

## Supporting Information to:

# *Convergence in the QM-only and QM/MM Modeling of Enzymatic Reactions: a Case Study for Acetylene Hydratase*

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The following data can be obtained electronically from the authors upon request.

For each stationary point: optimized Cartesian coordinates for models M3a and M4 (full system, 30942 atoms) and for the corresponding QM regions (157 atoms for M3a, 408 atoms for M4). Data will be provided as an archive file containing two pdb files for each stationary point and a given model (M3a or M4) as well as the CHARMM parameter file.

**Table S1.** Electrostatic contribution of selected groups and residues to the energy of Int2 relative to Int1 (QM region M3a, 157 atoms, RI-BP86/def2-SVP).

Selected residue/group	Distance to W*(Å)	QM energy (kcal/mol)	Energy Difference
No selection (Original model)		3.5	0
Cys12	8.6	21.0	17.5
SFE <sup>a</sup>	11.3	-4.4	-7.9
Cys16	14.3	9.7	6.2
Cys9	12.8	9.1	5.6
Asp699	11.6	-1.5	-5.0
Lys172	10.8	-1.3	-4.8
Cys46	14.6	7.0	3.5
Cryw471 <sup>b</sup>	7.2	6.6	3.1
Lys48	11.8	0.6	-2.9
Asp298	8.9	1.3	-2.2
Cryw276	8.8	1.3	-2.2
Ile14	8.6	1.4	-2.1
Arg673	13.9	5.4	1.9
Glu607	12.1	1.8	-1.7
Cryw207	5.4	5.1	1.6
Ribose-base <sup>c</sup>	10.8	5.1	1.5
Asn114	9.0	4.9	1.4
Asn178	9.7	4.9	1.4
His616	13.7	4.8	1.3
Asn15	11.2	2.2	-1.3
Trp293	5.1	4.7	1.2
Cryw204	5.5	4.7	1.2
Wz2-2590 <sup>d</sup>	7.9	2.5	-1.0
Thr111	8.1	4.4	0.9
Ile113	7.0	4.4	0.9
Arg678	14.6	4.4	0.9
Cryw131	9.6	4.4	0.9
Ser613	10.7	4.3	0.8
Ser11	11.0	2.7	-0.8
His385	14.9	4.2	0.7
Trp472	6.5	4.2	0.7
Cryw162	8.2	4.2	0.7
Wz1-1419 <sup>c</sup>	8.4	4.2	0.7
Phe611	6.3	4.1	0.6
Cryw43	8.2	4.1	0.6
Gly422	9.6	2.9	-0.6
Cryw259	11.3	2.9	-0.6
Met140	7.0	4.0	0.5
Gly143	8.5	4.0	0.5
Asp608	14.4	4.0	0.5
Cryw20	9.9	3.0	-0.5
Cryw39	10.3	3.0	-0.5
Wz1-1423	10.0	3.0	-0.5
Tyr156	9.3	3.9	0.4
Met299	6.2	3.9	0.4
Cryw46	10.1	3.9	0.4
Cryw66	8.8	3.9	0.4
Cryw73	10.5	3.9	0.4
Cryw632	11.4	3.9	0.4

Ser296	9.0	3.1	-0.4
Arg314	14.3	3.1	-0.4
Gln612	5.4	3.1	-0.4
Wz1-261	10.7	3.1	-0.4
Ala294	7.7	3.8	0.3
Met138	6.5	3.8	0.3
Cryw105	10.8	3.8	0.3
Wz1-1146	10.7	3.8	0.3
Wz1-1415	5.9	3.8	0.3
Cryw49	7.6	3.2	-0.3
Cryw620	9.9	3.2	-0.3
Ala146	12.5	3.7	0.2
Glu473	14.7	3.7	0.2
Leu719	9.9	3.7	0.2
Cryw2	11.5	3.7	0.2
Cryw177	9.8	3.7	0.2
Cryw245	8.8	3.7	0.2
Cryw257	8.6	3.7	0.2
Wz1-1416	11.1	3.7	0.2
Wz1-2707	8.4	3.7	0.2
Glu112	10.8	3.3	-0.2
Ser136	9.3	3.3	-0.2
Ser137	6.9	3.3	-0.2
Tyr139	8.4	3.6	0.1
Thr297	11.3	3.6	0.1
Met387	11.0	3.6	0.1
Gly388	11.3	3.6	0.1
Met391	11.8	3.6	0.1
Wz1-1420	9.0	3.6	0.1
Ile142	6.3	3.4	-0.1
Thr145	9.0	3.4	-0.1
Ile170	11.5	3.4	-0.1
Val295	5.4	3.4	-0.1
Gly604	11.0	3.4	-0.1
Cryw37	10.2	3.4	-0.1
Cryw98	10.9	3.4	-0.1
Cryw197	10.7	3.4	-0.1
Wz1-188	10.5	3.4	-0.1
Asn144	8.8	3.5	0
Ser417	10.6	3.5	0
Ala603	10.7	3.5	0
Leu605	11.5	3.5	0
Cryw246	10.6	3.5	0
Cryw279	10.8	3.5	0
Wz2-2377	10.5	3.5	0

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a: Iron-sulfur cluster

b: Crystal water molecule with segment ID Cryw and residue ID 471 in Charmm format.

c: Guanosine nucleoside of pterin molecule.

d: Solvent water molecule with segment ID Wz2 and residue ID 2590 in Charmm format.

e: Solvent water molecule with segment ID Wz1 and residue ID 1419 in Charmm format.

## QM region M4, 408 QM atoms

For snapshot BS100, the following residues (within 15 Å to tungsten, 2311 atoms) were allowed to move during the geometry optimizations:

Val8, Cys9, Gln10, Ser11, Cys12, Asp13, Ile14, Asn15, Cys16, Cys46, Lys48, Ser109, Gln110, Thr111, Glu112, Ile113, Asn114, Gln115, Gln116, Trp134, Thr135, Ser136, Ala137, Met138, Tyr139, Met140, Cys141, Ile142, Gly143, Asn144, Thr145, Ala146, Gly147, Val148, Hse149, Tyr156, Ser157, Phe158, Ala159, Phe161, Phe169, Ile170, Gly171, Lys172, Asn173, Leu174, Ser175, Hse177, Asn178, Trp179, Val180, Ser181, Gln182, Ile291, Pro292, Trp293, Ala294, Val295, Ser296, Thr297, Asp298, Met299, Gln300, Ser303, Ala306, Ile307, Gln310, Arg314, Phe362, Leu363, Hsp385, Asn386, Met387, Gly388, Ala389, Met391, Pro394, Leu415, Ala416, Ser417, Asn418, Ala419, Met421, Gly422, Tyr423, Ala424, Arg465, Gln469, Asn471, Trp472, Glu473, Gly474, Ile475, Phe602, Ala603, Gly604, Leu605, Arg606, Glu607, Asp608, Asn610, Phe611, Gln612, Ser613, Cys614, Tyr615, Hsp616, Arg673, Ile674, Pro675, Hsp676, Gly677, Arg678, Asn698, Asp699, Ala700, Leu703, Gln714, Leu716, Pro717, Asn718, Leu719, Arg720, SFE, PTA1, Cryw2, Cryw6, Cryw20, Cryw21, Cryw35, Cryw37, Cryw39, Cryw43, Cryw46, Cryw49, Cryw66, Cryw68, Cryw73, Cryw80, Cryw85, Cryw91, Cryw96, Cryw98, Cryw105, Cryw119, Cryw131, Cryw137, Cryw141, Cryw145, Cryw148, Cryw150, Cryw156, Cryw162, Cryw177, Cryw197, Cryw204, Cryw207, Cryw219, Cryw225, Cryw228, Cryw239, Cryw245, Cryw246, Cryw257, Cryw259, Cryw276, Cryw279, Cryw291, Cryw305, Cryw471, Cryw472, Cryw487, Cryw488, Cryw491, Cryw492, Cryw494, Cryw578, Cryw620, Cryw632, Cryw651, Cryw719, Wz1-188, Wz1-261, Wz1-298, Wz1-411, Wz1-650, Wz1-717, Wz1-734, Wz1-818, Wz1-1146, Wz1-1149, Wz1-1152, Wz1-1170, Wz1-1190, Wz1-1199, Wz1-1270, Wz1-1285, Wz1-1415, Wz1-1416, Wz1-1419, Wz1-1420, Wz1-1423, Wz1-2470, Wz1-2707, Wz2-43, Wz2-1262, Wz2-1267, Wz2-1640, Wz2-2267, Wz2-2377, Wz1-2408, Wz2-2409, Wz2-2590, Wz2-2591.

Notice: In the previous QM/MM geometry optimizations, the iron-sulfur cluster SFE was fixed.

**Table S2. Details of QM region M4**

Residue ID	Composition	Atom numbers
Cys9	Side chain -CH <sub>2</sub> S <sup>-</sup>	138-141
Ser11	Backbone -CHCO-	163,164,170,171
Cys12	All	172-180
Asp13	All	181-193
Ile14	All	194-212
Asn15	Backbone -NHCH-	213-216
Cys16	Side chain -CH <sub>2</sub> S <sup>-</sup>	231-234
Cys46	Side chain -CH <sub>2</sub> S <sup>-</sup>	675-678
Lys48	Side chain -CH <sub>2</sub> NH <sub>3</sub> <sup>+</sup>	711-717
Met138	Side chain -CH <sub>2</sub> CH <sub>2</sub> SCH <sub>3</sub>	2165-2175
Met140	Backbone -CHCO-	2201,2202,2214,2215
Cys141	All	2216-2225
Ile142	Backbone -NHCH-	2226-2229
Lys172	Side chain -CH <sub>2</sub> NH <sub>3</sub> <sup>+</sup>	2668-2674
Trp179	Side chain 3-methylene-indole	2770-2787
Gln182	Side chain -CH <sub>2</sub> CONH <sub>2</sub>	2824-2831
Trp293	Side chain -indole	4595-4609
Trp472	Side chain -indole	7354-7368
Arg606	Side chain -CH <sub>2</sub> CH <sub>2</sub> NHC(NH <sub>2</sub> )NH <sub>2</sub>	9503-9517
Gln617	Side chain -CH <sub>2</sub> CONH <sub>2</sub>	9599-9606
His676	Side chain imidazolium	10599-10607
Asp699	Side chain -CH <sub>2</sub> COO <sup>-</sup>	10921-10926
Arg720	Side chain -NHC(NH <sub>2</sub> )NH <sub>2</sub>	11239-11247
SFE	Fe <sub>4</sub> S <sub>4</sub>	11399-11406
PTA	Tungsten-complex without ribose-base	11407-11485,11502,11519

The following water molecules are also included:

Cryw35, Cryw43, Cryw49, Cryw131, Cryw137, Cryw204, Cryw207, Cryw257, Cryw259, Cryw276, Cryw291, Cryw471, Cryw620, Wz1-188, Wz1-261, Wz1-734, Wz1-818, Wz1-1152, Wz1-1170, Wz1-1190, Wz1-1415, Wz1-1416, Wz1-1419, Wz1-1420, Wz1-1423, Wz2-1262, Wz2-1267, Wz2-2590, Wz2-2591

**Table S3.** Calculated QM, MM, and QM/MM energies (in hartree) of optimized stationary points for snapshot BS100 (QM region **M4**, 408 QM atoms, RI-BP86/def2-SVP for geometry optimizations) for vinyl alcohol formation.

	RI-BP86/def2-SVP:MM			B3LYP/def2-SVP:MM <sup>a</sup>	B3LYP/def2-SVP:MM <sup>b</sup>
	QM	MM	QM/MM	QM/MM	QM/MM
Int1	-21747.19945	-130.559799	-21877.75925	-21868.70412	-21868.42165
TS1	-21747.18584	-130.560505	-21877.74634	-21868.68548	-21868.40152
Int2	-21747.19779	-130.558831	-21877.75662	-21868.69965	-21868.41647
Int2b	-21747.18921	-130.560139	-21877.74935	-21868.68637	-21868.40683
TS2	-21747.18831	-130.560592	-21877.7489	-21868.68404	-21868.40408
Int3	-21747.23733	-130.553522	-21877.79085	-21868.73379	-21868.44237

a: electronic embedding; b: mechanical embedding

**Table S4.** Calculated QM (B3LYP/def2-SVP) energies (in hartree) of optimized stationary points for snapshot BS100 (QM region **M4**, 408 QM atoms) using QM/MM geometries for vinyl alcohol formation.

	Gas phase	CPCM( $\epsilon=4$ )
Int1	-21735.67066	-21743.69223
TS1	-21735.65410	-21743.66700
Int2	-21735.66762	-21743.68924
Int2b	-21735.65011	-21743.66648
TS2	-21735.64747	-21743.66440
Int3	-21735.70157	-21743.72200

**Table S5.** Spin density of various atoms in **Int1** at the QM(B3LYP/def2-SVP)/MM level for various QM regions.

	<b>M4</b>	<b>M5</b>	<b>M6</b>	<b>M7</b>
Fe1	3.657	3.655	3.656	3.655
Fe2	3.744	3.745	3.745	3.745
Fe3	3.802	3.800	3.800	3.800
Fe4	3.704	3.697	3.696	3.699
S1	0.457	0.458	0.457	0.458
S2	0.395	0.397	0.397	0.396
S3	0.364	0.353	0.353	0.354
S4	0.385	0.387	0.387	0.387
S-Cys9	0.113	0.113	0.114	0.113
S-Cys12	0.098	0.100	0.099	0.101
S-Cys16	0.094	0.097	0.097	0.096
S-Cys46	0.081	0.082	0.082	0.082
Tungsten	0	0	0	0
Other atoms	0.106	0.116	0.117	0.114
Total	17	17	17	17

**Table S6.** Calculated QM, MM, and QM/MM relative energies (in kcal/mol) with QM region **M4** at QM/MM geometries optimized with QM region **M3a**.

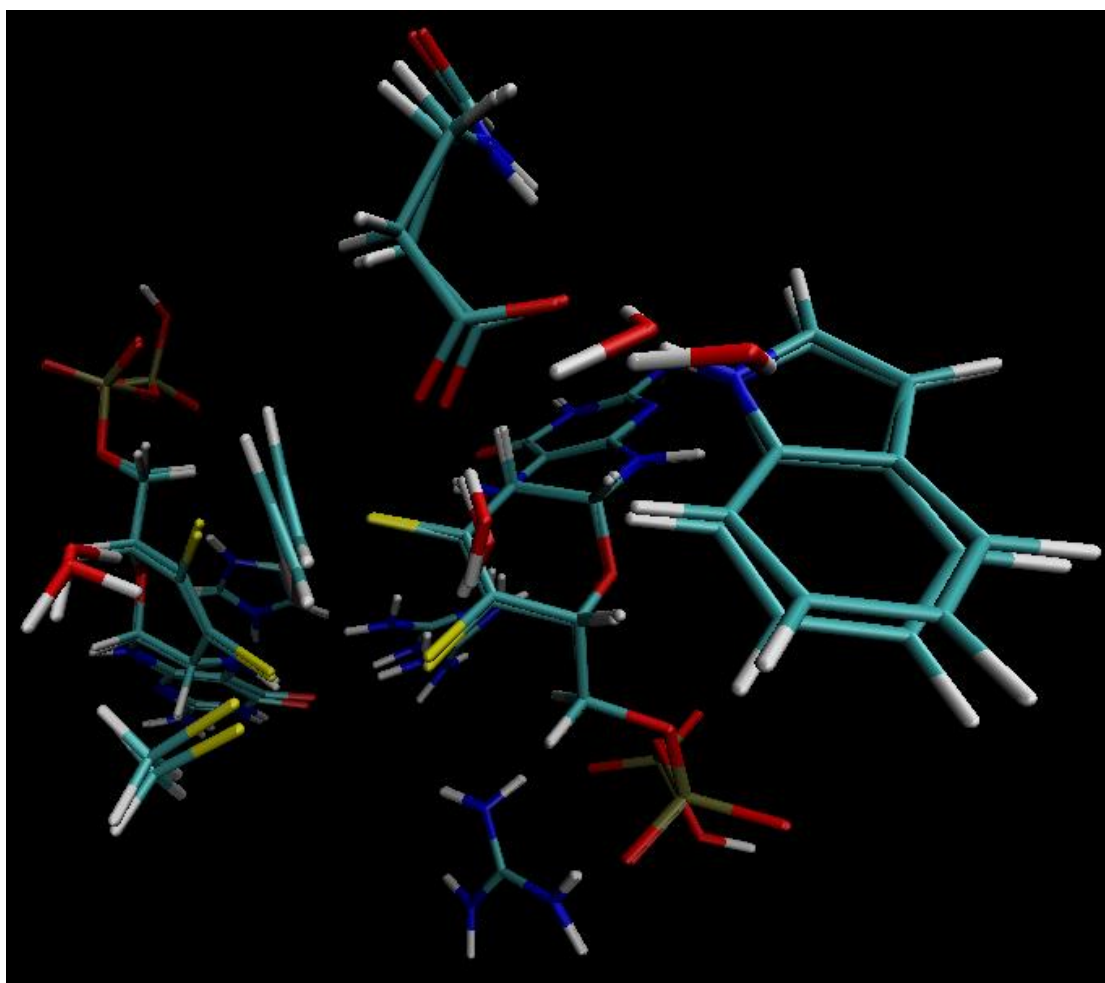
	QM(B3LYP/def2-SVP)/MM			QM/MM( <b>M3a</b> ) <sup>a</sup>	QM/MM( <b>M4</b> ) <sup>b</sup>
	QM	MM	QM/MM		
Int1	0	0	0	0	0
TS1	17.0	-0.2	16.8	13.0	11.7
Int2	8.7	0.3	9.0	4.2	2.8
Int2b	8.9	-1.5	7.4	6.1	11.1
TS2	11.5	-2.3	9.2	9.1	12.6
Int3	-18.7	-0.6	-19.3	-21.1	-18.6

<sup>a</sup>: QM/MM relative energies with QM region **M3a** at QM/MM geometries optimized with QM region **M3a**. QM= B3LYP/def2-SVP.

<sup>b</sup>: QM/MM relative energies with QM region **M4** at QM/MM geometries optimized with QM region **M4**. QM= B3LYP/def2-SVP.

**Table S7.** RMSD (in Å) of QM region **M3a** from QM/MM geometries with models **M3a** and **M4**.

	RMSD
Int1	0.41
TS1	0.36
Int2	0.34
Int2b	0.28
TS2	0.28
Int3	0.32



*Figure S1. Overlay of Int1 of QM region M3a from QM/MM geometry optimization with model M3a and from QM/MM geometry optimization with model M4.*



## QM region M5, 533 QM atoms

**Table S8.** Modification and addition of residues on the basis of QM region M4.

Residue ID	Composition	Atom numbers
Met138	All	2161-2177
Ile142	All	2226-2244
Trp179	All	2766-2789
Trp293	All	4588-4611
Val295	All	4622-4637
Met299	All	4675-4691
Trp472	All	7347-7370
Arg606	All	9496-9519
Phe611	All	9572-9591
Gln612	All	9592-9608

**Table S9.** Calculated QM, MM, and QM/MM energies (in hartree) of optimized stationary points for snapshot BS100 (QM region M5, 533 QM atoms) on the basis of QM/MM geometries obtained with QM region M4 for vinyl alcohol formation.

	B3LYP/def2-SVP:MM <sup>a</sup>			B3LYP/def2SVP:MM <sup>b</sup>
	QM	MM	QM/MM	QM/MM
Int1	-24940.91932	-130.357124	-25071.27645	-25071.33251
TS1	-24940.90112	-130.359582	-25071.26070	-25071.31400
Int2	-24940.91749	-130.358581	-25071.27607	-25071.33107
Int2b	-24940.90388	-130.355665	-25071.25955	-25071.31560
TS2	-24940.90103	-130.355995	-25071.25703	-25071.31242
Int3	-24940.95602	-130.350979	-25071.30700	-25071.35299

a: electronic embedding; b: mechanical embedding

## QM region M6, 576 QM atoms

**Table S10.** Modification and addition of residues on the basis of QM region M5.

Residue ID	Composition	Atom numbers
Ile113	All	1765-1783
Ala137	All	2151-2160
Met140	All	2199-2215

**Table S11.** Calculated QM, MM, and QM/MM energies (in hartree) of optimized stationary points for snapshot BS100 (QM region M6, 576 QM atoms) on the basis of QM/MM geometries obtained with QM region M4 for vinyl alcohol formation.

	B3LYP/def2-SVP:MM <sup>a</sup>			B3LYP/def2SVP:MM <sup>b</sup>
	QM	MM	QM/MM	QM/MM
Int1	-26124.92236	-130.255227	-26255.17758	-26255.43620
TS1	-26124.90562	-130.256999	-26255.16262	-26255.41746
Int2	-26124.92263	-130.255460	-26255.17809	-26255.43397
Int2b	-26124.90850	-130.251898	-26255.16040	-26255.41870
TS2	-26124.90565	-130.252234	-26255.15788	-26255.41569
Int3	-26124.95946	-130.249105	-26255.20857	-26255.45897

a: electronic embedding; b: mechanical embedding

## QM region M7, 657 QM atoms

**Table S12.** Modification and addition of residues on the basis of QM region M5.

Residue ID	Composition	Atom numbers
Thr111	All	1736-1749
Gly143	All	2245-2251
Ala294	All	4612-4621
Asp298	All	4663-4674
His676	All	10592-10609
Arg720	All	11226-11249

The following water molecules are also added: Cryw66, Cryw162, Cryw245, Wz1-2707

**Table S13.** Calculated QM, MM, and QM/MM energies (in hartree) of optimized stationary points for snapshot BS100 (QM region M7, 657 QM atoms) on the basis of QM/MM geometries obtained with QM region M4 for vinyl alcohol formation.

	B3LYP/def2-SVP:MM <sup>a</sup>			B3LYP/def2SVP:MM <sup>b</sup>
	QM	MM	QM/MM	QM/MM
Int1	-28254.07689	-129.760609	-28383.83750	-28384.06859
TS1	-28254.06047	-129.761073	-28383.82155	-28384.05258
Int2	-28254.07638	-129.760520	-28383.83690	-28384.07109
Int2b	-28254.06182	-129.757195	-28383.81902	-28384.05411
TS2	-28254.05949	-129.757280	-28383.81677	-28384.05123
Int3	-28254.11412	-129.755253	-28383.86937	-28384.09795

a: electronic embedding; b: mechanical embedding

**Table S14.** QM-only (B3LYP/def2-SVP, gas phase) and QM(B3LYP/def2-SVP)/MM relative energies (in kcal/mol) for QM region **M7** at QM/MM geometries optimized with QM region **M4**. The energy of **Int2** is set to zero.

	QM-only	QM/MM
Int1	3.0	-0.4
TS1	10.6	9.6
Int2	0	0
Int2b	10.3	11.2
TS2	12.2	12.6
Int3	-20.1	-20.4
MAD		1.2

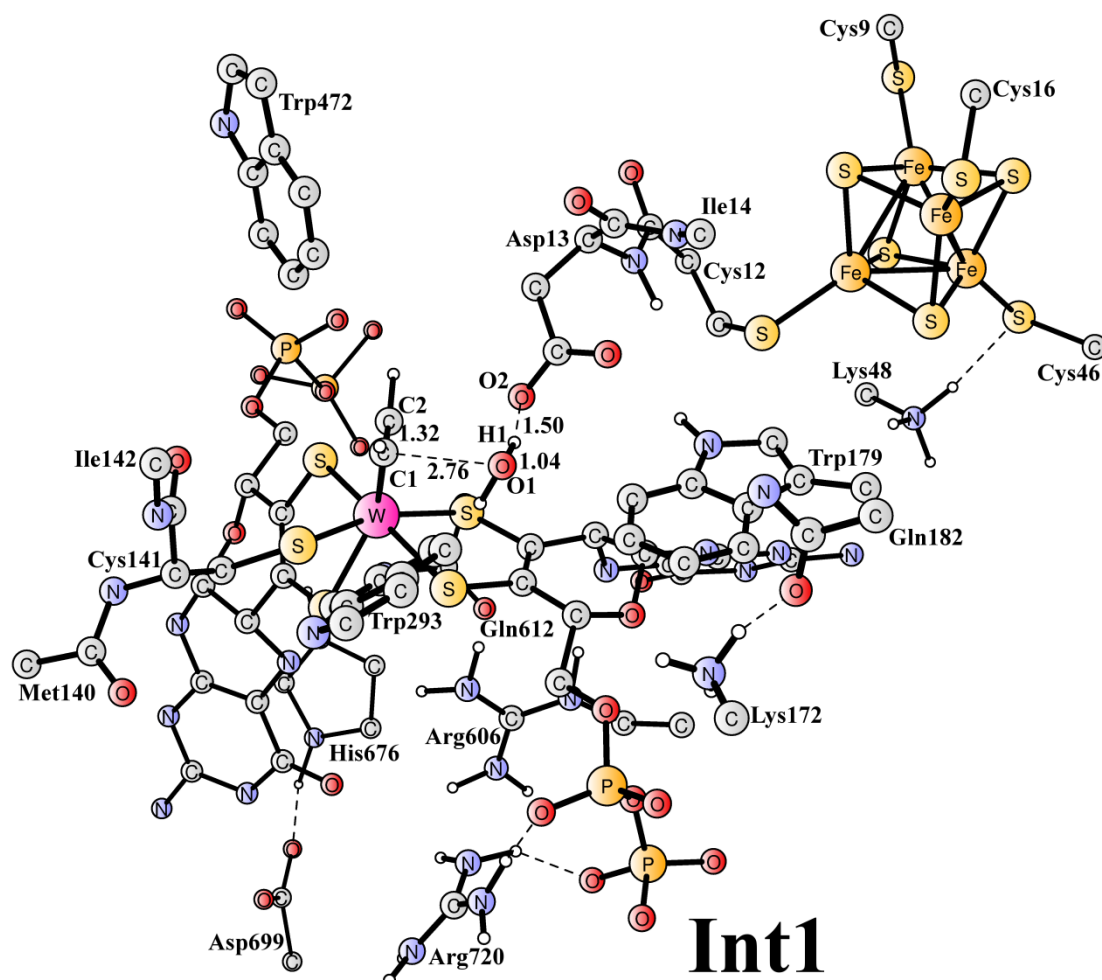
**Table S15.** QM and QM/MM (B3LYP/def2-SVP) relative energies (in kcal/mol) using different QM regions on the basis of QM/MM geometries obtained with QM region **M4**.

		Int1	TS1	Int2	Int2b	TS2	Int3
M4	QM <sup>a</sup>	0	10.4	1.9	12.9	14.6	-19.4
	QM <sup>b</sup>	0	12.1	2.2	11.4	13.1	-22.6
	QM/MM	0	11.7	2.8	11.1	12.6	-18.6
M5	QM <sup>a</sup>	0	9.8	0.3	9.9	11.7	-18.7
	QM <sup>b</sup>	0	11.4	1.2	9.7	11.5	-23.0
	QM/MM	0	9.9	0.2	10.6	12.2	-19.2
M6	QM <sup>a</sup>	0	10.1	0.9	9.4	11.2	-21.2
	QM <sup>b</sup>	0	10.5	-0.2	8.7	10.5	-23.3
	QM/MM	0	9.4	-0.3	10.8	12.4	-19.4
M7	QM <sup>a</sup>	0	7.6	-3.0	7.3	9.2	-23.1
	QM <sup>b</sup>	0	10.3	0.3	9.5	10.9	-23.4
	QM/MM	0	10.0	0.4	11.6	13.0	-20.0

<sup>a</sup>: From QM gas-phase calculations; <sup>b</sup>: QM energies of QM/MM calculations, with polarization from the MM point charges.

## QM region M3c, 352 QM atoms

We also tried to use QM region **M3c** (352 atoms, total charge of -5, details shown in **Table S16**) for QM(RI-BP86/def2-SVP)/MM geometry optimizations. The optimized structure for **Int1** is shown in **Figure S2**, and the QM/MM relative energies of all stationary points are displayed in **Table S17**. For model **M3c**, we observed quite large MM energy contributions, with a mean absolute value of 2.9 kcal/mol, which are partially due to the large movement of the side chains of Ile14 and Met138, and of a number of water molecules around the active site in the second step of the reaction. These two residues and the relevant water molecules are thus included in QM region **M4**. The mean absolute change of MM energies then drops to 1.1 kcal/mol.



**Figure S2.** Optimized structure of the enzyme-acetylene complex (**Int1**) using QM region **M3c**, RI-BP86/MM. For clarity, some unimportant water molecules and hydrogen atoms are not shown. All bond lengths are given in Å.

**Table S16.** Difference between QM regions **M3c** and **M4**.

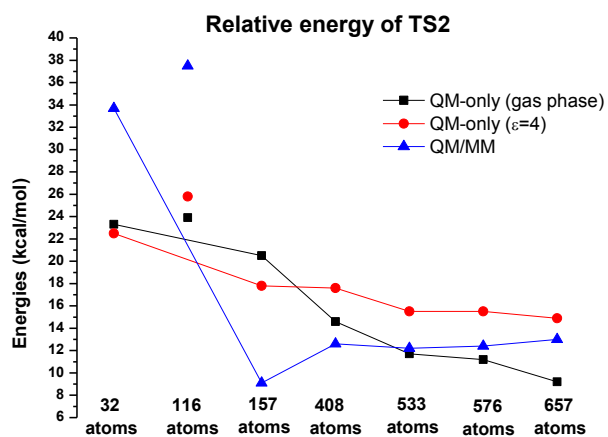
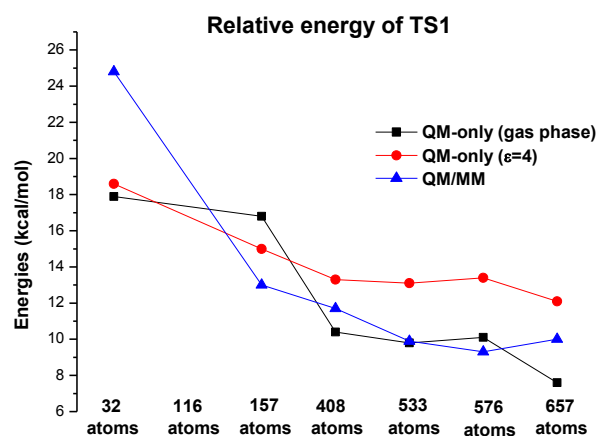
	<b>M3c</b>	<b>M4</b>
Ser11	no	Backbone -CHCO-
Cys12	-CO-CH-CH <sub>2</sub> -S <sup>-</sup>	full
Ile14	Backbone -NH-CH-	full
Asn15	no	Backbone -CHNH-
Met138	no	Side chain -CH <sub>2</sub> CH <sub>2</sub> SCH <sub>3</sub>

Six water molecules are not included in **M3c** but are included in **M4**: Cyrw43, Cryw131, Cryw259, Wz1-734, Wz1-818, Wz2-1262.

**Table S17.** Calculated QM, MM, and QM/MM relative energies (in kcal/mol) on the basis of QM/MM geometries obtained with QM region **M3c**.

	RI-BP86/def2-SVP:MM		
	QM	MM	QM/MM
Int1	0	0	0
TS1	10.2	-0.7	9.5
Int2	3.1	-0.3	2.8
Int2b	12.3	-4.5	7.8
TS2	12.6	-4.5	8.1
Int3	-25.7	4.3	-21.4

## Convergence of QM/MM and QM-only energies



**Figure S3.** Relative energy of *TS1* and *TS2* as function of the size of the QM region. The results for QM model **M2** (116 atoms) are only shown as points because this model has been introduced independently in a QM-only study and is not part of the systematic sequence of QM/MM models considered here. See Table S18 for the corresponding numerical results.

**Table S18.** QM-only (B3LYP/def2-SVP, gas phase and in solvation (CPCM,  $\epsilon=4$ )) and QM (B3LYP/def2-SVP)/MM relative energies (in kcal/mol) calculated with different QM regions.

		Int1	TS1	Int2	Int2b	TS2	Int3
<b>M1<sup>a</sup></b> (32 atoms)	QM-only gas phase	0	17.9	12.1	17.7	23.3	-7.1
	QM-only CPCM	0	18.6	11.7	16.1	22.5	-6.4
	QM/MM	0	24.8	19.9	27.2	33.7	7.6
<b>M2<sup>a</sup></b> (116 atoms)	QM-only gas phase	0	-	-	25.3	23.9	5.6
	QM-only CPCM	0	-	-	26.1	25.8	6.7
	QM/MM	0	-	-	29.5	37.5	10.1
<b>M2<sup>b</sup></b> (QM-only model,116 atoms)	Gas phase	0	14.5	7.6	-	16.7	-20.3
	CPCM	0	15.2	8.1	-	15.8	-19.7
<b>M3<sup>a</sup></b> (157 atoms)	QM-only gas phase	0	16.6	16.2	19.4	20.5	-19.7
	QM-only CPCM	0	15.0	11.1	16.0	17.8	-21.0
	QM/MM	0	13.0	4.2	6.1	9.1	-21.1
<b>M4<sup>a</sup></b> (408 atoms)	QM-only gas phase	0	10.4	1.9	12.9	14.6	-19.4
	QM-only CPCM	0	13.3	4.8	16.0	17.6	-18.9
	QM/MM	0	11.7	2.8	11.1	12.6	-18.6
<b>M5<sup>c</sup></b> (533 atoms)	QM-only gas phase	0	9.8	0.3	9.9	11.7	-20.7
	QM-only CPCM	0	13.1	4.4	14.0	15.5	-19.3
	QM/MM	0	9.9	0.2	10.6	12.2	-19.2
<b>M6<sup>c</sup></b> (576 atoms)	QM-only gas phase	0	10.1	0.9	9.4	11.2	-21.2
	QM-only CPCM	0	13.4	5.0	14.2	15.5	-20.1
	QM/MM	0	9.3	-0.3	10.8	12.4	-19.4
<b>M7<sup>c</sup></b> (657 atoms)	QM-only gas phase	0	7.6	-3.0	7.3	9.2	-23.1
	QM-only CPCM	0	12.1	3.1	13.5	14.9	-20.7
	QM/MM	0	10.0	0.4	11.6	13.0	-20.0

a: using QM/MM geometries optimized for the given QM region.

b: using QM-only geometries optimized in the previous QM-only study.

c: using QM/MM geometries optimized for QM region **M4**.



## Cartesian Coordinates for QM region of model M4

### Int1

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C	11.382	11.181	-6.768
H	12.158	11.673	-7.386
H	10.893	10.393	-7.379
S	10.142	12.426	-6.196
C	7.571	12.239	-3.023
H	7.323	12.502	-1.974
C	6.303	11.494	-3.535
O	5.161	11.929	-3.328
N	6.478	10.301	-4.204
H	7.427	9.915	-4.207
C	5.430	9.302	-4.264
H	4.846	9.399	-3.320
C	4.353	9.510	-5.354
H	3.412	9.043	-4.998
H	4.176	10.600	-5.401
S	4.620	8.862	-7.072
C	6.130	7.933	-4.145
O	7.148	7.821	-3.449
N	5.549	6.893	-4.797
H	4.780	7.075	-5.455
C	6.017	5.529	-4.658
H	6.830	5.551	-3.904
C	4.884	4.630	-4.143
H	5.271	3.593	-4.053
H	4.592	4.959	-3.125
C	3.662	4.590	-5.079
O	3.823	4.908	-6.305
O	2.579	4.193	-4.557
C	6.649	4.925	-5.923
O	7.215	3.820	-5.836
N	6.578	5.620	-7.092
H	6.005	6.477	-7.130
C	6.998	4.972	-8.330
H	6.853	3.880	-8.190
C	6.159	5.385	-9.572
H	5.105	5.345	-9.219
C	6.466	6.807	-10.048
H	5.790	7.100	-10.873
H	6.346	7.570	-9.253
H	7.504	6.890	-10.433
C	6.302	4.343	-10.704
H	7.304	4.441	-11.166
H	6.273	3.323	-10.268
C	5.232	4.451	-11.794
H	5.320	3.594	-12.490
H	4.209	4.406	-11.367
H	5.322	5.397	-12.369
C	8.505	5.103	-8.532
O	9.130	4.375	-9.340
N	9.147	6.018	-7.766
H	8.553	6.667	-7.233
C	10.583	6.110	-7.517
H	10.744	7.014	-6.898
C	11.076	9.275	-11.153
H	11.058	10.064	-10.375
H	11.621	9.683	-12.030
S	9.349	8.872	-11.667
C	5.549	15.156	-10.896
H	4.541	15.590	-11.028
H	5.644	14.318	-11.614
S	5.730	14.543	-9.152

C	3.146	13.590	-6.228
H	4.198	13.384	-5.955
H	2.529	12.766	-5.825
N	3.041	13.545	-7.720
H	2.985	12.544	-8.062
H	2.172	13.987	-8.070
H	3.887	13.974	-8.228
C	1.058	-1.296	2.119
H	1.005	-1.595	1.058
H	1.695	-0.390	2.173
C	1.660	-2.435	2.943
H	1.680	-2.208	4.023
H	1.108	-3.393	2.817
S	3.424	-2.751	2.546
C	3.282	-3.231	0.792
H	4.308	-3.472	0.454
H	2.625	-4.118	0.664
H	2.903	-2.408	0.158
C	-5.283	-2.994	1.009
H	-5.605	-4.045	0.843
C	-4.627	-2.553	-0.317
O	-5.253	-2.498	-1.388
N	-3.284	-2.230	-0.286
H	-2.736	-2.410	0.566
C	-2.578	-1.709	-1.443
H	-3.177	-2.004	-2.330
C	-2.504	-0.171	-1.371
H	-3.531	0.237	-1.354
H	-1.982	0.136	-0.442
S	-1.532	0.445	-2.810
C	-1.176	-2.350	-1.500
O	-0.201	-1.856	-0.908
N	-1.089	-3.517	-2.205
H	-1.971	-3.940	-2.524
C	0.121	-4.293	-2.501
H	-0.156	-4.926	-3.362
C	-2.052	1.678	-14.816
H	-1.434	0.872	-15.249
H	-2.040	2.517	-15.533
N	-1.404	2.127	-13.560
H	-1.287	1.347	-12.884
H	-0.423	2.510	-13.832
H	-1.921	2.923	-13.054
C	2.556	7.277	-12.259
H	1.608	7.413	-12.815
H	3.183	6.578	-12.855
C	2.334	6.661	-10.901
C	2.855	6.979	-9.648
H	3.477	7.827	-9.336
N	2.503	6.017	-8.715
H	2.911	5.893	-7.771
C	1.764	5.038	-9.350
C	1.620	5.419	-10.724
C	0.919	4.558	-11.599
H	0.817	4.790	-12.670
C	0.381	3.376	-11.079
H	-0.140	2.679	-11.736
C	1.225	3.850	-8.833
H	1.363	3.554	-7.785
C	0.525	3.025	-9.718
H	0.093	2.081	-9.352
C	2.736	3.766	-15.873
H	2.012	4.216	-16.577
H	3.390	3.071	-16.437
C	1.960	2.984	-14.820
O	0.728	3.199	-14.663
N	2.640	2.057	-14.126

H	2.214	1.554	-13.323
H	3.661	1.940	-14.300
C	-0.820	-3.329	-9.202
C	-1.710	-4.279	-8.703
H	-2.032	-5.234	-9.135
N	-2.235	-3.854	-7.496
H	-2.992	-4.316	-6.949
C	-1.714	-2.613	-7.191
C	-0.796	-2.255	-8.234
C	-0.141	-0.998	-8.175
H	0.567	-0.691	-8.963
C	-0.449	-0.125	-7.131
H	0.045	0.856	-7.078
C	-2.003	-1.744	-6.125
H	-2.705	-2.033	-5.330
C	-1.374	-0.496	-6.122
H	-1.588	0.202	-5.303
C	8.301	-2.075	-1.202
C	8.257	-1.626	0.111
H	9.030	-1.632	0.889
N	6.980	-1.157	0.404
H	6.675	-0.594	1.221
C	6.207	-1.201	-0.744
C	6.996	-1.817	-1.769
C	6.399	-1.999	-3.042
H	6.957	-2.486	-3.859
C	5.094	-1.544	-3.263
H	4.661	-1.661	-4.267
C	4.909	-0.707	-0.963
H	4.365	-0.161	-0.178
C	4.362	-0.889	-2.238
H	3.350	-0.502	-2.431
C	-4.120	9.264	-6.968
H	-4.816	8.687	-7.606
H	-3.104	8.861	-7.150
C	-4.490	9.122	-5.488
H	-3.970	9.854	-4.832
H	-5.570	9.303	-5.324
N	-4.162	7.788	-4.993
H	-3.135	7.583	-5.052
C	-4.922	7.052	-4.175
N	-6.132	7.460	-3.763
H	-6.794	6.807	-3.307
H	-6.510	8.404	-3.976
N	-4.473	5.812	-3.826
H	-4.828	5.391	-2.968
H	-3.490	5.582	-4.017
C	-1.034	8.643	-0.107
H	-0.460	9.042	-0.961
H	-0.393	7.913	0.428
C	-2.280	7.943	-0.651
O	-2.779	8.209	-1.765
N	-2.799	6.995	0.168
H	-3.614	6.418	-0.082
H	-2.486	6.920	1.149
C	-5.139	8.756	1.536
H	-4.330	8.868	0.813
C	-6.496	8.956	1.405
N	-4.930	8.292	2.817
H	-3.982	7.956	3.168
N	-7.082	8.621	2.612
H	-8.181	8.692	2.799
C	-6.115	8.220	3.453
H	-6.274	7.876	4.481
C	-11.940	9.050	2.220
H	-12.665	8.327	1.805
H	-11.847	9.888	1.498

C	-10.559	8.369	2.311
O	-9.612	9.027	2.857
O	-10.480	7.219	1.791
N	-9.674	3.780	-5.539
H	-9.999	4.376	-4.763
C	-8.476	4.096	-6.147
N	-8.108	3.632	-7.338
H	-7.105	3.689	-7.699
H	-8.757	3.211	-8.021
N	-7.674	4.939	-5.490
H	-7.191	5.637	-6.097
H	-7.790	5.105	-4.469
Fe	6.736	12.438	-9.225
Fe	8.566	11.695	-7.737
Fe	8.098	10.179	-10.148
Fe	6.272	10.219	-7.985
S	6.392	12.277	-6.916
S	9.005	12.343	-9.990
S	5.802	10.548	-10.315
S	8.473	9.316	-7.926
W	-0.795	2.811	-2.720
C	0.763	1.699	-3.498
C	1.263	2.566	-2.644
H	1.029	0.841	-4.126
H	2.196	2.879	-2.161
S	-0.185	3.259	-0.449
S	-3.124	3.020	-1.713
S	-1.807	3.047	-4.980
S	-0.542	5.256	-3.077
C	-1.626	3.536	0.513
C	-2.876	3.405	-0.032
C	-1.473	4.675	-5.573
C	-0.881	5.610	-4.766
C	-1.411	3.917	1.962
H	-1.138	3.010	2.560
O	-2.608	4.479	2.522
C	-4.120	3.561	0.818
H	-4.743	2.637	0.689
C	-3.736	3.614	2.311
H	-3.418	2.588	2.598
C	-0.274	4.915	2.081
H	0.625	4.453	1.632
H	-0.520	5.821	1.483
C	-1.778	4.948	-7.038
H	-1.072	4.355	-7.673
O	-1.644	6.336	-7.366
C	-0.431	6.950	-5.325
H	0.628	7.113	-5.013
C	-0.407	6.875	-6.871
H	0.419	6.191	-7.170
C	-3.197	4.524	-7.365
H	-3.366	3.498	-6.980
H	-3.904	5.216	-6.861
C	-5.949	4.645	2.638
N	-9.094	5.709	3.886
H	-9.963	6.009	3.432
H	-9.144	5.162	4.761
N	-6.958	4.847	3.522
C	-8.042	5.454	3.060
N	-8.154	5.878	1.759
H	-9.029	6.429	1.526
C	-7.168	5.656	0.793
O	-7.335	6.045	-0.398
C	-6.004	4.997	1.280
N	-4.888	4.760	0.444
H	-5.173	4.727	-0.543
N	-4.824	4.022	3.131

H	-4.876	3.724	4.117
C	-0.417	9.335	-6.788
N	-0.066	12.829	-7.482
H	-0.771	13.582	-7.350
H	0.195	12.724	-8.471
N	-0.100	10.487	-7.455
C	-0.388	11.636	-6.869
N	-0.969	11.696	-5.630
H	-1.103	12.610	-5.155
C	-1.276	10.552	-4.853
O	-1.774	10.682	-3.711
C	-0.962	9.311	-5.494
N	-1.294	8.070	-4.893
H	-1.394	8.153	-3.867
N	-0.171	8.161	-7.451
H	0.056	8.244	-8.453
O	-0.038	5.225	3.448
O	1.700	6.027	5.172
O	2.174	6.296	2.572
O	0.332	7.705	3.656
O	-0.997	9.780	4.153
O	0.032	8.402	6.155
P	0.137	8.947	4.747
P	1.210	6.262	3.766
O	-3.395	4.549	-8.792
O	-4.935	4.516	-10.823
O	-5.759	3.470	-8.564
O	-5.359	6.070	-8.767
O	-7.489	6.795	-7.488
O	-6.486	8.284	-9.451
P	-6.759	6.932	-8.828
P	-4.949	4.546	-9.287
O	1.484	9.897	4.574
O	-7.716	5.986	-9.830
O	3.953	-0.982	-13.020
H	4.202	-1.578	-12.250
H	3.064	-0.632	-12.755
O	-8.115	5.644	-2.813
H	-9.068	5.876	-2.850
H	-7.870	5.651	-1.831
O	-2.506	7.164	3.082
H	-1.611	7.461	3.376
H	-2.510	6.179	3.193
O	-2.588	4.214	-12.223
H	-2.050	4.905	-11.771
H	-3.432	4.219	-11.694
O	-7.574	9.873	-4.082
H	-7.160	10.618	-3.564
H	-7.809	10.324	-4.924
O	2.930	4.321	0.822
H	2.696	5.032	1.495
H	2.233	4.428	0.143
O	3.165	1.374	1.393
H	2.590	0.964	0.696
H	3.100	2.346	1.222
O	-4.225	10.633	-2.450
H	-3.827	9.748	-2.270
H	-3.525	11.030	-3.020
O	10.642	1.062	-4.546
H	10.729	2.046	-4.480
H	9.855	1.018	-5.141
O	3.356	1.059	-9.841
H	4.140	1.148	-10.546
H	3.522	1.774	-9.160
O	7.638	1.074	-11.924
H	7.885	1.827	-12.526
H	8.245	1.256	-11.144

O	5.019	5.915	-0.572
H	4.431	5.290	-0.090
H	5.358	6.486	0.157
O	6.684	1.294	-8.658
H	7.431	1.542	-8.066
H	5.890	1.751	-8.269
O	1.797	0.381	-11.915
H	2.203	0.789	-11.087
H	0.841	0.247	-11.717
O	7.340	-1.431	-8.322
H	7.495	-1.326	-7.358
H	7.001	-0.528	-8.559
O	9.642	5.546	-11.810
H	9.567	6.530	-11.661
H	9.567	5.153	-10.904
O	8.443	3.353	-13.329
H	7.675	3.864	-13.654
H	8.945	4.030	-12.807
O	5.017	1.176	-11.722
H	4.753	0.408	-12.303
H	6.031	1.170	-11.679
O	1.197	2.688	-6.045
H	1.648	3.437	-5.479
H	0.268	2.634	-5.711
O	9.564	1.889	-10.264
H	9.976	1.413	-9.497
H	9.255	2.746	-9.873
O	3.243	1.218	-5.617
H	3.515	1.605	-4.761
H	2.333	1.670	-5.798
O	4.854	-2.336	-10.908
H	4.478	-3.242	-10.776
H	4.510	-1.875	-10.080
O	3.677	-1.227	-8.809
H	3.510	-0.257	-9.186
H	2.800	-1.601	-8.595
O	7.138	-0.374	-5.721
H	7.087	-0.544	-4.758
H	6.163	-0.521	-6.044
O	8.634	1.590	-6.507
H	8.219	2.455	-6.236
H	7.985	0.865	-6.190
O	10.801	0.866	-7.966
H	10.039	1.202	-7.408
H	11.500	1.573	-7.959
O	4.340	2.529	-7.747
H	4.202	3.465	-7.435
H	4.025	2.009	-6.951
O	4.738	-0.919	-6.377
H	4.493	-1.096	-7.332
H	4.099	-0.212	-6.090
O	1.454	0.345	-0.554
H	0.882	-0.437	-0.756
H	0.815	1.090	-0.573
h	11.905	10.670	-5.960
h	8.506	11.680	-3.044
h	7.652	13.214	-3.502
h	10.963	5.231	-6.996
h	11.173	6.329	-8.407
h	11.594	8.409	-10.743
h	6.264	15.909	-11.227
h	2.788	14.528	-5.803
h	0.053	-0.978	2.396
h	-4.718	-2.934	1.939
h	-6.210	-2.446	1.178
h	0.971	-3.732	-2.889
h	0.317	-5.050	-1.742

h	-3.067	1.309	-14.669
h	3.032	8.258	-12.253
h	3.394	4.543	-15.485
h	-0.357	-3.268	-10.187
h	9.122	-2.572	-1.719
h	-4.137	10.301	-7.303
h	-1.220	9.455	0.596
h	-7.042	9.358	0.551
h	-12.338	9.507	3.125
h	-10.285	3.020	-5.759
h	2.351	9.613	4.840
h	-7.751	6.107	-10.772

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C	11.381	11.202	-6.762
H	12.153	11.710	-7.372
H	10.906	10.414	-7.382
S	10.122	12.431	-6.192
C	7.574	12.284	-3.051
H	7.334	12.577	-2.008
C	6.314	11.508	-3.529
O	5.166	11.905	-3.282
N	6.501	10.331	-4.222
H	7.464	9.997	-4.312
C	5.479	9.307	-4.270
H	4.870	9.443	-3.347
C	4.421	9.449	-5.394
H	3.471	9.012	-5.024
H	4.258	10.535	-5.520
S	4.687	8.695	-7.073
C	6.203	7.961	-4.074
O	7.177	7.886	-3.314
N	5.697	6.897	-4.753
H	4.951	7.057	-5.445
C	6.228	5.561	-4.599
H	7.110	5.652	-3.933
C	5.204	4.645	-3.921
H	5.658	3.645	-3.760
H	4.956	5.044	-2.913
C	3.954	4.446	-4.766
O	3.896	4.784	-5.969
O	2.994	3.852	-4.120
C	6.751	4.917	-5.892
O	7.304	3.804	-5.817
N	6.603	5.582	-7.070
H	6.087	6.478	-7.095
C	7.021	4.937	-8.311
H	6.882	3.844	-8.171
C	6.178	5.347	-9.550
H	5.124	5.300	-9.198
C	6.478	6.771	-10.024
H	5.802	7.064	-10.849
H	6.351	7.529	-9.224
H	7.517	6.863	-10.402
C	6.327	4.312	-10.688
H	7.328	4.421	-11.152
H	6.307	3.289	-10.259
C	5.254	4.420	-11.775
H	5.343	3.567	-12.476
H	4.233	4.368	-11.344
H	5.338	5.368	-12.347
C	8.530	5.071	-8.512
O	9.157	4.328	-9.304

N	9.171	5.998	-7.759
H	8.586	6.688	-7.266
C	10.605	6.092	-7.507
H	10.761	6.999	-6.891
C	11.019	9.218	-11.140
H	11.002	10.014	-10.369
H	11.528	9.634	-12.035
S	9.284	8.774	-11.607
C	5.566	15.157	-10.866
H	4.552	15.580	-10.994
H	5.660	14.306	-11.569
S	5.761	14.579	-9.112
C	3.167	13.569	-6.199
H	4.216	13.372	-5.909
H	2.549	12.751	-5.786
N	3.083	13.489	-7.691
H	3.054	12.481	-8.014
H	2.210	13.907	-8.062
H	3.924	13.927	-8.194
C	1.021	-1.236	2.080
H	0.961	-1.492	1.008
H	1.656	-0.330	2.166
C	1.641	-2.410	2.843
H	1.678	-2.236	3.934
H	1.084	-3.361	2.687
S	3.395	-2.713	2.403
C	3.213	-3.204	0.655
H	4.233	-3.432	0.293
H	2.565	-4.101	0.555
H	2.806	-2.387	0.030
C	-5.301	-2.989	0.995
H	-5.626	-4.039	0.831
C	-4.646	-2.552	-0.334
O	-5.270	-2.516	-1.406
N	-3.309	-2.208	-0.300
H	-2.760	-2.382	0.553
C	-2.599	-1.702	-1.462
H	-3.204	-1.993	-2.345
C	-2.497	-0.165	-1.396
H	-3.515	0.265	-1.373
H	-1.960	0.137	-0.475
S	-1.534	0.430	-2.848
C	-1.206	-2.361	-1.513
O	-0.234	-1.886	-0.901
N	-1.117	-3.520	-2.229
H	-1.995	-3.938	-2.564
C	0.095	-4.299	-2.511
H	-0.176	-4.937	-3.370
C	-1.915	1.761	-14.704
H	-1.263	0.978	-15.133
H	-1.887	2.620	-15.397
N	-1.319	2.189	-13.413
H	-1.209	1.394	-12.753
H	-0.340	2.596	-13.652
H	-1.861	2.971	-12.910
C	2.526	7.216	-12.154
H	1.555	7.355	-12.668
H	3.116	6.500	-12.767
C	2.364	6.629	-10.770
C	2.934	7.022	-9.561
H	3.544	7.900	-9.318
N	2.659	6.100	-8.566
H	3.061	6.113	-7.622
C	1.907	5.074	-9.101
C	1.680	5.384	-10.486
C	0.906	4.489	-11.262
H	0.728	4.680	-12.332



C	0.386	3.344	-10.646
H	-0.235	2.646	-11.218
C	1.409	3.909	-8.491
H	1.631	3.674	-7.440
C	0.639	3.051	-9.285
H	0.224	2.131	-8.848
C	2.732	3.773	-15.840
H	1.999	4.228	-16.531
H	3.364	3.063	-16.407
C	1.978	3.028	-14.747
O	0.783	3.332	-14.485
N	2.637	2.039	-14.123
H	2.232	1.557	-13.296
H	3.642	1.878	-14.350
C	-0.813	-3.323	-9.186
C	-1.707	-4.279	-8.703
H	-2.020	-5.232	-9.146
N	-2.249	-3.861	-7.502
H	-3.007	-4.328	-6.962
C	-1.736	-2.620	-7.185
C	-0.805	-2.253	-8.212
C	-0.152	-0.994	-8.133
H	0.570	-0.683	-8.906
C	-0.479	-0.132	-7.086
H	0.014	0.847	-6.997
C	-2.049	-1.758	-6.120
H	-2.766	-2.053	-5.341
C	-1.424	-0.509	-6.100
H	-1.655	0.187	-5.284
C	8.330	-2.100	-1.214
C	8.268	-1.632	0.092
H	9.032	-1.623	0.879
N	6.984	-1.168	0.363
H	6.666	-0.592	1.165
C	6.226	-1.237	-0.794
C	7.031	-1.862	-1.799
C	6.451	-2.083	-3.074
H	7.024	-2.584	-3.872
C	5.140	-1.658	-3.316
H	4.710	-1.817	-4.316
C	4.924	-0.768	-1.037
H	4.352	-0.223	-0.272
C	4.391	-0.993	-2.311
H	3.364	-0.649	-2.500
C	-4.117	9.252	-6.986
H	-4.806	8.686	-7.641
H	-3.099	8.853	-7.168
C	-4.498	9.075	-5.512
H	-4.011	9.813	-4.838
H	-5.586	9.218	-5.361
N	-4.133	7.744	-5.040
H	-3.099	7.571	-5.100
C	-4.853	6.992	-4.197
N	-6.051	7.389	-3.740
H	-6.714	6.735	-3.290
H	-6.441	8.330	-3.948
N	-4.369	5.760	-3.874
H	-4.667	5.311	-3.007
H	-3.401	5.536	-4.138
C	-0.988	8.645	-0.107
H	-0.393	9.043	-0.947
H	-0.363	7.908	0.438
C	-2.225	7.955	-0.684
O	-2.659	8.189	-1.832
N	-2.816	7.061	0.148
H	-3.615	6.475	-0.130
H	-2.528	6.985	1.136

C	-5.152	8.759	1.567
H	-4.331	8.859	0.854
C	-6.507	8.960	1.419
N	-4.958	8.297	2.850
H	-4.013	7.961	3.206
N	-7.107	8.628	2.620
H	-8.208	8.701	2.795
C	-6.150	8.226	3.472
H	-6.322	7.882	4.499
C	-11.964	9.064	2.217
H	-12.693	8.345	1.801
H	-11.871	9.906	1.500
C	-10.585	8.379	2.304
O	-9.634	9.040	2.840
O	-10.512	7.225	1.794
N	-9.688	3.788	-5.534
H	-10.020	4.387	-4.764
C	-8.495	4.112	-6.146
N	-8.125	3.647	-7.337
H	-7.124	3.707	-7.698
H	-8.771	3.220	-8.018
N	-7.701	4.963	-5.491
H	-7.208	5.653	-6.098
H	-7.808	5.123	-4.467
Fe	6.812	12.499	-9.267
Fe	8.528	11.664	-7.710
Fe	8.051	10.055	-10.020
Fe	6.319	10.039	-8.090
S	6.312	12.119	-6.980
S	9.029	12.250	-9.986
S	5.759	10.637	-10.319
S	8.543	9.275	-7.824
W	-0.785	2.768	-2.714
C	0.784	1.756	-3.696
C	1.195	2.414	-2.584
H	0.886	0.743	-4.112
H	2.111	2.648	-2.026
S	-0.212	3.184	-0.448
S	-3.137	3.062	-1.754
S	-1.778	3.039	-5.029
S	-0.482	5.238	-3.098
C	-1.650	3.559	0.477
C	-2.901	3.452	-0.074
C	-1.468	4.684	-5.585
C	-0.869	5.612	-4.774
C	-1.433	3.937	1.927
H	-1.154	3.031	2.523
O	-2.627	4.497	2.493
C	-4.145	3.606	0.779
H	-4.769	2.685	0.638
C	-3.758	3.638	2.272
H	-3.444	2.607	2.545
C	-0.299	4.940	2.041
H	0.595	4.489	1.571
H	-0.563	5.852	1.461
C	-1.793	4.970	-7.044
H	-1.105	4.376	-7.697
O	-1.653	6.361	-7.370
C	-0.425	6.957	-5.333
H	0.636	7.123	-5.028
C	-0.411	6.888	-6.878
H	0.406	6.196	-7.185
C	-3.218	4.557	-7.357
H	-3.395	3.539	-6.956
H	-3.916	5.266	-6.864
C	-5.970	4.669	2.617
N	-9.110	5.721	3.886

H	-9.983	6.017	3.436
H	-9.158	5.167	4.757
N	-6.976	4.861	3.506
C	-8.063	5.469	3.052
N	-8.184	5.896	1.754
H	-9.063	6.443	1.526
C	-7.199	5.688	0.784
O	-7.376	6.084	-0.403
C	-6.028	5.035	1.263
N	-4.913	4.811	0.422
H	-5.201	4.790	-0.564
N	-4.843	4.041	3.100
H	-4.891	3.735	4.084
C	-0.408	9.346	-6.789
N	-0.043	12.840	-7.481
H	-0.750	13.590	-7.352
H	0.216	12.731	-8.470
N	-0.086	10.496	-7.456
C	-0.372	11.646	-6.869
N	-0.956	11.705	-5.632
H	-1.088	12.619	-5.156
C	-1.267	10.562	-4.855
O	-1.767	10.695	-3.715
C	-0.952	9.320	-5.494
N	-1.282	8.078	-4.895
H	-1.394	8.153	-3.869
N	-0.164	8.173	-7.455
H	0.047	8.259	-8.460
O	-0.043	5.232	3.409
O	1.696	6.033	5.131
O	2.158	6.322	2.530
O	0.314	7.714	3.637
O	-1.005	9.788	4.156
O	0.030	8.395	6.144
P	0.130	8.948	4.738
P	1.199	6.274	3.728
O	-3.416	4.563	-8.785
O	-4.947	4.527	-10.819
O	-5.782	3.489	-8.561
O	-5.372	6.089	-8.769
O	-7.504	6.813	-7.496
O	-6.502	8.297	-9.464
P	-6.774	6.948	-8.835
P	-4.967	4.562	-9.283
O	1.478	9.896	4.566
O	-7.724	5.992	-9.834
O	3.935	-0.980	-13.028
H	4.185	-1.594	-12.272
H	3.049	-0.630	-12.752
O	-8.121	5.651	-2.819
H	-9.063	5.921	-2.862
H	-7.885	5.664	-1.835
O	-2.531	7.172	3.069
H	-1.633	7.457	3.366
H	-2.538	6.183	3.153
O	-2.551	4.242	-12.096
H	-2.064	4.969	-11.639
H	-3.427	4.244	-11.621
O	-7.543	9.796	-4.051
H	-7.132	10.549	-3.543
H	-7.795	10.244	-4.889
O	2.919	4.381	0.722
H	2.677	5.072	1.411
H	2.211	4.480	0.053
O	3.106	1.368	1.246
H	2.530	0.949	0.553
H	3.027	2.339	1.083

O	-4.211	10.587	-2.459
H	-3.815	9.698	-2.299
H	-3.508	10.993	-3.019
O	10.661	1.045	-4.552
H	10.734	2.029	-4.482
H	9.874	0.989	-5.147
O	3.363	1.015	-9.821
H	4.145	1.110	-10.535
H	3.540	1.719	-9.135
O	7.623	1.074	-11.922
H	7.878	1.825	-12.526
H	8.235	1.245	-11.143
O	5.046	5.883	-0.676
H	4.415	5.298	-0.196
H	5.395	6.452	0.049
O	6.738	1.245	-8.680
H	7.482	1.483	-8.079
H	5.942	1.689	-8.281
O	1.794	0.399	-11.898
H	2.209	0.779	-11.060
H	0.844	0.244	-11.689
O	7.365	-1.481	-8.354
H	7.529	-1.383	-7.390
H	7.037	-0.572	-8.584
O	9.648	5.502	-11.796
H	9.556	6.487	-11.643
H	9.588	5.106	-10.891
O	8.454	3.337	-13.330
H	7.704	3.868	-13.666
H	8.963	4.003	-12.798
O	5.008	1.155	-11.706
H	4.742	0.396	-12.298
H	6.024	1.156	-11.672
O	1.362	2.568	-5.364
H	2.170	3.456	-4.761
H	0.450	2.818	-5.642
O	9.568	1.854	-10.263
H	9.983	1.367	-9.504
H	9.267	2.707	-9.858
O	3.405	1.092	-5.629
H	3.752	1.356	-4.753
H	2.485	1.553	-5.660
O	4.851	-2.373	-10.954
H	4.476	-3.280	-10.825
H	4.504	-1.921	-10.123
O	3.673	-1.300	-8.843
H	3.507	-0.322	-9.191
H	2.801	-1.676	-8.613
O	7.147	-0.440	-5.744
H	7.099	-0.642	-4.786
H	6.188	-0.639	-6.081
O	8.643	1.529	-6.510
H	8.243	2.399	-6.232
H	7.991	0.807	-6.195
O	10.816	0.820	-7.968
H	10.053	1.150	-7.410
H	11.507	1.536	-7.963
O	4.403	2.451	-7.716
H	4.287	3.380	-7.404
H	4.108	1.925	-6.911
O	4.779	-1.102	-6.425
H	4.538	-1.244	-7.386
H	4.146	-0.393	-6.130
O	1.695	0.079	-0.818
H	0.938	-0.557	-0.862
H	1.441	0.769	-1.475
h	11.909	10.689	-5.958

h	8.513	11.731	-3.061
h	7.634	13.245	-3.560
h	10.987	5.216	-6.982
h	11.195	6.310	-8.397
h	11.576	8.371	-10.739
h	6.270	15.911	-11.217
h	2.799	14.514	-5.800
h	0.015	-0.938	2.373
h	-4.736	-2.928	1.926
h	-6.226	-2.437	1.163
h	0.948	-3.741	-2.897
h	0.289	-5.053	-1.749
h	-2.930	1.372	-14.616
h	3.013	8.191	-12.186
h	3.404	4.547	-15.468
h	-0.347	-3.255	-10.169
h	9.155	-2.599	-1.723
h	-4.133	10.295	-7.300
h	-1.184	9.456	0.595
h	-7.045	9.361	0.560
h	-12.356	9.517	3.127
h	-10.297	3.027	-5.758
h	2.344	9.610	4.832
h	-7.757	6.106	-10.777

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C	11.375	11.196	-6.768
H	12.145	11.704	-7.381
H	10.900	10.407	-7.385
S	10.117	12.425	-6.196
C	7.590	12.287	-3.040
H	7.358	12.587	-1.998
C	6.330	11.503	-3.502
O	5.184	11.882	-3.224
N	6.512	10.338	-4.218
H	7.475	10.022	-4.353
C	5.493	9.310	-4.249
H	4.891	9.460	-3.324
C	4.425	9.435	-5.364
H	3.483	8.992	-4.985
H	4.251	10.518	-5.496
S	4.679	8.677	-7.045
C	6.220	7.969	-4.036
O	7.169	7.894	-3.245
N	5.748	6.906	-4.742
H	5.024	7.074	-5.456
C	6.294	5.576	-4.583
H	7.206	5.687	-3.963
C	5.317	4.671	-3.827
H	5.776	3.670	-3.686
H	5.122	5.079	-2.809
C	4.028	4.471	-4.597
O	3.904	4.685	-5.812
O	3.057	4.008	-3.834
C	6.764	4.909	-5.885
O	7.306	3.791	-5.814
N	6.592	5.566	-7.066
H	6.107	6.479	-7.087
C	7.014	4.926	-8.308
H	6.879	3.832	-8.170
C	6.170	5.336	-9.547
H	5.115	5.286	-9.197
C	6.466	6.763	-10.016

H	5.790	7.055	-10.842
H	6.333	7.519	-9.216
H	7.506	6.860	-10.391
C	6.326	4.306	-10.688
H	7.327	4.422	-11.150
H	6.311	3.281	-10.263
C	5.255	4.412	-11.777
H	5.350	3.562	-12.480
H	4.233	4.353	-11.349
H	5.336	5.363	-12.345
C	8.523	5.064	-8.509
O	9.151	4.319	-9.297
N	9.163	5.995	-7.759
H	8.583	6.699	-7.280
C	10.598	6.091	-7.507
H	10.753	6.999	-6.892
C	11.013	9.215	-11.136
H	10.998	10.011	-10.366
H	11.519	9.632	-12.033
S	9.277	8.768	-11.598
C	5.565	15.154	-10.865
H	4.552	15.577	-10.993
H	5.659	14.304	-11.570
S	5.758	14.574	-9.112
C	3.160	13.574	-6.191
H	4.209	13.375	-5.903
H	2.540	12.758	-5.776
N	3.072	13.490	-7.683
H	3.043	12.481	-8.003
H	2.196	13.904	-8.050
H	3.910	13.929	-8.187
C	1.018	-1.231	2.076
H	0.951	-1.493	1.005
H	1.646	-0.319	2.150
C	1.647	-2.394	2.847
H	1.696	-2.202	3.934
H	1.092	-3.347	2.704
S	3.399	-2.703	2.393
C	3.201	-3.194	0.648
H	4.220	-3.404	0.268
H	2.566	-4.100	0.550
H	2.771	-2.382	0.031
C	-5.290	-2.992	0.986
H	-5.612	-4.044	0.824
C	-4.632	-2.559	-0.344
O	-5.258	-2.525	-1.416
N	-3.295	-2.219	-0.311
H	-2.748	-2.391	0.543
C	-2.581	-1.720	-1.474
H	-3.188	-2.007	-2.357
C	-2.458	-0.185	-1.411
H	-3.469	0.264	-1.390
H	-1.920	0.108	-0.487
S	-1.483	0.399	-2.859
C	-1.194	-2.390	-1.525
O	-0.224	-1.940	-0.890
N	-1.103	-3.534	-2.265
H	-1.977	-3.943	-2.620
C	0.113	-4.309	-2.541
H	-0.151	-4.948	-3.401
C	-1.886	1.783	-14.671
H	-1.226	1.008	-15.102
H	-1.855	2.649	-15.355
N	-1.301	2.202	-13.371
H	-1.198	1.401	-12.716
H	-0.322	2.607	-13.601
H	-1.845	2.982	-12.865

C	2.530	7.228	-12.166
H	1.556	7.357	-12.676
H	3.120	6.509	-12.773
C	2.380	6.661	-10.771
C	2.941	7.096	-9.573
H	3.537	7.991	-9.353
N	2.686	6.196	-8.556
H	3.068	6.279	-7.609
C	1.954	5.141	-9.061
C	1.720	5.411	-10.454
C	0.958	4.485	-11.204
H	0.772	4.648	-12.277
C	0.455	3.349	-10.559
H	-0.156	2.627	-11.114
C	1.473	3.984	-8.422
H	1.703	3.791	-7.365
C	0.715	3.093	-9.191
H	0.310	2.181	-8.730
C	2.737	3.777	-15.823
H	2.000	4.229	-16.512
H	3.367	3.064	-16.391
C	1.991	3.038	-14.720
O	0.803	3.353	-14.441
N	2.650	2.043	-14.105
H	2.249	1.563	-13.275
H	3.652	1.876	-14.340
C	-0.814	-3.343	-9.189
C	-1.706	-4.303	-8.711
H	-2.014	-5.256	-9.156
N	-2.252	-3.890	-7.510
H	-3.009	-4.359	-6.970
C	-1.744	-2.648	-7.189
C	-0.813	-2.275	-8.213
C	-0.168	-1.012	-8.130
H	0.554	-0.694	-8.901
C	-0.506	-0.154	-7.083
H	-0.027	0.832	-6.997
C	-2.063	-1.791	-6.121
H	-2.779	-2.094	-5.344
C	-1.449	-0.539	-6.097
H	-1.683	0.152	-5.278
C	8.324	-2.097	-1.213
C	8.260	-1.634	0.094
H	9.022	-1.630	0.883
N	6.978	-1.163	0.362
H	6.658	-0.592	1.168
C	6.223	-1.224	-0.797
C	7.028	-1.851	-1.802
C	6.448	-2.066	-3.078
H	7.017	-2.573	-3.875
C	5.139	-1.632	-3.320
H	4.710	-1.792	-4.320
C	4.925	-0.746	-1.041
H	4.354	-0.199	-0.275
C	4.391	-0.964	-2.316
H	3.363	-0.616	-2.499
C	-4.124	9.252	-6.976
H	-4.819	8.685	-7.624
H	-3.109	8.849	-7.163
C	-4.497	9.085	-5.498
H	-3.996	9.823	-4.833
H	-5.582	9.242	-5.339
N	-4.140	7.754	-5.022
H	-3.108	7.576	-5.084
C	-4.866	6.997	-4.189
N	-6.074	7.386	-3.750
H	-6.727	6.731	-3.288

H	-6.466	8.323	-3.963
N	-4.374	5.772	-3.858
H	-4.700	5.302	-3.012
H	-3.394	5.563	-4.087
C	-0.992	8.650	-0.105
H	-0.393	9.047	-0.943
H	-0.372	7.908	0.440
C	-2.231	7.967	-0.688
O	-2.666	8.213	-1.832
N	-2.823	7.067	0.136
H	-3.620	6.480	-0.145
H	-2.530	6.979	1.122
C	-5.156	8.754	1.566
H	-4.336	8.851	0.851
C	-6.510	8.959	1.419
N	-4.962	8.289	2.848
H	-4.016	7.950	3.200
N	-7.110	8.626	2.620
H	-8.210	8.700	2.795
C	-6.154	8.220	3.471
H	-6.326	7.875	4.497
C	-11.970	9.068	2.218
H	-12.700	8.349	1.802
H	-11.877	9.910	1.502
C	-10.592	8.381	2.304
O	-9.639	9.040	2.840
O	-10.522	7.227	1.796
N	-9.687	3.787	-5.528
H	-10.013	4.379	-4.749
C	-8.493	4.109	-6.138
N	-8.125	3.647	-7.330
H	-7.124	3.705	-7.693
H	-8.772	3.219	-8.010
N	-7.696	4.956	-5.481
H	-7.203	5.648	-6.085
H	-7.808	5.119	-4.458
Fe	6.799	12.490	-9.262
Fe	8.515	11.654	-7.703
Fe	8.041	10.044	-10.011
Fe	6.306	10.025	-8.084
S	6.298	12.105	-6.976
S	9.017	12.238	-9.980
S	5.748	10.622	-10.313
S	8.529	9.262	-7.814
W	-0.773	2.738	-2.700
C	0.846	1.808	-3.823
C	1.156	2.373	-2.566
H	0.799	0.714	-4.019
H	2.066	2.607	-1.994
S	-0.219	3.142	-0.428
S	-3.136	3.087	-1.767
S	-1.696	3.006	-5.076
S	-0.457	5.248	-3.108
C	-1.658	3.555	0.478
C	-2.907	3.467	-0.082
C	-1.453	4.679	-5.598
C	-0.878	5.614	-4.777
C	-1.444	3.932	1.929
H	-1.165	3.028	2.527
O	-2.639	4.492	2.495
C	-4.152	3.618	0.768
H	-4.777	2.698	0.619
C	-3.771	3.637	2.263
H	-3.458	2.603	2.528
C	-0.312	4.937	2.041
H	0.581	4.483	1.573
H	-0.575	5.847	1.458



C	-1.790	4.968	-7.052
H	-1.109	4.377	-7.714
O	-1.660	6.360	-7.383
C	-0.442	6.962	-5.339
H	0.621	7.126	-5.034
C	-0.426	6.896	-6.884
H	0.395	6.209	-7.188
C	-3.216	4.549	-7.355
H	-3.384	3.531	-6.952
H	-3.914	5.255	-6.860
C	-5.981	4.667	2.612
N	-9.118	5.724	3.890
H	-9.991	6.017	3.441
H	-9.164	5.166	4.759
N	-6.986	4.858	3.503
C	-8.073	5.469	3.053
N	-8.194	5.900	1.757
H	-9.073	6.447	1.530
C	-7.210	5.696	0.786
O	-7.390	6.100	-0.400
C	-6.038	5.041	1.259
N	-4.922	4.825	0.419
H	-5.207	4.808	-0.568
N	-4.856	4.035	3.092
H	-4.902	3.730	4.076
C	-0.422	9.355	-6.791
N	-0.045	12.848	-7.481
H	-0.752	13.599	-7.350
H	0.205	12.738	-8.472
N	-0.098	10.505	-7.459
C	-0.378	11.655	-6.870
N	-0.959	11.714	-5.632
H	-1.088	12.628	-5.154
C	-1.272	10.570	-4.854
O	-1.769	10.706	-3.714
C	-0.961	9.328	-5.494
N	-1.291	8.086	-4.896
H	-1.401	8.157	-3.869
N	-0.184	8.182	-7.461
H	0.018	8.271	-8.468
O	-0.055	5.235	3.409
O	1.691	6.033	5.126
O	2.147	6.316	2.524
O	0.309	7.716	3.634
O	-1.006	9.792	4.158
O	0.026	8.393	6.143
P	0.126	8.947	4.737
P	1.190	6.272	3.723
O	-3.420	4.552	-8.784
O	-4.947	4.525	-10.818
O	-5.790	3.486	-8.565
O	-5.373	6.085	-8.768
O	-7.503	6.809	-7.489
O	-6.504	8.293	-9.459
P	-6.775	6.944	-8.829
P	-4.970	4.557	-9.281
O	1.476	9.895	4.568
O	-7.728	5.990	-9.829
O	3.948	-0.970	-13.009
H	4.196	-1.588	-12.255
H	3.059	-0.626	-12.738
O	-8.125	5.633	-2.809
H	-9.066	5.906	-2.849
H	-7.882	5.657	-1.825
O	-2.540	7.163	3.066
H	-1.641	7.442	3.365
H	-2.552	6.173	3.139

O	-2.534	4.235	-12.050
H	-2.063	4.973	-11.594
H	-3.422	4.237	-11.594
O	-7.550	9.806	-4.065
H	-7.139	10.555	-3.553
H	-7.800	10.259	-4.902
O	2.895	4.364	0.702
H	2.650	5.055	1.390
H	2.158	4.418	0.058
O	3.110	1.339	1.209
H	2.532	0.918	0.517
H	3.024	2.310	1.050
O	-4.215	10.606	-2.454
H	-3.813	9.719	-2.294
H	-3.516	11.015	-3.017
O	10.668	1.045	-4.556
H	10.739	2.030	-4.483
H	9.883	0.987	-5.153
O	3.363	0.994	-9.782
H	4.147	1.092	-10.495
H	3.541	1.689	-9.090
O	7.620	1.073	-11.911
H	7.872	1.821	-12.518
H	8.241	1.241	-11.139
O	5.004	5.851	-0.696
H	4.350	5.281	-0.226
H	5.366	6.404	0.035
O	6.764	1.231	-8.693
H	7.509	1.466	-8.091
H	5.969	1.663	-8.281
O	1.800	0.401	-11.879
H	2.210	0.772	-11.037
H	0.850	0.233	-11.674
O	7.381	-1.497	-8.361
H	7.546	-1.398	-7.398
H	7.057	-0.588	-8.594
O	9.643	5.498	-11.793
H	9.550	6.483	-11.637
H	9.586	5.100	-10.889
O	8.449	3.333	-13.329
H	7.700	3.863	-13.670
H	8.956	4.000	-12.799
O	5.010	1.148	-11.660
H	4.743	0.398	-12.264
H	6.026	1.153	-11.635
O	1.318	2.484	-5.066
H	2.268	3.689	-4.393
H	0.463	2.724	-5.528
O	9.580	1.849	-10.264
H	9.998	1.361	-9.508
H	9.275	2.699	-9.856
O	3.523	1.151	-5.494
H	3.868	1.259	-4.585
H	2.605	1.580	-5.464
O	4.853	-2.376	-10.938
H	4.476	-3.284	-10.820
H	4.502	-1.934	-10.104
O	3.652	-1.330	-8.821
H	3.486	-0.351	-9.165
H	2.781	-1.713	-8.597
O	7.166	-0.447	-5.754
H	7.114	-0.657	-4.797
H	6.207	-0.637	-6.094
O	8.655	1.523	-6.520
H	8.253	2.391	-6.239
H	8.007	0.798	-6.202
O	10.830	0.814	-7.972

H	10.068	1.144	-7.414
H	11.522	1.528	-7.967
O	4.445	2.430	-7.667
H	4.356	3.370	-7.391
H	4.206	1.947	-6.821
O	4.788	-1.074	-6.431
H	4.510	-1.234	-7.381
H	4.170	-0.365	-6.114
O	1.677	0.076	-0.858
H	0.938	-0.580	-0.895
H	1.353	0.810	-1.443
h	11.906	10.686	-5.964
h	8.529	11.733	-3.053
h	7.643	13.245	-3.557
h	10.981	5.216	-6.982
h	11.189	6.309	-8.397
h	11.573	8.370	-10.738
h	6.269	15.909	-11.215
h	2.794	14.520	-5.793
h	0.012	-0.934	2.370
h	-4.726	-2.927	1.916
h	-6.216	-2.443	1.151
h	0.964	-3.746	-2.923
h	0.308	-5.061	-1.777
h	-2.900	1.388	-14.597
h	3.013	8.204	-12.206
h	3.409	4.553	-15.458
h	-0.348	-3.271	-10.172
h	9.148	-2.599	-1.721
h	-4.137	10.294	-7.295
h	-1.189	9.458	0.598
h	-7.049	9.360	0.561
h	-12.362	9.520	3.129
h	-10.296	3.025	-5.750
h	2.342	9.607	4.834
h	-7.759	6.104	-10.771

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## Int2b

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C	11.391	11.205	-6.736
H	12.166	11.713	-7.344
H	10.914	10.421	-7.359
S	10.137	12.437	-6.161
C	7.593	12.238	-2.993
H	7.362	12.527	-1.948
C	6.332	11.462	-3.465
O	5.186	11.875	-3.234
N	6.507	10.268	-4.131
H	7.458	9.899	-4.208
C	5.436	9.302	-4.218
H	4.809	9.463	-3.311
C	4.419	9.523	-5.368
H	3.433	9.144	-5.032
H	4.329	10.619	-5.483
S	4.694	8.767	-7.043
C	6.052	7.902	-4.017
O	7.034	7.737	-3.284
N	5.404	6.899	-4.666
H	4.682	7.143	-5.359
C	5.650	5.486	-4.487
H	6.459	5.384	-3.733
C	4.374	4.818	-3.922
H	4.519	3.726	-3.779
H	4.192	5.239	-2.908

C	3.196	5.075	-4.858
O	3.393	5.559	-5.983
O	1.967	4.842	-4.462
C	6.159	4.777	-5.765
O	6.345	3.537	-5.733
N	6.423	5.536	-6.863
H	6.102	6.521	-6.859
C	6.888	4.925	-8.111
H	6.743	3.834	-7.979
C	6.074	5.344	-9.377
H	5.010	5.295	-9.052
C	6.372	6.779	-9.821
H	5.711	7.076	-10.657
H	6.213	7.521	-9.013
H	7.419	6.889	-10.173
C	6.277	4.335	-10.534
H	7.277	4.498	-10.982
H	6.297	3.303	-10.130
C	5.221	4.420	-11.641
H	5.344	3.571	-12.341
H	4.190	4.350	-11.237
H	5.295	5.369	-12.212
C	8.398	5.072	-8.327
O	9.001	4.321	-9.127
N	9.069	6.010	-7.613
H	8.524	6.737	-7.127
C	10.520	6.103	-7.440
H	10.705	7.014	-6.839
C	11.007	9.176	-11.106
H	10.999	9.982	-10.345
H	11.511	9.580	-12.010
S	9.264	8.738	-11.558
C	5.566	15.156	-10.864
H	4.552	15.578	-10.997
H	5.663	14.303	-11.563
S	5.756	14.586	-9.107
C	3.166	13.576	-6.190
H	4.216	13.381	-5.905
H	2.550	12.757	-5.775
N	3.073	13.498	-7.681
H	3.039	12.491	-8.006
H	2.195	13.915	-8.041
H	3.910	13.937	-8.187
C	1.097	-1.206	2.068
H	1.015	-1.493	1.005
H	1.710	-0.282	2.115
C	1.762	-2.340	2.852
H	1.881	-2.097	3.923
H	1.198	-3.297	2.791
S	3.485	-2.678	2.313
C	3.197	-3.238	0.601
H	4.198	-3.400	0.157
H	2.610	-4.181	0.571
H	2.678	-2.475	-0.008
C	-5.154	-2.970	0.928
H	-5.445	-4.026	0.741
C	-4.484	-2.497	-0.383
O	-5.091	-2.461	-1.464
N	-3.154	-2.128	-0.319
H	-2.619	-2.326	0.537
C	-2.413	-1.627	-1.467
H	-3.024	-1.879	-2.358
C	-2.237	-0.099	-1.377
H	-3.230	0.387	-1.378
H	-1.711	0.168	-0.438
S	-1.205	0.495	-2.791
C	-1.049	-2.341	-1.528

O	-0.051	-1.901	-0.928
N	-1.010	-3.499	-2.248
H	-1.905	-3.885	-2.576
C	0.176	-4.307	-2.561
H	-0.129	-4.932	-3.419
C	-1.922	1.768	-14.692
H	-1.267	0.988	-15.120
H	-1.897	2.626	-15.386
N	-1.323	2.200	-13.403
H	-1.219	1.407	-12.739
H	-0.345	2.594	-13.654
H	-1.855	2.988	-12.895
C	2.529	7.229	-12.180
H	1.576	7.367	-12.727
H	3.138	6.510	-12.771
C	2.320	6.651	-10.799
C	2.763	7.104	-9.557
H	3.304	8.020	-9.286
N	2.471	6.188	-8.567
H	2.784	6.222	-7.581
C	1.840	5.102	-9.135
C	1.710	5.363	-10.543
C	1.099	4.382	-11.359
H	0.999	4.529	-12.445
C	0.637	3.203	-10.762
H	0.200	2.412	-11.381
C	1.372	3.915	-8.537
H	1.489	3.746	-7.457
C	0.763	2.969	-9.371
H	0.379	2.032	-8.942
C	2.723	3.769	-15.891
H	1.994	4.256	-16.564
H	3.347	3.074	-16.487
C	1.959	2.988	-14.831
O	0.778	3.316	-14.533
N	2.591	1.943	-14.278
H	2.167	1.398	-13.500
H	3.595	1.775	-14.512
C	-0.842	-3.381	-9.184
C	-1.731	-4.364	-8.750
H	-2.019	-5.310	-9.225
N	-2.302	-3.990	-7.549
H	-3.054	-4.479	-7.021
C	-1.808	-2.758	-7.179
C	-0.867	-2.342	-8.176
C	-0.226	-1.084	-8.030
H	0.517	-0.737	-8.767
C	-0.568	-0.277	-6.944
H	-0.063	0.686	-6.786
C	-2.144	-1.951	-6.078
H	-2.871	-2.296	-5.329
C	-1.525	-0.703	-5.988
H	-1.749	-0.053	-5.132
C	8.334	-2.092	-1.201
C	8.281	-1.641	0.111
H	9.047	-1.647	0.896
N	7.003	-1.168	0.392
H	6.686	-0.612	1.208
C	6.240	-1.216	-0.763
C	7.037	-1.832	-1.780
C	6.455	-2.012	-3.062
H	7.021	-2.510	-3.867
C	5.156	-1.547	-3.299
H	4.730	-1.634	-4.309
C	4.943	-0.725	-0.996
H	4.379	-0.188	-0.219
C	4.414	-0.899	-2.278

H	3.402	-0.513	-2.468
C	-4.195	9.258	-6.887
H	-4.930	8.681	-7.479
H	-3.200	8.813	-7.089
C	-4.511	9.176	-5.389
H	-3.927	9.900	-4.783
H	-5.571	9.417	-5.179
N	-4.219	7.847	-4.865
H	-3.201	7.617	-4.936
C	-5.019	7.099	-4.102
N	-6.277	7.472	-3.814
H	-6.921	6.838	-3.310
H	-6.659	8.405	-4.062
N	-4.561	5.886	-3.679
H	-5.097	5.397	-2.964
H	-3.545	5.718	-3.635
C	-0.992	8.662	-0.105
H	-0.394	9.061	-0.943
H	-0.372	7.919	0.437
C	-2.235	7.986	-0.685
O	-2.703	8.271	-1.806
N	-2.792	7.045	0.118
H	-3.586	6.456	-0.167
H	-2.484	6.936	1.096
C	-5.135	8.734	1.551
H	-4.322	8.828	0.828
C	-6.489	8.951	1.420
N	-4.931	8.262	2.829
H	-3.985	7.917	3.175
N	-7.079	8.618	2.626
H	-8.180	8.696	2.815
C	-6.117	8.201	3.465
H	-6.282	7.856	4.493
C	-11.922	9.034	2.223
H	-12.642	8.304	1.811
H	-11.834	9.866	1.494
C	-10.534	8.366	2.317
O	-9.600	9.029	2.882
O	-10.432	7.227	1.779
N	-9.679	3.782	-5.528
H	-10.012	4.384	-4.760
C	-8.483	4.101	-6.137
N	-8.112	3.634	-7.326
H	-7.111	3.690	-7.691
H	-8.759	3.206	-8.007
N	-7.686	4.951	-5.483
H	-7.205	5.651	-6.091
H	-7.812	5.123	-4.464
Fe	6.830	12.518	-9.245
Fe	8.543	11.681	-7.682
Fe	8.051	10.062	-9.988
Fe	6.327	10.084	-8.061
S	6.334	12.161	-6.948
S	9.045	12.249	-9.964
S	5.766	10.659	-10.298
S	8.540	9.291	-7.786
W	-0.627	2.854	-2.804
C	1.072	1.803	-3.829
C	1.376	2.722	-2.772
H	1.115	0.703	-3.686
H	2.221	2.774	-2.058
S	-0.089	3.298	-0.524
S	-3.010	3.040	-1.839
S	-1.459	2.991	-5.187
S	-0.794	5.368	-3.115
C	-1.551	3.590	0.403
C	-2.795	3.431	-0.155

C	-1.397	4.683	-5.692
C	-0.999	5.673	-4.842
C	-1.366	3.935	1.868
H	-1.079	3.019	2.446
O	-2.579	4.455	2.435
C	-4.050	3.550	0.692
H	-4.664	2.626	0.531
C	-3.683	3.568	2.191
H	-3.344	2.542	2.453
C	-0.255	4.953	2.026
H	0.655	4.511	1.586
H	-0.507	5.866	1.441
C	-1.747	4.953	-7.143
H	-1.048	4.398	-7.817
O	-1.695	6.351	-7.465
C	-0.550	7.015	-5.389
H	0.514	7.149	-5.076
C	-0.502	6.944	-6.932
H	0.356	6.289	-7.201
C	-3.159	4.465	-7.415
H	-3.256	3.425	-7.043
H	-3.874	5.112	-6.864
C	-5.901	4.583	2.538
N	-9.035	5.663	3.807
H	-9.894	6.000	3.361
H	-9.096	5.112	4.679
N	-6.909	4.780	3.425
C	-7.985	5.413	2.979
N	-8.089	5.868	1.686
H	-8.954	6.431	1.464
C	-7.101	5.659	0.719
O	-7.258	6.085	-0.462
C	-5.946	4.971	1.188
N	-4.827	4.755	0.352
H	-5.098	4.756	-0.639
N	-4.789	3.928	3.014
H	-4.827	3.644	4.004
C	-0.493	9.406	-6.835
N	-0.030	12.894	-7.501
H	-0.737	13.646	-7.378
H	0.219	12.782	-8.493
N	-0.145	10.552	-7.498
C	-0.392	11.703	-6.898
N	-0.964	11.769	-5.657
H	-1.070	12.682	-5.173
C	-1.297	10.629	-4.883
O	-1.781	10.765	-3.737
C	-1.024	9.385	-5.535
N	-1.374	8.152	-4.935
H	-1.441	8.230	-3.905
N	-0.294	8.233	-7.514
H	-0.066	8.323	-8.517
O	-0.041	5.243	3.402
O	1.681	6.019	5.155
O	2.179	6.321	2.562
O	0.325	7.716	3.649
O	-1.000	9.792	4.156
O	0.031	8.408	6.152
P	0.132	8.955	4.744
P	1.204	6.272	3.748
O	-3.413	4.507	-8.832
O	-4.968	4.517	-10.835
O	-5.787	3.460	-8.576
O	-5.363	6.057	-8.763
O	-7.495	6.794	-7.491
O	-6.482	8.278	-9.449
P	-6.760	6.927	-8.828

P	-4.972	4.533	-9.297
O	1.482	9.903	4.572
O	-7.717	5.983	-9.832
O	3.998	-1.199	-13.112
H	4.228	-1.701	-12.274
H	3.066	-0.899	-12.957
O	-8.166	5.612	-2.800
H	-9.123	5.828	-2.828
H	-7.889	5.664	-1.825
O	-2.509	7.129	3.054
H	-1.614	7.411	3.362
H	-2.514	6.140	3.123
O	-2.539	4.245	-12.081
H	-2.062	4.972	-11.613
H	-3.422	4.240	-11.619
O	-7.652	9.917	-4.116
H	-7.217	10.642	-3.587
H	-7.868	10.381	-4.957
O	2.912	4.333	0.760
H	2.692	5.050	1.429
H	2.122	4.320	0.175
O	3.139	1.376	1.308
H	2.582	0.993	0.576
H	3.079	2.353	1.171
O	-4.208	10.685	-2.418
H	-3.798	9.800	-2.266
H	-3.530	11.097	-3.004
O	10.561	1.048	-4.546
H	10.639	2.033	-4.477
H	9.749	0.990	-5.101
O	3.190	0.619	-10.153
H	4.011	0.765	-10.814
H	3.326	1.400	-9.538
O	7.567	1.077	-11.946
H	7.839	1.825	-12.546
H	8.137	1.267	-11.142
O	4.871	5.786	-0.801
H	4.288	5.186	-0.276
H	5.251	6.360	-0.096
O	6.726	1.086	-8.848
H	7.345	1.432	-8.164
H	5.878	1.582	-8.715
O	1.701	0.132	-12.260
H	2.139	0.426	-11.392
H	0.759	-0.032	-12.021
O	7.345	-1.607	-8.359
H	7.489	-1.473	-7.396
H	7.021	-0.710	-8.632
O	9.542	5.477	-11.671
H	9.471	6.468	-11.532
H	9.472	5.096	-10.762
O	8.429	3.349	-13.314
H	7.695	3.899	-13.654
H	8.923	3.989	-12.740
O	4.944	1.032	-11.898
H	4.747	0.262	-12.502
H	5.956	1.077	-11.801
O	1.447	2.097	-5.191
H	1.796	4.188	-3.667
H	0.666	2.568	-5.590
O	9.493	1.930	-10.276
H	9.901	1.435	-9.520
H	9.156	2.751	-9.839
O	3.899	1.938	-6.029
H	4.597	2.480	-5.592
H	2.974	2.099	-5.626
O	4.883	-2.400	-10.879



H	4.495	-3.305	-10.779
H	4.589	-1.994	-10.008
O	3.672	-1.421	-8.708
H	3.400	-0.582	-9.267
H	2.853	-1.902	-8.479
O	7.174	-0.519	-5.786
H	7.120	-0.697	-4.823
H	6.173	-0.549	-6.090
O	8.428	1.609	-6.506
H	7.884	2.370	-6.183
H	7.894	0.779	-6.209
O	10.704	0.934	-7.940
H	9.949	1.292	-7.397
H	11.417	1.627	-7.947
O	4.256	2.441	-8.549
H	4.012	3.362	-8.770
H	4.034	2.326	-7.563
O	4.725	-0.633	-6.371
H	4.414	-0.932	-7.276
H	4.332	0.270	-6.218
O	1.712	0.263	-0.816
H	1.020	-0.441	-0.883
H	1.358	0.982	-1.385
h	11.918	10.688	-5.934
h	8.533	11.687	-3.013
h	7.646	13.200	-3.502
h	10.922	5.232	-6.924
h	11.095	6.299	-8.345
h	11.567	8.335	-10.698
h	6.270	15.910	-11.216
h	2.798	14.521	-5.789
h	0.089	-0.922	2.372
h	-4.606	-2.911	1.869
h	-6.100	-2.454	1.089
h	1.034	-3.764	-2.956
h	0.363	-5.066	-1.801
h	-2.935	1.375	-14.602
h	3.019	8.202	-12.200
h	3.400	4.525	-15.493
h	-0.362	-3.286	-10.158
h	9.153	-2.596	-1.716
h	-4.189	10.284	-7.255
h	-1.188	9.470	0.600
h	-7.032	9.353	0.565
h	-12.324	9.498	3.123
h	-10.289	3.021	-5.748
h	2.347	9.615	4.838
h	-7.753	6.103	-10.774

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C	11.392	11.208	-6.736
H	12.166	11.716	-7.343
H	10.915	10.424	-7.360
S	10.137	12.438	-6.161
C	7.588	12.232	-2.998
H	7.355	12.520	-1.952
C	6.328	11.455	-3.472
O	5.181	11.871	-3.249
N	6.505	10.257	-4.130
H	7.455	9.886	-4.201
C	5.433	9.291	-4.221
H	4.805	9.451	-3.315
C	4.420	9.514	-5.373

H	3.433	9.134	-5.041
H	4.330	10.610	-5.488
S	4.702	8.760	-7.048
C	6.049	7.892	-4.023
O	7.036	7.727	-3.297
N	5.396	6.887	-4.665
H	4.659	7.122	-5.344
C	5.647	5.475	-4.485
H	6.466	5.379	-3.740
C	4.381	4.804	-3.907
H	4.534	3.714	-3.757
H	4.203	5.231	-2.895
C	3.190	5.046	-4.835
O	3.382	5.541	-5.961
O	1.976	4.785	-4.435
C	6.152	4.767	-5.764
O	6.333	3.526	-5.737
N	6.421	5.528	-6.860
H	6.104	6.515	-6.854
C	6.890	4.921	-8.108
H	6.746	3.829	-7.979
C	6.079	5.342	-9.375
H	5.013	5.301	-9.051
C	6.386	6.775	-9.820
H	5.724	7.078	-10.653
H	6.237	7.517	-9.010
H	7.433	6.876	-10.176
C	6.274	4.332	-10.531
H	7.276	4.487	-10.979
H	6.287	3.299	-10.128
C	5.220	4.425	-11.639
H	5.338	3.576	-12.340
H	4.188	4.359	-11.235
H	5.300	5.374	-12.207
C	8.399	5.070	-8.325
O	9.002	4.322	-9.127
N	9.069	6.009	-7.610
H	8.524	6.729	-7.117
C	10.521	6.103	-7.439
H	10.705	7.015	-6.839
C	11.007	9.177	-11.105
H	10.998	9.980	-10.341
H	11.513	9.584	-12.006
S	9.266	8.739	-11.561
C	5.566	15.156	-10.864
H	4.552	15.578	-10.997
H	5.663	14.302	-11.563
S	5.756	14.585	-9.107
C	3.167	13.575	-6.188
H	4.218	13.380	-5.902
H	2.553	12.755	-5.773
N	3.076	13.495	-7.679
H	3.044	12.488	-8.003
H	2.197	13.911	-8.040
H	3.912	13.935	-8.185
C	1.095	-1.211	2.069
H	1.014	-1.500	1.006
H	1.709	-0.288	2.113
C	1.757	-2.344	2.856
H	1.871	-2.101	3.927
H	1.193	-3.301	2.792
S	3.482	-2.682	2.324
C	3.202	-3.237	0.610
H	4.204	-3.403	0.171
H	2.610	-4.178	0.575
H	2.689	-2.470	-0.001
C	-5.156	-2.967	0.929

H	-5.448	-4.023	0.741
C	-4.488	-2.494	-0.383
O	-5.095	-2.461	-1.464
N	-3.159	-2.117	-0.319
H	-2.624	-2.317	0.537
C	-2.418	-1.620	-1.468
H	-3.030	-1.873	-2.358
C	-2.239	-0.092	-1.381
H	-3.230	0.397	-1.386
H	-1.716	0.176	-0.441
S	-1.202	0.501	-2.793
C	-1.055	-2.335	-1.528
O	-0.057	-1.893	-0.930
N	-1.016	-3.495	-2.245
H	-1.911	-3.882	-2.573
C	0.170	-4.303	-2.558
H	-0.135	-4.927	-3.417
C	-1.924	1.767	-14.696
H	-1.269	0.987	-15.126
H	-1.899	2.626	-15.389
N	-1.324	2.197	-13.407
H	-1.219	1.403	-12.745
H	-0.346	2.592	-13.658
H	-1.857	2.984	-12.899
C	2.529	7.226	-12.172
H	1.575	7.363	-12.717
H	3.136	6.507	-12.763
C	2.321	6.648	-10.790
C	2.773	7.095	-9.549
H	3.320	8.007	-9.279
N	2.482	6.178	-8.559
H	2.792	6.208	-7.571
C	1.839	5.098	-9.127
C	1.703	5.364	-10.533
C	1.079	4.390	-11.347
H	0.974	4.540	-12.433
C	0.607	3.215	-10.749
H	0.154	2.431	-11.366
C	1.365	3.915	-8.528
H	1.490	3.743	-7.450
C	0.741	2.977	-9.360
H	0.352	2.041	-8.931
C	2.723	3.774	-15.884
H	1.992	4.259	-16.557
H	3.347	3.079	-16.479
C	1.960	2.994	-14.822
O	0.776	3.315	-14.532
N	2.598	1.958	-14.259
H	2.173	1.414	-13.481
H	3.604	1.794	-14.490
C	-0.844	-3.384	-9.189
C	-1.733	-4.369	-8.756
H	-2.018	-5.315	-9.231
N	-2.305	-3.997	-7.555
H	-3.056	-4.487	-7.028
C	-1.813	-2.764	-7.183
C	-0.871	-2.346	-8.180
C	-0.233	-1.087	-8.032
H	0.509	-0.738	-8.769
C	-0.576	-0.282	-6.945
H	-0.069	0.680	-6.783
C	-2.149	-1.959	-6.082
H	-2.876	-2.307	-5.333
C	-1.532	-0.711	-5.989
H	-1.755	-0.062	-5.132
C	8.335	-2.092	-1.196
C	8.280	-1.640	0.116

H	9.047	-1.645	0.900
N	7.002	-1.170	0.397
H	6.685	-0.611	1.211
C	6.238	-1.219	-0.758
C	7.036	-1.834	-1.775
C	6.455	-2.016	-3.057
H	7.022	-2.512	-3.862
C	5.155	-1.553	-3.294
H	4.730	-1.641	-4.305
C	4.941	-0.729	-0.991
H	4.378	-0.191	-0.215
C	4.413	-0.906	-2.273
H	3.401	-0.520	-2.463
C	-4.193	9.258	-6.891
H	-4.928	8.681	-7.483
H	-3.198	8.814	-7.093
C	-4.510	9.177	-5.394
H	-3.924	9.899	-4.787
H	-5.570	9.418	-5.184
N	-4.219	7.847	-4.870
H	-3.201	7.616	-4.941
C	-5.020	7.099	-4.110
N	-6.277	7.472	-3.819
H	-6.922	6.838	-3.316
H	-6.659	8.407	-4.064
N	-4.564	5.883	-3.690
H	-5.098	5.397	-2.971
H	-3.549	5.714	-3.650
C	-0.991	8.663	-0.107
H	-0.394	9.063	-0.945
H	-0.368	7.921	0.434
C	-2.233	7.983	-0.686
O	-2.700	8.262	-1.810
N	-2.789	7.044	0.119
H	-3.582	6.453	-0.164
H	-2.482	6.939	1.098
C	-5.134	8.733	1.549
H	-4.322	8.827	0.824
C	-6.488	8.950	1.420
N	-4.928	8.261	2.827
H	-3.982	7.916	3.171
N	-7.077	8.617	2.626
H	-8.178	8.695	2.816
C	-6.113	8.201	3.464
H	-6.277	7.856	4.492
C	-11.918	9.031	2.223
H	-12.639	8.301	1.811
H	-11.830	9.862	1.493
C	-10.530	8.363	2.319
O	-9.598	9.026	2.885
O	-10.427	7.225	1.781
N	-9.679	3.780	-5.529
H	-10.011	4.382	-4.760
C	-8.484	4.100	-6.139
N	-8.114	3.633	-7.329
H	-7.113	3.689	-7.694
H	-8.762	3.206	-8.010
N	-7.686	4.949	-5.485
H	-7.206	5.649	-6.093
H	-7.811	5.121	-4.467
Fe	6.828	12.517	-9.246
Fe	8.543	11.682	-7.684
Fe	8.052	10.063	-9.990
Fe	6.329	10.082	-8.062
S	6.334	12.159	-6.949
S	9.044	12.251	-9.966
S	5.766	10.659	-10.300

S	8.544	9.293	-7.789
W	-0.630	2.861	-2.818
C	1.084	1.796	-3.821
C	1.395	2.758	-2.801
H	1.142	0.703	-3.641
H	2.207	2.766	-2.047
S	-0.083	3.299	-0.536
S	-3.005	3.036	-1.847
S	-1.452	2.994	-5.193
S	-0.791	5.362	-3.123
C	-1.545	3.589	0.395
C	-2.788	3.431	-0.163
C	-1.394	4.682	-5.698
C	-0.997	5.673	-4.847
C	-1.358	3.934	1.858
H	-1.072	3.017	2.436
O	-2.571	4.454	2.426
C	-4.043	3.551	0.684
H	-4.658	2.627	0.522
C	-3.675	3.567	2.183
H	-3.336	2.541	2.443
C	-0.248	4.952	2.018
H	0.663	4.513	1.577
H	-0.502	5.865	1.434
C	-1.748	4.955	-7.148
H	-1.049	4.401	-7.822
O	-1.696	6.354	-7.467
C	-0.548	7.016	-5.391
H	0.516	7.149	-5.078
C	-0.500	6.946	-6.934
H	0.356	6.289	-7.203
C	-3.160	4.467	-7.417
H	-3.256	3.427	-7.045
H	-3.875	5.114	-6.867
C	-5.893	4.583	2.532
N	-9.027	5.659	3.803
H	-9.886	5.998	3.357
H	-9.088	5.109	4.675
N	-6.900	4.780	3.420
C	-7.977	5.411	2.974
N	-8.082	5.866	1.682
H	-8.948	6.429	1.460
C	-7.094	5.658	0.714
O	-7.252	6.084	-0.467
C	-5.939	4.971	1.182
N	-4.820	4.756	0.345
H	-5.093	4.758	-0.645
N	-4.779	3.928	3.007
H	-4.818	3.644	3.997
C	-0.494	9.407	-6.836
N	-0.032	12.896	-7.499
H	-0.736	13.649	-7.372
H	0.216	12.785	-8.492
N	-0.146	10.553	-7.498
C	-0.393	11.704	-6.897
N	-0.964	11.769	-5.656
H	-1.071	12.682	-5.171
C	-1.297	10.629	-4.883
O	-1.781	10.763	-3.736
C	-1.024	9.386	-5.536
N	-1.374	8.151	-4.936
H	-1.440	8.231	-3.906
N	-0.293	8.235	-7.516
H	-0.067	8.325	-8.519
O	-0.035	5.241	3.394
O	1.684	6.018	5.150
O	2.184	6.322	2.558

O	0.326	7.714	3.646
O	-0.999	9.789	4.155
O	0.032	8.403	6.150
P	0.134	8.952	4.742
P	1.208	6.271	3.743
O	-3.415	4.508	-8.834
O	-4.971	4.517	-10.836
O	-5.788	3.459	-8.577
O	-5.365	6.057	-8.763
O	-7.496	6.794	-7.490
O	-6.483	8.279	-9.447
P	-6.761	6.927	-8.827
P	-4.974	4.533	-9.299
O	1.482	9.901	4.572
O	-7.719	5.984	-9.832
O	3.995	-1.179	-13.107
H	4.226	-1.687	-12.272
H	3.066	-0.874	-12.946
O	-8.165	5.612	-2.804
H	-9.122	5.827	-2.831
H	-7.887	5.664	-1.829
O	-2.505	7.128	3.053
H	-1.610	7.412	3.358
H	-2.506	6.139	3.121
O	-2.542	4.243	-12.083
H	-2.064	4.969	-11.615
H	-3.425	4.239	-11.622
O	-7.650	9.917	-4.118
H	-7.215	10.641	-3.587
H	-7.864	10.382	-4.958
O	2.917	4.329	0.761
H	2.698	5.048	1.429
H	2.135	4.328	0.165
O	3.138	1.376	1.308
H	2.582	0.993	0.577
H	3.079	2.353	1.170
O	-4.208	10.680	-2.418
H	-3.797	9.795	-2.268
H	-3.530	11.093	-3.002
O	10.567	1.051	-4.544
H	10.646	2.035	-4.475
H	9.754	0.994	-5.097
O	3.201	0.648	-10.141
H	4.022	0.790	-10.804
H	3.338	1.428	-9.524
O	7.578	1.076	-11.941
H	7.847	1.825	-12.542
H	8.149	1.267	-11.139
O	4.880	5.796	-0.784
H	4.301	5.188	-0.264
H	5.257	6.367	-0.074
O	6.731	1.091	-8.835
H	7.354	1.436	-8.152
H	5.885	1.589	-8.698
O	1.707	0.153	-12.241
H	2.145	0.451	-11.374
H	0.764	-0.012	-12.002
O	7.359	-1.601	-8.350
H	7.505	-1.468	-7.387
H	7.032	-0.705	-8.621
O	9.542	5.479	-11.672
H	9.472	6.470	-11.535
H	9.471	5.099	-10.762
O	8.431	3.349	-13.312
H	7.692	3.895	-13.650
H	8.923	3.992	-12.740
O	4.956	1.044	-11.888

H	4.754	0.275	-12.491
H	5.969	1.084	-11.792
O	1.442	2.043	-5.195
H	1.779	4.068	-3.629
H	0.691	2.568	-5.582
O	9.501	1.931	-10.272
H	9.908	1.436	-9.516
H	9.163	2.753	-9.836
O	3.914	1.925	-6.008
H	4.610	2.475	-5.575
H	2.989	2.082	-5.607
O	4.880	-2.392	-10.880
H	4.493	-3.297	-10.779
H	4.583	-1.983	-10.011
O	3.677	-1.402	-8.712
H	3.409	-0.556	-9.263
H	2.854	-1.875	-8.480
O	7.184	-0.521	-5.776
H	7.128	-0.699	-4.812
H	6.183	-0.556	-6.082
O	8.430	1.612	-6.498
H	7.881	2.371	-6.178
H	7.899	0.780	-6.200
O	10.707	0.932	-7.935
H	9.953	1.292	-7.393
H	11.421	1.624	-7.942
O	4.266	2.457	-8.525
H	4.032	3.383	-8.733
H	4.047	2.332	-7.539
O	4.737	-0.642	-6.368
H	4.429	-0.931	-7.276
H	4.347	0.262	-6.209
O	1.708	0.267	-0.817
H	1.015	-0.436	-0.883
H	1.348	0.991	-1.375
h	11.918	10.689	-5.935
h	8.530	11.684	-3.017
h	7.641	13.196	-3.504
h	10.924	5.232	-6.923
h	11.095	6.298	-8.345
h	11.567	8.335	-10.698
h	6.270	15.910	-11.215
h	2.799	14.520	-5.788
h	0.088	-0.925	2.372
h	-4.608	-2.909	1.870
h	-6.102	-2.450	1.091
h	1.028	-3.759	-2.953
h	0.357	-5.063	-1.799
h	-2.937	1.374	-14.606
h	3.019	8.199	-12.194
h	3.400	4.531	-15.489
h	-0.363	-3.288	-10.162
h	9.153	-2.595	-1.711
h	-4.187	10.284	-7.259
h	-1.188	9.470	0.598
h	-7.032	9.352	0.565
h	-12.322	9.496	3.123
h	-10.290	3.019	-5.748
h	2.348	9.614	4.838
h	-7.754	6.104	-10.773

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C	11.384	11.176	-6.769
H	12.158	11.665	-7.392
H	10.891	10.387	-7.375
S	10.147	12.424	-6.196
C	7.606	12.262	-3.010
H	7.370	12.542	-1.963
C	6.341	11.501	-3.495
O	5.197	11.905	-3.241
N	6.512	10.325	-4.194
H	7.467	9.967	-4.275
C	5.464	9.327	-4.246
H	4.884	9.444	-3.303
C	4.381	9.533	-5.332
H	3.438	9.084	-4.963
H	4.221	10.625	-5.395
S	4.616	8.861	-7.047
C	6.151	7.955	-4.103
O	7.132	7.828	-3.359
N	5.592	6.929	-4.798
H	4.868	7.147	-5.498
C	6.021	5.554	-4.650
H	6.824	5.554	-3.885
C	4.850	4.695	-4.143
H	5.195	3.641	-4.068
H	4.570	5.028	-3.124
C	3.637	4.731	-5.090
O	3.859	4.872	-6.339
O	2.493	4.594	-4.563
C	6.647	4.934	-5.910
O	7.181	3.813	-5.821
N	6.603	5.634	-7.077
H	6.068	6.515	-7.116
C	7.022	4.985	-8.315
H	6.872	3.894	-8.174
C	6.187	5.404	-9.557
H	5.132	5.355	-9.209
C	6.489	6.831	-10.018
H	5.822	7.128	-10.849
H	6.353	7.588	-9.220
H	7.532	6.928	-10.387
C	6.339	4.379	-10.703
H	7.337	4.497	-11.169
H	6.326	3.352	-10.283
C	5.260	4.496	-11.784
H	5.356	3.658	-12.501
H	4.241	4.427	-11.351
H	5.333	5.454	-12.339
C	8.529	5.110	-8.516
O	9.151	4.377	-9.321
N	9.174	6.024	-7.751
H	8.586	6.691	-7.232
C	10.610	6.112	-7.506
H	10.775	7.015	-6.887
C	11.072	9.262	-11.161
H	11.053	10.060	-10.392
H	11.614	9.663	-12.044
S	9.344	8.847	-11.665
C	5.547	15.162	-10.902
H	4.540	15.601	-11.030
H	5.638	14.328	-11.625
S	5.735	14.539	-9.163
C	3.155	13.588	-6.243
H	4.208	13.385	-5.970
H	2.541	12.761	-5.842



N	3.054	13.545	-7.735
H	3.004	12.546	-8.079
H	2.184	13.986	-8.085
H	3.903	13.978	-8.241
C	1.093	-1.362	2.149
H	1.067	-1.662	1.088
H	1.740	-0.464	2.219
C	1.657	-2.507	2.991
H	1.618	-2.296	4.075
H	1.111	-3.463	2.825
S	3.438	-2.808	2.671
C	3.377	-3.226	0.896
H	4.410	-3.500	0.609
H	2.697	-4.084	0.707
H	3.063	-2.371	0.269
C	-5.229	-2.973	0.939
H	-5.544	-4.024	0.760
C	-4.562	-2.521	-0.379
O	-5.177	-2.469	-1.455
N	-3.220	-2.190	-0.333
H	-2.680	-2.389	0.521
C	-2.492	-1.692	-1.488
H	-3.094	-1.970	-2.377
C	-2.363	-0.160	-1.413
H	-3.371	0.295	-1.421
H	-1.860	0.127	-0.467
S	-1.351	0.481	-2.817
C	-1.107	-2.363	-1.537
O	-0.121	-1.880	-0.951
N	-1.034	-3.532	-2.237
H	-1.920	-3.948	-2.556
C	0.174	-4.308	-2.547
H	-0.113	-4.946	-3.401
C	-1.984	1.728	-14.765
H	-1.337	0.936	-15.182
H	-1.965	2.570	-15.478
N	-1.379	2.186	-13.490
H	-1.253	1.406	-12.816
H	-0.405	2.602	-13.747
H	-1.923	2.971	-12.999
C	2.496	7.194	-12.164
H	1.532	7.344	-12.687
H	3.090	6.486	-12.781
C	2.312	6.580	-10.793
C	2.890	6.918	-9.569
H	3.529	7.769	-9.303
N	2.578	5.980	-8.602
H	3.014	5.869	-7.665
C	1.802	4.996	-9.173
C	1.592	5.347	-10.551
C	0.801	4.489	-11.351
H	0.631	4.707	-12.417
C	0.247	3.345	-10.763
H	-0.396	2.682	-11.349
C	1.260	3.836	-8.589
H	1.448	3.589	-7.537
C	0.475	3.015	-9.406
H	0.022	2.103	-8.989
C	2.665	3.838	-15.883
H	1.942	4.320	-16.566
H	3.293	3.138	-16.468
C	1.897	3.063	-14.824
O	0.693	3.346	-14.581
N	2.554	2.062	-14.215
H	2.154	1.565	-13.394
H	3.571	1.943	-14.416
C	-0.791	-3.252	-9.162

C	-1.664	-4.230	-8.685
H	-1.957	-5.187	-9.132
N	-2.219	-3.828	-7.484
H	-2.974	-4.308	-6.950
C	-1.737	-2.576	-7.164
C	-0.813	-2.183	-8.188
C	-0.199	-0.905	-8.105
H	0.512	-0.570	-8.880
C	-0.553	-0.050	-7.059
H	-0.101	0.950	-6.974
C	-2.074	-1.725	-6.097
H	-2.784	-2.047	-5.322
C	-1.488	-0.458	-6.075
H	-1.735	0.232	-5.258
C	8.288	-2.076	-1.229
C	8.233	-1.627	0.083
H	8.999	-1.634	0.868
N	6.957	-1.150	0.364
H	6.646	-0.590	1.183
C	6.194	-1.190	-0.790
C	6.989	-1.812	-1.807
C	6.401	-1.997	-3.085
H	6.962	-2.492	-3.894
C	5.101	-1.533	-3.318
H	4.671	-1.653	-4.324
C	4.901	-0.685	-1.022
H	4.357	-0.127	-0.243
C	4.366	-0.868	-2.302
H	3.360	-0.475	-2.518
C	-4.108	9.250	-6.999
H	-4.814	8.677	-7.630
H	-3.096	8.844	-7.198
C	-4.456	9.101	-5.514
H	-3.918	9.823	-4.863
H	-5.532	9.292	-5.333
N	-4.137	7.760	-5.032
H	-3.113	7.548	-5.093
C	-4.903	7.026	-4.214
N	-6.092	7.460	-3.768
H	-6.771	6.811	-3.330
H	-6.455	8.413	-3.968
N	-4.486	5.769	-3.897
H	-4.833	5.326	-3.047
H	-3.548	5.464	-4.179
C	-0.982	8.642	-0.113
H	-0.389	9.038	-0.955
H	-0.354	7.909	0.434
C	-2.216	7.942	-0.688
O	-2.643	8.159	-1.840
N	-2.808	7.053	0.151
H	-3.605	6.465	-0.127
H	-2.525	6.987	1.141
C	-5.150	8.755	1.570
H	-4.333	8.858	0.853
C	-6.506	8.955	1.430
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H	-4.002	7.960	3.205
N	-7.099	8.621	2.633
H	-8.200	8.692	2.813
C	-6.138	8.220	3.481
H	-6.304	7.874	4.507
C	-11.953	9.055	2.222
H	-12.681	8.334	1.807
H	-11.859	9.893	1.501
C	-10.574	8.371	2.313
O	-9.626	9.026	2.862
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H	-10.011	4.387	-4.770
C	-8.495	4.114	-6.163
N	-8.132	3.652	-7.358
H	-7.132	3.713	-7.722
H	-8.782	3.224	-8.035
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H	-7.214	5.659	-6.120
H	-7.802	5.124	-4.488
Fe	6.736	12.424	-9.237
Fe	8.564	11.692	-7.737
Fe	8.099	10.161	-10.134
Fe	6.281	10.204	-7.983
S	6.384	12.267	-6.915
S	9.009	12.324	-9.996
S	5.800	10.522	-10.317
S	8.480	9.305	-7.906
W	-0.965	2.882	-2.786
C	0.753	1.989	-4.089
C	1.262	2.415	-2.825
H	0.563	0.913	-4.259
H	1.487	1.633	-2.083
S	-0.228	3.335	-0.570
S	-3.183	2.979	-1.742
S	-2.030	3.214	-4.975
S	-0.411	5.219	-3.200
C	-1.654	3.596	0.442
C	-2.909	3.424	-0.069
C	-1.505	4.734	-5.628
C	-0.805	5.632	-4.852
C	-1.423	3.958	1.893
H	-1.140	3.040	2.469
O	-2.616	4.502	2.481
C	-4.142	3.582	0.790
H	-4.772	2.662	0.667
C	-3.743	3.632	2.280
H	-3.419	2.606	2.564
C	-0.288	4.956	2.024
H	0.607	4.506	1.554
H	-0.541	5.877	1.454
C	-1.815	5.019	-7.090
H	-1.121	4.409	-7.720
O	-1.650	6.403	-7.422
C	-0.367	6.973	-5.409
H	0.697	7.147	-5.123
C	-0.389	6.916	-6.954
H	0.417	6.224	-7.286
C	-3.240	4.620	-7.415
H	-3.441	3.614	-6.995
H	-3.933	5.349	-6.946
C	-5.958	4.657	2.623
N	-9.100	5.709	3.888
H	-9.971	6.006	3.438
H	-9.146	5.160	4.763
N	-6.964	4.851	3.511
C	-8.052	5.457	3.056
N	-8.172	5.885	1.757
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N	-4.906	4.787	0.427
H	-5.194	4.765	-0.559
N	-4.827	4.037	3.108
H	-4.874	3.734	4.093
C	-0.401	9.371	-6.844
N	-0.066	12.873	-7.500

H	-0.758	13.630	-7.336
H	0.188	12.789	-8.493
N	-0.098	10.531	-7.504
C	-0.384	11.673	-6.902
N	-0.959	11.715	-5.659
H	-1.095	12.623	-5.173
C	-1.253	10.562	-4.890
O	-1.748	10.679	-3.745
C	-0.931	9.330	-5.543
N	-1.240	8.078	-4.951
H	-1.335	8.148	-3.924
N	-0.152	8.206	-7.522
H	0.039	8.300	-8.530
O	-0.041	5.229	3.397
O	1.686	6.007	5.144
O	2.176	6.307	2.550
O	0.328	7.706	3.643
O	-1.006	9.774	4.154
O	0.033	8.390	6.147
P	0.133	8.942	4.741
P	1.205	6.261	3.738
O	-3.427	4.595	-8.842
O	-4.984	4.537	-10.857
O	-5.781	3.500	-8.583
O	-5.389	6.101	-8.804
O	-7.508	6.817	-7.502
O	-6.523	8.311	-9.471
P	-6.790	6.959	-8.848
P	-4.984	4.576	-9.321
O	1.476	9.898	4.570
O	-7.748	6.008	-9.842
O	3.969	-0.943	-13.090
H	4.217	-1.561	-12.338
H	3.086	-0.594	-12.806
O	-8.105	5.664	-2.830
H	-9.056	5.905	-2.867
H	-7.864	5.669	-1.847
O	-2.518	7.176	3.068
H	-1.622	7.469	3.363
H	-2.519	6.188	3.159
O	-2.614	4.267	-12.202
H	-2.108	4.982	-11.746
H	-3.472	4.261	-11.697
O	-7.537	9.872	-4.087
H	-7.129	10.612	-3.557
H	-7.765	10.331	-4.926
O	2.932	4.303	0.815
H	2.686	5.028	1.468
H	2.250	4.383	0.116
O	3.184	1.394	1.395
H	2.533	1.002	0.760
H	3.126	2.367	1.225
O	-4.187	10.575	-2.466
H	-3.789	9.686	-2.310
H	-3.489	10.981	-3.033
O	10.632	1.059	-4.549
H	10.723	2.043	-4.483
H	9.844	1.017	-5.142
O	3.481	1.235	-10.036
H	4.236	1.309	-10.760
H	3.665	1.929	-9.337
O	7.724	1.072	-11.953
H	7.979	1.836	-12.539
H	8.301	1.257	-11.149
O	4.993	5.896	-0.601
H	4.417	5.266	-0.113
H	5.338	6.467	0.125

O	6.724	1.292	-8.710
H	7.472	1.544	-8.119
H	5.939	1.781	-8.342
O	1.804	0.443	-11.960
H	2.242	0.893	-11.172
H	0.857	0.315	-11.722
O	7.324	-1.440	-8.337
H	7.478	-1.326	-7.374
H	7.009	-0.533	-8.588
O	9.678	5.550	-11.794
H	9.589	6.536	-11.652
H	9.599	5.162	-10.886
O	8.474	3.386	-13.319
H	7.756	3.959	-13.658
H	9.012	4.028	-12.788
O	5.121	1.244	-11.986
H	4.819	0.408	-12.451
H	6.124	1.163	-11.827
O	1.106	2.617	-5.283
H	1.902	3.312	-2.797
H	1.554	3.533	-5.068
O	9.587	1.897	-10.249
H	9.999	1.418	-9.483
H	9.281	2.755	-9.857
O	3.392	1.372	-5.660
H	3.830	1.652	-4.832
H	2.469	1.804	-5.606
O	4.862	-2.303	-10.973
H	4.495	-3.205	-10.800
H	4.522	-1.803	-10.167
O	3.713	-1.045	-8.936
H	3.601	-0.086	-9.351
H	2.813	-1.372	-8.747
O	7.116	-0.359	-5.751
H	7.059	-0.544	-4.791
H	6.147	-0.500	-6.086
O	8.626	1.608	-6.523
H	8.207	2.471	-6.248
H	7.977	0.884	-6.214
O	10.810	0.871	-7.954
H	10.049	1.214	-7.400
H	11.513	1.575	-7.950
O	4.405	2.604	-7.859
H	4.297	3.531	-7.508
H	4.086	2.081	-7.068
O	4.711	-0.877	-6.455
H	4.497	-1.001	-7.425
H	4.094	-0.155	-6.164
O	1.223	0.436	-0.320
H	0.705	-0.347	-0.641
H	0.587	1.187	-0.346
h	11.909	10.667	-5.961
h	8.542	11.703	-3.032
h	7.674	13.230	-3.507
h	10.987	5.231	-6.986
h	11.196	6.330	-8.398
h	11.595	8.402	-10.744
h	6.264	15.914	-11.231
h	2.793	14.523	-5.816
h	0.087	-1.024	2.397
h	-4.674	-2.919	1.876
h	-6.162	-2.434	1.106
h	1.014	-3.743	-2.951
h	0.379	-5.059	-1.784
h	-2.997	1.341	-14.653
h	2.987	8.168	-12.181
h	3.350	4.588	-15.489

h	-0.317	-3.182	-10.141
h	9.114	-2.572	-1.739
h	-4.127	10.289	-7.330
h	-1.180	9.453	0.587
h	-7.049	9.355	0.573
h	-12.348	9.512	3.129
h	-10.293	3.027	-5.762
h	2.343	9.613	4.834
h	-7.779	6.118	-10.785

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## Geometry optimization procedure

Unless noted otherwise, all optimizations were carried out at the QM/MM level with the HDLC optimizer as implemented in the ChemShell package using standard options and convergence criteria (*Phys. Chem. Chem. Phys.* 2001, 2, 2177). The geometries of **Int1**, **Int2**, **Int2b**, and **Int3** were obtained from unconstrained energy minimizations. The transition states **TS1** and **TS2** were determined from reaction profiles along suitably defined reaction coordinates, which were computed by performing energy minimizations at appropriately chosen values (see below) of the reaction coordinate (subjected to a harmonic restraint). The highest point of these energy profiles represents an approximation to the corresponding transition state. The spacing between the points on the reaction profile was chosen such that the computed energy of the transition state is accurate to within 0.1 kcal/mol (as confirmed by comparisons for the model **M1** where precise transition state searches are still technically feasible). In the following, we provide further details on the specific geometry optimizations that have been carried out in the present work.

Starting from the structure of **Int1** from QM/MM model **M3a** (157 atoms, *J. Chem. Theory Comput.* 2012, 8, 3793), the geometry of **Int1** was optimized by energy minimization using model **M4** with 408 atoms in the QM region. The energy profile was then computed for the first step of the reaction, using the same reaction coordinate ( $R1 = d_{C-O} - d_{O-H}$ ) as in our previous paper; R1 was scanned between 0.80 Å to 0.40 Å with a step size of 0.10 Å. The highest point (approximate transition state **TS1**) was found at R1 = 0.60 Å. Starting from the structure at R = 0.40 Å, the geometry of **Int2** was obtained by energy minimization with a very small stepsize (maxstep= 0.1 Bohr). Another analogous energy minimization was performed starting from the structure at R1 = 0.80 Å, which led to the same minimum structure of **Int1** that had been obtained initially (i.e., differences in energy of less than 0.01 kcal/mol and in coordinates of less than 0.001 Å).

Starting from **Int2**, the carboxylic hydroxyl group of Asp13 was manually rotated into the orientation typical of **Int2b**, and the resulting geometry was then optimized to obtain the minimum structure of **Int2b**. The energy profile was then computed using the same reaction coordinate ( $R2 = d_{C-H} - d_{O-H}$ ) for the second proton transfer step as in our previous paper; R2 was scanned between 0.90 Å to 0.20 Å with a step size of 0.10 Å. The highest point (approximate transition state **TS2**) was found at R2 = 0.50 Å. Starting from the structure at R2 = 0.20 Å, the geometry of **Int3** was obtained by energy minimization with a very small stepsize (maxstep= 0.1 Bohr). Another analogous energy minimization was performed starting from the structure at R2 = 0.90 Å, which led to the same minimum structure of **Int2b** that had been obtained initially.

In order to confirm that all stationary points for model **M4** correspond to the same local minimum, we generated overlays of all optimized structures and checked the deviations for individual atoms and the overall root-mean-square deviations (RMSD) from the **Int1** reference structure. The active optimized region for model **M4** consists of the 408 QM atoms and the surrounding 1928 MM atoms, while the remaining outer MM atoms are kept fixed during the optimizations and thus provide a scaffold. The overall integrity and similarity of the computed structures is indicated by the RMSD values for the active part of the MM region, which are less than 0.05 Å for all

stationary points (Table S18). The deviations for individual MM atoms are always less than 0.10 Å. The different stationary points for model **M4** thus belong to the same local minimum as far as the MM region is concerned. For the QM region (408 atoms), the deviations between different stationary points must be larger, of course, because the reactions occur in the QM region. The RMSD values for the QM region range between 0.15 and 0.27 Å, and become somewhat smaller when the attacking water molecule is not included (Table S18). Careful visual inspection (using overlays of the optimized QM regions) confirms that the different stationary points for model **M4** belong to the same local minimum, also as far as the QM region is concerned. In particular, they share the same hydrogen-bonding interactions, with one trivial exception: when going from **Int2** to **Int2b** by rotation of Asp13, one hydrogen bond between Asp13 and a water molecule is disrupted to allow the conformational change that enables the following proton transfer – during this process, the system remains in the same local minimum since the disruption of the hydrogen bond is part of the corresponding reaction.

For the sake of completeness, we note that further comparisons were done for the optimized stationary points obtained with models **M3a** and **M4**. All QM atoms in model **M3a** were included in the RMSD evaluation. The results are given in **Table S7** (page S7), and the overlay of **Int1** for **M3a** and **M4** is shown in **Figure S1** (page S8).

**Table S19.** Comparison of the optimized QM/MM geometries of model **M4**: RMSD values (in Å) of the QM region (408 atoms) and the active part of the MM region (1928 atoms) relative to **Int1**

	RMSD		
	MM region	QM region <sup>a</sup>	QM region <sup>b</sup>
<b>Int1</b>	0	0	0
<b>TS1</b>	0.031	0.148	0.137
<b>Int2</b>	0.033	0.184	0.165
<b>Int2b</b>	0.042	0.274	0.250
<b>TS2</b>	0.040	0.271	0.247
<b>Int3</b>	0.041	0.210	0.133

<sup>a</sup>: 408 atoms with attacking water molecule;

<sup>b</sup>: 405 atoms without attacking water molecule.