.91673	-0.59581	-0.09117
H	-6.05001	0.78097	-0.74330
H	-2.85390	-1.32480	0.62478

Prod_CH3_ciclohex_g_6.log

64			
H	4.60337	-0.26063	0.25984
H	3.66293	-2.89223	-0.95098
H	3.76606	-1.53705	1.09803
C	3.60861	-0.62202	0.52970
H	2.38880	-3.02240	1.15573
H	3.39573	0.50342	2.36334
C	2.67932	-2.41039	-0.90714
H	2.14867	-1.49025	2.67041
H	1.66467	-4.08394	-0.02142
C	3.46031	-0.31878	-1.91049
C	1.84850	-3.03285	0.21064
N	2.82837	-0.93712	-0.71022
C	2.91122	0.43243	1.38309
H	2.19284	-2.55541	-1.87246
H	3.00745	1.40694	0.90489
C	1.19379	-1.01780	2.44221
H	0.79021	-0.67987	3.40005
H	0.24055	-2.95747	2.41495
N	1.45146	0.14923	1.53889
N	0.53529	-2.31947	0.39099
C	0.22526	-2.03412	1.82432
H	1.20228	1.82813	2.84687
C	-0.54571	-3.13348	-0.23298
C	0.74422	1.38703	1.95477
H	-0.79281	-1.64533	1.85600
Fe	0.69402	-0.31617	-0.53363
H	-0.28704	1.12449	2.20277
C	0.74309	2.38282	0.81196
N	0.75641	1.84952	-0.43081
H	0.71778	4.16600	2.00890
C	0.71886	3.75779	1.00551
C	0.75216	2.66148	-1.50783
H	0.76999	2.17042	-2.47328
C	0.70488	4.59839	-0.10694
C	0.72605	4.04256	-1.38453
H	0.68776	5.67398	0.02362
H	0.72649	4.66442	-2.27036
H	-1.49001	-2.59815	-0.19503
H	-0.65521	-4.08827	0.29074
H	-0.29491	-3.32326	-1.27564
H	3.56856	0.75481	-1.75283
H	2.82615	-0.49025	-2.77763
H	4.45083	-0.75062	-2.08393
O	-1.45854	0.19177	0.01557
O	0.40806	-0.59969	-2.29935
H	-0.35486	-0.65427	-2.88275
C	-2.85487	-0.31677	0.15339
H	-1.54139	1.08269	-0.34869
C	-3.46355	-0.60879	-1.21297
H	-3.45645	0.31397	-1.80792
H	-2.85875	-1.34579	-1.75069
C	-3.68139	0.68230	0.95621
H	-3.22974	0.84231	1.93996
H	-3.67979	1.64868	0.43257
C	-4.91556	-1.10478	-1.06506
H	-5.34243	-1.26593	-2.05730
H	-4.91662	-2.08139	-0.56607
C	-5.13532	0.19123	1.10179
H	-5.71517	0.94635	1.63688
H	-5.15100	-0.70967	1.72655
C	-5.76766	-0.11423	-0.26181
H	-6.77387	-0.51588	-0.12309
H	-5.88151	0.81624	-0.83076
H	-2.74431	-1.23836	0.72851

