Handling Methane: A Ni(I) F_{430}-like Cofactor Derived From VB_{12} is Active in Methyl-Coenzyme M Reductase

Jue Wu, and Shi-Lu Chen[*]

Key Laboratory of Cluster Science of Ministry of Education, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081 (China)

E-mail: shlchen@bit.edu.cn

Contents

Computational Details

Density functional calculations

All calculations were performed using the unrestricted B3LYP hybrid functional[S1] with Grimme's empirical D3-dispersion correction[S2] included. Geometry optimizations were carried out with the LACVP** basis set as implemented in the Jaguar 8.7 package.[S3] Based on the optimized geometries, more accurate energies were obtained using larger basis sets, that is, lacv3p+ for Ni and cc-pvtz(-f)+ for the other atoms. Solvation effects were calculated at the same level of theory as in the optimizations by performing single-point calculations using a dielectric cavity and a dielectric constant of 4. Using Gaussian 09,[S4] frequency calculations were performed to obtain zero-point energies (ZPE) and to characterize the nature of stationary points, in which the contributions of frozen atoms in vibrational analysis can be excluded to ensure that the fixation of atoms does not generate extra imaginary frequencies. The general modeling method employed here has been carefully examined and successfully applied to a large number of metalloenzymes,[S5] especially the enzymes containing Ni cofactors,[S6] such as the methyl-coenzyme M reductase with a F_{430} cofactor[S7] and the lactate racemase with a Ni pincer cofactor.[S8]

Molecular Dynamics Simulations

Molecular dynamics (MD) simulations were performed starting from the crystallographic structure of MCR (PDB entry: 1HBN).[S9] The F ring of the F_{430} cofactor was modified to its propionyloxy precursor (referred to as $F_{430\text{-NoF*}}$, as shown in Fig. 4). Bonded and atom/atom force fields parameters for methylated His257, Arg271, Glu400, and Cys452 were taken from the Generalized AMBER Force Field (GAFF) using Antechamber module[S10] of AmberTools 17. The force field for $F_{430\text{-NoF*}}$ and the Gln147 ligand were taken from Metal Centre Parameter Builder (MCPB) using MCPB.py v3.0.[S11] The rest of protein were described by the Amber ff14SB force field.[S12] The MCR protein was inserted into a box of TIP3P water[S13] molecules based on a minimum clearance of 12 Å between solute atoms and the sides of the box. To neutralize the system, 10 sodium ions were added.

The PMEMD.CUDA[S14] module of AMBER 16[S15] was used to run the MD simulations. Four minimization steps, composed of 10000 cycles of steepest descent and 10000 cycles of conjugate gradient, were performed as follows: (1) in the first step, all heavy atoms of the protein (i.e., non-hydrogen atoms) were restrained with 500 kcal/mol·Å² harmonic force constant; (2) in the following three steps, only the backbone atoms of the protein were restrained, with 500, 125, and 25 kcal/mol·Å² force constant, respectively. Then, the fifth minimization step, composed of 2000 cycles of steepest descent and 8000 cycles of conjugate gradient, was performed without any constraints.

The system was gradually heated up from 0 to 298 K in 50 K increments by performing seven 100-ps consecutive simulations in the NVT ensemble. Subsequently, the 20-ps simulation employing 1 bar pressure in the NPT ensemble was carried out. In these simulations, heavy atoms were restrained using harmonic position restraints with a force constant of 10 kcal/mol·Å². The system was then evolved without constraints for 100 ns at 298 K and the temperature was then increased in step of about 5 K, until 333 K. These additional simulations were run for 25 ns except for 100 ns at the 333 K.

The periodic boundary conditions were applied in all equilibration molecular simulations. The particle mesh Ewald (PME) algorithm[S16] was used for the treatment of the long-range interactions beyond a 10 Å cutoff. The SHAKE algorithm[S17] was used to constrain the bonds involving the hydrogen atoms. During this procedure, the Langevin thermostat[S18] with collision frequency of 2 ps⁻¹ and the Berendsen barostat[S19] with a pressure relaxation time of 2 ps were used to maintain the temperature and density of the system. The time step in all simulations is 2 fs. The root mean square displacement (RMSD) of the enzyme backbone relative to the starting crystal structure (Fig. S12 in the ESI) was calculated using the cpptraj[S20] in the AmberTools 17 package.
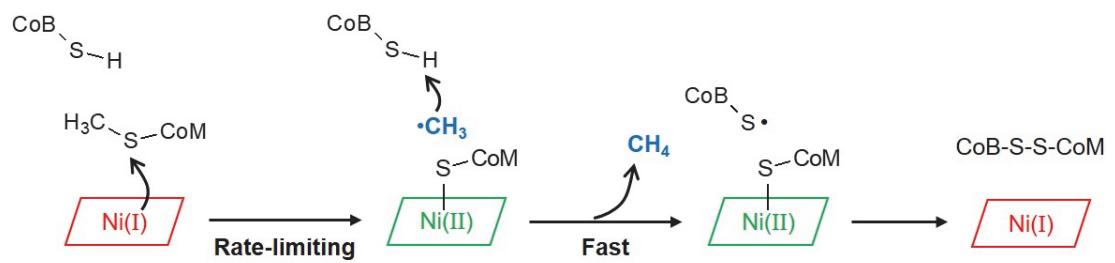
Scheme S1. Catalytic mechanism for the MCR reaction.
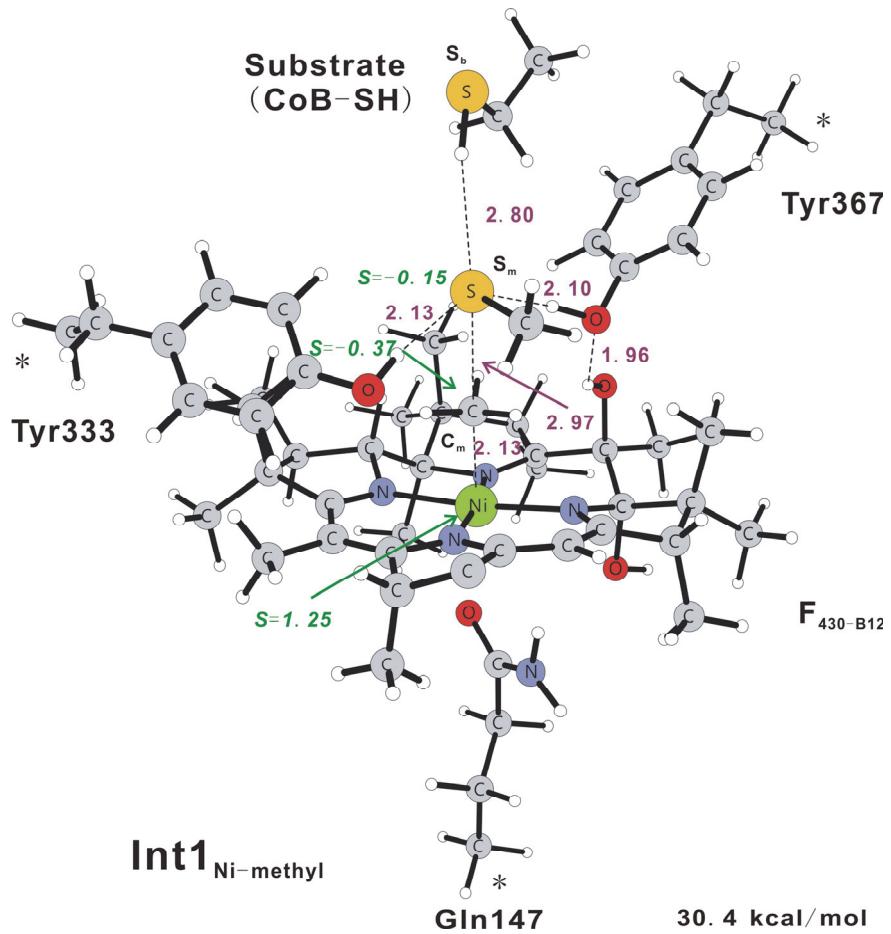
Fig. S1 Optimized structures of a methyl-Ni($F_{430-B12}$) intermediate (**Int1$_{Ni-methyl}$**) using the $F_{430-B12}$ cofactor. Asterisks indicate atoms that are fixed to their X-ray positions. All distances are given in angstrom (Å). The unpaired spin population is indicated by "S". S_m=The sulphur of CH_3-SCoM; C_m=The methyl carbon of CH_3-SCoM; S_b=The sulphur of CoB-SH. For clarity, several atoms in the porphyrinoid are omitted. Its energy relative to the enzyme-substrate complex of Fig. 2 is calculated to be 30.4 kcal/mol.
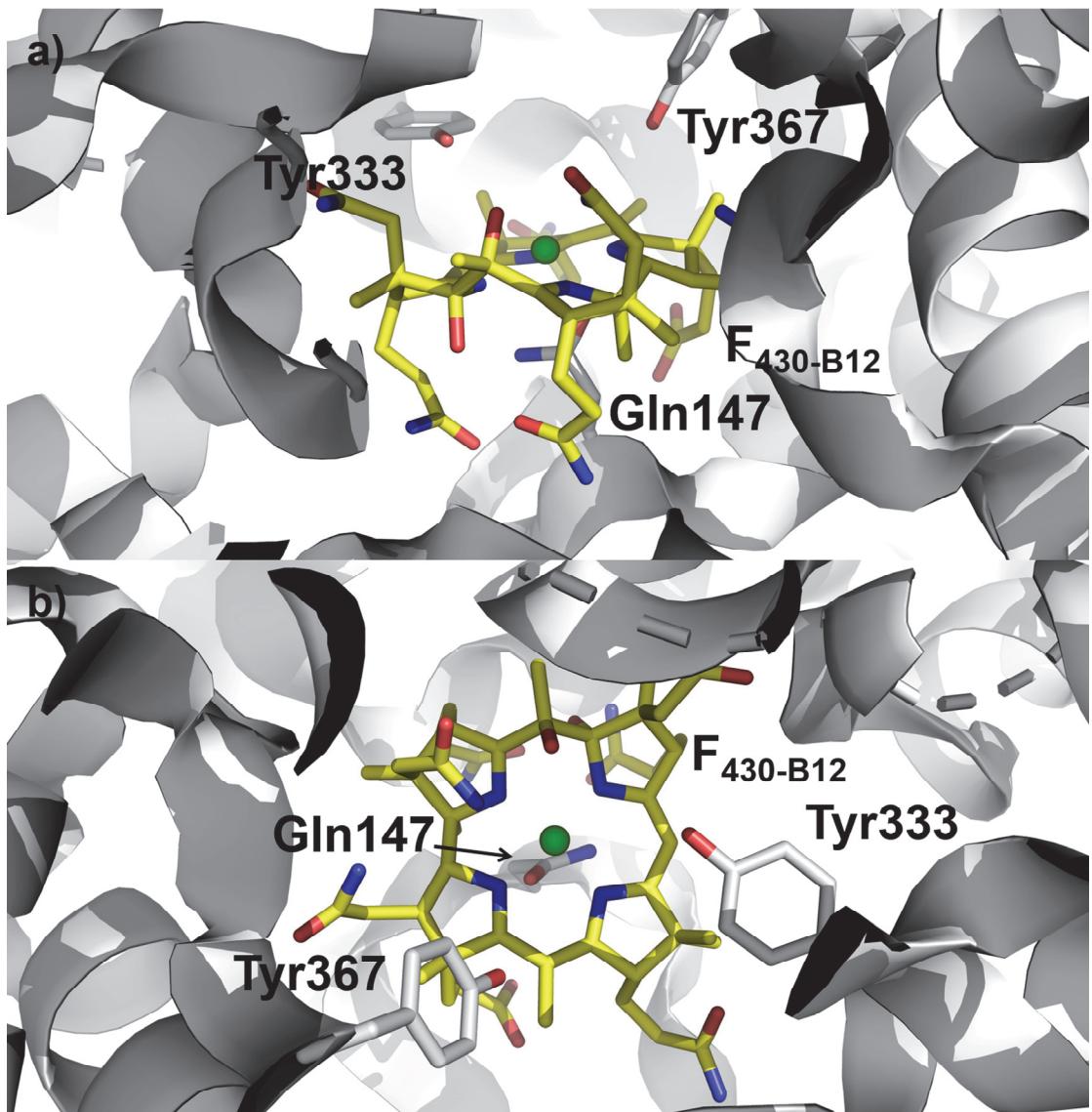
Fig. S2 Structure of the MCR active site with a $F_{430-B12}$ cofactor embedded from the different views a) and b), predicted by a docking simulation. The long adenosyl tail has been hydrolyzed to a propionyloxy.
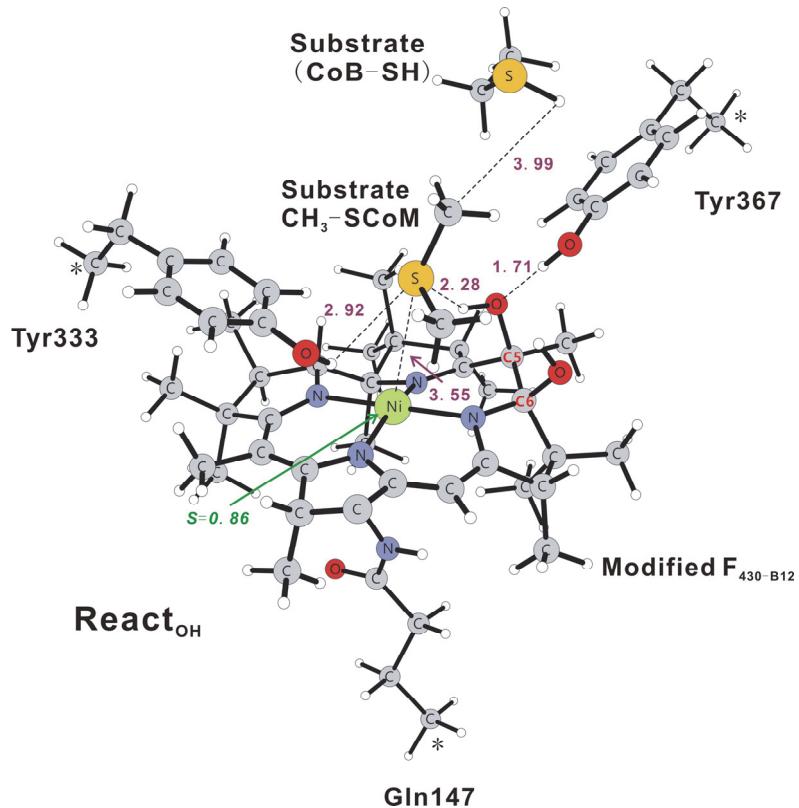
Fig. S3 Optimized structure of the MCR active site with a modified Ni(I) $F_{430-B12}$ cofactor bound (**React$_{OH}$**). The C6 hydroxyl is changed towards the β side (R configuration).
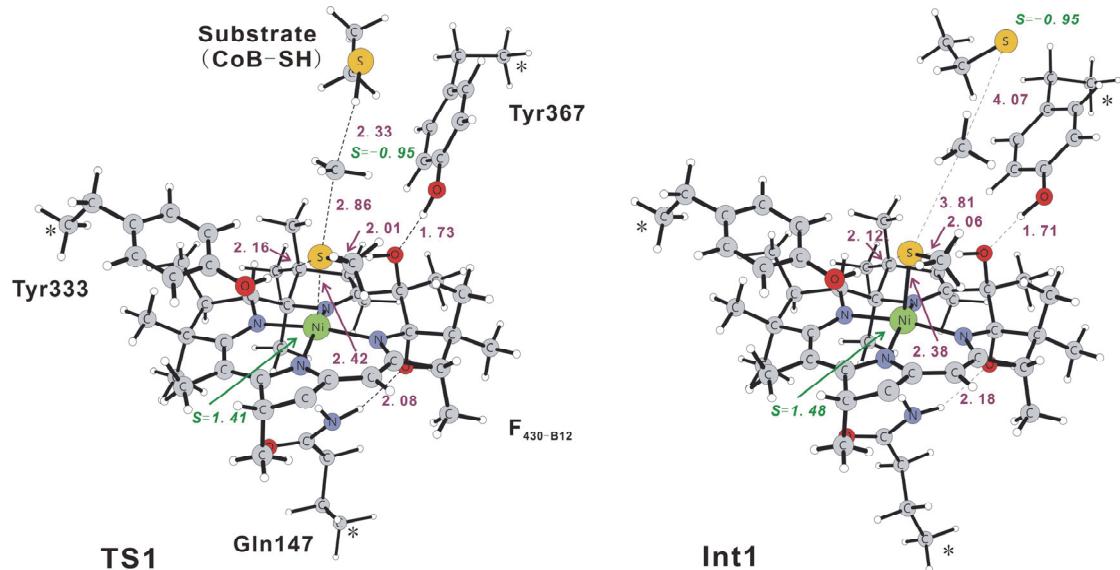
Fig. S4 Optimized structures of the transition state for methane formation (**TS1**) and the resulting CoM-S-Ni(F$_{430\text{-}B12}$) intermediate (**Int1**) in the MCR reaction using the F$_{430\text{-}B12}$ cofactor. Asterisks indicate atoms that are fixed to their X-ray positions. All distances are given in angstrom (Å). The unpaired spin population is indicated by "S". S$_m$=The sulphur of CH$_3$-SCoM; C$_m$=The methyl carbon of CH$_3$-SCoM; S$_b$=The sulphur of CoB-SH. For clarity, several atoms in the porphyrinoid are omitted.
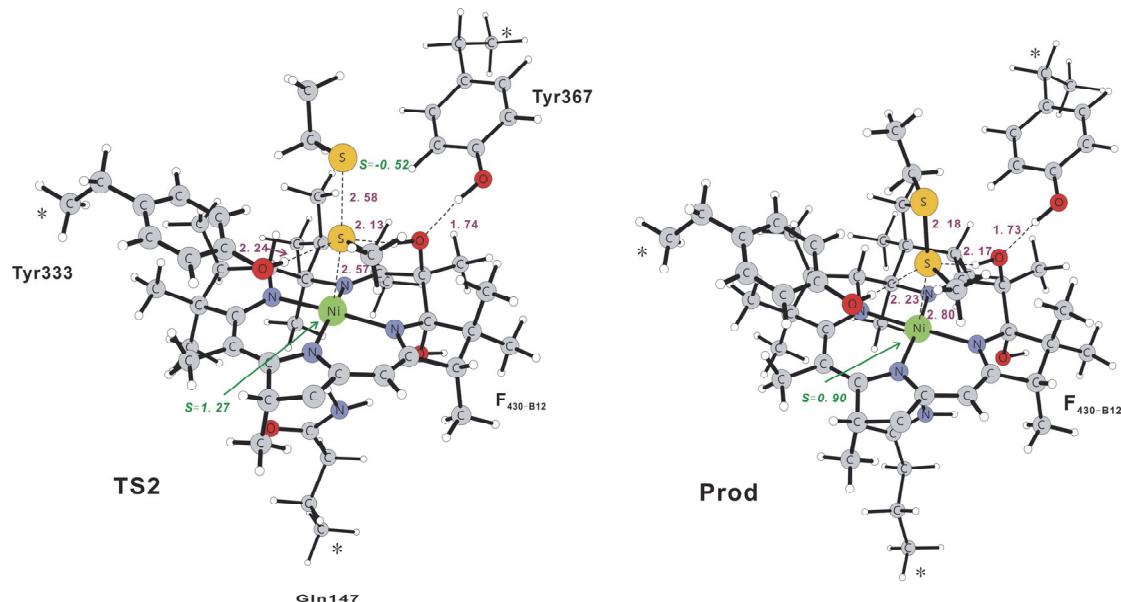
Fig. S5 Optimized structures of the transition state for the S-S bonding (**TS2**) and the final enzyme-product complex (**Prod**).
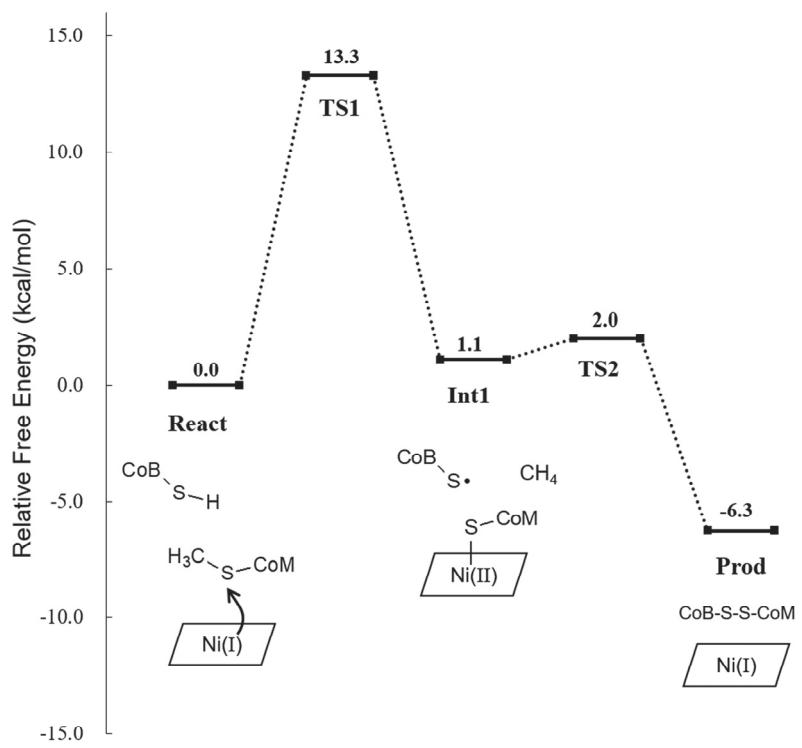
Fig. S6 Potential energy profile for the MCR reaction using a $F_{430\text{-}B12}$ cofactor.
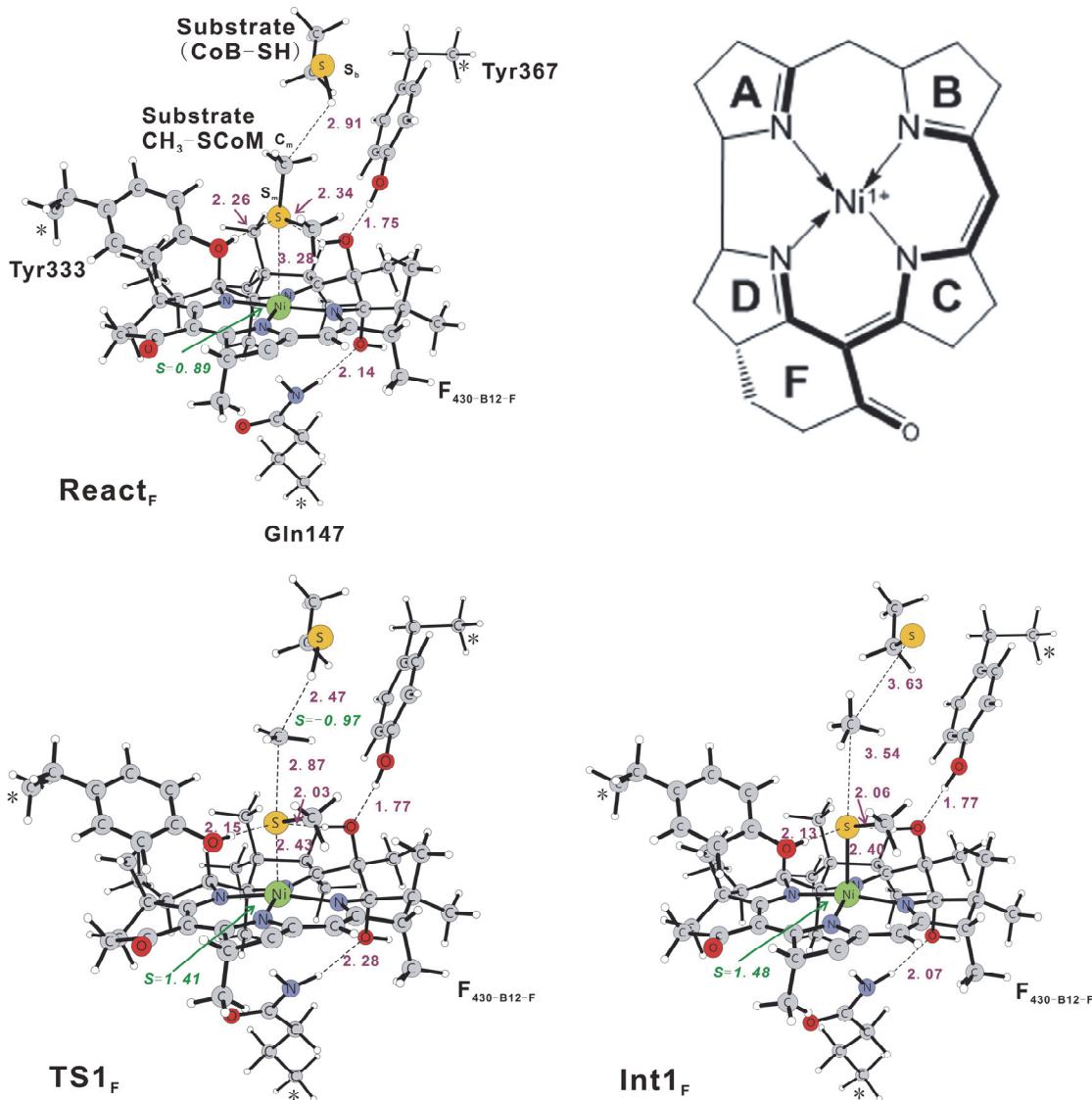
Fig. S7 Optimized structure of the MCR active site with a $F_{430-B12-F}$ cofactor bound (**React$_F$**), the schematic structure of $F_{430-B12-F}$ (upper right), the transition state for methane formation (**TS1$_F$**), and the resulting CoM-S-Ni($F_{430-B12-F}$) intermediate (**Int1$_F$**).
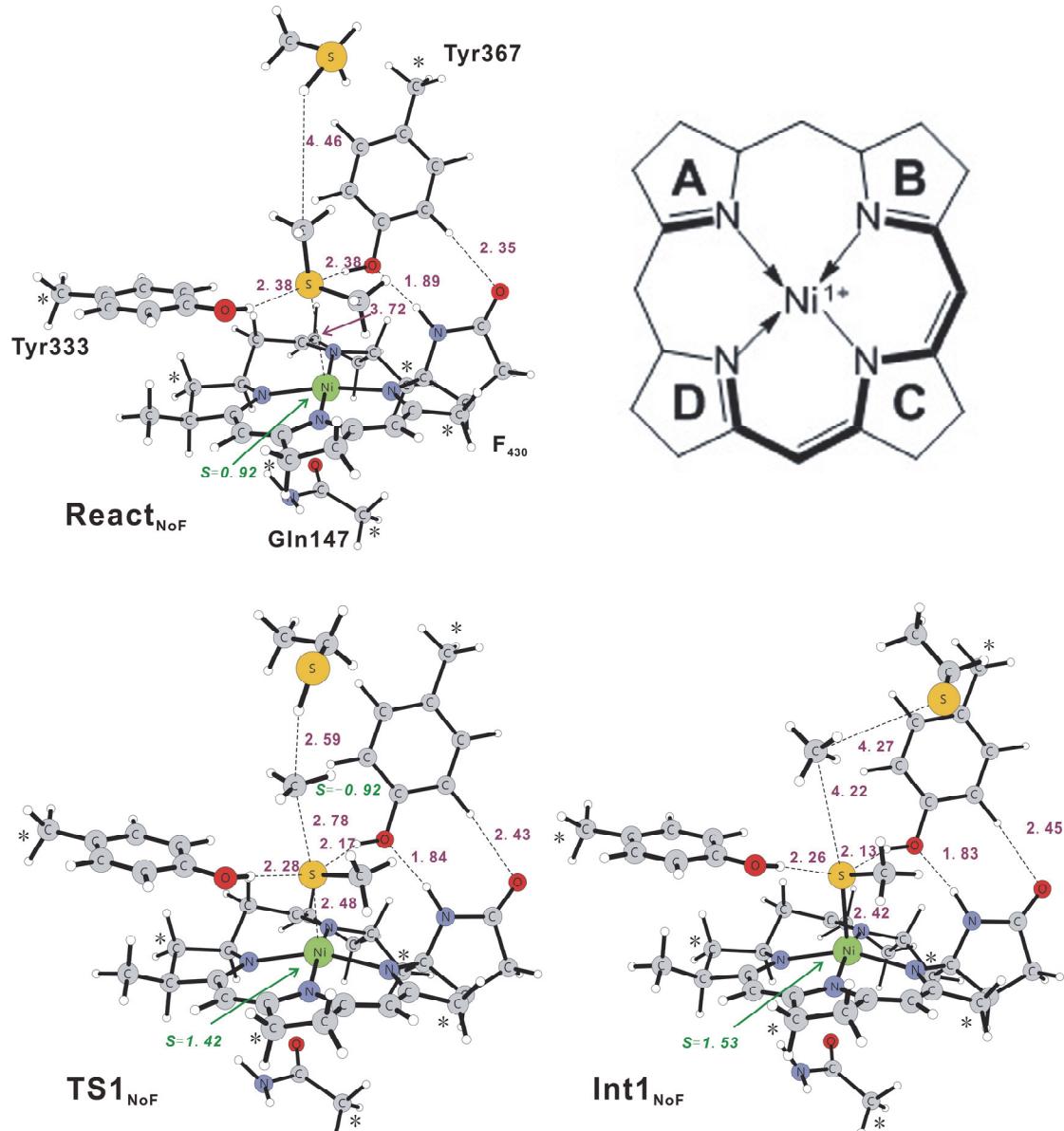
Fig. S8 Optimized structure of the MCR active site with a $F_{430\text{-NoF}}$ cofactor bound (**React$_{NoF}$**), the schematic structure of $F_{430\text{-NoF}}$ (upper right), the transition state for methane formation (**TS1$_{NoF}$**), and the resulting CoM-S-Ni($F_{430\text{-NoF}}$) intermediate (**Int1$_{NoF}$**).
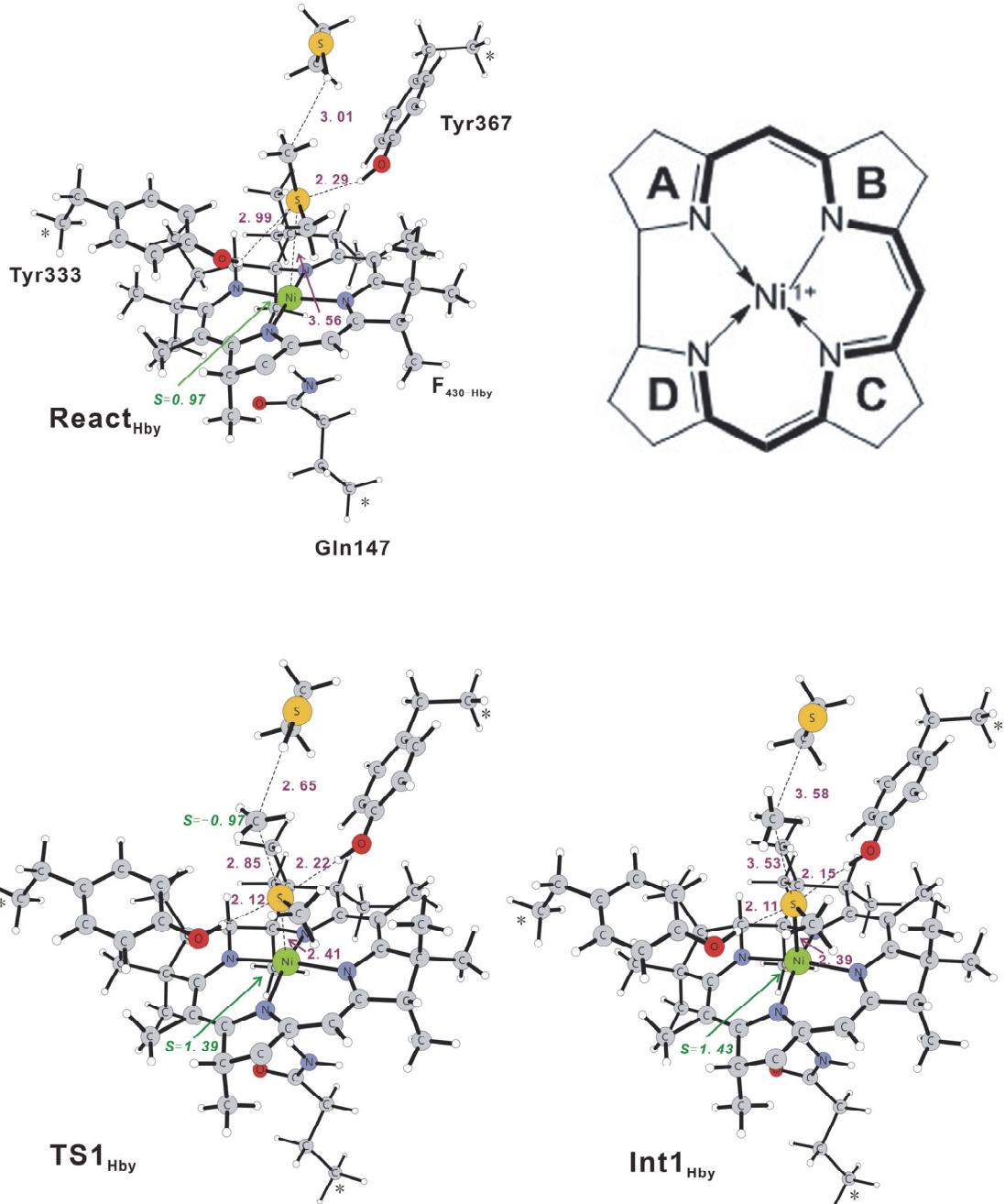
Fig. S9 Optimized structure of the MCR active site with a $F_{430-Hby}$ cofactor bound (**React_Hby**), the schematic structure of $F_{430-Hby}$ (upper right), the transition state for methane formation (**TS1_Hby**), and the resulting CoM-S-Ni($F_{430-Hby}$) intermediate (**Int1_Hby**).
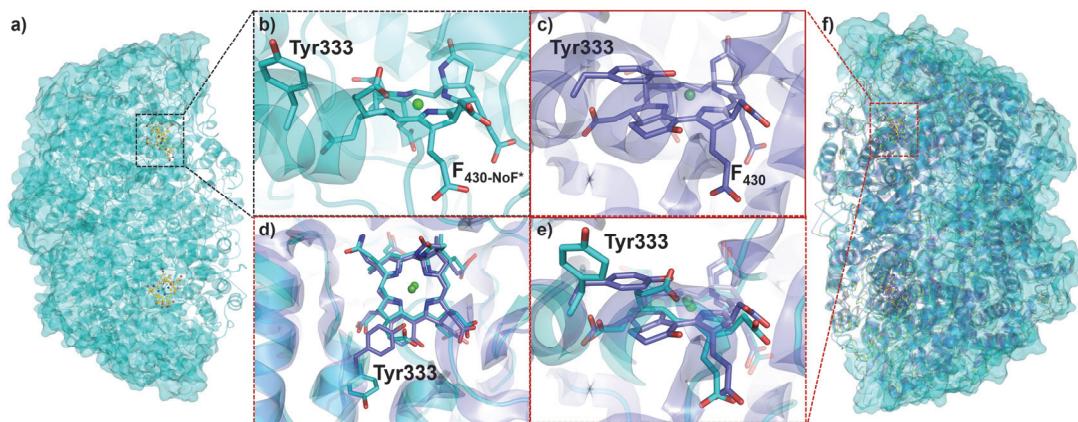
Fig. S10 Structure of MCR in the MD simulation with the F_{430} F ring modified to its propionyloxy precursor. a) The MCR structure in the final frame of 100 ns MD simulation at 60 °C. b) The positions of Tyr333 and modified F_{430} ($F_{430-NoF*}$) from the final MD frame. c) The crystal structure of MCR containing a native F_{430} (PDB code: 1HBN).[S9] d) and e) Superimposition between the final MD frame (cyan) and the crystal structure (purple) from the different views. f) Superimposition of all MCR structures between MD (cyan) and crystal (purple).
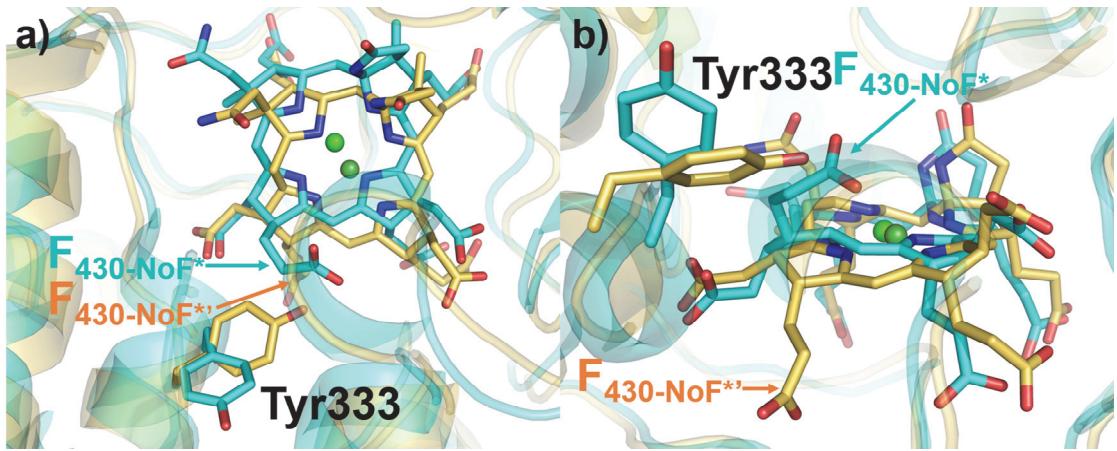
Fig. S11 Structures of the MCR active sites in the MD simulations using a modified F_{430} with the propionyloxy (the precursor of **F** ring) changed to the α face (the opposite side to Tyr333) ($F_{430\text{-NoF}*'}$, in yellow). The one with the propionyloxy locating in the β face (the same side of Tyr333, a natural orientation in F_{430}) ($F_{430\text{-NoF}*}$, in cyan) is shown also. Two different views are given in a) and b).
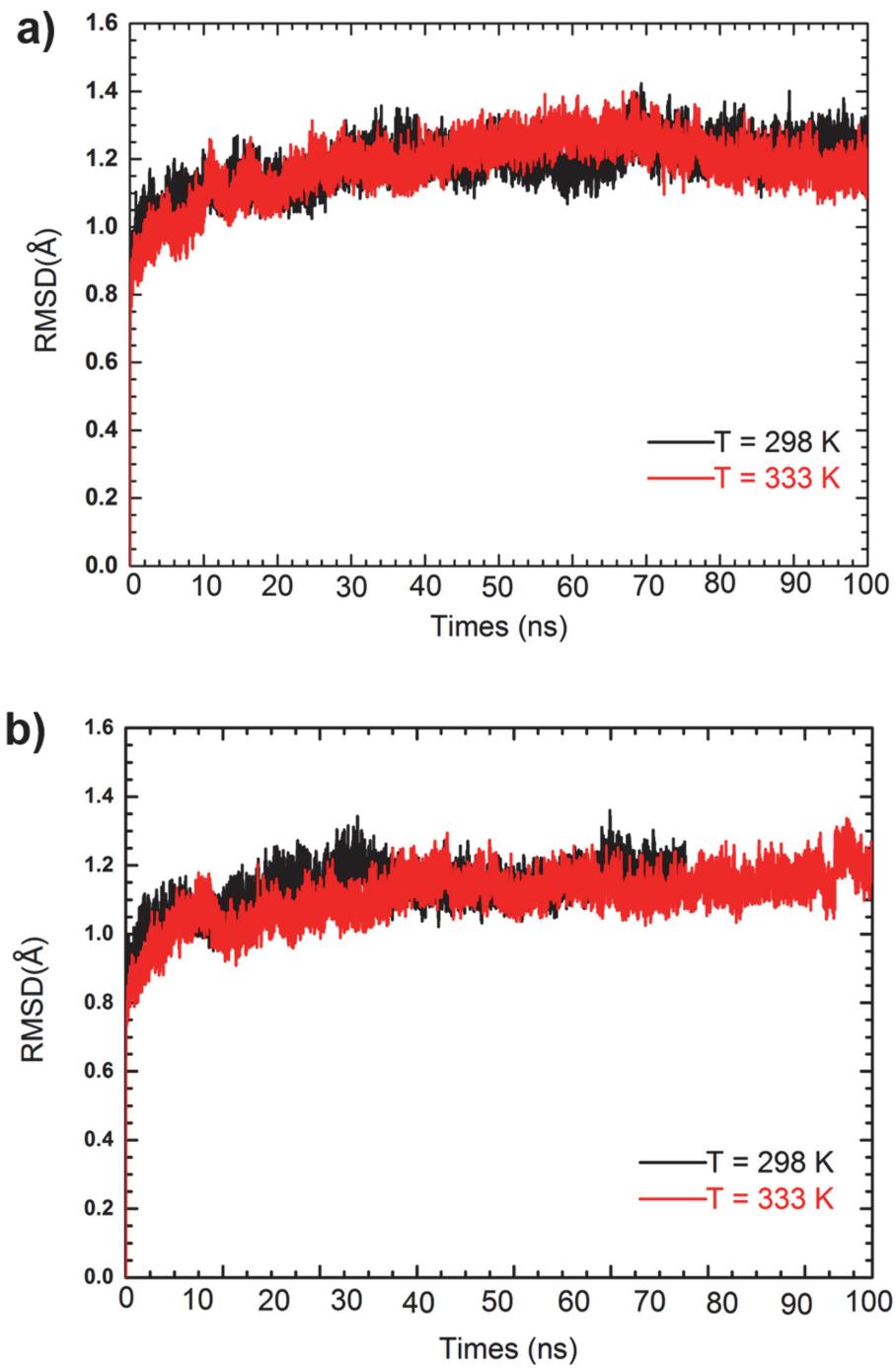
Fig. S12 Root mean square deviation (RMSD) of the protein backbone in the molecular dynamics (MD) simulations of the MCR protein with the F_{430} **F** ring modified to its propionyloxy precursor in the β side (R configuration) (a) and the α side (S configuration) (b).

Table S1. Unpaired spin populations of stationary points in the MCR methane Formation.

Entry	Complex[a]	Spin			
		Ni	S_m[b]	C_m[c]	S_b[d]
1	React	0.87	0.00	0.00	0.00
2	TS1	1.41	0.15	-0.95	-0.04
3	Int1	1.48	0.18	0.00	-0.95
4	TS2	1.27	-0.04	-	-0.52
5	Prod	0.90	-0.02	-	-0.05
6	React$_F$	0.89	0.00	0.00	0.00
7	TS1$_F$	1.41	0.16	-0.97	-0.02
8	Int1$_F$	1.48	0.19	-0.00	-0.97
9	React$_{NoF}$	0.92	0.00	0.00	0.00
10	TS1$_{NoF}$	1.42	0.16	-0.92	-0.02
11	Int1$_{NoF}$	1.53	0.20	-0.00	-0.97
12	React$_{F430}$[e]	0.91	0.00	0.00	0.00
13	TS1$_{F430}$[e]	1.40	0.17	-0.90	-0.02
14	Int1$_{F430}$[e]	1.56	0.17	0.00	-0.97
15	React$_{Hby}$	0.97	0.00	0.00	0.00
16	TS1$_{Hby}$	1.37	0.16	-0.97	-0.01
17	Int1$_{Hby}$	1.43	0.12	-0.38	-0.66

[a] Abbreviations signify reacting state (React), TS for methane formation (TS1), CoM-S-Ni(II) intermediate (Int1), transition state for the S-S bonding (TS2) and the final enzyme-product complex (Prod); subscripts indicate the $F_{430-B12-F}$ (F), $F_{430-NoF}$ (NoF), F_{430} (F430) cofactors, and $F_{430-Hby}$ (Hby) cofactors. [b] The sulphur of CH_3-SCoM. [c] The methyl carbon of CH_3-SCoM. [d] The sulphur of CoB-SH. [e] These data are taken from the previous calculations of F_{430}.[S7c]

Cartesian Coordinates of Optimized Structures

The abbreviations used here are consistent with those in the text.

React

Ni	0.45701870	-2.18069955	2.00785910
N	1.42438829	-1.11938847	0.64059809
C	2.46288850	-1.00004456	-1.49166577
C	2.29297380	0.44495013	-0.86680709
C	1.44225444	0.12593340	0.35603937
N	-0.00247890	-0.51423214	2.99756822
C	0.46735384	1.07083482	1.09734136
C	0.46481232	0.82330068	2.66397174
C	-0.40717842	1.77592114	3.58975350
C	-0.60746030	0.84708785	4.83322127
C	-0.54138565	-0.53313835	4.20568513
N	-0.03338268	-3.41808860	3.46823324
C	-0.96084892	-1.68835280	4.90724495
C	-0.69412003	-3.01347722	4.57658311
C	-1.12932777	-4.21940097	5.40528952
C	-0.09685858	-5.28200904	4.91554535
C	0.27390144	-4.76332947	3.52107986
N	1.05569830	-3.71775619	0.90976916
C	0.90452450	-5.50363793	2.53418401
C	1.36806381	-4.93521407	1.27246831
C	2.48104864	-4.51729027	-0.86800128
C	1.61665229	-3.32430241	-0.38752007
H	-1.47493322	-1.50917691	5.84551366
H	0.76007729	-3.18425102	-1.05411067
C	-3.19189671	-1.86160335	1.81707426
H	-2.39094508	-2.05340965	2.53313645
H	-3.94369227	-2.65041873	1.89015293
H	-3.63830460	-0.88615208	2.03013697
S	-2.43471706	-1.85553495	0.15571183
C	-3.83159653	-1.21231805	-0.83450266
H	-3.51166001	-1.20936072	-1.87886309
H	-4.07001168	-0.18990358	-0.52903315
H	-4.70432142	-1.86335509	-0.73653537
S	-5.71628102	0.34812624	-3.79206563
C	-3.94592419	0.58716129	-4.27263133
H	-3.43128126	-0.37851350	-4.23186472
H	-3.48538989	1.26070751	-3.55067727
C	-3.86455400	1.18191800	-5.67637300
H	-4.34519413	2.16381489	-5.70700442
H	-2.81501124	1.30783751	-5.96481180
H	-4.34486533	0.53742588	-6.42084583
C	2.32031344	-1.92272885	-0.21808172
C	3.62469807	-2.10660519	0.58585244
H	3.41680887	-2.70300422	1.47531510
H	4.40096572	-2.61045008	0.00722615
H	4.01800247	-1.14628749	0.92204680
C	1.27317332	-1.19079272	-2.45957837
H	1.32796452	-0.44616777	-3.26189148
H	1.27428618	-2.17728354	-2.92953424
H	0.31376320	-1.05950036	-1.94682676
C	3.76966385	-1.20281724	-2.26569062
H	3.83185627	-2.23003478	-2.64138283
H	3.81561839	-0.53192972	-3.13127633
H	4.65663164	-1.01930003	-1.65533600
O	1.85829105	0.87048164	3.07404888

H	2.14655096	1.79133361	3.09048047
C	-1.80694926	2.04346775	2.99804997
H	-2.30882873	1.11097407	2.73071526
H	-2.42071835	2.55666262	3.74657989
H	-1.78806025	2.67235453	2.10815994
C	0.24101155	3.11792952	3.96401752
H	0.30157676	3.80163210	3.11454035
H	-0.36519801	3.61342385	4.73008303
H	1.24293274	3.00439646	4.38954126
C	-1.13866752	-3.97816293	6.91883678
H	-1.93752139	-3.28173863	7.19476465
H	-1.32640621	-4.91501392	7.45517399
H	-0.19305256	-3.56198245	7.27568745
C	-2.54679774	-4.62985534	4.93320449
H	-2.88045509	-5.52395316	5.47369034
H	-3.26519404	-3.82598963	5.12859724
H	-2.55596042	-4.84866397	3.86111629
C	1.06043086	-6.99695545	2.76289545
H	0.41041256	-7.56241466	2.08518096
H	2.08380159	-7.34772590	2.61072403
H	0.78285533	-7.28440086	3.77539798
C	2.33246339	-5.61614803	0.26781610
C	1.81029390	-6.95924674	-0.28175495
H	1.85430833	-7.74474566	0.47122151
H	0.77881827	-6.88714537	-0.63073698
H	2.43213423	-7.29270899	-1.11791742
C	3.71144671	-5.82779132	0.93821978
H	3.67605416	-6.58901439	1.72100713
H	4.43632353	-6.16062485	0.18511873
H	4.08248394	-4.91025843	1.40277467
C	0.76159825	2.53539777	0.76256696
H	1.67901350	2.88019726	1.24475957
H	0.87449957	2.67076942	-0.31386244
H	-0.06253137	3.17121756	1.08239936
O	-0.81280444	0.79335950	0.52272950
H	-1.04111994	-0.16224439	0.59553350
H	-1.60103403	1.01952359	5.26548363
C	0.42663216	0.97238432	5.96869839
H	0.38038508	1.95565893	6.44805196
H	0.22762172	0.21617068	6.73410570
H	1.43960441	0.81085328	5.59259349
C	1.17787168	-5.36585385	5.77922300
H	1.66435240	-4.38706063	5.84746498
H	0.95344802	-5.71404850	6.79259720
H	1.90175222	-6.05234269	5.33308563
H	-0.57544395	-6.26461595	4.87726287
H	3.53273133	-4.22161486	-0.89503598
C	2.10879812	-4.95056675	-2.29119338
H	2.25372508	-4.11679942	-2.98673291
H	2.73420379	-5.77498751	-2.64677708
H	1.06347904	-5.26471905	-2.35699363
C	3.58178978	1.22662932	-0.54513152
H	3.34604484	2.21726704	-0.14814026
H	4.20628861	0.71479492	0.18997718
H	4.17758275	1.37205592	-1.45119622
H	1.71285916	1.06159467	-1.56585750
H	-5.52404035	0.33999227	-2.45929227
C	0.03880500	-8.95451900	-3.01748400
C	-1.45489891	-8.59932598	-2.87404606
C	-1.69219823	-7.62073992	-1.74370556
C	-2.01868111	-8.05557897	-0.45287545

C	-1.49796258	-6.24639917	-1.93614593
C	-2.12841421	-7.16134350	0.61237910
C	-1.59163843	-5.33993225	-0.88274086
C	-1.90137969	-5.79836148	0.40409445
O	-2.01933504	-4.95644877	1.47341266
C	-2.33178300	6.38467200	-4.58248000
C	-2.62334567	4.91055515	-4.91812160
C	-2.76687052	4.07446895	-3.66594475
C	-3.97116780	4.06070575	-2.94734011
C	-1.69125609	3.34762162	-3.14506005
C	-4.09708646	3.37066114	-1.74530409
C	-1.80130439	2.63705289	-1.94976062
C	-3.00537543	2.66166062	-1.23087369
O	-3.16711931	2.00587882	-0.04855144
H	-2.03368363	-9.51544070	-2.70380931
H	-1.81700281	-8.17225550	-3.81810441
H	-2.17636504	-9.11700360	-0.27250832
H	-1.26009033	-5.87741527	-2.93225111
H	-2.37144924	-7.50203586	1.61433772
H	-1.44167622	-4.27837155	-1.04310780
H	-1.41820289	-4.20054144	1.36364921
H	0.41865692	-9.40991377	-2.09660336
H	-3.54146199	4.84782964	-5.51616982
H	-1.81676505	4.50915750	-5.54415218
H	-0.74829624	3.32625738	-3.68852726
H	-4.83039052	4.60056650	-3.33936479
H	-0.97558678	2.04349445	-1.57406805
H	-5.03253045	3.36284304	-1.19466102
H	-2.31159422	1.60266057	0.21565112
H	-1.40525142	6.47374915	-4.00496520
H	0.63413027	-8.05495126	-3.20770118
H	0.20562474	-9.65698082	-3.84224237
H	-3.13982185	6.81043247	-3.97794717
H	-2.22899511	6.99063059	-5.49011945
C	7.27036300	-0.96856400	5.68488600
C	6.04420584	-1.85895767	5.45349308
C	5.19353326	-1.42280380	4.24655916
C	4.03432902	-2.39614114	4.03464961
O	4.24002225	-3.59137532	3.82426484
N	2.78440606	-1.87189138	4.15334183
H	5.41116797	-1.85755694	6.35081977
H	6.34769187	-2.89860062	5.28938182
H	4.83350605	-0.39475652	4.38079887
H	5.80962077	-1.44389001	3.33836615
H	2.61036272	-0.88776849	3.98203762
H	2.01555418	-2.48183690	3.89184324
H	6.97894152	0.07224842	5.87148874
H	7.93401328	-0.97479427	4.81177548
H	7.85165866	-1.31147739	6.54772056

TS1

Ni	0.34498200	-2.17618200	2.28925900
N	1.51935000	-1.09582600	1.04966000
C	2.51727600	-0.95658100	-1.09844300
C	2.36676500	0.47725500	-0.45160800
C	1.52504400	0.14851200	0.77393000
N	0.02522600	-0.51643500	3.37676100
C	0.54460500	1.10280400	1.49908600
C	0.49928100	0.82597900	3.06090500
C	-0.40051700	1.76260300	3.97334500

C	-0.62352700	0.82095200	5.20406600
C	-0.54552100	-0.54974400	4.56423300
N	-0.05518500	-3.41848900	3.78034000
C	-1.00795700	-1.71259300	5.22976700
C	-0.76075400	-3.03107800	4.86791900
C	-1.25681500	-4.25153000	5.63445700
C	-0.20257100	-5.30706400	5.18219000
C	0.22832800	-4.77281800	3.81347000
N	1.14815100	-3.68810500	1.28696600
C	0.89006900	-5.50701400	2.84917900
C	1.39547600	-4.92248700	1.60921700
C	2.50376900	-4.48670600	-0.53031200
C	1.67735800	-3.28356600	-0.01301800
H	-1.55493600	-1.54652900	6.15041800
H	0.80068200	-3.12531900	-0.64898300
C	-2.99376600	-1.66186900	2.11666700
H	-2.57695500	-1.53976600	3.11654700
H	-3.69052700	-2.50350000	2.12574700
H	-3.53205800	-0.75601400	1.82881800
S	-1.64054600	-1.98971000	0.91124600
C	-3.49205000	-1.16854800	-1.10087700
H	-2.83253100	-1.37347300	-1.93295600
H	-3.51562300	-0.17875900	-0.66479300
H	-4.19472300	-1.92698300	-0.78326200
S	-5.53460600	0.23113200	-3.67983600
C	-3.82010600	0.57889600	-4.27500100
H	-3.25838600	-0.35986200	-4.27873900
H	-3.34256400	1.26810900	-3.57651200
C	-3.86455400	1.18191800	-5.67637300
H	-4.42210900	2.12405100	-5.67887100
H	-2.84752500	1.39653300	-6.02227100
H	-4.33531300	0.50183300	-6.39336900
C	2.39752500	-1.89649300	0.16535600
C	3.71433600	-2.10671600	0.93744900
H	3.52873900	-2.73615500	1.80862600
H	4.47398200	-2.59181200	0.32284900
H	4.11881200	-1.15913800	1.29399900
C	1.30671400	-1.12806600	-2.04395100
H	1.35023500	-0.36945700	-2.83257700
H	1.30018700	-2.10449100	-2.53268500
H	0.35574100	-1.00572400	-1.51464000
C	3.80678700	-1.15582100	-1.89988200
H	3.85694500	-2.17838900	-2.28811500
H	3.83683200	-0.47669700	-2.75881200
H	4.70615800	-0.98182400	-1.30567300
O	1.88257600	0.85923300	3.50613300
H	2.17081400	1.77842800	3.56560400
C	-1.78497400	2.02335200	3.34227300
H	-2.27478900	1.09054400	3.05651800
H	-2.41972200	2.53327200	4.07470200
H	-1.74175100	2.65042400	2.45229000
C	0.22869300	3.10370000	4.37950300
H	0.30354000	3.79753800	3.54070500
H	-0.40069000	3.58358100	5.13586800
H	1.22014800	2.99225500	4.82870500
C	-1.36780300	-4.05414100	7.14927200
H	-2.18253900	-3.36361100	7.38921600
H	-1.59543400	-5.00627500	7.63979700
H	-0.44787100	-3.65472900	7.58320500
C	-2.64198900	-4.63505100	5.05431200
H	-3.01887100	-5.53173000	5.55915900

H	-3.36284100	-3.82630000	5.21184100
H	-2.57994400	-4.84097900	3.98203200
C	1.03610400	-7.00171600	3.06681900
H	0.37020700	-7.55640000	2.39689600
H	2.05335100	-7.35733200	2.89299600
H	0.77803600	-7.29315200	4.08285900
C	2.32079900	-5.61312200	0.57391800
C	1.74158300	-6.91577000	-0.01137400
H	1.73064600	-7.71691700	0.72531200
H	0.72423600	-6.78499700	-0.38046500
H	2.36605900	-7.26144200	-0.84003100
C	3.69693800	-5.89738200	1.22252600
H	3.64648800	-6.69795000	1.96317200
H	4.40468700	-6.21208800	0.44675300
H	4.09846200	-5.01528800	1.72862100
C	0.88385800	2.56841400	1.20932500
H	1.79646300	2.88963800	1.71591800
H	1.01470000	2.72191900	0.13771700
H	0.06084300	3.20730500	1.52420800
O	-0.70472100	0.87286000	0.86271600
H	-0.95591700	-0.10107700	0.89116300
H	-1.62574000	0.98412400	5.61873700
C	0.39056500	0.93069700	6.35909300
H	0.33031500	1.90660600	6.84932400
H	0.18138800	0.16409300	7.11054700
H	1.41035900	0.77994200	5.99813400
C	1.03208800	-5.39087900	6.10258400
H	1.49839700	-4.40688400	6.21675200
H	0.76459800	-5.76428000	7.09536900
H	1.78888200	-6.05392300	5.67777600
H	-0.67524300	-6.29006600	5.11083700
H	3.56381800	-4.22309800	-0.54578300
C	2.11651900	-4.86743300	-1.96419900
H	2.29327900	-4.02226100	-2.63722900
H	2.71277200	-5.70355400	-2.33993100
H	1.06080700	-5.14233600	-2.03744600
C	3.66348200	1.24422500	-0.13050200
H	3.44041500	2.23198600	0.27823400
H	4.29064800	0.71871700	0.59196700
H	4.24900400	1.39274600	-1.04172300
H	1.78052800	1.10873600	-1.13015600
H	-5.14853000	-0.31247100	-2.49872600
C	0.03880500	-8.95451900	-3.01748400
C	-1.43314200	-8.55552700	-2.81114200
C	-1.62214000	-7.60500800	-1.64911000
C	-1.84076400	-8.07969600	-0.34791600
C	-1.53979800	-6.21763500	-1.82634200
C	-1.97215900	-7.21076000	0.73314500
C	-1.66525600	-5.33013900	-0.75719400
C	-1.88773900	-5.82524000	0.53766700
O	-2.04502400	-5.02053300	1.61719000
C	-2.33178300	6.38467200	-4.58248000
C	-2.47515000	4.87192400	-4.84001400
C	-2.60217100	4.07173000	-3.56114700
C	-3.81969300	4.02850100	-2.86355500
C	-1.51491900	3.38520500	-3.00870000
C	-3.94452600	3.35621100	-1.65250700
C	-1.62251400	2.69549500	-1.79846000
C	-2.83797200	2.69839400	-1.09873200
O	-3.00269500	2.07814400	0.10174500
H	-2.03265300	-9.45983900	-2.64957700

H	-1.81333600	-8.09294800	-3.73032000
H	-1.91150100	-9.15185000	-0.17764900
H	-1.38185700	-5.81764500	-2.82597100
H	-2.15247600	-7.58218900	1.73704200
H	-1.61846300	-4.25799400	-0.91580900
H	-1.81674200	-4.09059600	1.37920100
H	0.43554700	-9.44669800	-2.12305000
H	-3.35543300	4.69753300	-5.47177000
H	-1.61031200	4.51686400	-5.41366000
H	-0.56339500	3.38088900	-3.53672900
H	-4.68977700	4.52903200	-3.28197900
H	-0.78108400	2.14205000	-1.39389000
H	-4.89036300	3.32002600	-1.12271400
H	-2.14863800	1.69680500	0.39678600
H	-1.43957500	6.59250600	-3.98235400
H	0.65679500	-8.06976200	-3.20548300
H	0.15326700	-9.63912900	-3.86504100
H	-3.19695200	6.76659400	-4.03054300
H	-2.25220300	6.94283600	-5.52174400
C	7.27036300	-0.96856400	5.68488600
C	6.03185400	-1.86423900	5.58968200
C	5.09000700	-1.47476800	4.43721100
C	3.92073700	-2.45211700	4.34932000
O	4.10853900	-3.65493000	4.17217000
N	2.68223000	-1.91720700	4.52864100
H	5.47300500	-1.82468300	6.53364600
H	6.32230200	-2.90994200	5.44468300
H	4.74089600	-0.44169000	4.55561300
H	5.63430800	-1.53340700	3.48645800
H	2.50606900	-0.93256700	4.36653500
H	1.89439300	-2.53692400	4.38027200
H	6.99313200	0.07904000	5.85170600
H	7.86044000	-1.01148100	4.76195000
H	7.91953200	-1.27680700	6.51079700

Int1

Ni	0.47161487	-2.26411189	2.08849214
N	1.34340605	-1.08103080	0.69158003
C	2.02421572	-0.84520956	-1.56654600
C	1.86108893	0.56952873	-0.87442924
C	1.22438706	0.16521505	0.44876478
N	0.24340476	-0.63526696	3.25152834
C	0.30585225	1.02797086	1.34554898
C	0.55405500	0.74062233	2.88709065
C	-0.24168926	1.60095176	3.95862477
C	-0.19009249	0.63312899	5.18787840
C	-0.11778006	-0.72285549	4.51552325
N	0.47217542	-3.53627976	3.61605441
C	-0.36939415	-1.92163333	5.22763558
C	-0.07766536	-3.21281953	4.80971202
C	-0.33169703	-4.47101005	5.63127013
C	0.71115456	-5.43705812	4.98885751
C	0.86798766	-4.86218310	3.57804532
N	1.24359142	-3.69957067	0.94503625
C	1.41878051	-5.53283759	2.50442200
C	1.65810562	-4.90377734	1.20813327
C	2.34742016	-4.36975032	-1.08253731
C	1.52048863	-3.24246891	-0.41549344
H	-0.76802554	-1.80240272	6.22866185
H	0.54270022	-3.14656808	-0.89940497

C	-2.88097257	-2.09067292	2.57417702
H	-2.40231867	-1.55654588	3.39640264
H	-3.18905547	-3.07633832	2.93343864
H	-3.76520959	-1.53783439	2.24635380
S	-1.72134306	-2.26968969	1.15527501
C	-4.29270901	-0.32255179	-0.86859595
H	-3.41299576	-0.20924135	-1.50671776
H	-4.24635095	0.42399769	-0.07355034
H	-4.28866338	-1.32682681	-0.43966071
S	-5.80616119	2.03814413	-3.82365659
C	-4.35711047	1.02181033	-4.23429128
H	-4.56299985	-0.02549936	-3.99007479
H	-3.58813048	1.36474294	-3.52842221
C	-3.86454600	1.18192800	-5.67638000
H	-3.62325885	2.22778885	-5.88875813
H	-2.96286715	0.57760176	-5.83647509
H	-4.62229366	0.85372399	-6.39488352
C	2.14896612	-1.80221869	-0.31837964
C	3.57183279	-1.91392683	0.26508065
H	3.54620334	-2.53229918	1.16390477
H	4.26515848	-2.36971138	-0.44351521
H	3.96405672	-0.93596187	0.54643358
C	0.70881358	-1.09970367	-2.33774342
H	0.58122897	-0.33172213	-3.10914796
H	0.70550963	-2.06961700	-2.84073385
H	-0.16443948	-1.05886344	-1.67718264
C	3.20210849	-0.93911368	-2.54147130
H	3.26993210	-1.95066973	-2.95652457
H	3.06508149	-0.24755534	-3.38047869
H	4.16117072	-0.70757382	-2.07252885
O	1.98660128	0.87582555	3.09080163
H	2.21081908	1.81473351	3.09225487
C	-1.72838848	1.77646701	3.57738371
H	-2.19306780	0.82156196	3.32272114
H	-2.26668660	2.20015220	4.43289887
H	-1.88137310	2.44763312	2.73260535
C	0.35749556	2.97817996	4.28153959
H	0.24201497	3.68317637	3.45624599
H	-0.16506881	3.40714459	5.14320320
H	1.41676749	2.93196511	4.55349652
C	-0.19013242	-4.27833497	7.14459882
H	-1.00646911	-3.66051944	7.53301616
H	-0.24176262	-5.24439481	7.65836745
H	0.75370165	-3.79651431	7.41158865
C	-1.76191393	-4.96627587	5.29885687
H	-1.97361900	-5.88788711	5.85377081
H	-2.50585439	-4.21601048	5.58740195
H	-1.87136388	-5.17217566	4.23057675
C	1.73355515	-7.00828471	2.67112760
H	1.02625405	-7.62174213	2.10205510
H	2.74128642	-7.26469554	2.33714297
H	1.66386441	-7.32601429	3.70996538
C	2.46431756	-5.50188985	0.02656531
C	1.92678577	-6.85982085	-0.46536699
H	2.13185627	-7.65561464	0.24897755
H	0.85056704	-6.83633333	-0.64082965
H	2.42014567	-7.14285360	-1.39971804
C	3.94929444	-5.64174681	0.43917893
H	4.09819235	-6.42360577	1.18703913
H	4.54597258	-5.90658125	-0.44201164
H	4.34028270	-4.71439831	0.86569296

C	0.47638333	2.51857320	1.03298776
H	1.43020484	2.90599145	1.39821071
H	0.42527347	2.69426347	-0.04172712
H	-0.33399638	3.08900636	1.48327263
O	-1.01392260	0.69674672	0.93074928
H	-1.20428384	-0.28560003	1.01700797
H	-1.12010918	0.71637862	5.76309041
C	0.98823215	0.80618194	6.16570966
H	0.94220582	1.77173491	6.67871988
H	0.95782866	0.01993759	6.92612614
H	1.94376313	0.73217165	5.64098904
C	2.08399004	-5.43077160	5.69266974
H	2.48419382	-4.41322087	5.75060187
H	2.01219451	-5.83492254	6.70730136
H	2.81087914	-6.02463403	5.13394850
H	0.30872255	-6.45338249	4.97479030
H	3.35970961	-4.01099725	-1.28656651
C	1.74475699	-4.79325893	-2.42759327
H	1.72119246	-3.93871138	-3.11215764
H	2.33589190	-5.57505925	-2.91365877
H	0.72111601	-5.16129765	-2.31313425
C	3.12870661	1.43211866	-0.71928936
H	2.88701743	2.39966827	-0.27307161
H	3.88556581	0.95590997	-0.09251674
H	3.57549496	1.62742203	-1.69834926
H	1.14244725	1.16250294	-1.45377743
H	-5.19644944	-0.16012829	-1.46165951
C	0.03880700	-8.95450900	-3.01747400
C	-1.43718127	-8.78515346	-2.60893219
C	-1.58965190	-7.85298431	-1.42662845
C	-1.56834811	-8.33438670	-0.11065420
C	-1.67074381	-6.46608801	-1.60704729
C	-1.61182691	-7.47221945	0.98320441
C	-1.70971245	-5.58537983	-0.52704509
C	-1.67501337	-6.08716698	0.78400187
O	-1.71752733	-5.28714645	1.87569124
C	-2.33178100	6.38465200	-4.58246600
C	-2.69659488	4.88994104	-4.68488216
C	-2.75210755	4.20257776	-3.33604435
C	-3.74092562	4.56090773	-2.40524390
C	-1.84652129	3.20640773	-2.96179624
C	-3.80503355	3.98054807	-1.14317224
C	-1.90843162	2.59305476	-1.70521064
C	-2.87514326	2.99955204	-0.77450947
O	-2.96191292	2.48754853	0.47850874
H	-1.86296164	-9.76737713	-2.36800392
H	-2.00768950	-8.39961731	-3.46364767
H	-1.51024164	-9.40740067	0.06213113
H	-1.70261921	-6.06202163	-2.61759107
H	-1.59912748	-7.85012442	2.00137815
H	-1.78671286	-4.51404170	-0.68190532
H	-1.60192094	-4.34323847	1.60396097
H	0.62572582	-9.36286594	-2.18740547
H	-3.67247414	4.78936024	-5.17894736
H	-1.96975730	4.37906825	-5.32881676
H	-1.08254874	2.88571448	-3.66814107
H	-4.47853421	5.31175496	-2.67840671
H	-1.22682465	1.79036289	-1.44117033
H	-4.57008774	4.26533068	-0.42776865
H	-2.28544263	1.78521899	0.60847328
H	-1.34630070	6.51376304	-4.12199553

H	0.47903513	-7.98772241	-3.28578767
H	0.14369456	-9.62864290	-3.87569439
H	-3.05851139	6.92405115	-3.96631799
H	-2.31238359	6.85548875	-5.57154982
C	7.27035200	-0.96856400	5.68487000
C	6.04731199	-1.82456551	5.34746582
C	5.54064491	-1.61966876	3.90421429
C	4.31889953	-2.50162682	3.67996140
O	4.42295588	-3.69429239	3.39555335
N	3.11898570	-1.90935841	3.93212990
H	5.22891304	-1.59493455	6.04213524
H	6.27912745	-2.88824102	5.47826660
H	5.30475473	-0.56031346	3.73563674
H	6.31289779	-1.91849711	3.18823902
H	2.97547839	-0.90989700	3.85581699
H	2.29519000	-2.48805588	3.81522857
H	7.04596270	0.10061306	5.58831293
H	8.10827005	-1.19282638	5.01419572
H	7.60830124	-1.14702352	6.71149059

TS2

Ni	0.07135600	-1.95278400	2.40145500
N	0.80192200	-0.57909600	1.14878800
C	1.63006700	-0.01875700	-0.99871200
C	1.34268500	1.28433400	-0.15314900
C	0.63224400	0.67900200	1.04616100
N	-0.36909700	-0.48744900	3.69039200
C	-0.37147400	1.37701100	1.98375300
C	-0.13140000	0.94240900	3.48820200
C	-0.99232900	1.62982300	4.63024800
C	-0.87988400	0.54399300	5.75312200
C	-0.70206500	-0.72708300	4.94596100
N	0.03176300	-3.39747000	3.74070200
C	-0.85220300	-2.00849000	5.53231200
C	-0.47589500	-3.23105700	4.98219300
C	-0.60683400	-4.57506200	5.68994300
C	0.44870200	-5.40911500	4.90260200
C	0.51151500	-4.68224100	3.55748400
N	0.82808900	-3.20930300	1.07659600
C	1.08191300	-5.20202900	2.41178000
C	1.31758400	-4.40973300	1.20923300
C	2.05435400	-3.56491100	-0.96504600
C	1.15802500	-2.56408900	-0.19131000
H	-1.22639800	-2.02074000	6.54944300
H	0.20286400	-2.43327900	-0.71366300
C	-3.38544600	-2.15100600	2.75324300
H	-2.78074200	-2.11361500	3.65465300
H	-3.93894000	-3.09154100	2.71951800
H	-4.07901600	-1.30739600	2.73211200
S	-2.25413200	-2.06068500	1.30899300
S	-4.24040300	-2.02586700	-0.34196100
C	-3.15903500	-2.01943800	-1.82005900
H	-2.55886900	-2.93798900	-1.84622300
H	-2.44115600	-1.18546900	-1.80217000
C	-4.06665800	-1.90615300	-3.03308400
H	-4.63207600	-0.97047800	-3.01337800
H	-3.46761900	-1.92469000	-3.95089600
H	-4.77649900	-2.73705300	-3.07353400
C	1.71042500	-1.12766200	0.12365400
C	3.09398200	-1.25591200	0.79025900

H	3.02886600	-1.95396700	1.62568700
H	3.84768900	-1.61974700	0.09035900
H	3.42981000	-0.29932100	1.19060500
C	0.39154300	-0.20850100	-1.91019400
H	0.32698400	0.63435600	-2.60639000
H	0.45454900	-1.12224700	-2.50456300
H	-0.56081100	-0.23900800	-1.35570300
C	2.88463900	0.05250200	-1.87340900
H	3.03224700	-0.89688300	-2.39917100
H	2.78429800	0.83653600	-2.63180600
H	3.78956400	0.25772200	-1.29833700
O	1.28740100	1.13479400	3.72635800
H	1.47627900	2.08169300	3.73841200
C	-2.48044900	1.73692800	4.22958100
H	-2.87136300	0.77303700	3.89672300
H	-3.06058800	2.06129500	5.10021700
H	-2.66058600	2.45300300	3.42789100
C	-0.49824300	3.00935000	5.09337400
H	-0.68720100	3.78623400	4.35094900
H	-1.03542100	3.30027300	6.00195900
H	0.56672100	3.01954100	5.34238600
C	-0.38386100	-4.51595700	7.20518600
H	-1.20077900	-3.97616300	7.69457500
H	-0.36617600	-5.52659800	7.62643300
H	0.55295100	-4.01806400	7.46644200
C	-2.02193900	-5.12923600	5.39071600
H	-2.13219100	-6.12615500	5.83272600
H	-2.79042000	-4.47926700	5.82195700
H	-2.19319300	-5.20916000	4.31313200
C	1.44745100	-6.67428900	2.40618500
H	0.82368100	-7.22377900	1.69440100
H	2.49395100	-6.85195900	2.14622300
H	1.29001500	-7.13340100	3.38021600
C	2.26482700	-4.77952300	0.03494200
C	1.99871500	-6.13548400	-0.64853600
H	2.28214900	-6.96941300	-0.01117900
H	0.95168800	-6.26594500	-0.92320700
H	2.60855200	-6.21580100	-1.55368800
C	3.71993300	-4.77233100	0.57037100
H	3.91938600	-5.64358700	1.19853900
H	4.41970100	-4.80619600	-0.27275300
H	3.93818500	-3.89145900	1.17611700
C	-0.32798400	2.89791800	1.80653600
H	0.58333200	3.33266700	2.22255700
H	-0.38140400	3.15850900	0.74873700
H	-1.18895500	3.35604200	2.28675200
O	-1.65718700	0.98509000	1.51398200
H	-1.73006800	-0.00161400	1.48827000
H	-1.82065200	0.49550400	6.31571800
C	0.26775700	0.70641500	6.76706600
H	0.12824100	1.59746200	7.38600200
H	0.30245200	-0.16285300	7.42979000
H	1.23032900	0.78064400	6.25688900
C	1.85618100	-5.40574800	5.53321600
H	2.20744300	-4.38189400	5.69202000
H	1.86427900	-5.93252400	6.49209300
H	2.57745800	-5.88507900	4.86807700
H	0.09728800	-6.43935300	4.80084100
H	3.03346300	-3.11968700	-1.16320900
C	1.43410600	-3.91904400	-2.32228000
H	1.32766500	-3.01751900	-2.93398000

H	2.05168600	-4.62009800	-2.88926300
H	0.44206800	-4.36328100	-2.20268900
C	2.54247300	2.17251000	0.22707700
H	2.20567800	3.06213700	0.76438500
H	3.26429600	1.65327600	0.85981300
H	3.06182100	2.51458700	-0.67203000
H	0.64548000	1.91997400	-0.71212400
C	0.03870600	-8.95415200	-3.01768000
C	-1.43354800	-8.61291400	-2.69610500
C	-1.62021100	-7.69190800	-1.49983500
C	-1.82043400	-8.20492100	-0.20901700
C	-1.57375600	-6.29621400	-1.63058400
C	-1.99464000	-7.37190500	0.89657700
C	-1.73008600	-5.44486600	-0.53196400
C	-1.96778200	-5.97846500	0.74416900
O	-2.20453100	-5.21263100	1.84491900
C	-2.33129100	6.38439000	-4.58285400
C	-2.80879300	4.91901800	-4.47714100
C	-2.95305500	4.37400100	-3.06090800
C	-3.86562100	4.93736900	-2.15208300
C	-2.20191400	3.28184100	-2.60801200
C	-4.02018300	4.44033800	-0.85930200
C	-2.34903900	2.76056700	-1.31634700
C	-3.26486600	3.33947100	-0.42253700
O	-3.47415000	2.88945700	0.84809400
H	-1.97997000	-9.54688200	-2.51711200
H	-1.89104900	-8.14998200	-3.57933700
H	-1.85604500	-9.28283100	-0.06754100
H	-1.41608400	-5.86013600	-2.61496900
H	-2.16976700	-7.77985100	1.88686800
H	-1.67922600	-4.36906700	-0.65605300
H	-2.05275500	-4.26372800	1.64402500
H	0.51339100	-9.45828200	-2.16922900
H	-3.77681800	4.83512000	-4.99006200
H	-2.11255200	4.27936800	-5.03273600
H	-1.49092000	2.81050300	-3.28412400
H	-4.47749000	5.77970000	-2.46681700
H	-1.77546100	1.89610300	-0.99972900
H	-4.73460800	4.87901700	-0.17008200
H	-2.90152600	2.11800100	1.05524000
H	-1.33982300	6.50363100	-4.13358500
H	0.61311400	-8.04364600	-3.22081100
H	0.11496400	-9.60927500	-3.89210000
H	-3.01335200	7.06137900	-4.05869100
H	-2.27572300	6.70719700	-5.62803400
C	7.27008600	-0.96845900	5.68488800
C	6.03172200	-1.82716000	5.44536900
C	4.98970500	-1.11952600	4.57308600
C	3.86994900	-2.07823900	4.19119300
O	4.10447100	-3.18822300	3.71427400
N	2.60795800	-1.62471500	4.40931400
H	5.57089900	-2.09218800	6.40601000
H	6.29601100	-2.77030900	4.95698700
H	4.59402000	-0.23405200	5.08516700
H	5.46479400	-0.77477100	3.64490000
H	2.39381300	-0.63679100	4.44834100
H	1.86483400	-2.20968400	4.05326300
H	7.01035700	-0.01976100	6.16901700
H	7.77445000	-0.73071500	4.74076800
H	7.98945800	-1.48472300	6.32769700

Prod

Ni	0.54045241	-1.42603482	1.66310777
N	0.95633361	-0.12100826	0.22399000
C	1.48185410	0.35585437	-2.04661989
C	1.19986957	1.68773614	-1.23665274
C	0.68594431	1.11722142	0.07790562
N	0.10766954	0.06194039	2.89725673
C	-0.25264799	1.79066225	1.10745894
C	0.19570981	1.48531306	2.59489601
C	-0.59570634	2.17732145	3.78477836
C	-0.27466199	1.17753274	4.94578417
C	-0.08649162	-0.12601736	4.19226123
N	0.68310285	-2.80859752	3.04510867
C	-0.08150093	-1.37404812	4.85511510
C	0.30936867	-2.60184893	4.32372061
C	0.33934763	-3.90906325	5.11256418
C	1.34224523	-4.73083641	4.24701926
C	1.20591372	-4.07525597	2.86787828
N	1.10192461	-2.73543299	0.29055885
C	1.64809227	-4.63075416	1.68049684
C	1.66525698	-3.90565790	0.41535187
C	2.03921715	-3.17076892	-1.88908873
C	1.22111166	-2.15711539	-1.04794995
H	-0.34222407	-1.35257291	5.90768733
H	0.19806772	-2.08567203	-1.43762750
C	-2.93610775	-1.86925145	2.58607869
H	-2.13804180	-1.71759500	3.31515354
H	-3.38865428	-2.85129069	2.74015009
H	-3.68570676	-1.07961802	2.66965152
S	-2.13520250	-1.81544077	0.94276177
S	-3.91750310	-2.10158585	-0.28372177
C	-3.18601269	-1.48515436	-1.85670799
H	-2.18371749	-1.91457985	-1.96650638
H	-3.09183278	-0.39625778	-1.80372579
C	-4.06665800	-1.90615300	-3.03308400
H	-5.07932048	-1.50120510	-2.93928370
H	-3.63902209	-1.52604971	-3.96764093
H	-4.13652037	-2.99602618	-3.10263647
C	1.75310356	-0.68292435	-0.88625633
C	3.21794555	-0.71881137	-0.40767763
H	3.30195024	-1.36020416	0.47117165
H	3.88560624	-1.10446641	-1.18085061
H	3.56345028	0.27602270	-0.12338698
C	0.17519888	0.03460306	-2.80197815
H	-0.04855712	0.83791105	-3.51315876
H	0.24137923	-0.89626874	-3.37000347
H	-0.67237461	-0.04688087	-2.11559529
C	2.62345093	0.46358849	-3.06333208
H	2.77217615	-0.49765273	-3.56805873
H	2.38691723	1.20706049	-3.83319229
H	3.57334509	0.74862935	-2.60624085
O	1.60542362	1.81826221	2.67427058
H	1.69420404	2.77685879	2.59699890
C	-2.12522685	2.14641261	3.57305410
H	-2.47388871	1.13469844	3.35314196
H	-2.61799066	2.48312093	4.49213653
H	-2.46447962	2.79359623	2.76422351
C	-0.16539488	3.61450555	4.11616854
H	-0.46995451	4.32417554	3.34398784
H	-0.64313903	3.93288250	5.04925276

H	0.91374493	3.70909156	4.26823917
C	0.73577597	-3.74961126	6.58504941
H	-0.05149963	-3.23324748	7.14447217
H	0.87322142	-4.73144878	7.05171457
H	1.66117867	-3.18050308	6.70466598
C	-1.06519965	-4.55462417	5.02121538
H	-1.07507779	-5.51059917	5.55835499
H	-1.82048573	-3.90314266	5.47485207
H	-1.34472838	-4.74165414	3.98075241
C	2.10833321	-6.07765318	1.69778248
H	1.43429873	-6.70804651	1.10778286
H	3.11987153	-6.20554846	1.30271154
H	2.11504804	-6.48955819	2.70531982
C	2.42764650	-4.32572018	-0.86936994
C	2.07261028	-5.72734863	-1.40727858
H	2.48160032	-6.51363301	-0.77464222
H	0.99527400	-5.88464940	-1.48208206
H	2.51151853	-5.86792464	-2.40031702
C	3.94859951	-4.26853713	-0.58421421
H	4.26000276	-5.05272094	0.10987789
H	4.50237309	-4.41218980	-1.52014557
H	4.24595286	-3.31808447	-0.13780486
C	-0.37194039	3.29255976	0.83881441
H	0.54627987	3.82283510	1.10153470
H	-0.58366258	3.47467228	-0.21547654
H	-1.19750640	3.71661615	1.40653638
O	-1.55032649	1.24715759	0.84905930
H	-1.55017839	0.26963410	0.95920366
H	-1.13982570	1.10067405	5.61621367
C	0.96132728	1.48800690	5.81015869
H	0.82751692	2.41016427	6.38461659
H	1.13167317	0.67181344	6.51876123
H	1.85303910	1.58954952	5.18741802
C	2.80866157	-4.61653801	4.71005612
H	3.11647020	-3.56713613	4.75257407
H	2.95319005	-5.06695335	5.69750576
H	3.47605694	-5.11156022	4.00142879
H	1.04113143	-5.78256342	4.23832217
H	2.96669800	-2.70731999	-2.23854800
C	1.25489942	-3.61211853	-3.13276480
H	1.03450243	-2.74668972	-3.76647398
H	1.81557340	-4.32274686	-3.74642774
H	0.30347688	-4.08028662	-2.86107646
C	2.37814369	2.66376545	-1.05387651
H	2.05275034	3.56564459	-0.52900991
H	3.19735320	2.22229142	-0.48196470
H	2.77150011	2.97749459	-2.02523539
H	0.39905030	2.24360536	-1.74010588
C	0.03870600	-8.95415200	-3.01768000
C	-1.38811999	-8.40140255	-2.83775002
C	-1.48802353	-7.43271351	-1.67770249
C	-1.40022031	-7.89444596	-0.35551428
C	-1.61539398	-6.05309775	-1.87252277
C	-1.42428695	-7.02076491	0.72725699
C	-1.63532762	-5.16012920	-0.80021309
C	-1.53395530	-5.64185926	0.51082266
O	-1.55843705	-4.83128926	1.60049159
C	-2.33129100	6.38439000	-4.58285400
C	-3.16959855	5.09773624	-4.70452109
C	-3.35273236	4.42005155	-3.36386260
C	-4.20221324	4.98063766	-2.39761081

C	-2.63860487	3.27141472	-3.00981135
C	-4.31682047	4.44105571	-1.12151368
C	-2.74585960	2.70894008	-1.73664907
C	-3.57500346	3.30525531	-0.77383115
O	-3.69158741	2.83310989	0.49341641
H	-2.08030158	-9.23991488	-2.68236424
H	-1.70722953	-7.90449025	-3.76217027
H	-1.30746349	-8.96309430	-0.17151977
H	-1.69557175	-5.66227191	-2.88528691
H	-1.35519459	-7.38223690	1.74889986
H	-1.74293648	-4.09501876	-0.97035428
H	-1.44474159	-3.89911462	1.32567455
H	0.36943230	-9.47952282	-2.11533171
H	-4.14833369	5.34522410	-5.13678499
H	-2.68538722	4.40876197	-5.40760038
H	-1.97976532	2.80327113	-3.73970417
H	-4.77820001	5.86902782	-2.65017945
H	-2.17832676	1.82367842	-1.47021399
H	-4.96667785	4.88577737	-0.37394351
H	-3.00952480	2.14437647	0.64373926
H	-1.33780172	6.16211553	-4.17821725
H	0.74848789	-8.14043562	-3.20295671
H	0.09214114	-9.65515294	-3.85840981
H	-2.81124819	7.09825297	-3.90497173
H	-2.20319616	6.87295515	-5.55571611
C	7.27008600	-0.96845900	5.68488800
C	6.05048044	-1.54589440	4.95908694
C	5.69580954	-0.77825813	3.66920376
C	4.46524136	-1.40914901	3.02498669
O	4.53082541	-2.48924014	2.43660786
N	3.28935015	-0.76479507	3.24092755
H	5.18000603	-1.53262769	5.62845103
H	6.22279075	-2.59496914	4.69233741
H	5.53135677	0.28313221	3.89743256
H	6.52501043	-0.84768876	2.95687847
H	3.22662224	0.21539701	3.47177960
H	2.44948339	-1.17059612	2.83764141
H	7.09624918	0.07096123	5.98809611
H	8.15671858	-0.98161363	5.03991488
H	7.50503802	-1.54453856	6.58644318

React$_F$

Ni	0.77611360	-2.13920995	2.14423806
N	2.10609735	-1.06140695	1.07639365
C	3.61697225	-0.87064539	-0.75780117
C	3.29095258	0.54818607	-0.13246550
C	2.17733301	0.18880907	0.83786321
N	0.18393655	-0.52746588	3.10458815
C	1.05735975	1.10589568	1.39685711
C	0.76060425	0.80311571	2.92978547
C	-0.22560147	1.74786872	3.73882935
C	-0.67903822	0.77166127	4.87805324
C	-0.56429940	-0.57699082	4.19168810
N	-0.18953699	-3.46438931	3.30297961
C	-1.16770142	-1.74687691	4.72973531
C	-0.97703194	-3.06564493	4.34417172
C	-1.63417830	-4.26909282	5.00942696
C	-0.69687862	-5.42000110	4.52083180
C	-0.05207049	-4.81785688	3.27380089

N	1.52082938	-3.57437660	1.08658132
C	0.69006414	-5.52215414	2.29756894
C	1.42653702	-4.86308922	1.23877769
C	3.23298397	-4.50294282	-0.26275562
C	2.41678624	-3.20728630	-0.02431305
H	-1.80973899	-1.58129974	5.58878875
H	1.78473219	-3.00005525	-0.89492741
C	-2.80790409	-1.43515187	1.31134617
H	-2.26472942	-1.57133714	2.24737451
H	-3.68851487	-2.08280510	1.30360833
H	-3.10368719	-0.39018821	1.19124507
S	-1.66611050	-1.90700302	-0.03921419
C	-2.69745386	-1.40883038	-1.46580513
H	-2.12990488	-1.61644113	-2.37548679
H	-2.89872002	-0.33765509	-1.39880241
H	-3.63473312	-1.97087795	-1.49146326
S	-5.38216838	0.22193607	-3.57581430
C	-3.70925575	0.53241920	-4.30296408
H	-3.17382987	-0.41869844	-4.37980718
H	-3.15862956	1.19245499	-3.63163667
C	-3.86205500	1.18075500	-5.67671700
H	-4.36054883	2.15077511	-5.59212638
H	-2.87456039	1.34264313	-6.12277140
H	-4.44282108	0.55255550	-6.36078913
C	3.14359737	-1.86271654	0.38554154
C	4.22774203	-2.17736278	1.43436606
H	3.80848170	-2.81271633	2.21733702
H	5.07886328	-2.69792412	0.98882813
H	4.59513309	-1.26484689	1.90821980
C	2.73846984	-1.01163248	-2.01891919
H	3.00712328	-0.23835644	-2.74757987
H	2.87583882	-1.98239101	-2.50363594
H	1.67495935	-0.89301994	-1.78240092
C	5.08692657	-1.02458087	-1.16481112
H	5.26644136	-2.01396388	-1.59515718
H	5.35153791	-0.28407018	-1.92821991
H	5.77565163	-0.89876840	-0.32712873
O	2.05569816	0.76369905	3.58069262
H	2.35601505	1.66853206	3.73021382
C	-1.48899210	2.10158559	2.92935425
H	-1.98835793	1.20386641	2.56212798
H	-2.19259439	2.63656543	3.57621037
H	-1.28993366	2.74156788	2.07034698
C	0.39728300	3.04140694	4.28475771
H	0.63635619	3.75202998	3.49036626
H	-0.31639943	3.53559877	4.95249821
H	1.30089767	2.86611829	4.87702517
C	-1.75985460	-4.13837505	6.53304528
H	-2.48515779	-3.36054932	6.79484832
H	-2.12165540	-5.07673486	6.96672453
H	-0.80776959	-3.88488433	7.00642597
C	-3.04253385	-4.45640153	4.39394152
H	-3.52652311	-5.33501761	4.83572549
H	-3.67144804	-3.58194404	4.59701067
H	-2.98464014	-4.60404715	3.31299306
C	0.77970677	-6.99719116	2.34843873
C	2.21069929	-5.60823621	0.16282645
C	1.25857251	-5.97716415	-0.99548779
H	0.41925212	-6.57793925	-0.64806039
H	0.83200003	-5.08542840	-1.46364165
H	1.78866694	-6.54824351	-1.76508371

C	2.84645311	-6.85913438	0.77788279
H	3.39901034	-7.42976684	0.01998555
H	3.57196660	-6.54927658	1.54155623
C	1.38729428	2.57880381	1.15515843
H	2.20346256	2.91673744	1.79720198
H	1.68279329	2.73331164	0.11559119
H	0.51521511	3.20301064	1.34242332
O	-0.08946034	0.82964885	0.58019611
H	-0.27679868	-0.13355812	0.58937200
H	-1.72575819	0.97329249	5.13984742
C	0.14258140	0.79374234	6.18112678
H	0.04466856	1.75366415	6.69838605
H	-0.21371292	0.01082263	6.85740946
H	1.20021012	0.60766014	5.98121473
C	0.41611852	-5.80115114	5.51974142
H	1.05129505	-4.94076072	5.75836964
H	-0.01064915	-6.18409023	6.45132974
H	1.04376344	-6.58364480	5.09263419
H	-1.26055427	-6.31859630	4.27523803
H	4.04179131	-4.53509957	0.47594085
C	3.83700492	-4.67411256	-1.65467236
H	4.64445706	-3.95688760	-1.82890165
H	4.26205544	-5.67695706	-1.77323720
H	3.09133817	-4.53377927	-2.44361132
C	4.45651698	1.29045290	0.55035168
H	4.12871801	2.26258284	0.92682678
H	4.86312374	0.72718050	1.39350077
H	5.26774384	1.47426228	-0.15966687
H	2.90908892	1.20381127	-0.92560738
H	-4.99940262	0.16683970	-2.28658699
C	0.03924500	-8.95516600	-3.01651900
C	-1.45603835	-9.02420472	-2.64935866
C	-1.82998383	-7.93921829	-1.66363022
C	-1.82653316	-8.17342393	-0.28151944
C	-2.08246197	-6.63437399	-2.10423769
C	-2.03392947	-7.14377647	0.63547819
C	-2.29536081	-5.59334693	-1.20356051
C	-2.24804063	-5.84253388	0.17362614
O	-2.41132961	-4.84432761	1.09092488
C	-2.33141000	6.38400300	-4.58291200
C	-2.43580907	4.87656068	-4.88446605
C	-2.44983787	4.03159975	-3.62722506
C	-3.62549000	3.88219796	-2.87639032
C	-1.29180862	3.40628144	-3.15036014
C	-3.65060459	3.14400765	-1.69635899
C	-1.29721285	2.65461453	-1.97400520
C	-2.48220492	2.52572530	-1.23753751
O	-2.55236068	1.79309951	-0.08836954
H	-1.68451007	-10.01059911	-2.22753182
H	-2.05800255	-8.92625927	-3.56203925
H	-1.63131109	-9.17675393	0.09143051
H	-2.10027668	-6.42525460	-3.17225919
H	-1.97890211	-7.32633004	1.70287908
H	-2.48516994	-4.58343847	-1.55721116
H	-2.11874806	-4.00166184	0.69283109
H	0.66254455	-9.07797921	-2.12393662
H	-3.34849670	4.68681947	-5.46418448
H	-1.59656763	4.57327094	-5.52270987
H	-0.36556224	3.49798696	-3.71444861
H	-4.54489936	4.34417616	-3.22906936
H	-0.39900250	2.15468205	-1.62223679

H	-4.56609266	3.02388587	-1.12590088
H	-1.65017185	1.51816942	0.18263855
H	-1.41149674	6.60646720	-4.03128638
H	0.28445088	-7.98285389	-3.45752909
H	0.31304516	-9.73623020	-3.73545453
H	-3.17452895	6.71571374	-3.96737305
H	-2.32918566	6.97520192	-5.50556908
C	1.76508554	-7.72928978	1.42480869
H	1.15144129	-8.22554768	0.66207373
H	2.20129059	-8.53217880	2.02734728
O	0.09447368	-7.70360126	3.09185610
C	7.27051500	-0.96889900	5.68434700
C	6.24988843	-1.97206218	5.13569281
C	4.80890426	-1.47139801	5.24897138
C	3.77633238	-2.54672734	4.89693318
O	4.07545634	-3.72951447	4.76122847
N	2.49250564	-2.09320699	4.79936002
H	6.32517609	-2.92648773	5.66669491
H	6.46809543	-2.20015223	4.08462482
H	4.60040622	-1.13815823	6.27596172
H	4.64169594	-0.59207493	4.61011508
H	2.32112014	-1.12563580	4.55023017
H	1.82488082	-2.74930830	4.41045199
H	7.09107037	-0.76272819	6.74654019
H	7.22045991	-0.01117236	5.15110475
H	8.29353018	-1.34851120	5.58816439

TS1$_F$

Ni	0.71830100	-2.08991100	2.38511400
N	2.17419200	-1.01993700	1.42393300
C	3.47979600	-0.87301900	-0.56217400
C	3.18121600	0.56179700	0.03104800
C	2.18867400	0.22088600	1.13122300
N	0.20587300	-0.46482900	3.41263900
C	1.09829000	1.16831900	1.69275800
C	0.77787600	0.86535800	3.21981000
C	-0.23385700	1.81596300	3.99002000
C	-0.70458600	0.85571800	5.13268300
C	-0.56700000	-0.49914900	4.47258300
N	-0.12971800	-3.39188500	3.66865100
C	-1.19605500	-1.65764700	5.00957300
C	-0.98834900	-2.97477200	4.64967500
C	-1.69915800	-4.16347100	5.27767400
C	-0.72583800	-5.31983500	4.89237300
C	0.01383100	-4.74614900	3.69118400
N	1.67993700	-3.55808100	1.54592900
C	0.83789600	-5.46910100	2.80782800
C	1.61467400	-4.83545600	1.76318700
C	3.46103600	-4.48742500	0.31563400
C	2.56547600	-3.22571800	0.41937300
H	-1.88254300	-1.47662600	5.82859900
H	1.93213500	-3.15258600	-0.46987000
C	-2.48537900	-1.41392200	1.53673700
H	-2.27988100	-1.33687700	2.60371700
H	-3.25261300	-2.17553100	1.38323800
H	-2.85100600	-0.45624900	1.16012200
S	-0.95146900	-1.90485600	0.63237200
C	-2.65360500	-1.37605700	-1.62147500
H	-1.98282300	-1.61846700	-2.43432000
H	-2.67257000	-0.37221200	-1.21908400

H	-3.32362500	-2.13232300	-1.23819900
S	-5.29442700	0.17117800	-3.53661900
C	-3.65647900	0.49978500	-4.32693800
H	-3.13664000	-0.45402500	-4.44764000
H	-3.06948200	1.13565700	-3.66092300
C	-3.86205500	1.18075500	-5.67671700
H	-4.37570500	2.13994500	-5.55655400
H	-2.89236300	1.37961200	-6.14541400
H	-4.45094900	0.55769100	-6.35692900
C	3.19968300	-1.80741800	0.68663500
C	4.39792000	-1.95184700	1.64084700
H	4.09361500	-2.51065200	2.52669200
H	5.22876800	-2.47997100	1.16908300
H	4.75590400	-0.97605000	1.97102100
C	2.44692300	-1.11379800	-1.68462100
H	2.56485000	-0.35072300	-2.46125000
H	2.58620700	-2.08693000	-2.16378500
H	1.41820300	-1.05915800	-1.31262300
C	4.88579600	-1.00385800	-1.15607600
H	5.03130300	-2.00239200	-1.57498800
H	5.02062300	-0.28780300	-1.97418300
H	5.67787400	-0.82730700	-0.42593900
O	2.05432600	0.82078800	3.90381100
H	2.39817500	1.71945900	3.98269000
C	-1.47807100	2.14714100	3.14006300
H	-1.95358200	1.24346200	2.75570300
H	-2.20621000	2.67608300	3.76373700
H	-1.25902400	2.78431900	2.28404600
C	0.36692600	3.11694900	4.54211500
H	0.60670600	3.83262300	3.75371200
H	-0.36235800	3.60013400	5.20023300
H	1.26572000	2.94946100	5.14281300
C	-1.96488600	-4.01485700	6.78063300
H	-2.70336100	-3.22843400	6.96622200
H	-2.37667200	-4.94541900	7.18366100
H	-1.05979600	-3.76824000	7.34118700
C	-3.04510800	-4.35106100	4.53238000
H	-3.53592000	-5.26387800	4.88611200
H	-3.71197700	-3.50406200	4.72551700
H	-2.88698400	-4.43264800	3.45510400
C	0.94828700	-6.94013500	2.91577200
C	2.47529500	-5.61213600	0.77249100
C	1.60459100	-6.11462200	-0.40043000
H	0.78257300	-6.74185100	-0.05833500
H	1.15139300	-5.28791700	-0.95187700
H	2.21306200	-6.69991500	-1.09712500
C	3.13787700	-6.77690800	1.51589000
H	3.76789100	-7.36400200	0.83636800
H	3.79119700	-6.37100700	2.29807400
C	1.49115700	2.63586200	1.49621200
H	2.32032000	2.93756300	2.14049000
H	1.77897600	2.80753200	0.45847100
H	0.63625500	3.27715100	1.69996300
O	-0.02021000	0.96688400	0.83648800
H	-0.24270500	-0.00994200	0.76666500
H	-1.75768300	1.04939100	5.37016200
C	0.09249500	0.89126900	6.45108400
H	-0.03272700	1.84954100	6.96306300
H	-0.26240600	0.10363000	7.12204000
H	1.15655000	0.72768500	6.26732500
C	0.30042700	-5.67771700	5.98813600

H	0.88861800	-4.80168300	6.28331100
H	-0.20366600	-6.06749600	6.87632600
H	0.98123800	-6.44747900	5.62554800
H	-1.26359800	-6.22435300	4.61324100
H	4.22551300	-4.42264500	1.09713500
C	4.14823700	-4.72461700	-1.02670400
H	4.97006300	-4.02004200	-1.18000500
H	4.57552200	-5.73193100	-1.07008300
H	3.45384500	-4.62046800	-1.86612800
C	4.39627300	1.38318600	0.50685900
H	4.09274400	2.37531200	0.84562400
H	4.93127900	0.90089200	1.32731200
H	5.10024400	1.52445200	-0.31685500
H	2.66998700	1.15929800	-0.73384100
H	-4.79159500	-0.45555300	-2.45045700
C	0.03924500	-8.95516600	-3.01651900
C	-1.43405800	-8.74112000	-2.62594400
C	-1.60239800	-7.68389800	-1.55657400
C	-1.66602600	-8.02356900	-0.19770000
C	-1.65198200	-6.32410200	-1.89186100
C	-1.76692800	-7.04939100	0.79491400
C	-1.76012800	-5.33420900	-0.91662600
C	-1.81252900	-5.69647100	0.43671500
O	-1.91478500	-4.77264400	1.42984100
C	-2.33141000	6.38400300	-4.58291200
C	-2.33684700	4.86545900	-4.84834000
C	-2.35473200	4.03611600	-3.58067900
C	-3.55212900	3.81701300	-2.88205600
C	-1.18443800	3.48053900	-3.04883800
C	-3.58409400	3.09046300	-1.69566300
C	-1.19554900	2.74448700	-1.86147500
C	-2.40009100	2.55826700	-1.17006900
O	-2.47822000	1.86233600	0.00088800
H	-1.85756600	-9.69075000	-2.27734000
H	-2.00505300	-8.45716700	-3.51889200
H	-1.62694100	-9.07106900	0.09328500
H	-1.61149700	-6.03214700	-2.93935400
H	-1.77941600	-7.31673900	1.84621500
H	-1.80039300	-4.28334000	-1.18742200
H	-1.54739400	-3.90910200	1.12351100
H	0.62739400	-9.26989600	-2.14775500
H	-3.21115600	4.61291000	-5.46161900
H	-1.45652400	4.60071900	-5.44685700
H	-0.24243400	3.61857500	-3.57560700
H	-4.48275600	4.21305400	-3.28142500
H	-0.28456500	2.30343700	-1.46661700
H	-4.51621700	2.91085900	-1.17141300
H	-1.57911600	1.62991000	0.30997700
H	-1.44779000	6.67373400	-4.00418700
H	0.47907400	-8.02501000	-3.39225900
H	0.14080500	-9.72042900	-3.79433800
H	-3.21488600	6.68075900	-4.00826900
H	-2.32813700	6.94965000	-5.52118600
C	2.06672800	-7.66712700	2.15466600
H	1.56597900	-8.28657700	1.40151700
H	2.50666800	-8.36805100	2.87075800
O	0.19070600	-7.63685000	3.59175500
C	7.27051500	-0.96889900	5.68434700
C	6.25565300	-1.97599100	5.13487000
C	4.80903800	-1.50835900	5.29921700
C	3.79060200	-2.59783300	4.96371000

O	4.11648400	-3.75260400	4.70481700
N	2.48164600	-2.20028300	5.00922700
H	6.36637100	-2.94267600	5.63571000
H	6.45051000	-2.17024800	4.07317800
H	4.62408400	-1.18606900	6.33337000
H	4.59949700	-0.63073000	4.67155300
H	2.23407300	-1.22610200	4.88265100
H	1.82229500	-2.88049200	4.65706900
H	7.11372900	-0.79440200	6.75513800
H	7.18829600	0.00103300	5.17813200
H	8.29648000	-1.32601500	5.55187100

Int1$_F$

Ni	0.66537879	-2.25319478	2.31641645
N	2.04592738	-1.13981167	1.30240348
C	3.58165280	-0.93117670	-0.50404373
C	3.18705329	0.48618175	0.08315083
C	2.07269441	0.10799845	1.04518967
N	0.16915051	-0.62307943	3.35926006
C	0.92430100	1.00989277	1.57513804
C	0.66142974	0.73154227	3.11867951
C	-0.36627021	1.63907849	3.91252944
C	-0.74410402	0.67782652	5.09143734
C	-0.55399162	-0.68378612	4.45311947
N	-0.00215964	-3.57496260	3.67636229
C	-1.07956934	-1.86902297	5.04401858
C	-0.81694492	-3.18355922	4.70136203
C	-1.41005072	-4.39580039	5.40243338
C	-0.42835113	-5.51924619	4.93752574
C	0.19165873	-4.92504451	3.67889373
N	1.65351169	-3.68688282	1.42797678
C	0.94888980	-5.62606223	2.71835880
C	1.63167930	-4.96754917	1.62690941
C	3.38242051	-4.55470189	0.07188248
C	2.49663378	-3.29946928	0.28730230
H	-1.72759410	-1.71004669	5.89882229
H	1.83292125	-3.15153103	-0.57161120
C	-2.64068969	-1.62422132	1.64134406
H	-2.41908719	-1.48877955	2.70095075
H	-3.42554126	-2.37939407	1.54748713
H	-3.00197314	-0.68428997	1.21568654
S	-1.13553086	-2.19182588	0.73679663
C	-3.60640378	-1.86842019	-1.77580615
H	-2.69297685	-2.11891899	-2.32038979
H	-3.50043203	-0.86808663	-1.34890665
H	-3.74606775	-2.58993855	-0.96881504
S	-5.58878315	0.53675639	-3.63116927
C	-3.87704735	0.58548333	-4.25837194
H	-3.47559973	-0.43164399	-4.27310778
H	-3.27168864	1.20360145	-3.59117148
C	-3.86205500	1.18075500	-5.67671700
H	-4.24417131	2.20597605	-5.67617746
H	-2.82976479	1.20686088	-6.04304099
H	-4.46084271	0.58469396	-6.37209134
C	3.14152819	-1.90951872	0.65910498
C	4.22009500	-2.13282063	1.73630075
H	3.83057585	-2.78351701	2.52185162
H	5.11055551	-2.60462998	1.31507464
H	4.51915281	-1.19126893	2.19967147
C	2.72081310	-1.14900827	-1.76644670

H	2.95738028	-0.38225088	-2.51255026
H	2.91349974	-2.12297203	-2.22532157
H	1.65029207	-1.08085494	-1.54359036
C	5.06145496	-1.03096610	-0.89180972
H	5.28894137	-2.02243791	-1.29354029
H	5.29983897	-0.30102460	-1.67344004
H	5.73630339	-0.85117588	-0.05254611
O	1.97107328	0.78018558	3.74593207
H	2.20134089	1.70186397	3.91452509
C	-1.65479861	1.88984060	3.10214322
H	-2.09780034	0.95626900	2.75223781
H	-2.38773662	2.39431731	3.74127483
H	-1.49915706	2.51830707	2.22698799
C	0.18489586	2.98384419	4.40947487
H	0.36952325	3.68152309	3.59054835
H	-0.55025671	3.45391602	5.07085759
H	1.10463646	2.88552340	4.99583288
C	-1.52972717	-4.22655376	6.92274410
H	-2.28545909	-3.47326980	7.16852059
H	-1.85004856	-5.16682853	7.38303795
H	-0.58555941	-3.92221792	7.38196347
C	-2.81435516	-4.65356515	4.79973378
H	-3.25689859	-5.53913691	5.26929924
H	-3.47536275	-3.79985232	4.98543304
H	-2.75649200	-4.82636580	3.72267736
C	1.09115794	-7.09780760	2.79540013
C	2.43351394	-5.70233079	0.55762224
C	1.48099297	-6.15491452	-0.57224057
H	0.68004931	-6.79039194	-0.19804533
H	0.99726935	-5.30368853	-1.05764842
H	2.03371883	-6.71693496	-1.33255643
C	3.13947555	-6.90000405	1.20190661
H	3.70962439	-7.46453495	0.45323274
H	3.85817174	-6.53308682	1.94659742
C	1.22972375	2.48877908	1.32306506
H	2.02576844	2.86196589	1.97067510
H	1.53077537	2.63684490	0.28450823
H	0.33405337	3.08613921	1.48567321
O	-0.19743539	0.71085315	0.75647476
H	-0.39231538	-0.27263697	0.74474749
H	-1.79840072	0.81938866	5.35788489
C	0.08970493	0.78951789	6.38264630
H	-0.05733533	1.76037542	6.86552074
H	-0.21421309	0.01340379	7.09152158
H	1.15433451	0.65654023	6.17676259
C	0.70112830	-5.84460626	5.93909684
H	1.33465067	-4.97243749	6.13422657
H	0.28740231	-6.19679638	6.88800948
H	1.32928833	-6.63772335	5.53414548
H	-0.95828691	-6.44112994	4.70285286
H	4.21010740	-4.51510655	0.78943530
C	3.95936259	-4.73717147	-1.33027494
H	4.72086221	-3.98277784	-1.54782845
H	4.43626871	-5.71839128	-1.42901088
H	3.18732015	-4.66321963	-2.10207079
C	4.31213251	1.29653112	0.75771881
H	3.94358043	2.26713391	1.09651844
H	4.73163931	0.77888206	1.62342671
H	5.12331876	1.48673496	0.04978990
H	2.78124211	1.10473901	-0.72708631
H	-4.46647091	-1.89849686	-2.44967899

C	0.03924500	-8.95516600	-3.01651900
C	-1.43415030	-8.91056596	-2.56358187
C	-1.66468717	-7.89654024	-1.46202390
C	-1.63604398	-8.26419038	-0.10935417
C	-1.84096234	-6.53922142	-1.76250343
C	-1.75055723	-7.31748498	0.90939414
C	-1.96655066	-5.57841700	-0.76122286
C	-1.90277775	-5.96413170	0.58555721
O	-1.98946054	-5.06172244	1.60075496
C	-2.33141000	6.38400300	-4.58291200
C	-2.33199379	4.86425390	-4.84361950
C	-2.37355775	4.03754277	-3.57256759
C	-3.55836838	3.93134584	-2.82720520
C	-1.24443750	3.36727784	-3.08745633
C	-3.61920386	3.19604111	-1.64764196
C	-1.28564256	2.61894647	-1.90829763
C	-2.47836045	2.53350296	-1.17671755
O	-2.58482178	1.82201066	-0.02153828
H	-1.73926067	-9.90744952	-2.22188363
H	-2.06770495	-8.67048269	-3.42725133
H	-1.50484693	-9.31149117	0.15627721
H	-1.87901526	-6.22450326	-2.80398922
H	-1.68485541	-7.60479242	1.95400967
H	-2.09860597	-4.52901612	-1.00728828
H	-1.66990605	-4.17703084	1.29250259
H	0.69293054	-9.22142471	-2.17819817
H	-3.19740739	4.61165367	-5.47119689
H	-1.44253203	4.59518351	-5.42686943
H	-0.31194706	3.41988067	-3.64664536
H	-4.45964356	4.42276446	-3.18744050
H	-0.40868692	2.08376721	-1.55333713
H	-4.54530430	3.10095639	-1.09046666
H	-1.71071091	1.46069217	0.23275007
H	-1.45628735	6.67619501	-3.99223077
H	0.35996713	-7.97460910	-3.38580970
H	0.19175413	-9.68902204	-3.81646143
H	-3.22352373	6.68266715	-4.02198200
H	-2.31508069	6.94789605	-5.52239453
C	2.10833742	-7.80482220	1.88617811
H	1.51817345	-8.35771708	1.14495998
H	2.59135788	-8.56312609	2.51026822
O	0.43070721	-7.80973188	3.55226525
C	7.27051500	-0.96889900	5.68434700
C	6.20730488	-1.96067817	5.20413240
C	4.78810504	-1.43747486	5.42477372
C	3.71305769	-2.49045489	5.15464631
O	3.94839431	-3.69566118	5.14428741
N	2.46096712	-1.98556539	4.97882320
H	6.30552189	-2.91838506	5.72519522
H	6.34825304	-2.18251574	4.13819351
H	4.66552849	-1.11447029	6.46899325
H	4.59296858	-0.54732790	4.81012030
H	2.31499281	-1.02081091	4.70760612
H	1.73702241	-2.64681797	4.73086477
H	7.16597387	-0.76647856	6.75712496
H	7.19060927	-0.00864662	5.15952935
H	8.28198170	-1.35446530	5.51678979

React$_{NoF}$

C	-0.08960200	7.77957500	-1.92406600

C	0.10433200	6.73920800	-0.84291300
C	-0.07803400	7.05853900	0.51178200
C	0.42932800	5.41458900	-1.15284900
C	0.03285100	6.09784200	1.51266400
C	0.54098700	4.43565400	-0.16278200
C	0.33112400	4.77002900	1.18076900
O	0.41309200	3.86468100	2.19625800
C	7.45009600	-2.64303900	-1.38324300
C	5.97973800	-2.37830200	-1.19427800
C	5.14495900	-3.38570400	-0.69005000
C	5.40308000	-1.14821900	-1.52299700
C	3.78102000	-3.18570100	-0.51722700
C	4.03342700	-0.92556800	-1.36239400
C	3.22884300	-1.94651900	-0.85608400
O	1.86963800	-1.79387700	-0.70560600
C	-5.86031900	-2.55887300	-0.49882500
C	-5.30495300	-1.34758400	-1.22585900
O	-4.69936300	-1.43330200	-2.28956300
N	-5.54185800	-0.15093500	-0.60256300
Ni	-1.94009400	-0.55377300	0.09731100
N	-1.05846400	-1.29129000	-1.73102400
C	-1.05443800	0.87346000	-2.84523500
C	-1.01041100	-0.62075400	-2.82784700
C	-1.04993400	-1.46876200	-4.08391800
C	-1.54500700	-2.79607900	-3.48351000
C	-1.00817700	-2.73352900	-2.08497200
N	-1.73708300	-2.40102600	0.91203600
C	-1.80648100	-3.64281900	-1.19981900
C	-1.32218400	-3.64384500	0.22357400
C	-1.88077700	-4.84997400	1.00953800
C	-2.08715800	-4.20384000	2.36036700
C	-2.12654800	-2.72619600	2.12413700
N	0.11948500	-3.85990200	0.34033200
C	0.49975800	-5.11567400	0.70768700
O	1.64947400	-5.52790400	0.80467200
C	-0.78340400	-5.92119100	0.95645800
N	-2.73221100	0.16887200	1.87742500
C	-2.52800100	-1.86608200	3.17386300
C	-2.78927500	-0.52570600	3.04730100
C	-3.23353000	0.35371400	4.20223800
C	-3.84315600	1.54967900	3.46525800
C	-3.30667500	1.39106900	2.04715400
N	-2.48934400	1.16378700	-0.83239800
C	-3.48274400	2.33663300	1.06253200
C	-3.12591800	2.19274100	-0.30541700
C	-3.57428300	3.21942500	-1.35395900
C	-2.68680100	2.82218700	-2.54330700
C	-2.40979100	1.34068100	-2.29803700
H	0.39334000	8.72964900	-1.66456000
H	0.32790500	7.44492200	-2.87996700
H	-0.32221100	8.08248100	0.78946700
H	0.59207700	5.13321100	-2.19205700
H	-0.11801500	6.35360100	2.55754500
H	0.77761400	3.40979000	-0.43406500
H	0.49449400	2.96067500	1.82849300
H	7.89131400	-3.11339600	-0.49597300
H	8.01159400	-1.72418700	-1.58377300
H	5.57377800	-4.34865100	-0.41957800
H	6.02512900	-0.35382400	-1.93144300
H	3.14921100	-3.97242200	-0.10935100
H	3.59075500	0.02808900	-1.64133400

H	1.63791400	-0.86591100	-0.49097000
H	-5.10715600	-2.91837200	0.21375600
H	-6.06089600	-3.35480000	-1.21923000
H	-5.76578800	-0.16344600	0.38378800
H	-4.92245100	0.60404700	-0.86900800
H	-0.25817400	1.29970700	-2.22287900
H	-0.92367400	1.24297100	-3.86923500
H	-1.20856800	-3.67925300	-4.03838500
H	0.04867600	-3.02712600	-2.05625500
H	-2.86414900	-3.35837400	-1.22459000
H	-1.72372400	-4.65949700	-1.60960500
H	-1.25499400	-4.43971400	3.04318200
H	-0.69245800	-6.52055600	1.86731500
H	-0.92386500	-6.61939700	0.12172700
H	-2.69275100	-2.32591700	4.14412000
H	-3.92695600	-0.15649200	4.87819000
H	-3.57980400	2.52051500	3.89791400
H	-4.62696700	2.99525500	-1.60000900
H	-1.74737100	3.39102000	-2.49722000
H	-3.19784200	0.72140300	-2.75428100
H	-6.77597100	-2.33092700	0.05714100
H	-2.35995200	0.65294500	4.79770600
H	-4.94081000	1.49487800	3.45421100
H	-3.14921900	3.01487700	-3.51753200
H	-1.70264400	-1.03943400	-4.85266400
H	-0.04194900	-1.55057600	-4.52060000
H	-2.64089900	-2.79393200	-3.46137900
H	-2.99081600	-4.55249400	2.87766700
H	-2.82962000	-5.18641900	0.57958100
H	7.63116000	-3.32384000	-2.22627900
H	-1.15411700	7.99492700	-2.08911200
C	1.14711100	-0.34165300	2.51010300
H	1.27902900	0.16547100	3.47016200
H	1.86803100	-1.15803300	2.41182400
H	0.13331700	-0.73974800	2.43912600
S	1.34571400	0.84822800	1.13730600
H	0.79502300	-3.14904400	0.06007200
C	3.04456100	1.44261300	1.48891500
H	3.29893200	2.17522100	0.71790400
H	3.76113400	0.61788800	1.44867600
H	3.08322100	1.93180300	2.46662500
H	7.42507900	2.18100400	1.85752500
S	8.56585200	1.45816800	1.90833800
C	8.48429000	0.80628300	0.18559200
H	9.33932300	0.12531100	0.11940000
H	7.57925700	0.20038000	0.08010600
H	8.56470000	1.41929000	-1.89289700
H	7.70851200	2.56337800	-0.84401200
H	9.47728300	2.47734500	-0.79443700
C	8.56495000	1.88102100	-0.89638100
H	-3.98044100	3.25830600	1.34591400
C	-3.48458800	4.69293500	-0.94745300
H	-3.75137600	5.33590500	-1.79508700
H	-4.17102000	4.93335500	-0.12776500
H	-2.46959000	4.95254300	-0.63041100

TS1$_{NoF}$

C	0.97826800	7.65809600	-1.96147200
C	0.90785700	6.53190300	-0.95511400
C	0.55483200	6.77368000	0.38206300

C	1.17030700	5.20673100	-1.32010700
C	0.44923500	5.74075300	1.30931200
C	1.06909600	4.15619900	-0.40448100
C	0.69793600	4.41441600	0.92316500
O	0.57467500	3.44477600	1.86531400
C	7.27297100	-3.56074200	-1.42779600
C	5.83854300	-3.16134300	-1.20550300
C	4.89369400	-4.11147000	-0.79414700
C	5.40235900	-1.84984600	-1.41902200
C	3.55762800	-3.77650000	-0.60685100
C	4.06359700	-1.49209000	-1.24426100
C	3.14221300	-2.45999600	-0.83901500
O	1.80677900	-2.18045900	-0.69346100
C	-5.93261500	-1.94286000	-0.45239200
C	-5.30468900	-0.76119600	-1.17039200
O	-4.57069400	-0.89911600	-2.14421500
N	-5.61932400	0.46641700	-0.65501600
Ni	-1.53344700	-0.33592800	0.17806900
N	-1.03742100	-1.22927300	-1.72964800
C	-0.78019600	0.90981500	-2.85872600
C	-0.91539500	-0.57670000	-2.82863300
C	-1.05180500	-1.42776800	-4.07396400
C	-1.69515900	-2.68525700	-3.46558800
C	-1.14894800	-2.67220900	-2.06649100
N	-1.73575100	-2.26779900	0.95498300
C	-2.03805900	-3.46946500	-1.16315100
C	-1.52259400	-3.55655800	0.24791900
C	-2.25469400	-4.66453900	1.03592800
C	-2.35287600	-4.00105200	2.38784800
C	-2.18468600	-2.53291300	2.15578100
N	-0.13476000	-3.99157300	0.33493900
C	0.05067200	-5.29561900	0.69300400
O	1.11901300	-5.88688400	0.75896800
C	-1.33689300	-5.89046300	0.97144200
N	-2.47781500	0.41533500	1.89402800
C	-2.49220700	-1.62662400	3.20071900
C	-2.61991600	-0.26967800	3.06181700
C	-2.99650800	0.64602300	4.20996800
C	-3.42737700	1.92007000	3.48012000
C	-2.92789200	1.69220100	2.05589400
N	-2.13861200	1.38262700	-0.82243800
C	-3.01705300	2.64421400	1.06931100
C	-2.68502000	2.45762400	-0.30227600
C	-3.03877700	3.50989300	-1.36207400
C	-2.17630800	3.03028300	-2.54163600
C	-2.06111500	1.53190200	-2.29071600
H	1.53750600	8.51695900	-1.57062600
H	1.46953800	7.33575900	-2.88589300
H	0.35551200	7.79396200	0.70479500
H	1.46551900	4.98508800	-2.34428900
H	0.17469400	5.93929900	2.34117800
H	1.28877400	3.13720800	-0.70934800
H	0.64156000	2.54840500	1.45386800
H	7.64327300	-4.20271100	-0.61950400
H	7.93104400	-2.68669200	-1.48526600
H	5.21153600	-5.13514700	-0.60716100
H	6.11547200	-1.09335000	-1.74037200
H	2.84235700	-4.51904700	-0.26160200
H	3.73334900	-0.47262700	-1.42329100
H	1.62419300	-1.24034200	-0.41897100
H	-5.22632700	-2.31125800	0.30184100

H	-6.11282800	-2.74440200	-1.17173000
H	-6.02182000	0.53458500	0.26902800
H	-5.02997000	1.23967600	-0.93443700
H	0.07829600	1.23873600	-2.26194500
H	-0.63266500	1.25317800	-3.88848700
H	-1.45943200	-3.60440800	-4.01191500
H	-0.12987900	-3.07593600	-2.03627600
H	-3.04854700	-3.04492100	-1.16144600
H	-2.10552900	-4.48505700	-1.57692600
H	-1.54840500	-4.34429800	3.05736300
H	-1.32251900	-6.49005700	1.88615700
H	-1.59968200	-6.56404600	0.14676100
H	-2.71563300	-2.05981300	4.17061300
H	-3.77186600	0.21460700	4.84986400
H	-3.00842500	2.83625200	3.90720200
H	-4.10339500	3.36368600	-1.61883000
H	-1.18629600	3.50067300	-2.47828300
H	-2.92463800	1.00216300	-2.72115200
H	-6.87073100	-1.68663100	0.05007400
H	-2.11468800	0.82028100	4.83962500
H	-4.51873300	2.03782300	3.47798500
H	-2.60710700	3.26879300	-3.51958700
H	-1.64761900	-0.93077800	-4.84721400
H	-0.05814800	-1.62729400	-4.50355600
H	-2.78342700	-2.55944600	-3.43977800
H	-3.28704300	-4.22066700	2.91982600
H	-3.24752800	-4.84745200	0.61299100
H	7.39740900	-4.12281900	-2.36374200
H	-0.02125100	8.02464300	-2.23318200
C	1.07195900	-0.48414600	2.33863100
H	1.71632300	0.12884100	2.97321600
H	1.55796300	-1.44743900	2.16135800
H	0.12512800	-0.65488800	2.85407000
S	0.76996200	0.38571300	0.74071700
H	0.64024300	-3.38808800	0.04746900
C	3.32756900	1.42828000	1.03348000
H	3.50562300	1.84614000	0.04982100
H	3.76004000	0.46663600	1.27832100
H	3.01486300	2.09485800	1.82773200
H	5.66213800	1.99025300	2.00676300
S	6.96306800	1.86714700	2.36901700
C	7.51714200	1.00092500	0.83827000
H	8.55645200	0.72398800	1.04326300
H	6.94878000	0.07187200	0.73199800
H	7.80169300	1.29505600	-1.29209300
H	6.38310200	2.13223600	-0.63305400
H	8.00468400	2.77408200	-0.32539600
C	7.42208000	1.85289200	-0.42550900
H	-3.40946500	3.61442700	1.35274200
C	-2.84417200	4.97508700	-0.96387800
H	-3.04015700	5.62525100	-1.82440200
H	-3.53320900	5.27490400	-0.16652600
H	-1.82250300	5.16113600	-0.62095700

Int1$_{NoF}$

C	-0.97293900	7.78387199	-1.89637499
C	-0.66289418	6.67718525	-0.90978387
C	-0.99457307	6.80262992	0.44759461
C	-0.06787583	5.47565212	-1.31591737
C	-0.77444818	5.76912001	1.35514738

C	0.16293715	4.42846067	-0.42069606
C	-0.20464792	4.56167092	0.92687647
O	-0.02225542	3.58210552	1.84888031
C	7.67483694	-1.75337401	-1.73104199
C	6.19384937	-1.68415708	-1.45407828
C	5.47987260	-2.84542864	-1.12683585
C	5.48705279	-0.47844358	-1.52741699
C	4.11060575	-2.81698905	-0.89139696
C	4.10969492	-0.42732056	-1.30018508
C	3.42174232	-1.60197598	-0.98726768
O	2.06520718	-1.62552125	-0.79820543
C	-5.52081899	-3.12982697	-0.33947100
C	-5.03624350	-1.81195272	-0.91073346
O	-4.33961385	-1.75016326	-1.92038239
N	-5.42556799	-0.70329910	-0.21325882
Ni	-1.52171638	-0.56800300	0.20326711
N	-0.94121040	-1.32916644	-1.75356309
C	-1.20489194	0.82604070	-2.85574182
C	-1.00438582	-0.65534988	-2.84520973
C	-0.99095465	-1.50732956	-4.09862412
C	-1.32445398	-2.88087200	-3.48829096
C	-0.74577269	-2.75904683	-2.10748028
N	-1.31119609	-2.52223172	0.93870851
C	-1.41069911	-3.74056629	-1.19163003
C	-0.84412226	-3.72412081	0.20268667
C	-1.28742229	-4.97477765	0.99297376
C	-1.48256797	-4.36409095	2.35992895
C	-1.65021542	-2.88981406	2.14884616
N	0.60771656	-3.84105195	0.23908813
C	1.08628145	-5.08265351	0.54517458
O	2.25789631	-5.43131239	0.54052614
C	-0.12602028	-5.96936874	0.87134933
N	-2.57990440	-0.06797152	1.95251238
C	-2.11512463	-2.08270961	3.21859640
C	-2.53343828	-0.78311510	3.11239383
C	-3.05943720	0.02481299	4.28439844
C	-3.81200999	1.15804498	3.57935897
C	-3.28466686	1.08150385	2.15086911
N	-2.53594916	0.98486390	-0.75463571
C	-3.58473132	2.01717067	1.19031813
C	-3.26630905	1.92253796	-0.19353481
C	-3.88955683	2.87949726	-1.21687415
C	-3.03545201	2.57472196	-2.45796398
C	-2.56725452	1.14217225	-2.22452091
H	-0.85677392	8.77407412	-1.44011692
H	-0.31185037	7.73984665	-2.76942718
H	-1.44355529	7.72900454	0.80273180
H	0.22850978	5.35227825	-2.35679521
H	-1.04053082	5.87603287	2.40314074
H	0.64064977	3.51045441	-0.75353647
H	0.18879507	2.71931871	1.41089366
H	8.19020217	-2.40050709	-1.01063938
H	8.14162547	-0.76316925	-1.68214901
H	6.00933945	-3.79289032	-1.04375323
H	6.01645886	0.44008941	-1.77460912
H	3.57777084	-3.71989544	-0.60271415
H	3.57054834	0.51449697	-1.36505309
H	1.69287856	-0.75603053	-0.46972662
H	-4.77863793	-3.50048824	0.37890197
H	-5.61233183	-3.86232437	-1.14419548
H	-5.79843234	-0.81402459	0.71934153

H	-4.88142024	0.13699289	-0.36355314
H	-0.41621984	1.33444175	-2.28855036
H	-1.18195229	1.20114279	-3.88506697
H	-0.91212210	-3.72225856	-4.05566233
H	0.33719880	-2.93185989	-2.11521758
H	-2.48910257	-3.54940081	-1.15626683
H	-1.26422888	-4.74223629	-1.61918946
H	-0.59888239	-4.52595349	2.99747494
H	0.06008566	-6.55711500	1.77528582
H	-0.27129177	-6.67972365	0.04825776
H	-2.20481268	-2.56595790	4.18662053
H	-3.67747608	-0.57117866	4.96258685
H	-3.64454376	2.14545289	4.02056903
H	-4.92186647	2.53059913	-1.39222293
H	-2.17173395	3.25347755	-2.47392196
H	-3.30588135	0.42563722	-2.61228119
H	-6.48105204	-3.03901825	0.17934801
H	-2.21214412	0.41025605	4.86666490
H	-4.89684942	0.98499381	3.58284896
H	-3.58005621	2.69631867	-3.40017947
H	-1.70488589	-1.14701217	-4.84769813
H	0.00841518	-1.48092736	-4.55992735
H	-2.41246666	-2.99673500	-3.42704398
H	-2.32575260	-4.78969143	2.91883650
H	-2.23015877	-5.36713374	0.59792165
H	7.88271128	-2.16106202	-2.73032340
H	-2.00567205	7.71997598	-2.26794321
C	1.14031814	-0.12993569	2.28637717
H	1.99758155	0.44906704	2.64113643
H	1.45049633	-1.16793006	2.13771321
H	0.35511255	-0.09907793	3.04643265
S	0.54269680	0.59885760	0.70424046
H	1.21988242	-3.07889747	-0.06678102
C	3.80321036	3.07914884	1.71561622
H	4.19280794	3.92748401	1.14454209
H	3.74736954	2.19930417	1.06766780
H	2.80119581	3.31922197	2.08214875
H	4.47125148	2.87025157	2.55683707
S	6.68246889	0.47416867	3.48490189
C	7.40730259	0.13769759	1.85179743
H	8.10216560	-0.70436615	1.97365014
H	6.58543040	-0.25099893	1.23257719
H	8.47898671	1.04672565	0.19884381
H	7.36967635	2.15253628	1.03671283
H	8.91238546	1.71205272	1.78668044
C	8.08179189	1.33382772	1.18129542
H	-4.16948825	2.87603124	1.50087401
C	-3.94064671	4.35684820	-0.81696413
H	-4.32533077	4.95677263	-1.65037921
H	-4.60376941	4.52653943	0.03888066
H	-2.94577661	4.73076634	-0.55813214

React$_{Hby}$

Ni	0.70416331	-2.19357021	1.73722285
N	1.44315161	-1.12763309	0.31680481
C	2.32930393	-0.92489820	-1.87672362
C	2.14995269	0.49742394	-1.21315352
C	1.41131147	0.15513212	0.08621053
N	0.21553569	-0.51427520	2.71887217
C	0.76159324	1.11325861	0.97043964

C	0.24922080	0.77485023	2.21864818
C	-0.46512755	1.71205289	3.23419843
C	-0.45426172	0.83260856	4.52939840
C	-0.29010090	-0.56244897	3.96310256
N	0.29950863	-3.44430521	3.19531919
C	-0.57304893	-1.72795591	4.68732158
C	-0.32066938	-3.05973833	4.32550138
C	-0.76162783	-4.27583283	5.13707133
C	0.22315730	-5.35326215	4.58486340
C	0.55749072	-4.80941778	3.19072864
N	1.18139588	-3.73655290	0.55042647
C	1.12041043	-5.53565198	2.15950434
C	1.53618018	-4.94551534	0.88251190
C	2.56341165	-4.46571934	-1.28273539
C	1.67119097	-3.30828263	-0.76572273
H	-1.03506359	-1.57310741	5.65706204
H	0.78112151	-3.20560949	-1.39260573
C	-2.87464142	-1.64648431	1.40287905
H	-2.06247107	-1.58134223	2.12820077
H	-3.32233453	-2.64053715	1.45967730
H	-3.61914432	-0.87032978	1.60057908
S	-2.13604835	-1.39932183	-0.25084102
C	-3.66712652	-1.52708173	-1.23842621
H	-3.39659239	-1.41226849	-2.28939808
H	-4.35706027	-0.72654862	-0.95710247
H	-4.13796805	-2.50302253	-1.09369700
S	-5.85165658	0.44056051	-3.89869429
C	-4.05351837	0.50741845	-4.32238602
H	-3.65367773	-0.51127973	-4.34471241
H	-3.53825571	1.07337557	-3.54687270
C	-3.86455400	1.18191800	-5.67637300
H	-4.23413532	2.21110458	-5.65125995
H	-2.79879635	1.21143157	-5.92888201
H	-4.38732287	0.64513050	-6.47578281
C	2.31026121	-1.86993512	-0.61521811
C	3.68119782	-2.00941609	0.08686762
H	3.56885657	-2.62935830	0.97881008
H	4.44121524	-2.46313358	-0.55280119
H	4.05017263	-1.03561539	0.41242936
C	1.08955878	-1.15544484	-2.76877058
H	1.04447701	-0.38357740	-3.54541144
H	1.11603661	-2.12453308	-3.27480810
H	0.16454724	-1.10213251	-2.18536204
C	3.58819830	-1.05950253	-2.74190736
H	3.67390137	-2.07911728	-3.13377739
H	3.54301103	-0.37939159	-3.60039806
H	4.50602450	-0.83864893	-2.19285355
C	-1.93818035	1.88145936	2.79306739
H	-2.44032521	0.91047728	2.74096021
H	-2.47756815	2.50095923	3.51971493
H	-2.03061983	2.34907992	1.81160002
C	0.16327873	3.09463934	3.47256386
H	-0.04531438	3.78764093	2.65749854
H	-0.26156128	3.53715125	4.38030044
H	1.24812048	3.03794461	3.60097829
C	-0.71739615	-4.07783612	6.65654426
H	-1.48721139	-3.36719047	6.97522362
H	-0.91727967	-5.02388598	7.17201083
H	0.25022695	-3.69968194	6.99688584
C	-2.20442948	-4.63312168	4.69965404
H	-2.54612479	-5.53634467	5.21980831

H	-2.89358492	-3.81768633	4.94470068
H	-2.25154937	-4.80942739	3.62080653
C	1.27159579	-7.03467710	2.34386117
H	0.60963146	-7.57569212	1.65839589
H	2.29195064	-7.38202785	2.16201238
H	1.00851527	-7.35082945	3.35190076
C	2.47267144	-5.59276663	-0.16610929
C	1.94150155	-6.92795145	-0.72296739
H	2.02010561	-7.73002730	0.00981456
H	0.89678066	-6.85492493	-1.02963380
H	2.53212653	-7.23857420	-1.58964665
C	3.87563492	-5.80177433	0.45188854
H	3.87449935	-6.58076432	1.21876695
H	4.57808425	-6.11087696	-0.33191824
H	4.25138391	-4.88940953	0.92307511
C	0.66906662	2.54928191	0.47957844
H	1.40022889	3.20874491	0.96067951
H	0.83533884	2.61945782	-0.59513443
H	-0.32148899	2.97364290	0.65414412
H	-1.40204627	0.94115591	5.06958968
C	0.69779883	1.10354463	5.51697261
H	0.62533351	2.09612604	5.97030562
H	0.68136328	0.36077192	6.32043103
H	1.66929324	1.03126582	5.01401072
C	1.52225437	-5.49445621	5.40381240
H	2.03231000	-4.52879528	5.48866723
H	1.32065139	-5.86902484	6.41250584
H	2.21445214	-6.18474930	4.91478810
H	-0.28330900	-6.32147907	4.53857117
H	3.60412121	-4.13637116	-1.31940546
C	2.18207462	-4.88393380	-2.70770968
H	2.28099224	-4.02993748	-3.38630559
H	2.83279593	-5.67536457	-3.09235382
H	1.14795186	-5.23628868	-2.76297074
C	3.42616570	1.32764373	-0.98768716
H	3.18204567	2.27823844	-0.50735341
H	4.14793238	0.81313932	-0.34968775
H	3.91832064	1.55326724	-1.93885943
H	1.49714971	1.09728261	-1.86066184
H	-5.70144126	0.25247465	-2.57379601
C	0.03880500	-8.95451900	-3.01748400
C	-1.43662526	-8.51102742	-2.94672937
C	-1.65111536	-7.45975147	-1.87937734
C	-1.93563539	-7.82107031	-0.55583098
C	-1.46942224	-6.09871531	-2.15907724
C	-2.00545167	-6.86903021	0.46045918
C	-1.53482351	-5.13348475	-1.15546304
C	-1.78686443	-5.52142246	0.16538770
O	-1.85752720	-4.61531487	1.18694670
C	-2.33178300	6.38467200	-4.58248000
C	-2.34911047	4.87201159	-4.88268049
C	-2.50971305	4.00108930	-3.64982347
C	-3.68946309	4.05500328	-2.89025112
C	-1.51469946	3.10917676	-3.23314316
C	-3.87126204	3.26111876	-1.76332519
C	-1.68257290	2.29481278	-2.10904856
C	-2.86670064	2.37017043	-1.36647319
O	-3.10302135	1.60750887	-0.26182499
H	-2.06986401	-9.38381650	-2.74410958
H	-1.74603173	-8.12032973	-3.92440024
H	-2.08617336	-8.87069014	-0.31145291

H	-1.26401071	-5.78801630	-3.18178669
H	-2.20792748	-7.15187007	1.48900998
H	-1.39685343	-4.07943274	-1.37616438
H	-1.18646979	-3.92121072	1.05179531
H	0.36959123	-9.35753886	-2.05439335
H	-3.17004652	4.65927409	-5.58171596
H	-1.42586916	4.59426214	-5.40564289
H	-0.58984328	3.03537607	-3.80204186
H	-4.49130614	4.72230690	-3.19786336
H	-0.91052220	1.59078242	-1.81236393
H	-4.79262401	3.29500169	-1.19062009
H	-2.46494045	0.86409702	-0.21044877
H	-1.49703813	6.64035094	-3.92119652
H	0.68793273	-8.10671100	-3.25903787
H	0.18572039	-9.72677062	-3.78148362
H	-3.25587948	6.69947635	-4.08673332
H	-2.22883710	6.96537411	-5.50539448
C	7.27036300	-0.96856400	5.68488600
C	6.14354862	-1.92082658	5.27174721
C	5.41402831	-1.46459005	3.99295565
C	4.31200070	-2.45647571	3.63330244
O	4.57009733	-3.56646481	3.17331007
N	3.04156483	-2.06939822	3.94436244
H	5.41183990	-2.00609295	6.08610356
H	6.53623667	-2.92900458	5.09728403
H	5.01495240	-0.45087017	4.13015293
H	6.11881461	-1.43711447	3.15459165
H	2.81019734	-1.09315723	4.05276042
H	2.28210632	-2.64834056	3.59901578
H	6.88552336	0.03781328	5.88921077
H	8.02311582	-0.88062606	4.89236934
H	7.77770729	-1.32177611	6.58924381

TS1$_{Hby}$

Ni	0.30481600	-1.48021400	1.41688200
N	1.34764200	-0.42755500	0.12134500
C	2.24371500	-0.28049600	-2.06810600
C	2.03810500	1.15639100	-1.44761200
C	1.28077500	0.83586300	-0.15572800
N	0.00860600	0.21396000	2.44767900
C	0.58218100	1.81112300	0.67766100
C	0.06658800	1.49835600	1.92441800
C	-0.61852200	2.45942300	2.93008900
C	-0.54110000	1.61665700	4.24565100
C	-0.44665300	0.20806800	3.70472300
N	0.06663300	-2.68299900	2.98773100
C	-0.75230900	-0.93223800	4.46409000
C	-0.53790400	-2.27104700	4.11529200
C	-0.97336400	-3.46677100	4.95411100
C	0.03628400	-4.54065700	4.44914100
C	0.36932700	-4.03868800	3.03966700
N	1.10113600	-3.01665300	0.42252200
C	0.99094900	-4.78161800	2.06043500
C	1.42840800	-4.21901400	0.77718700
C	2.44832600	-3.80517000	-1.40530000
C	1.58166100	-2.62418900	-0.90076800
H	-1.19135100	-0.74627100	5.43773300
H	0.68145400	-2.52973100	-1.51509300
C	-3.04516900	-1.18503800	1.50383400
H	-2.56671300	-0.95066800	2.45563300

H	-3.59815900	-2.12165700	1.61026700
H	-3.73850900	-0.38268100	1.24198000
S	-1.76199500	-1.35442000	0.18950200
C	-3.96107100	-1.66442800	-1.59171800
H	-3.37636400	-1.91376800	-2.46613500
H	-4.18058200	-0.63085900	-1.36787900
H	-4.39560000	-2.45744500	-0.99869200
S	-5.94955300	0.39949500	-4.01965000
C	-4.14425100	0.36743500	-4.41721700
H	-3.84053400	-0.67414500	-4.55148800
H	-3.59551200	0.78263800	-3.57136700
C	-3.86484000	1.18153900	-5.67602000
H	-4.16951800	2.22403400	-5.54287500
H	-2.79034400	1.17736200	-5.88724800
H	-4.38941900	0.77327500	-6.54581800
C	2.22578100	-1.19026400	-0.78162500
C	3.58849000	-1.30293500	-0.06738800
H	3.47725900	-1.87390700	0.85598700
H	4.34161400	-1.79591000	-0.68492800
H	3.96858600	-0.31697100	0.20366000
C	1.01806400	-0.56284900	-2.96509900
H	0.93853200	0.20670700	-3.74052000
H	1.09691100	-1.52681800	-3.47355100
H	0.08579700	-0.56333100	-2.39162500
C	3.51241700	-0.42022900	-2.91579400
H	3.61767600	-1.44933800	-3.27547500
H	3.46211800	0.23143500	-3.79509800
H	4.41995300	-0.16596300	-2.36497600
C	-2.10893100	2.59841700	2.53768600
H	-2.60199900	1.62299500	2.52097500
H	-2.62380400	3.23712000	3.26450800
H	-2.23172900	3.02875500	1.54327000
C	0.00803700	3.85155000	3.10674600
H	-0.24460400	4.52190200	2.28628500
H	-0.38108800	4.31038600	4.02208900
H	1.09776600	3.80717000	3.18619100
C	-0.96944300	-3.22902800	6.46710500
H	-1.76062500	-2.52703700	6.74899000
H	-1.16376500	-4.16574400	6.99947900
H	-0.01746700	-2.82483500	6.82072200
C	-2.40029100	-3.85517400	4.48771500
H	-2.74153300	-4.73793200	5.04019000
H	-3.10468900	-3.03915200	4.67790500
H	-2.41650300	-4.08517600	3.41830300
C	1.18949700	-6.26492900	2.30535700
H	0.57391700	-6.85136500	1.61674800
H	2.22796900	-6.57908300	2.17489900
H	0.89789900	-6.55440300	3.31280900
C	2.36670200	-4.89712400	-0.25417600
C	1.86030200	-6.25815900	-0.76835000
H	1.95059300	-7.03357500	-0.00967400
H	0.81875200	-6.21715900	-1.08741600
H	2.46799900	-6.58334100	-1.61750300
C	3.77140000	-5.07088800	0.37115000
H	3.77738000	-5.82732100	1.15960400
H	4.47296300	-5.40017800	-0.40429600
H	4.14019500	-4.14157200	0.81093600
C	0.45570700	3.22063300	0.12503600
H	1.20940600	3.90554500	0.53029200
H	0.55303700	3.23076900	-0.95990000
H	-0.52708500	3.64370800	0.33365800

H	-1.44521800	1.75830500	4.84819600
C	0.69101800	1.88079600	5.13524500
H	0.67633100	2.88494900	5.56640600
H	0.71860300	1.16023500	5.95869700
H	1.61604800	1.77533300	4.55617700
C	1.33088400	-4.62136700	5.28319400
H	1.81306300	-3.64026300	5.34311300
H	1.12876300	-4.97188400	6.29955200
H	2.04586100	-5.30654100	4.82188000
H	-0.44889100	-5.52023000	4.43169000
H	3.49206000	-3.49147300	-1.47707700
C	2.02004700	-4.25682800	-2.80691900
H	2.12112600	-3.42593100	-3.51247300
H	2.64392400	-5.07206800	-3.18359100
H	0.97810100	-4.58866000	-2.82470900
C	3.29453500	2.01577500	-1.21949000
H	3.02198500	2.98013100	-0.78372900
H	4.01053000	1.53974800	-0.54631100
H	3.80274500	2.21298200	-2.16770800
H	1.38659900	1.72995300	-2.11625800
H	-5.86083800	-0.40235600	-2.93664000
C	0.03876800	-8.95446000	-3.01758700
C	-1.34683500	-8.28607000	-3.08699900
C	-1.54565600	-7.21761600	-2.03218500
C	-1.72568700	-7.56691500	-0.68483100
C	-1.53372500	-5.85316100	-2.34855000
C	-1.88090100	-6.60120000	0.30528100
C	-1.68763400	-4.86758300	-1.37021100
C	-1.86564300	-5.23844600	-0.02846600
O	-2.04055800	-4.33905800	0.96775300
C	-2.33227700	6.38456700	-4.58263300
C	-2.42228800	4.88594700	-4.92853000
C	-2.52137500	3.97645700	-3.71935300
C	-3.62254500	4.05418100	-2.85088300
C	-1.54561400	3.01429500	-3.43543700
C	-3.74194900	3.22083600	-1.74439400
C	-1.65183500	2.16390600	-2.33145300
C	-2.75140900	2.26662000	-1.47059300
O	-2.91261200	1.49225300	-0.36837400
H	-2.11949200	-9.05837900	-2.97737300
H	-1.48970900	-7.84904600	-4.08242600
H	-1.74636800	-8.61845000	-0.40626700
H	-1.40716200	-5.54856700	-3.38541000
H	-2.02882400	-6.87743900	1.34461400
H	-1.69769000	-3.81443400	-1.63313100
H	-1.85510200	-3.42365600	0.63564300
H	0.19860700	-9.41953600	-2.03903200
H	-3.29554300	4.72021500	-5.57429000
H	-1.54831300	4.59929100	-5.52572400
H	-0.68462200	2.91594400	-4.09360000
H	-4.41242800	4.77343600	-3.05357000
H	-0.88715300	1.42280100	-2.13166800
H	-4.60363000	3.27591000	-1.08738400
H	-2.27629200	0.73717300	-0.34657400
H	-1.44863800	6.58915400	-3.96904800
H	0.83286000	-8.21417700	-3.16196400
H	0.14631300	-9.72945300	-3.78423100
H	-3.21022200	6.71336800	-4.01736800
H	-2.26911300	6.99392500	-5.49035100
C	7.27033400	-0.96865300	5.68501600
C	6.13556900	-1.78161500	5.05739100

C	5.10523900	-0.90167800	4.33460400
C	4.04748000	-1.74770400	3.63321200
O	4.35557800	-2.69332500	2.91043900
N	2.75194600	-1.41464000	3.87767700
H	5.62382800	-2.36740200	5.83187400
H	6.52807200	-2.50310400	4.33384700
H	4.65038000	-0.18810900	5.03301400
H	5.61127600	-0.31292700	3.55817800
H	2.48823500	-0.58128000	4.37779400
H	2.02281000	-1.90956300	3.37851600
H	6.88944100	-0.25506900	6.42505800
H	7.81371700	-0.39656300	4.92395100
H	7.99124100	-1.61901500	6.19064000

Int1$_{Hby}$

Ni	0.28130420	-1.45372877	0.99394447
N	1.27858179	-0.41050599	-0.35862762
C	2.17103347	-0.28735374	-2.55180005
C	1.98998122	1.15679187	-1.93688213
C	1.25593378	0.85787756	-0.62652800
N	0.12092633	0.26794481	2.03641745
C	0.62131154	1.85176753	0.23354528
C	0.16290747	1.54997349	1.50362372
C	-0.46098280	2.52292280	2.53638642
C	-0.33139317	1.68648872	3.85171451
C	-0.25916275	0.27337566	3.31638504
N	0.24701706	-2.62711159	2.61662998
C	-0.50208118	-0.85838731	4.10999302
C	-0.28802772	-2.19933115	3.77283107
C	-0.65193491	-3.38044690	4.66548566
C	0.32073173	-4.46243191	4.10724546
C	0.55655066	-3.98036639	2.67123029
N	1.05648205	-3.00669045	-0.02143507
C	1.10498559	-4.73744447	1.66035660
C	1.44795853	-4.18794261	0.34448447
C	2.33964291	-3.79476507	-1.89786053
C	1.48672748	-2.61585102	-1.36399914
H	-0.88484407	-0.66148304	5.10538527
H	0.56560499	-2.51294541	-1.94608991
C	-3.06633336	-1.20957074	1.45953145
H	-2.56288156	-0.75302889	2.31376498
H	-3.43052726	-2.19724803	1.75417647
H	-3.91570244	-0.58712656	1.16836817
S	-1.90736913	-1.35420969	0.02989737
C	-4.99556355	-1.63595708	-1.64837654
H	-4.21939297	-2.04843445	-2.29638660
H	-4.72360025	-0.61422118	-1.37498706
H	-5.05789583	-2.24618405	-0.74461844
S	-6.14038720	0.50920954	-4.26962420
C	-4.33773307	0.33347020	-4.48172572
H	-4.09388686	-0.72081253	-4.64502317
H	-3.84253495	0.67972272	-3.57195762
C	-3.86484000	1.18153900	-5.67602000
H	-4.08818808	2.23959516	-5.51494012
H	-2.77861915	1.08156956	-5.77581328
H	-4.33224584	0.85717600	-6.61091314
C	2.14322497	-1.18839695	-1.25995867
C	3.50898949	-1.30794330	-0.54807868
H	3.39376771	-1.83619475	0.40114401
H	4.24812962	-1.84452352	-1.14678254

H	3.91510674	-0.32175804	-0.31856629
C	0.93850775	-0.55156477	-3.44373102
H	0.88586957	0.20331871	-4.23602422
H	0.98304362	-1.52964897	-3.92954265
H	0.00602888	-0.50396448	-2.87268635
C	3.43682849	-0.45496072	-3.40006949
H	3.51890966	-1.48739592	-3.75787228
H	3.40097918	0.19672609	-4.28053534
H	4.35094659	-0.22038260	-2.85032737
C	-1.96620749	2.67791476	2.20495575
H	-2.46975792	1.70821079	2.17544482
H	-2.45119531	3.30044865	2.96658652
H	-2.12231861	3.14314890	1.22957356
C	0.18536426	3.90969934	2.67806083
H	-0.09449181	4.57818543	1.86427398
H	-0.16179356	4.37771491	3.60589583
H	1.27717955	3.85563196	2.71455698
C	-0.53366243	-3.10941637	6.16899067
H	-1.30663622	-2.40631636	6.49641672
H	-0.67921739	-4.03584542	6.73494086
H	0.43969614	-2.69199092	6.44084643
C	-2.10972918	-3.78242596	4.31948908
H	-2.40664857	-4.65008046	4.92057177
H	-2.80095520	-2.96187850	4.53881752
H	-2.20592383	-4.04282903	3.26118347
C	1.32496132	-6.21767140	1.90798754
H	0.68655474	-6.81407334	1.24873159
H	2.36081702	-6.52461754	1.73996091
H	1.07378889	-6.50181978	2.92824286
C	2.36261240	-4.85359671	-0.71362546
C	1.88642435	-6.24837886	-1.16520550
H	2.05841097	-7.00169084	-0.39783264
H	0.82491558	-6.26085223	-1.41766880
H	2.45288310	-6.56768540	-2.04485668
C	3.79924168	-4.95629817	-0.14562407
H	3.86507671	-5.68522803	0.66648260
H	4.48073853	-5.28475016	-0.93956613
H	4.15504801	-4.00142813	0.24907591
C	0.50043778	3.26419872	-0.31371362
H	1.26782779	3.93847206	0.08282348
H	0.57830930	3.27823187	-1.40038796
H	-0.47575999	3.69479237	-0.08741772
H	-1.21054892	1.83087711	4.48968780
C	0.93513669	1.95193450	4.69213724
H	0.94236199	2.95924576	5.11721576
H	0.98895372	1.23627621	5.51935824
H	1.83829337	1.83665839	4.08054724
C	1.66751377	-4.53960826	4.85542615
H	2.15928777	-3.56087774	4.86836090
H	1.52996753	-4.87228851	5.88911746
H	2.34625586	-5.23846087	4.36002794
H	-0.16740147	-5.44027881	4.13349715
H	3.36848195	-3.46314647	-2.06122108
C	1.80935451	-4.29815600	-3.24644869
H	1.83279945	-3.48641401	-3.98102848
H	2.41692598	-5.11292243	-3.65097805
H	0.77656764	-4.65042440	-3.16770819
C	3.26012315	2.00417814	-1.74544136
H	3.00897152	2.97253674	-1.30660039
H	3.98712769	1.52245674	-1.08788261
H	3.74803594	2.19192385	-2.70652122

H	1.32337038	1.73093750	-2.59225571
H	-5.95778879	-1.64479478	-2.16856099
C	0.03876800	-8.95446000	-3.01758700
C	-1.39856000	-8.39895052	-3.07407487
C	-1.63484058	-7.29929526	-2.05896855
C	-1.78413144	-7.60491124	-0.69767124
C	-1.65491079	-5.94718713	-2.42276655
C	-1.93126682	-6.60899766	0.26367810
C	-1.79616935	-4.93229090	-1.47444131
C	-1.93053839	-5.25962359	-0.11679786
O	-2.07081425	-4.32437184	0.85082100
C	-2.33227700	6.38456700	-4.58263300
C	-2.32853183	4.87955181	-4.91375852
C	-2.52146403	3.96620660	-3.71583237
C	-3.64644306	4.09323331	-2.88470777
C	-1.62335084	2.93274871	-3.42436869
C	-3.86982611	3.23392124	-1.81442249
C	-1.83295263	2.05583733	-2.35703542
C	-2.96328832	2.20024383	-1.54122039
O	-3.22851685	1.38559303	-0.49293698
H	-2.10683055	-9.22043062	-2.90213770
H	-1.60338905	-8.02072551	-4.08326793
H	-1.78205476	-8.64738389	-0.38428556
H	-1.55576617	-5.67654257	-3.47254918
H	-2.04935619	-6.85151116	1.31583347
H	-1.81816844	-3.88721574	-1.76945102
H	-1.92921993	-3.41845295	0.47199744
H	0.26355368	-9.34986660	-2.02093588
H	-3.12105834	4.67822932	-5.64925084
H	-1.38607372	4.62176990	-5.41282140
H	-0.74289704	2.79648424	-4.05098952
H	-4.37797440	4.87120282	-3.09016636
H	-1.12804167	1.25993279	-2.14130442
H	-4.75296447	3.32673671	-1.19021770
H	-2.60554001	0.61458900	-0.46473100
H	-1.52786570	6.63175093	-3.88137794
H	0.76801488	-8.16561239	-3.23025003
H	0.18383462	-9.76111945	-3.74528759
H	-3.27730017	6.69178261	-4.12329380
H	-2.19233923	6.98302766	-5.48915395
C	7.27033400	-0.96865300	5.68501600
C	6.18970493	-1.73503671	4.90722665
C	5.28557832	-0.81397907	4.06910874
C	4.27260687	-1.61060845	3.24392884
O	4.62108407	-2.51394547	2.48717607
N	2.96607966	-1.26487608	3.41059969
H	5.56535446	-2.30710323	5.60668718
H	6.64479474	-2.46635880	4.23074625
H	4.78539021	-0.08050103	4.71492637
H	5.90194706	-0.24829261	3.35809548
H	2.67333582	-0.49065438	3.98445206
H	2.25190011	-1.74008158	2.87140102
H	6.82553620	-0.24879802	6.38238324
H	7.92501949	-0.41078020	5.00492622
H	7.89742687	-1.65303920	6.26596859

Reactmodified F430-B12

Ni	0.40161942	-2.39331054	1.41507199
N	1.34485455	-1.31889288	0.02725795
C	2.46432821	-1.20783282	-2.07023599

C	2.17483246	0.24328677	-1.51182975
C	1.28884064	-0.08909601	-0.32010430
N	-0.20152185	-0.70302733	2.31179166
C	0.17325504	0.78562990	0.25509274
C	-0.13454253	0.68724471	1.80931704
C	0.78465365	1.40861496	2.85240659
C	0.21009755	0.73012628	4.14623127
C	-0.14413037	-0.66015706	3.63129554
N	0.16157609	-3.58708450	2.98236820
C	-0.34446312	-1.76687391	4.50500969
C	-0.25486412	-3.11160672	4.18495273
C	-0.55882821	-4.26220307	5.13921355
C	0.31707039	-5.39505783	4.51836928
C	0.51602255	-4.91740888	3.07143268
N	1.17773985	-3.91059434	0.40876952
C	1.09905686	-5.67338778	2.06570220
C	1.53189991	-5.10797602	0.79198244
C	2.65284478	-4.68342476	-1.34057097
C	1.72022293	-3.52890123	-0.89815717
H	-0.53967907	-1.52186491	5.54282328
H	0.85949263	-3.45852060	-1.57223454
C	-3.34554830	-2.03763887	1.79996704
H	-2.43961101	-2.17345385	2.39363324
H	-4.07676356	-2.80658386	2.05924991
H	-3.75839860	-1.04412479	2.00151352
S	-2.86478366	-2.18767554	0.04369977
C	-4.35116087	-1.50568228	-0.77580120
H	-4.18973881	-1.56797670	-1.85351826
H	-4.49577958	-0.45621510	-0.51099867
H	-5.23413570	-2.09660270	-0.51966228
S	-5.74117151	0.37616641	-3.72639227
C	-4.10003826	0.18152899	-4.54748115
H	-4.09452605	-0.84657841	-4.92417707
H	-3.32317355	0.26053391	-3.78152585
C	-3.86455400	1.18191800	-5.67637300
H	-3.92689852	2.20684511	-5.30485260
H	-2.86679019	1.03916340	-6.11177086
H	-4.60808046	1.05712886	-6.46955799
C	2.33357831	-2.08725854	-0.76500115
C	3.62023749	-2.15477668	0.07682379
H	3.43826812	-2.72441817	0.98576355
H	4.44275303	-2.63503734	-0.45561850
H	3.95011053	-1.16010661	0.37954608
C	1.32872318	-1.50958035	-3.07393587
H	1.37907985	-0.80045723	-3.90809147
H	1.40047880	-2.51452331	-3.49572135
H	0.34321200	-1.40386711	-2.60735962
C	3.81163218	-1.35140368	-2.78634672
H	3.95732906	-2.38534265	-3.11802529
H	3.84641352	-0.71183495	-3.67575066
H	4.65951989	-1.08456526	-2.15190815
O	-1.41657867	1.29413291	1.98464705
H	-2.07389030	0.71446573	1.57928446
C	0.62959704	2.93351015	2.95160102
H	-0.42201612	3.22512026	2.92232103
H	1.05632228	3.28031486	3.89961351
H	1.15924984	3.46289255	2.15634876
C	2.25931543	1.03600561	2.61669918
H	2.89325124	1.45778447	3.40315527
H	2.41001873	-0.04648948	2.59003436
H	2.61473499	1.44638295	1.66632182

C	-0.27665726	-3.95272252	6.61374851
H	-0.97910201	-3.20072061	6.98818969
H	-0.40589711	-4.85047989	7.22771297
H	0.73657993	-3.57323271	6.76899158
C	-2.05578397	-4.62390388	4.96923974
H	-2.31235301	-5.46718893	5.62160300
H	-2.69218037	-3.77487459	5.24115933
H	-2.27583361	-4.90704772	3.93660930
C	1.25720354	-7.16666916	2.29679169
H	0.65904150	-7.72931800	1.57205866
H	2.29149402	-7.51566952	2.21788858
H	0.89900506	-7.46186466	3.28189458
C	2.53989950	-5.76407501	-0.18525022
C	2.09008182	-7.14106950	-0.71071606
H	2.18707912	-7.91331978	0.05104525
H	1.05096718	-7.12665956	-1.04305925
H	2.71618317	-7.45308533	-1.55139611
C	3.91361121	-5.89405546	0.51491879
H	3.89155447	-6.63992615	1.31333394
H	4.66790317	-6.21440476	-0.21437577
H	4.23813168	-4.94951678	0.96131709
C	0.30031869	2.24980815	-0.16096852
H	1.21609972	2.69476890	0.22731084
H	0.30943577	2.33705472	-1.24845640
H	-0.55366193	2.80852291	0.22260810
O	-1.00369658	0.30370453	-0.44969732
H	-1.22387009	-0.62301652	-0.19290039
H	-0.72030546	1.25601532	4.39508738
C	1.11984099	0.75107806	5.37670079
H	1.42480063	1.77508505	5.61742574
H	0.60487910	0.35021554	6.25470657
H	2.03009686	0.16122984	5.22822349
C	1.68481070	-5.57915536	5.20541026
H	2.25099636	-4.64234349	5.20030946
H	1.56791504	-5.90795036	6.24293246
H	2.28630694	-6.32476253	4.68019969
H	-0.23233178	-6.34103656	4.55538489
H	3.68799113	-4.33258585	-1.35589153
C	2.32641199	-5.16619054	-2.75850673
H	2.44575395	-4.34483492	-3.47250971
H	2.99272806	-5.97030362	-3.08418516
H	1.29613663	-5.52776378	-2.83435468
C	3.39037573	1.12754348	-1.17240791
H	3.06586431	2.11108236	-0.82244715
H	4.02353092	0.69099732	-0.39719830
H	4.00793992	1.28495923	-2.06174920
H	1.58344858	0.79358383	-2.25417977
H	-5.45163952	1.53919230	-3.10516424
C	0.03880500	-8.95451900	-3.01748400
C	-1.46470968	-8.68520531	-2.81564750
C	-1.71447337	-7.72299343	-1.67450341
C	-2.17711036	-8.15817633	-0.42757003
C	-1.40615454	-6.36255075	-1.81629886
C	-2.31492876	-7.27780392	0.64638023
C	-1.52305866	-5.47257964	-0.75354082
C	-1.97453922	-5.93307589	0.48997026
O	-2.11734196	-5.10643621	1.56786171
C	-2.33178300	6.38467200	-4.58248000
C	-3.43771097	5.32928423	-4.74955695
C	-3.44290638	4.33363448	-3.61044813
C	-4.43666791	4.33001278	-2.62494155

C	-2.41087043	3.39292731	-3.49618564
C	-4.40225530	3.43496574	-1.55449412
C	-2.36777452	2.47969316	-2.44884507
C	-3.35909120	2.50796144	-1.45469383
O	-3.33947246	1.65438489	-0.39928569
H	-1.98436133	-9.63204538	-2.62489932
H	-1.88599297	-8.28094786	-3.74585486
H	-2.42656799	-9.20797462	-0.28752583
H	-1.06026084	-5.99319746	-2.78009537
H	-2.66898276	-7.61884165	1.61465204
H	-1.26999119	-4.42566911	-0.86957862
H	-1.51945901	-4.34557719	1.47878780
H	0.48455803	-9.37233880	-2.10899554
H	-4.41405471	5.82356487	-4.81755684
H	-3.29155794	4.80069118	-5.70153590
H	-1.63405143	3.36039669	-4.25772674
H	-5.25524914	5.04350038	-2.69106189
H	-1.58192257	1.73453578	-2.38965772
H	-5.16800142	3.44510641	-0.78483428
H	-2.48457030	1.16521616	-0.41648821
H	-1.34509833	5.91202759	-4.53092237
H	0.57432242	-8.02908028	-3.25254592
H	0.20899969	-9.66122255	-3.83803195
H	-2.47473439	6.95171960	-3.65634156
H	-2.32458501	7.09277813	-5.41899592
C	7.27036300	-0.96856400	5.68488600
C	6.38457996	-2.02611125	5.01243927
C	5.06609814	-1.45878821	4.46514381
C	4.31487468	-2.47947513	3.60717433
O	4.90430388	-3.22297949	2.82529233
N	2.96140591	-2.49543204	3.73897863
H	6.15620834	-2.82919657	5.72518445
H	6.91487814	-2.49855640	4.17938407
H	4.43174163	-1.08319108	5.27870701
H	5.27692988	-0.59985776	3.81170837
H	2.44987534	-1.86767131	4.33987512
H	2.40402257	-3.06172937	3.11072316
H	6.75579497	-0.48656763	6.52470278
H	7.55284219	-0.18202959	4.97498973
H	8.19224341	-1.41555917	6.07168996

Int1$_{Ni-methyl}$

Ni	1.73201139	-0.97412469	1.17061738
N	2.79840040	-0.03119150	-0.26877801
C	3.62141423	-0.06878986	-2.50932299
C	3.56441016	1.40519647	-1.94275808
C	2.81590298	1.19126634	-0.63288244
N	1.16023958	0.77278290	1.93889527
C	1.92107649	2.26577657	0.03886169
C	1.72190559	2.07626307	1.60185924
C	0.76318881	3.10866023	2.35835301
C	0.31242672	2.23680480	3.57693861
C	0.41215643	0.82870311	3.01986786
N	0.88220582	-2.13157228	2.53155059
C	-0.15560949	-0.27983482	3.70742480
C	0.08018486	-1.64070340	3.48646193
C	-0.52918126	-2.76660170	4.32283259
C	0.41384197	-3.95537378	3.93908018
C	1.00433505	-3.50318401	2.60075625
N	2.32008197	-2.56592761	0.16993968

C	1.61167917	-4.32668724	1.66789205
C	2.18449165	-3.83406398	0.41739169
C	3.36437235	-3.59911424	-1.66804110
C	2.73116589	-2.27462092	-1.20743640
H	-0.80833281	-0.02766536	4.53574950
H	1.81045218	-2.09592492	-1.77395623
C	-0.11470921	-1.18212919	0.13208808
H	-0.76629331	-0.63559663	0.80182211
H	-0.24934885	-2.25514176	0.13104893
H	0.06032227	-0.72208914	-0.83500472
S	-2.86830716	-1.58190403	-0.89839140
C	-3.75985352	-1.12603182	0.65373647
H	-3.46181218	-1.77795012	1.48045232
H	-4.83913838	-1.22692348	0.50676435
H	-3.54066885	-0.08889281	0.92457530
S	-4.90417089	-1.06545169	-4.39873495
C	-3.47353189	0.06466371	-4.71018131
H	-2.64025409	-0.52008787	-5.11380837
H	-3.16217634	0.47957067	-3.75062623
C	-3.86455400	1.18191800	-5.67637300
H	-4.63801546	1.82092245	-5.23995990
H	-2.99462764	1.80806603	-5.89925547
H	-4.24519151	0.78076861	-6.62296606
C	3.55448264	-0.93290570	-1.18453857
C	4.92674568	-1.19743364	-0.53978887
H	4.78394424	-1.69577595	0.41975374
H	5.55310567	-1.81785673	-1.18540864
H	5.45465940	-0.26311362	-0.34461473
C	2.35554346	-0.25921666	-3.37209840
H	2.37662859	0.43817387	-4.21690974
H	2.28441658	-1.26959236	-3.78279665
H	1.44505028	-0.05425449	-2.79930007
C	4.85536267	-0.33316217	-3.38048965
H	4.85091050	-1.35850470	-3.75959165
H	4.85654898	0.33400468	-4.24978080
H	5.79533900	-0.18359759	-2.84585515
O	3.03493073	2.08170397	2.19813485
H	3.43472585	2.94482012	2.03307980
C	-0.51462896	3.46361405	1.56603984
H	-1.10174592	2.57795504	1.31312564
H	-1.14036529	4.11383609	2.18883709
H	-0.30955107	3.98609298	0.63157208
C	1.44981331	4.40999622	2.80668392
H	1.65946980	5.07670490	1.96736442
H	0.78709897	4.95791681	3.48541873
H	2.38414696	4.23145979	3.34525418
C	-0.58473439	-2.44770300	5.82358934
H	-1.30980055	-1.65171912	6.02045002
H	-0.90974700	-3.32767143	6.38907910
H	0.38325830	-2.12568686	6.21843151
C	-1.95750417	-3.04809739	3.80177446
H	-2.41677999	-3.85144193	4.39032024
H	-2.58598941	-2.15619392	3.89646515
H	-1.94618401	-3.35871766	2.75418426
C	1.66970780	-5.81924591	1.93399485
H	1.24774572	-6.39601880	1.10784685
H	2.69817738	-6.16518220	2.09151303
H	1.09970284	-6.09684899	2.81984382
C	2.58651187	-4.67405329	-0.82135373
C	1.29526617	-5.13923001	-1.52713785
H	0.70124616	-5.78959082	-0.88426742

H	0.65575433	-4.29688600	-1.80751006
H	1.53245448	-5.70354588	-2.43448200
C	3.51642946	-5.87338899	-0.56459176
H	2.98624476	-6.74781882	-0.18474815
H	3.98858792	-6.17073452	-1.50833565
H	4.31493658	-5.61794358	0.14073959
C	2.45024910	3.67596679	-0.26387015
H	3.41400510	3.88384410	0.20958979
H	2.56508206	3.80082237	-1.34140186
H	1.72283803	4.41594317	0.06202950
O	0.72079871	2.18744846	-0.70625401
H	0.07845163	1.54726582	-0.34495410
H	-0.72655636	2.46918772	3.83899891
C	1.16610627	2.35683456	4.85548290
H	1.08666750	3.35561515	5.29485008
H	0.82258059	1.63557587	5.60462432
H	2.21596899	2.15349425	4.63059346
C	1.56712915	-4.19904763	4.93340706
H	2.17195102	-3.29288459	5.05045127
H	1.19326565	-4.49542538	5.91825689
H	2.22592308	-4.99198679	4.56898727
H	-0.17575409	-4.87076363	3.83840080
H	4.40057686	-3.62352777	-1.31049082
C	3.36165388	-3.85035246	-3.17486682
H	4.03508107	-3.16248912	-3.69227585
H	3.69821347	-4.86652320	-3.40693355
H	2.36335189	-3.72568381	-3.60466841
C	4.91865573	2.12418658	-1.77192122
H	4.78289095	3.14287171	-1.40485407
H	5.57766747	1.60579727	-1.07167391
H	5.43633174	2.19349862	-2.73270336
H	2.94757425	2.01991683	-2.60951715
H	-4.48461942	-1.48751450	-3.18192542
C	0.03880500	-8.95451900	-3.01748400
C	-1.29406589	-9.00507187	-2.24316737
C	-1.56518582	-7.73570265	-1.46036630
C	-1.32786754	-7.65147280	-0.08208832
C	-2.02624350	-6.57993075	-2.10701682
C	-1.51568449	-6.46035627	0.62001357
C	-2.21740809	-5.38057870	-1.42511248
C	-1.93752526	-5.30587908	-0.05114918
O	-2.04440590	-4.15554245	0.65488077
C	-2.33178300	6.38467200	-4.58248000
C	-2.99557256	5.00834990	-4.76940764
C	-2.67834025	4.03399696	-3.65286880
C	-3.38657699	4.06227861	-2.44463440
C	-1.66545529	3.07649645	-3.79350397
C	-3.11481951	3.15242363	-1.42194627
C	-1.38797410	2.15946102	-2.78246468
C	-2.12219802	2.18703392	-1.59291533
O	-1.84933241	1.30273813	-0.57204102
H	-1.28607111	-9.86538667	-1.56212805
H	-2.11188549	-9.18180426	-2.95434642
H	-0.98690704	-8.53475778	0.45539078
H	-2.23914597	-6.61656874	-3.17403527
H	-1.32331332	-6.40034074	1.68696425
H	-2.57573852	-4.49469816	-1.94101850
H	-2.30619691	-3.39943979	0.06104503
H	0.88068691	-8.81378653	-2.32984934
H	-4.08305888	5.13935345	-4.83896534
H	-2.67707269	4.57856907	-5.72718582

H	-1.09362108	3.03693275	-4.71864538
H	-4.17908958	4.79569297	-2.30858187
H	-0.60068689	1.42231085	-2.89833643
H	-3.67706879	3.16151777	-0.49292074
H	-2.09003813	0.36648100	-0.84318310
H	-1.24132718	6.28805630	-4.53647590
H	0.04368994	-8.11469256	-3.72065794
H	0.20885200	-9.87690777	-3.58487329
H	-2.66133249	6.85139726	-3.64762656
H	-2.58072876	7.06172990	-5.40759917
C	7.27036300	-0.96856400	5.68488600
C	5.80256381	-1.19870312	5.30669637
C	5.40935947	-0.47036863	4.00798598
C	3.97294119	-0.70019078	3.55683176
O	3.71236995	-1.03382221	2.39724771
N	3.02030241	-0.53438341	4.50525626
H	5.16465199	-0.86728072	6.13660004
H	5.60986365	-2.27223814	5.18658282
H	5.54812202	0.61374227	4.12956099
H	6.05116677	-0.78596150	3.18081661
H	3.25008055	-0.11126258	5.39006538
H	2.04310696	-0.54117308	4.23763443
H	7.47731006	0.09748965	5.83580350
H	7.94150141	-1.32826708	4.89667174
H	7.52821002	-1.49457145	6.60985782

References cited in ESI:

S1 (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, 37, 785–789; (b) A. D. Becke, *J. Chem. Phys*. **1993**, 98, 1372–1377; (c) A. D. Becke, *J. Chem. Phys*. **1993**, 98, 5648–5652.

S2 (a) S. Grimme, *J. Comput. Chem.* **2004**, 25, 1463–1473; (b) S. Grimme, *J. Comput. Chem*. **2006**, 27, 1787–1799; (c) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, 132, 154104; (d) L. Goerigk, S. Grimme, *Phys. Chem. Chem. Phys*. **2011**, 13, 6670–6688.

S3 Jaguar, version 8.7, Schrodinger, LLC, New York, NY, **2015**.

S4 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, **2013**.

S5 (a) P. E. M. Siegbahn, *J. Comput. Chem*. **2001**, 22, 1634–1645; (b) P. E. M. Siegbahn, *Q. Rev. Biophys.* **2003**, 36, 91–145; (c) F. Himo, P. E. M. Siegbahn, *Chem. Rev.* **2003**, 103, 2421–2456; (d) F. Himo, *Theor. Chem. Acc*. **2006**, 116, 232–240; (e) F. Himo, P. E. M. Siegbahn, *J. Biol. Inorg. Chem*. **2009**, 14, 643–651; (f) P. E. M. Siegbahn, M. R. A Blomberg, *Chem. Rev*. **2010**, 110, 7040–7061.

S6 (a) P. E. M. Siegbahn, S. L. Chen, R. Z. Liao, *Inorganics* **2019**, 7, 95; (b) T. H. Zhang, X. Y. Zhang and L. W. Chung, *Asian J. Org. Chem*. **2018**, 7, 522-536.

S7 (a) V. Pelmenschikov, M. R. A. Blomberg, P. E. M. Siegbahn and R. H. Crabtree, *J. Am. Chem. Soc.* **2002**, 124, 4039-4049; (b) S. L. Chen, V. Pelmenschikov, M. R. A. Blomberg and P. E. M. Siegbahn, *J. Am. Chem. Soc.* **2009,** 131, 9912 –9913; (c) S. L. Chen, M. R. A. Blomberg, P. E. M. Siegbahn, *Chem. Eur. J.* **2012**, 18, 6309-6315; (d) S. L. Chen, M. R. A. Blomberg, P. E. M. Siegbahn, *Phys. Chem. Chem. Phys*. **2014**, 16, 14029–14035.

S8 (a) X. Zhang, L. W. Chung, *Chem. Eur. J.* **2017**, 23, 3623-3630; (b) M. J. Yu, S. L. Chen, *Chem. Eur. J.* **2017**, 23, 7545-7557.

S9 W. Grabarse, F. Mahlert, E. C. Duin, M. Goubeaud, S. Shima, R. K. Thauer, V. Lamzin and U. Ermler, *J. Mol. Biol.* **2001**, 309, 315–330.

S10 J. Wang, R. M. Wolf, J. W. Caldwell, P. A. Kollman and D. A. Case, *J. Comput. Chem.* **2004**, 25, 1157–1174.

S11 P. F. Li, K. M. Merz, *J. Chem. Inf. Model.* **2016**, 56, 599-604.

S12 J. A. Maier, C. Martinez, K. Kasavajhala, L. Wickstrom, K. E. Hauser and C. Simmerling, *J. Chem. Theory Comput*. **2015**, 11, 3696–3713.

S13 W. L. Jorgensen, J. Chandrasekhar, J. D. Madura, R. W. Impey and M. L. Klein, *J. Chem. Phys*. **1983**, 79, 926–935.

S14 (a) A. W. Götz, M. J. Williamson, D, Xu, D. Poole, S. L. Grand and R. C. Walker, J. *Chem. Theory Comput*. **2012**, 8, 1542–1555; (b) S. L. Grand, A. W. Götz, R. C. Walker, *Comput. Phys. Commun.* **2013**, 184, 374–380.

S15 D. A. Case, T. A. Darden, T. E. Cheatham, C. L. Simmerling, J. Wang, R. E. Duke, R. Luo, M. Crowley, R. C. Walker, W. Zhang, K. M. Merz, B. Wang, S. Hayik, A. Roitberg, G. Seabra, I. Kolossváry, K. F. Wong, F. Paesani, J. Vanicek, X. Wu, S. R. Brozell, T. Steinbrecher, H. Gohlke, L. Yang, C. Tan, J. Mongan, V. Hornak, G. Cui, D. H. Mathews, M. G. Seetin, C. Sagui, V. Babin, P. A. Kollman, *AMBER 16*, University of California, San Francisco, **2016**.

S16 T. Darden, D. York, L. Pedersen, *J. Chem. Phys.* **1993**, 98, 10089–10092.

S17 J.-P. Ryckaert, G. Ciccotti, H. J. C. Berendsen, *J. Comput. Phys.* **1977**, 23, 327–341.

S18 J. A. Izaguirre, D. P. Catarello, J. M. Wozniak and R. D. Skeel, *J. Chem. Phys.* **2001**, 114, 2090–2098.

S19 H. J. C. Berendsen, J. P. M. Postma, W. F. van Gunsteren, A. DiNola and J. R. Haak, *J. Chem. Phys.* **1984**, 81, 3684–3690.

S20 D. R. Roe, T. E. Cheatham, *J. Chem. Theory Comput.* **2013**, 9, 3084–3095.

The complete references 2, 3, 5, 6, 8, 9, 12, 15, 18, 20-23, and 26-28 in the text:

2 (a) P. N. Evans, J. A. Boyd, A. O. Leu, B. J. Woodcroft, D. H. Parks, P. Hugenholtz and G. W. Tyson, *Nature Rev. Microbiol*. **2019**, 17, 219-232; (b) R. K. Thauer, A. K. Kaster, H. Seedorf, W. Buckel and R. Hedderich, *Nature Rev. Microbiol*. **2008**, 6, 579-591.

3 K. Nauhaus, M. Albrecht, M. Elvert, A. Boetius and F. Widdel, *Environ. Microbiol*. **2007**, 9, 187-196.

5 K. F. Ettwig, B. Zhu, D. Speth, J. T. Keltjens, M. S. M. Jetten and B. Kartal, *Proc. Natl Acad. Sci*. *USA* **2016**, 113, 12792-12796.

6 M. F. Haroon, S. Hu, Y. Shi, M. Imelfort, J. Keller, P. Hugenholtz, Z. Yuan and G. W. Tyson, *Nature* **2013**, 500, 567-570.

8 B. Shen, L. Dong, S. H. Xiao, X. G. Lang, K. J. Huang, Y. B. Peng, C. M. Zhou, S. Ke and P. J. Liu, *Nature Comm*. **2016**, 7, 10317.

9 N. J. Planavsky, C. T. Reinhard, X. Wang, D. Thomson, P. McGoldrick, R. H. Rainbird, T. Johnson, W. W. Fischer and T. W. Lyons, *Science* **2014**, 346, 635-638.

12 (a) K. D. Nguyen, B. Y. Park, T. Luong, H. Sato, V. J. Garza and M. J. Krische, *Science* **2016**, 354, 300; (b) S. J. Moore, S. T. Sowa, C. Schuchardt, E. Deery, A. D. Lawrence, J. V. Ramos, S. Billig, C. Birkemeyer, P. T. Chivers, M. J. Howard, S. E. Rigby, G. Layer and M. J. Warren, *Nature* **2017**, 543, 78-82.

15 (a) A. Sluijs, H. Brinkhuis, S. Schouten, S. M. Bohaty, C. M. John, J. C. Zachos, G. J. Reichart, J. S. S. Damsté, E. M. Crouch and G. R. Dickens, *Nature* **2007**, 450, 1218-1221.

18 C. Kieninger, E. Deery, A. D. Lawrence, M. Podewitz, K. Wurst, E. Nemoto-Smith, F. J. Widner, J. A. Baker, S. Jockusch, C. R. Kreutz, K. R. Liedl, K. Gruber, M. J. Warren, B. Kräutler, *Angew. Chem. Int. Ed*. **2019**, 58, 10756 – 10760.

20 (a) V. Pelmenschikov, M. R. A. Blomberg, P. E. M. Siegbahn and R. H. Crabtree, *J. Am. Chem. Soc.* **2002**, 124, 4039-4049; (b) S. L. Chen, V. Pelmenschikov, M. R. A. Blomberg and P. E. M. Siegbahn, *J. Am. Chem. Soc.* **2009**, 131, 9912 –9913; (c) S. L. Chen, M. R. A. Blomberg and P. E. M. Siegbahn, *Chem. Eur. J.* **2012**, 18, 6309-6315.

21 (a) T. Wongnate, D. Sliwa, B. Ginovska, D. Smith, M. W. Wolf, N. Lehnert, S. Raugei and S. W. Ragsdale, *Science* **2016**, 352, 953–958; (b) T. J. Lawton, A. C. Rosenzweig, *Science* **2016,** 352, 892-893; (c) S. Shima, *Angew. Chem. Int. Ed*. **2016**, 55, 13648-13649.

22 S. Scheller, M. Goenrich, R. K. Thauer and B. Jaun, *J. Am. Chem. Soc*. **2013**, 135, 14975–14984.

23 W. Grabarse, F. Mahlert, E. C. Duin, M. Goubeaud, S. Shima, R. K. Thauer, V. Lamzin and U. Ermler, *J. Mol. Biol.* **2001**, 309, 315–330.

26 D. A. Case, T. A. Darden, T. E. Cheatham, C. L. Simmerling, J. Wang, R. E. Duke, R. Luo, M. Crowley, R. C. Walker, W. Zhang, K. M. Merz, B. Wang, S. Hayik, A. Roitberg, G. Seabra, I. Kolossváry, K. F. Wong, F. Paesani, J. Vanicek, X. Wu, S. R. Brozell, T. Steinbrecher, H. Gohlke, L. Yang, C. Tan, J. Mongan, V. Hornak, G. Cui, D. H. Mathews, M. G. Seetin, C. Sagui, V. Babin, P. A. Kollman, *AMBER 16*, University of California, San Francisco, **2016**.

27 S. C. Chen, N. Musat, O. J. Lechtenfeld, H. Paschke, M. Schmidt, N. Said, D. Popp, F. Calabrese, H. Stryhanyuk, U. Jaekel, Y. G. Zhu, S. B. Joye, H. H. Richnow, F. Widdel and F. Musat, *Nature* **2019**, *568*, 108-111.

28 R. L. Pérez, G. Wegener, K. Knittel, F. Widdel, K. J. Harding, V. Krukenberg, D. V. Meier, M. Richter, H. E. Tegetmeyer, D. Riedel, H. H. Richnow, L. Adrian, T. Reemtsma, O. J. Lechtenfeld and F. Musat, *Nature* **2016**, *539*, 396-401.