

Supporting Information

Enzyme Mimic Ammonium Polymer as a Single Catalyst for Glucose Dehydration to 5-hydroxymethylfurfural **

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Experimental Section

General Information

All solvents and chemicals used were obtained from commercial suppliers, unless otherwise indicated. NMR spectra were recorded on Bruker AV-400 (400 MHz) instrument. Progress of the reaction (conversion) was typically monitored by SU-300 Sugar Analyzer (TOA-DKK Corp.). Poly-benzyl chloride (P-BnCl) was purchased from Aldrich (Product No.: 63868). HMF yield was analyzed by both NMR and HPLC (Agilent Technologies, 1200 series). HPLC working conditions: column (Agilent Hi-Plex H, 7.7 × 300 mm, 8 μm), solvent 10mM H₂SO₄, flow rate 0.7 ml/min, 25 °C, UV detector: 280 nm. HMF retention time: 36.5 min.

Catalyst synthesis

PolyBnCl resin (1 g, 5.5 mmol Cl/g) and aq. NH₃ (5.78 mmol) respectively in DMF (15 mL) were stirred at 80 °C for 24 h. The resins were washed with DMF (15 mL X 5), DMF/H₂O (1:1 v/v, 15 mL X 5), MeOH (10 mL X 5), filtered and dried under vacuum at 50 °C for 24 h.

After synthesis, the catalysts were stirred in dilute HCl (5M, 28 mL) solution for 1 h, washed with MeOH, filtered and dried under vacuum at 50 °C for 6 h. The ammonium loading was analyzed by elemental analysis. The catalyst has the same morphology as purchased P-BnCl resin. No BET parameters could be measured for both catalyst and original P-BnCl resin. Elemental analysis (%): C, 73.45; H, 6.28; N, 1.00, Cl, 12.26. R-NH₃Cl loading of the catalyst is 0.7 mmol/g.

Glucose dehydration in DMSO

To a 4 mL sealed tube equipped with stirrer bar, glucose (0.18 g, 1 mmol), DMSO (2 mL), H₂O (0.24 mL) and PBnNH₃Cl (0.14 g, 10 mol%) were added. The reaction mixture was stirred at 120 °C for 10 h and then cooled to room temperature. Mesitylene (0.06 g, 0.5 mmol) was added as an internal standard and the composition was analyzed by NMR. The HMF yield was further confirmed by HPLC.

Glucose dehydration to HMF in biphasic solvent system

The two-phase system consists of a reactive NaCl-saturated aqueous layer (mixture of DMSO–water) and an extracting organic layer (MIBK). To a 20 mL sealed tube equipped with stirrer bar, glucose (0.18 g, 1 mmol), P-BnNH₃Cl (0.14 g, 10 mol%), DMSO and NaCl-saturated water (2 mL, 7:3 v/v), MIBK (8mL) were added. The reaction mixture was stirred at 140 °C for 10 h and then cooled to room temperature. Aliquots of the aqueous and organic phases were taken and analysed using HPLC, and confirmed by NMR with mesitylene as an internal standard. Glucose conversion was measured by Sugar Analyzer.

Elemental analysis for used catalyst: C, 72.41; H, 7.00; N, 0.95; Cl, 1.62. In addition, 0.43 mmol of Cl⁻ was detected in reaction mixture (after reaction) by titration.

Recycling experiment

After performing the dehydration reaction as described above, the washed catalyst was simply dried under vacuum at 50 °C for 2 h and used directly or regenerated with HCl for next batch of reaction. For catalyst regeneration, the catalyst was stirred in HCl (2M) solution for 1 h, washed with MeOH, filtered and dried under vacuum at 50 °C for 6 h.

Hot filtration experiment

After performing the dehydration reaction as described above for 1 hour, the solid catalyst was filtered out. A small portion of reaction solution was taken for HPLC analysis and 9% HMF yield was observed. The remaining solution was kept for further reaction at the same condition for another 2 hours. Then, the reaction mixture was analyzed again by using HPLC and the result showed 10% of HMF yield.

Computational method

All computations were conducted using M062x density functional^[24] implemented in Gaussian09 programs. Pre-optimization were performed at 6-31G(d) basis set for all atoms. The energies were further improved by using 6-311++G(d,p) in water solvent (IEFPCM model). Free energies were computed at 298.15 K and 1 atm. All reactants and intermediates had no imaginary vibrational frequency while only one imaginary frequency was detected for transition states. Additionally, intrinsic reaction coordinate (IRC) calculations were executed to guarantee the accuracy of transition states.

Table S1. Solvent screening for glucose dehydration with P-BnNH₃Cl as catalyst.

Solvent	Glucose conversion (%)	Furfural Selectivity (%)	Furfural yield (%) HMF : DFF	Formic acid (%)
DMSO	100	39	35 : 4	12
DMF	87	18	16 : 0	17
GVL	98	7	7 : 0	3
DMA	53	30	16 : 0	3
MeCN	99	9	9 : 0	2
2-propanol	96	6	6 (3:3) : 0 ^a	trace
3-pentanol	95	20	19 (13:6) : 0 ^a	3
TEAC	96	15	14 : 0	5
[BMIM]Cl	85	12	10 : 0	trace

Typical reaction conditions: Glucose (0.18 g), P-BnNH₃Cl (0.14 g), solvent (2 mL), 120 °C, 10 h.

^a Numbers in parentheses represent yield of HMF : HMF ether

Table S2. Time analysis for glucose dehydration process in DMSO.

Time (h)	Glucose conversion (%) ^a	Fructose (%) ^a
1.0	48	-
2.0	66	-
2.5	73	4
3.0	78	3
4.0	81	3
5.0	83	2
6.0	85	-
7.0	86	-

Typical reaction conditions: Glucose (0.18 g), P-BnNH₃Cl (0.07 g), DMSO (2 mL), 120 °C.

^a Determined from sugar analyzer

Table S3. Control experiments for glucose dehydration to HMF in DMSO.

Catalyst	Solvent	Conversion (%) ^a	HMF yield (%) ^b	DFF yield (%) ^b
BnNH ₃ Cl	DMSO/H ₂ O (12 vol%)	59	17	0
BnNH ₃ Cl	DMSO	83	18	2
NH ₄ Cl	DMSO	80	15	2
-----	DMSO	<10	0	0

Typical reaction conditions: Glucose (0.18 g), catalyst (10 mol%), solvent (2 mL), 120 °C, 10 h.

^a Determined from sugar analyzer; ^b NMR yield.

Table S4. Catalyst recycling in biphasic system.^a

Run	HMF yield %	Glucose Conversion %	Selectivity %
1	51.2	89.0	57.5
2	11.6	20.0	58.0
3 ^b	45.9	69.6	65.9
4 ^b	42.0	60.0	70.0

^a Conditions: Glucose (180 mg), P-BnNH₃Cl (140 mg, 10 mol%), water (0.6 mL), DMSO (1.4 mL), MIBK (8 mL), 140 °C, 10 h. ^b Recycled catalyst was acidified by HCl.

Table S5. pH value of the reaction solution.^a

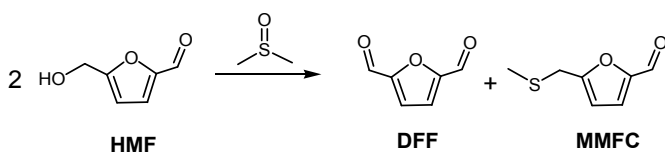
Before reaction	1h	2h	3h	4h	5h	6h
2.14	1.81 (46°C)	1.57 (60 °C)	1.74 (60° C)	1.33 (60° C)	1.41 (40°C)	1.82 (36°C)

^a pH value measured at different reaction time (temperature at measurement was also indicated).

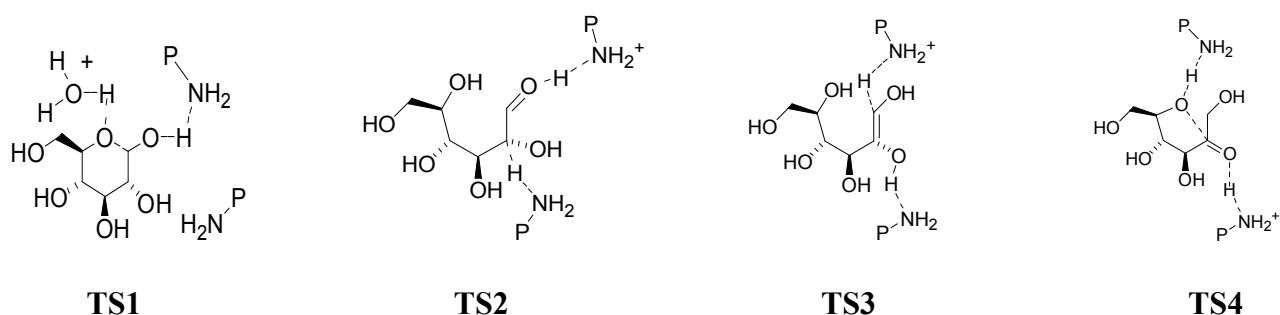
Table S6. Glucose dehydration to HMF in biphasic system with other solid catalysts.

Entry	Catalyst ^a	Temp (°C)	Time (h)	Yield (%)
1	PMF	140	16	13
2	PMF	160	9	26
3	PEI	140	10	0
4	PEI	160	6	0

^a Catalyst (10 mol%) was acidified before reaction.



Scheme S1. HMF oxidized with DMSO to form DFF and 5-((methylthio)methyl)furan-2-carbaldehyde (observed in the reaction mixture). A control reaction has also been carried by heating HMF in pure DMSO. 10% of HMF was converted to DFF in 10 hours at 120 °C.



Scheme S2. Structures of calculated transition states **TS1-4**.

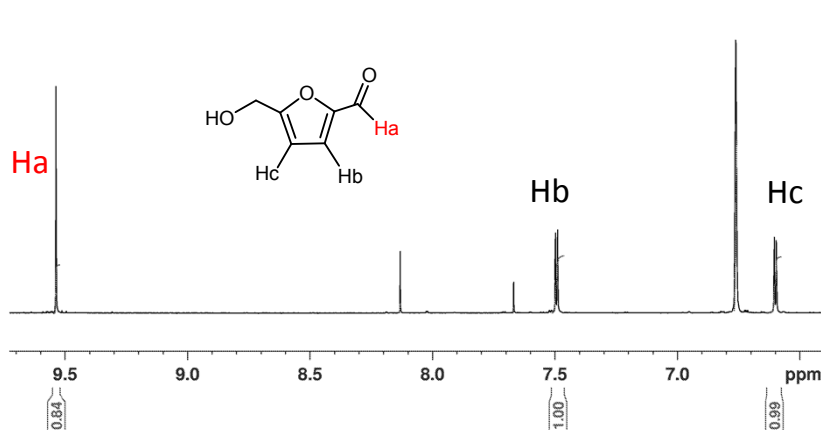
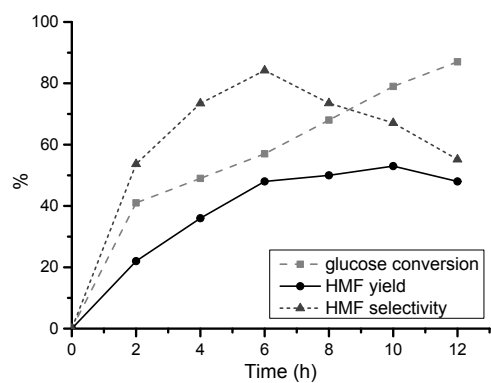
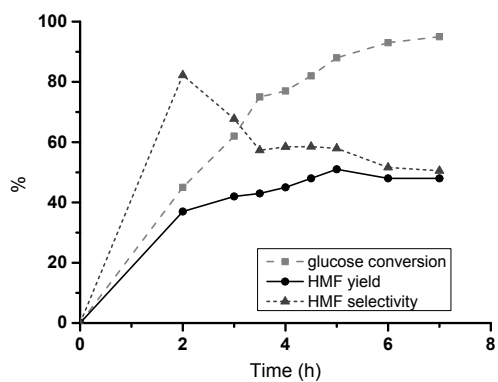


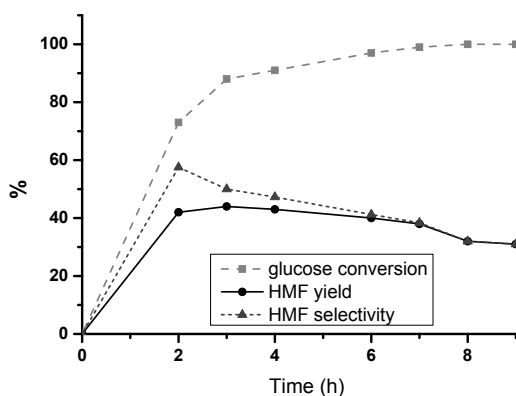
Figure S1. Glucose dehydration in DMSO/D₂O (12 vol%) with P-BnNH₃Cl catalyst. Substantial quantity of deuterium was found at C-1 of HMF.



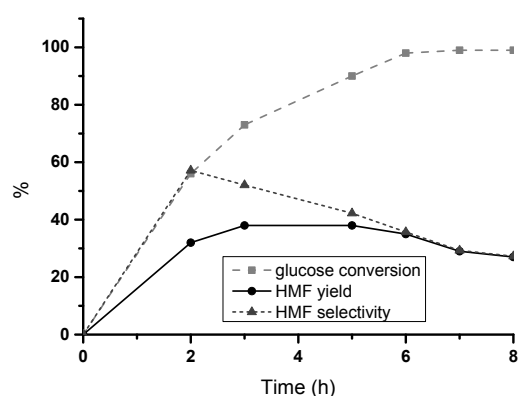
water 0.6 ml, DMSO 1.4 ml, MIBK 8 ml, 140 °C



water 0.6 ml, DMSO 1.4 ml, MIBK 8 ml, 160 °C



water 0.8 ml, DMSO 1.2 ml, MIBK 8 ml, 160 °C



water 1.0 ml, DMSO 1.0 ml, MIBK 8 ml, 160 °C

Figure S2. Glucose dehydration in biphasic system. Screening conditions: Glucose (1 mmol), catalyst (10 mol%).

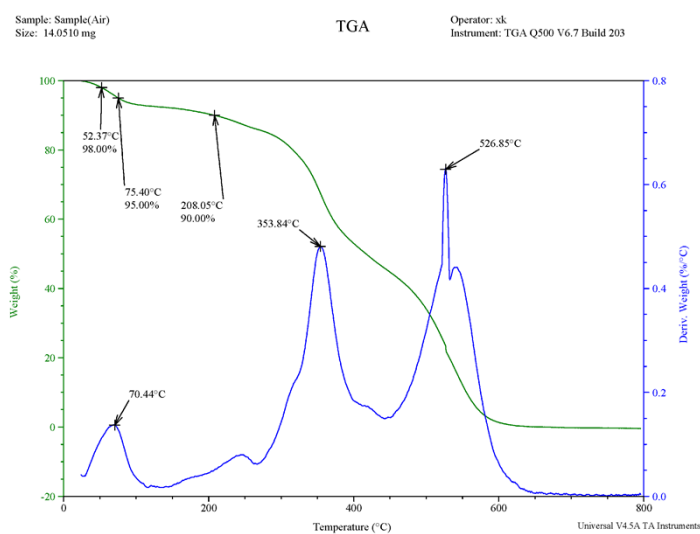


Figure S3. Thermogravimetric analysis (TGA) of synthesized catalyst. The catalyst is stable up to 200 °C in air. The small weight lost at 52 °C is due to the solvent evaporation.

DMSO-d₆ (500μL) + D₂O (150μL)

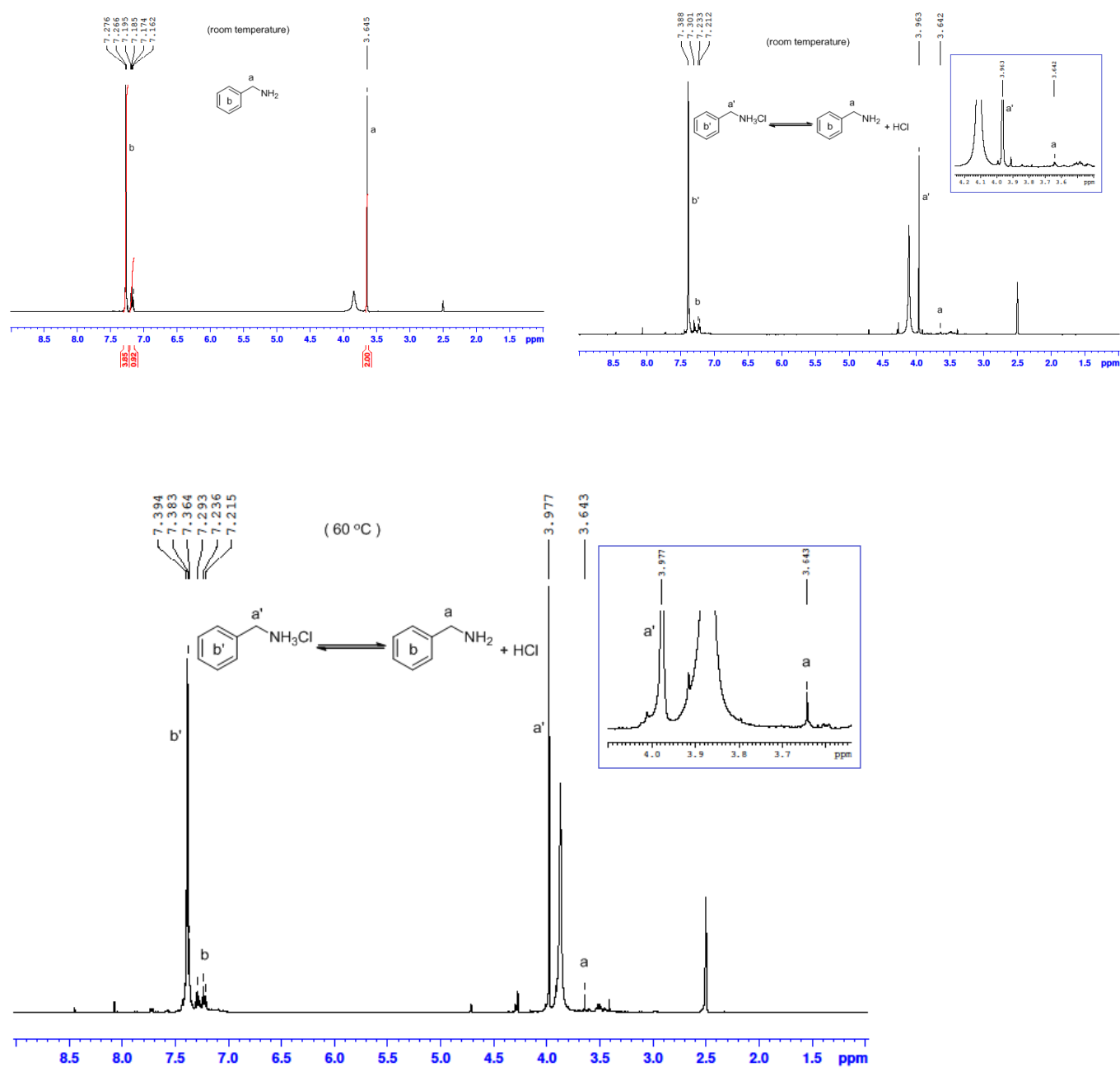


Figure S4. ¹H NMR of benzyl amine, benzyl ammonium (25 °C) and benzyl ammonium (60 °C) in DMSO/H₂O. Benzyl ammonium clearly shows the equilibrium to benzyl amine at 60 °C (60 °C is our equipment's limitation). At reaction condition of 140 °C, this equilibrium will be more apparent. This is also corresponded to the pH value changes during the reaction.

Table S7. Raw energy data for the isomerization of glucose into fructose.

	E (Eh)	ZPE (Eh)	E+ZPE (Eh)	ΔE (Kcal mol ⁻¹)	$\Delta(E+ZPE)$ (Kcal mol ⁻¹)	G (Eh)	ΔG (Kcal mol ⁻¹)
glucose	-687.1406	0.2009	-686.9397			-686.9768	
fructose	-687.1340	0.1989	-686.9350			-686.9728	
P-NH3+	-327.3020	0.1627	-327.1394			-327.1712	
P-NH2	-326.8498	0.1470	-326.7028			-326.7347	
H3O+	-76.8170	0.0352	-76.7818			-76.8009	
H2O	-76.4198	0.0216	-76.3982			-76.4158	
Reference	-1417.6571	0.5300	-1417.1270	0.0000	0.0000	-1417.2470	0.0000
1	-1417.7334	0.5350	-1417.1984	-47.8633	-44.7778	-1417.2677	-13.0058
TS1	-1417.7299	0.5331	-1417.1968	-45.7070	-43.7750	-1417.2648	-11.1866
2	-1417.7456	0.5368	-1417.2088	-55.5364	-51.3240	-1417.2797	-20.5051
3	-1341.3059	0.5122	-1340.7937	-43.0371	-40.7140	-1417.2700	-14.4214
TS2	-1341.2779	0.5072	-1340.7707	-25.5013	-26.2870	-1417.2448	1.3893
4	-1341.3041	0.5117	-1340.7924	-41.9226	-39.8656	-1417.2728	-16.1722
5	-1341.3087	0.5121	-1340.7966	-44.8130	-42.5363	-1417.2756	-17.9342
TS3	-1341.2726	0.5049	-1340.7677	-22.1463	-24.3932	-1417.2496	-1.6077
6	-1341.3155	0.5114	-1340.8041	-49.1012	-47.2295	-1417.2848	-23.7180
7	-1341.3183	0.5106	-1340.8076	-50.8073	-49.4521	-1417.2876	-25.4926
TS4	-1341.2978	0.5072	-1340.7906	-37.9523	-38.7606	-1417.2679	-13.0986
8	-1341.3231	0.5116	-1340.8115	-53.8437	-51.8473	-1417.2926	-28.6113
9	-1417.7055	0.5302	-1417.1754	-30.4059	-30.3212	-1417.2944	-29.7546

XYZ coordinates of optimized geometries

Glucose

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C      0.81552300 -1.50443500 -0.17930000
C      1.49211300 -0.21688900 -0.64461100
C      0.94282400  0.96202200  0.14576300
C     -0.56694000  1.00653300  0.03250200
C     -1.15286900 -0.31912000  0.50288800
C     -2.64935600 -0.40804400  0.27166600
O     -0.58522900 -1.39431700 -0.25200700
O      1.26361600 -1.72026400  1.13292500
O      2.89711800 -0.29709900 -0.51805000
O      1.44469200  2.19004600 -0.34782200
O     -2.96171200 -0.31506100 -1.10599800
H      1.07732200 -2.34248500 -0.82765500
H      1.27630500 -0.06432900 -1.70487100
H      1.21030000  0.83881700  1.20469000
H     -0.83887200  1.15872500 -1.02060100
H     -0.93488300 -0.44858300  1.56905800
H     -3.01751400 -1.34883100  0.69567400
H     -3.14030900  0.42430800  0.77613200
H      1.05753400 -2.62331100  1.39391300
H      3.07095300 -0.64606000  0.36535800
H      2.40619900  2.12977900 -0.33163600
H     -2.42638900 -0.98208500 -1.54979500
O     -1.10914000  2.03020100  0.84364900
H     -0.62317800  2.83559600  0.63470200

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Fructose

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C      2.50415100 -0.99431600 -0.19113700
C      1.42177900 -0.12482900 -0.80249500
C      0.97235000  1.05716100  0.07717600
C     -0.52958200  1.04774300 -0.13381900
C     -0.80694700 -0.45259800 -0.22678300
C     -2.15069600 -0.80528800 -0.84009800
O     -0.69932300 -1.04748000  1.05354300

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O	2.16989900	-1.42774700	1.11188100
O	0.24100600	-0.94032400	-1.00555400
O	1.50667200	2.30275400	-0.31586700
O	-3.18436800	-0.43765900	0.05855200
H	2.68347500	-1.84482700	-0.85946900
H	3.42999800	-0.41761800	-0.11753500
H	1.18158600	0.84518500	1.12953000
H	-0.74554200	1.51176400	-1.10554900
H	1.74456400	0.25316700	-1.77598300
H	-2.25364700	-0.31575900	-1.81352800
H	-2.20650000	-1.88645800	-0.97278500
H	1.23462400	-1.67518000	1.11298000
H	2.38515800	2.39582100	0.06326100
H	-3.10949000	0.51083600	0.22324100
O	-1.30763900	1.62083400	0.89140200
H	-1.09811900	2.55920800	0.94146100
H	-1.52240900	-0.86641400	1.52565300

P-NH₃⁺

C	-0.38665100	-0.00026900	-0.33899100
C	0.29879600	-1.20649300	-0.19359700
C	1.65855800	-1.20560800	0.09621900
C	2.33800700	0.00028200	0.24164600
C	1.65813900	1.20590700	0.09589100
C	0.29839200	1.20624000	-0.19394900
H	-0.22950600	-2.14628600	-0.31553500
H	2.18692400	-2.14491200	0.20330600
H	3.39836400	0.00049200	0.46342400
H	2.18618600	2.14541800	0.20273500
H	-0.23021200	2.14582900	-0.31617900
C	-1.86139400	-0.00053100	-0.62630800
H	-2.17357400	-0.88907000	-1.17096200
H	-2.17362500	0.88727800	-1.17214600
N	-2.64214700	0.00034200	0.66628700
H	-2.42078200	0.82553200	1.22929100
H	-3.65091400	0.00033400	0.49626500
H	-2.42092100	-0.82417400	1.23032200

P-NH₂

C	-1.87712800	1.00253500	-0.09625200
C	-0.51856300	1.29086300	-0.02671300
C	0.42506100	0.26784700	0.09033200
C	-0.01955300	-1.05335500	0.12489400
C	-1.37928900	-1.34533300	0.05000900
C	-2.31283400	-0.31972500	-0.05812200
H	-2.59570300	1.80884300	-0.18778500
H	-0.18279000	2.32260000	-0.06643800
H	0.71089500	-1.84870600	0.20679500
H	-1.70966100	-2.37753800	0.07632700
H	-3.37069300	-0.54681800	-0.11742900
C	1.89569000	0.61047500	0.20624000
H	2.11543700	0.84077500	1.25399900
H	2.08143100	1.53245500	-0.36046200
N	2.75395600	-0.50565200	-0.19054000
H	2.67005000	-0.65292000	-1.19229500
H	3.72303900	-0.25897800	-0.02125800

H₃O⁺

O	-0.00001300	-0.00009000	-0.08264300
H	0.01210300	0.92814300	0.22022400
H	0.79836000	-0.47415500	0.22044200
H	-0.81036300	-0.45326900	0.22047600

H ₂ O			
O	0.00000000	0.00000000	0.11884800
H	0.00000000	0.75457300	-0.47539000
H	0.00000000	-0.75457300	-0.47539000

I			
C	0.02674900	0.93570600	-0.80687200
C	-1.08075000	1.98764700	-0.89534500
C	-0.45876400	3.37825800	-0.93324200
C	0.40156800	3.60291800	0.29418800
C	1.47123000	2.52113000	0.36242800
C	2.40428300	2.66678800	1.55081000
O	0.81790000	1.23539100	0.40277300
O	0.82695600	0.97443300	-1.90442900
O	-1.87125300	1.82751200	-2.04031900
O	-1.46040700	4.37433200	-0.93284700
O	1.71678100	2.76345600	2.80628300
H	-0.36997700	-0.06369300	-0.59860600
H	-1.69361500	1.91424800	0.01459600
H	0.16738200	3.46064900	-1.83139800
H	-0.24861400	3.53180900	1.17897000
H	2.08220300	2.55293200	-0.54377500
H	3.05399800	1.79411600	1.62209300
H	3.01701800	3.55513900	1.40160000
H	1.37055200	0.12662500	-1.91593600
H	-2.69348300	1.33963300	-1.77103100
H	-2.07429200	4.13869300	-1.63854400
H	1.38266200	3.65852800	2.93595400
O	1.06430700	4.84751200	0.26545600
H	0.40144900	5.51471500	0.05401500
H	0.43589400	0.79230800	1.66696600
H	-0.54530800	0.61739900	3.03592600
H	0.82088000	1.51992700	3.04355300
C	4.18602400	-2.03882800	-0.22800100
C	5.44631300	-1.96791600	-0.82323600
C	6.38159900	-2.97864000	-0.62536800
C	6.06508800	-4.07355900	0.17398800
C	4.81158200	-4.15172900	0.77435700
C	3.87865200	-3.13909600	0.57383300
H	5.69753400	-1.11184300	-1.44185000
H	7.35817900	-2.90882200	-1.08992200
H	6.79394400	-4.85967100	0.33151200
H	4.56167000	-4.99945800	1.40150600
H	2.90313200	-3.20058800	1.04616000
C	3.15356500	-0.96969500	-0.49527800
H	3.64306700	-0.00564300	-0.65512700
H	2.48706900	-0.85838700	0.36246000
N	2.31212500	-1.23880300	-1.67915400
H	1.79511000	-2.10358400	-1.54320800
H	2.90590800	-1.39124200	-2.49084300
O	0.37057800	0.66215800	2.72606000
C	-6.15237200	-2.40428000	1.65770700
C	-5.14475000	-1.55053600	1.22359200
C	-4.49655700	-1.77488600	0.00721800
C	-4.87297500	-2.87321900	-0.76571200
C	-5.88055000	-3.73132300	-0.33359500
C	-6.52298300	-3.49746200	0.87805200
H	-6.64528100	-2.22131500	2.60525400
H	-4.85402500	-0.70202200	1.83575800
H	-4.37240700	-3.05867900	-1.71069000
H	-6.16151700	-4.58332100	-0.94159300
H	-7.30603200	-4.16547300	1.21637100

C	-3.44698700	-0.80473200	-0.48364700
H	-2.79485200	-1.29359600	-1.21085000
H	-2.82279800	-0.47876400	0.35264000
N	-4.00218600	0.40376400	-1.12181900
H	-4.62299300	0.12896600	-1.87906900
H	-4.58071100	0.90805100	-0.45516800

TS1

C	0.13694500	0.54760900	-0.73268600
C	-0.94795200	1.59622100	-0.94695200
C	-0.33484000	2.96232800	-1.24981200
C	0.45739600	3.48420000	-0.06801700
C	1.59034700	2.52940400	0.28346500
C	2.48720300	3.07408200	1.38815600
O	1.00543500	1.26100600	0.64578100
O	1.00698900	0.43206800	-1.66022000
O	-1.73453700	1.21136300	-2.04216500
O	-1.35963200	3.90205200	-1.49726700
O	1.75836500	3.71910700	2.42706900
H	-0.16427100	-0.35449000	-0.19002900
H	-1.55850600	1.67227400	-0.03705500
H	0.32436700	2.86939800	-2.12232800
H	-0.22675800	3.55144800	0.79019300
H	2.20175800	2.32472600	-0.59799200
H	3.04140800	2.25208800	1.84294700
H	3.19780900	3.77064800	0.94053200
H	1.66624300	-0.53704100	-1.52447600
H	-2.61831800	0.90423000	-1.69098300
H	-1.93123400	3.51048900	-2.16864300
H	1.48441000	4.58335300	2.09688600
O	1.04028700	4.74354300	-0.32575200
H	0.34612700	5.30674500	-0.68753500
H	0.47156900	1.36086600	1.50658700
H	-1.02041700	1.95390700	3.00338500
H	0.40414600	2.58322200	3.05916300
C	4.56992800	-2.09237100	-0.05851300
C	5.68310500	-2.15968200	-0.89743300
C	6.65009300	-3.14109000	-0.70858800
C	6.51249300	-4.06319300	0.32514200
C	5.40789300	-3.99913400	1.16926400
C	4.44058300	-3.01724800	0.97764000
H	5.79476200	-1.43647600	-1.69910100
H	7.51221600	-3.18259400	-1.36340600
H	7.26660700	-4.82662200	0.47501100
H	5.30018100	-4.71193500	1.97799800
H	3.58092600	-2.96708200	1.63807500
C	3.49769500	-1.06345200	-0.31021900
H	3.92829000	-0.14520100	-0.71336900
H	2.96697200	-0.80918700	0.60813800
N	2.47927600	-1.52822200	-1.28891600
H	1.99662400	-2.35166600	-0.93415100
H	2.92956900	-1.80984400	-2.15830600
O	-0.08519500	1.75836800	2.88880800
C	-6.80744500	-2.14304300	1.61375700
C	-5.65550600	-1.43728500	1.28323000
C	-4.93887000	-1.74925400	0.12611900
C	-5.39458800	-2.78313400	-0.69182900
C	-6.54682400	-3.49177800	-0.36435800
C	-7.25580600	-3.17202800	0.78938400
H	-7.35309500	-1.89411300	2.51631800
H	-5.30562300	-0.63933900	1.93096500
H	-4.84061700	-3.03671300	-1.59012000

H	-6.88795200	-4.29475400	-1.00701900
H	-8.15136900	-3.72436200	1.04796400
C	-3.72287700	-0.94380100	-0.26750800
H	-3.07288100	-1.54188700	-0.91021100
H	-3.14633000	-0.67033600	0.61914300
N	-4.04250400	0.30189500	-0.99225300
H	-4.67495900	0.09193500	-1.76099800
H	-4.54658900	0.93844000	-0.38088500

2

C	-0.13829300	0.33458500	-1.42705700
C	-0.98683000	1.53441300	-1.04672300
C	-0.20776100	2.84931800	-1.05493200
C	0.66226600	3.05583600	0.17441000
C	1.75538700	2.00021000	0.33905300
C	2.83919600	2.47762800	1.30777500
O	1.16273400	0.76736400	0.72228200
O	0.80304100	0.41000600	-2.18752300
O	-1.99464600	1.60617000	-2.03627900
O	-1.12504500	3.92890900	-1.05090200
O	2.31235700	3.15198800	2.44961100
H	-0.48772400	-0.64378800	-1.05937400
H	-1.42837300	1.36768000	-0.05648200
H	0.42092900	2.88807000	-1.95352500
H	0.01039100	3.01248100	1.05897600
H	2.23338400	1.81896300	-0.62899600
H	3.39196300	1.61055300	1.67317000
H	3.53021900	3.13762800	0.77917900
H	1.86041500	-1.03211200	-2.33333800
H	-2.85647400	1.32043200	-1.61155000
H	-1.80659900	3.70059300	-1.69560000
H	1.98895800	4.00452600	2.12980300
O	1.29168600	4.32739500	0.10602700
H	0.60860700	4.96108800	-0.14367200
H	0.77323400	0.87442300	1.61405100
H	-0.50679300	1.78374400	3.43469200
H	0.98393400	2.14158100	3.24249300
C	4.42829600	-1.93693200	-0.34949900
C	5.67357700	-2.11998200	-0.95190000
C	6.58751900	-3.01658900	-0.40998600
C	6.26257400	-3.73199500	0.73913400
C	5.02448900	-3.54845400	1.34744900
C	4.10938300	-2.65257300	0.80470200
H	5.93100600	-1.55446300	-1.84156000
H	7.55387700	-3.15258400	-0.88017000
H	6.97637800	-4.42833400	1.16272900
H	4.77250700	-4.09911000	2.24549000
H	3.14593600	-2.50325900	1.28118500
C	3.42363300	-0.99478800	-0.95203100
H	3.90298600	-0.15305200	-1.45132900
H	2.71699400	-0.61785700	-0.21118600
N	2.59695100	-1.68813100	-2.00253800
H	2.14082200	-2.51953700	-1.62105900
H	3.16651500	-1.98678600	-2.79629500
O	0.35538500	1.39826100	3.25573400
C	-6.45252400	-2.12598100	1.93528200
C	-5.33801600	-1.48368500	1.40659200
C	-5.10260200	-1.48623400	0.03063900
C	-6.00162300	-2.14603700	-0.80759300
C	-7.11774000	-2.79011500	-0.28218300
C	-7.34541100	-2.78029500	1.09068700
H	-6.62237600	-2.12047300	3.00544500

H	-4.63970000	-0.97907500	2.06722200
H	-5.82330800	-2.15795500	-1.87819200
H	-7.80671300	-3.30225400	-0.94345600
H	-8.21282900	-3.28269900	1.50183400
C	-3.92352600	-0.73775800	-0.54439300
H	-3.61636600	-1.18769000	-1.49109300
H	-3.07358000	-0.79746000	0.13962200
N	-4.18998200	0.69242500	-0.79663400
H	-5.01106500	0.78479500	-1.38999700
H	-4.42199300	1.15769400	0.07703500

3

C	1.18815200	-2.36431300	1.38855800
C	1.79209700	-1.64241200	0.19774400
C	2.95727200	-0.73090200	0.62597900
C	3.24516200	0.31202600	-0.46429900
C	2.27167000	1.49344600	-0.37860900
C	2.71102100	2.54448900	0.64286000
O	2.10296500	2.11253800	-1.64154800
O	0.66774900	-1.78519800	2.31207800
O	2.20980400	-2.55601000	-0.78468100
O	4.12262100	-1.53808100	0.75590800
O	3.77159500	3.32775300	0.11756500
H	1.24566900	-3.46691800	1.36690500
H	0.62162600	0.51262800	-2.50176700
H	2.71959200	-0.23669600	1.57324400
H	3.11633800	-0.16678300	-1.44329900
H	1.29000300	1.10386600	-0.10135900
H	1.88277700	3.22935300	0.83095500
H	2.99250700	2.07297900	1.59051300
H	-0.11261600	-0.11524100	2.72983800
H	3.10012500	-2.84239600	-0.53741100
H	4.29282500	-1.73286800	1.68242100
H	4.51373100	2.71817300	0.00951200
O	4.57234600	0.79534600	-0.33353900
H	5.12109100	0.03793200	-0.09300200
C	-1.50375900	-1.85839800	-1.53450600
C	-2.79247200	-1.33064100	-1.42669800
C	-3.70429400	-1.86299500	-0.52039300
C	-3.33596600	-2.93008200	0.29651700
C	-2.05744100	-3.47018900	0.18960900
C	-1.15049900	-2.93940600	-0.72550900
H	-3.08730500	-0.49492600	-2.05533700
H	-4.70001000	-1.44104600	-0.44643500
H	-4.04395400	-3.34157300	1.00612500
H	-1.76651700	-4.30735400	0.81395700
H	-0.15806800	-3.37035300	-0.82550800
C	-0.49941200	-1.22531600	-2.47031100
H	-0.90663400	-1.19987900	-3.48855800
H	0.40832300	-1.83273400	-2.48760400
N	-0.14316600	0.11075300	-1.96482500
H	0.99913100	-1.02807200	-0.24549300
H	2.79501900	2.78487200	-1.69905200
H	-0.93166700	0.74053700	-2.08891000
C	-2.37674500	1.32302000	0.70303300
C	-3.72980100	1.29586500	1.03918400
C	-4.57870900	2.30517700	0.59867000
C	-4.07869600	3.34486700	-0.18038600
C	-2.72859000	3.37769600	-0.51687700
C	-1.87894600	2.36822900	-0.07663400
H	-4.11889400	0.47671900	1.63519100
H	-5.63014300	2.27720800	0.85783600

H	-4.74221400	4.12720900	-0.52857800
H	-2.33888200	4.18301400	-1.12727000
H	-0.82831500	2.38379400	-0.35451000
C	-1.44844000	0.24055300	1.17514200
H	-0.64345700	0.09390700	0.45543700
H	-1.96040300	-0.70973400	1.33254900
N	-0.81002800	0.60596300	2.48970200
H	-1.50248000	0.65912100	3.23955000
H	-0.34110800	1.51316600	2.44121300

TS2

C	-1.35101200	-0.64015500	1.53156400
C	-0.61743800	-1.53095900	0.70203400
C	0.78143800	-1.95483000	1.09303800
C	1.67131900	-2.17825700	-0.13525100
C	2.20369000	-0.83603600	-0.67928400
C	3.63995200	-0.56096200	-0.23774100
O	2.14164700	-0.78788500	-2.09877500
O	-0.88200000	0.29815400	2.20511800
O	-1.35573800	-2.60668100	0.15207000
O	0.72608700	-3.22232500	1.76458800
O	4.53380400	-1.40579100	-0.94521500
H	-2.44714800	-0.74198800	1.46885800
H	0.09128400	-0.78102100	-2.29536800
H	1.24182100	-1.21065100	1.75141500
H	1.05981500	-2.64918000	-0.91510400
H	1.56399300	-0.02123600	-0.31668600
H	3.90306400	0.46275500	-0.50257000
H	3.73859800	-0.68496600	0.84567400
H	0.51754100	0.88946700	2.57348900
H	-1.17777800	-3.37696600	0.70666400
H	0.51374800	-3.07776500	2.69177200
H	4.35149400	-2.29793000	-0.62102100
O	2.75898600	-3.03277900	0.18962900
H	2.42987800	-3.64737400	0.85857900
C	-3.08979600	-0.31953000	-1.30240100
C	-3.16843500	1.00718300	-0.87709100
C	-4.12397700	1.40050900	0.05314800
C	-5.02965500	0.46894500	0.55366000
C	-4.97597600	-0.85054200	0.11375000
C	-4.00668900	-1.24297600	-0.80415500
H	-2.47963100	1.74554800	-1.27335000
H	-4.16412400	2.43224900	0.38196800
H	-5.77577900	0.77180800	1.27850000
H	-5.68043400	-1.57904400	0.49765700
H	-3.94077200	-2.27889600	-1.11524600
C	-2.00917000	-0.75068100	-2.26624300
H	-2.15776000	-0.29483500	-3.24827600
H	-2.02318400	-1.83352900	-2.37627600
N	-0.67155700	-0.38086100	-1.74358500
H	-0.57887100	-0.77017800	-0.51151600
H	2.94851900	-1.21561400	-2.41573600
H	-0.52961200	0.62918700	-1.75676800
C	1.09858100	2.88518900	0.81514500
C	2.35768200	2.79457400	0.21794500
C	2.48094800	2.76918900	-1.16630800
C	1.34633500	2.86435600	-1.96675400
C	0.09086600	2.98008500	-1.37657700
C	-0.03673600	2.97189900	0.01091600
H	3.24965000	2.75777500	0.83715000
H	3.46132400	2.69539200	-1.62129700
H	1.44094000	2.86228000	-3.04571000

H	-0.78722000	3.09718200	-2.00238300
H	-1.01605200	3.05599300	0.47067600
C	0.98212100	2.91811900	2.31605200
H	-0.02814100	3.17301300	2.63074700
H	1.68341800	3.62832300	2.75210800
N	1.28090200	1.56890000	2.89333100
H	1.28038200	1.59599300	3.91411200
H	2.19903800	1.23565100	2.59768700

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C	0.56341900	-2.01691500	-1.17809100
C	0.90462100	-1.68781300	0.06909700
C	-0.05696700	-1.41533500	1.18842300
C	-0.35441900	0.06581500	1.42439100
C	-0.61695800	0.87111600	0.13588900
C	-1.64809500	1.96873700	0.35767500
O	0.60603800	1.47422800	-0.28560600
O	-0.68917600	-2.11086000	-1.68376300
O	2.24294900	-1.54170400	0.39937500
O	0.48326300	-1.88454100	2.42402000
O	-1.20136400	2.83790700	1.38530200
H	1.33222500	-2.23029700	-1.91403400
H	2.04278100	0.82664000	-1.16426100
H	-1.00549500	-1.91464700	0.98232000
H	0.52211300	0.51013700	1.91271200
H	-0.93030500	0.22625100	-0.68628700
H	-1.72653900	2.56178500	-0.55535200
H	-2.62941600	1.54523600	0.58987400
H	-1.40932600	-1.85162300	-1.05382900
H	2.32802100	-1.76096800	1.33825900
H	0.30420200	-2.82707800	2.50598700
H	-1.32747400	2.35908100	2.21395900
O	-1.48534900	0.17544700	2.28091300
H	-1.29880800	-0.35216100	3.06691500
C	5.26720000	0.76242900	-0.21738000
C	6.24297500	1.46957800	-0.91833000
C	7.55133800	0.99863800	-0.96191200
C	7.88843000	-0.18161800	-0.30690200
C	6.91739700	-0.89138100	0.39443200
C	5.61084700	-0.41986800	0.43966700
H	5.97913100	2.39055200	-1.42709500
H	8.30668700	1.55396000	-1.50445200
H	8.90781400	-0.54679000	-0.33960700
H	7.17846700	-1.80728700	0.91020700
H	4.85321200	-0.96886000	0.98897500
C	3.84189900	1.24199300	-0.19820300
H	3.76535200	2.30710100	-0.41013700
H	3.35334100	1.02748400	0.75176700
N	3.03251400	0.52465400	-1.23803500
H	3.05065000	-0.48019200	-1.03045800
H	0.73450800	2.25288500	0.27514100
H	3.38665100	0.69108800	-2.18043400
C	-5.08319900	-0.10234500	-0.90298200
C	-6.08813300	-1.04785100	-0.68154400
C	-7.34996500	-0.65412600	-0.25408300
C	-7.62561200	0.69588800	-0.04406100
C	-6.63522600	1.64495900	-0.26925500
C	-5.37069400	1.24599100	-0.69766700
H	-5.88202800	-2.10031300	-0.85233100
H	-8.12082700	-1.39794400	-0.09009700
H	-8.60929900	1.00461800	0.28876400
H	-6.84441800	2.69667700	-0.11336200

H	-4.60396300	1.99207700	-0.88049700
C	-3.70368600	-0.55155200	-1.32971600
H	-3.10323800	0.31847800	-1.60900000
H	-3.77062500	-1.18978100	-2.21392200
N	-2.96823400	-1.30849000	-0.29848000
H	-3.48041500	-2.15820700	-0.07248300
H	-2.93488200	-0.77292100	0.56974100

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C	0.75978100	-0.32628100	2.00295900
C	0.70058500	-0.07613600	0.69499800
C	0.99165900	1.27346000	0.09782500
C	-0.11034700	1.75284100	-0.84949000
C	-1.41852900	2.04251800	-0.10674900
C	-1.46546500	3.44994200	0.49130300
O	-2.53789800	1.86788300	-0.96278900
O	1.15794600	0.64476300	2.89057100
O	0.51085200	-1.08609800	-0.20842600
O	2.22789300	1.21292200	-0.63781900
O	-1.71180500	4.40511100	-0.52825500
H	0.56520000	-1.31701500	2.39944600
H	3.09450500	0.97546900	2.45180800
H	1.14982100	2.01855000	0.88066500
H	-0.30296500	0.96153100	-1.58398600
H	-1.52074900	1.30877500	0.69823400
H	-2.30319900	3.51323700	1.18609800
H	-0.54242200	3.67095900	1.03682000
H	0.86086400	0.42169200	3.77820900
H	-0.45638400	-1.07988800	-0.53129200
H	2.19585400	0.41702800	-1.19000300
H	-0.93035300	4.38990200	-1.09612100
O	0.31992500	2.93036800	-1.51727700
H	1.22709100	2.78209500	-1.80950800
C	4.67850400	-1.14812400	0.43072400
C	6.01699400	-0.98130200	0.07910200
C	6.45629900	-1.34817000	-1.18876200
C	5.55950300	-1.88255300	-2.10896200
C	4.22330800	-2.05710700	-1.75899400
C	3.78192700	-1.69261700	-0.49117400
H	6.71727800	-0.56924800	0.79827000
H	7.49809600	-1.21990900	-1.45579500
H	5.90268200	-2.17007100	-3.09538700
H	3.52493000	-2.48145000	-2.47038600
H	2.74029900	-1.83815900	-0.21659200
C	4.17717800	-0.70182400	1.77622100
H	4.92562700	-0.80874500	2.55845000
H	3.28111100	-1.24967600	2.06084600
N	3.78990900	0.75564500	1.72463700
H	3.36426000	0.97966800	0.80419500
H	-2.67705200	2.71799700	-1.40221000
H	4.60103000	1.36284200	1.84995000
C	-4.27701500	-1.53039500	0.20173700
C	-5.02535500	-0.39551100	-0.12498000
C	-6.39948700	-0.48796600	-0.30982400
C	-7.04381200	-1.71588800	-0.16734900
C	-6.30622700	-2.84847500	0.15888700
C	-4.92812700	-2.75412400	0.34148300
H	-4.51984000	0.55982800	-0.23854500
H	-6.97126800	0.39767800	-0.56172300
H	-8.11561500	-1.78685300	-0.30990000
H	-6.80085700	-3.80608700	0.27210200
H	-4.35432500	-3.63940100	0.59582100

C	-2.77945200	-1.41830700	0.37278200
H	-2.37310600	-2.35644400	0.75616600
H	-2.54774900	-0.64349100	1.10901800
N	-2.05599300	-1.07935000	-0.86822300
H	-2.39883700	-0.18870800	-1.23038800
H	-2.25818500	-1.77964200	-1.57761300

TS3

C	1.26441500	-2.24442400	-0.65980900
C	0.41039600	-1.18380500	-0.29749700
C	-0.66572500	-1.44709500	0.75666600
C	-2.01582900	-1.70404600	0.07383100
C	-2.08532200	-3.00921600	-0.71975000
C	-2.15251100	-4.24939900	0.17581200
O	-3.21794400	-2.98719300	-1.57097700
O	0.87111700	-3.54045000	-0.26894400
O	0.56908400	-0.01766700	-0.73404500
O	-0.88176300	-0.30301300	1.57828800
O	-3.45174700	-4.38514800	0.73779000
H	1.70042500	-2.17825500	-1.65918900
H	2.37044700	-1.67061200	0.07929800
H	-0.38955100	-2.30532200	1.37131100
H	-2.19827700	-0.88780100	-0.63882100
H	-1.20087700	-3.07511800	-1.35605600
H	-1.98481400	-5.13594900	-0.43715100
H	-1.37783400	-4.21473600	0.94625400
H	1.61663800	-3.97290700	0.15566400
H	-0.18922400	1.27351700	-0.22971600
H	-0.23570200	-0.29557300	2.29132300
H	-3.58836700	-3.59704800	1.27949800
O	-3.04460800	-1.70984800	1.05481600
H	-2.81640200	-1.02847500	1.70020600
C	5.16860500	0.54659200	-0.28161000
C	6.45269300	0.00118600	-0.28765800
C	7.54591000	0.76923800	0.09887100
C	7.36320700	2.09119900	0.49431200
C	6.08535500	2.64279900	0.50085500
C	4.99325400	1.87303700	0.11359900
H	6.59679100	-1.02710900	-0.60341500
H	8.53991400	0.33854300	0.08583600
H	8.21512400	2.69128100	0.79111200
H	5.93953600	3.67323100	0.80198300
H	3.99769900	2.30515400	0.11117100
C	3.98026800	-0.29858700	-0.66038600
H	4.26005500	-1.05930300	-1.39050200
H	3.17765400	0.30406900	-1.08699400
N	3.39436000	-1.01300200	0.50288800
H	3.09771700	-0.35332600	1.22073400
H	-3.95081700	-3.31479200	-1.03429800
H	4.07394300	-1.63987000	0.93030200
C	-3.19240900	2.76919700	-0.54826900
C	-4.11966900	1.96459100	0.11721700
C	-5.28757100	2.51901400	0.62784500
C	-5.53868400	3.87965200	0.47126900
C	-4.62029800	4.68418800	-0.19538600
C	-3.44937700	4.13005700	-0.70320900
H	-3.93303700	0.90034600	0.23381900
H	-6.00403800	1.88905200	1.14067800
H	-6.45142600	4.31003100	0.86549000
H	-4.81545200	5.74198700	-0.32310900
H	-2.73386900	4.75550900	-1.22601700
C	-1.91374900	2.16646500	-1.06256000

H	-1.46723600	2.76751400	-1.85237800
H	-2.07709600	1.16087500	-1.44883300
N	-0.89494500	2.03670000	0.02688800
H	-1.32359400	1.69679400	0.89098900
H	-0.43510100	2.92511200	0.22210900

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C	0.70891000	2.37922700	1.48107900
C	-0.64940200	2.00104700	0.92043100
C	-1.33226000	0.72707100	1.42127900
C	-0.99604500	-0.45539100	0.49780600
C	0.47452100	-0.86232700	0.47988100
C	0.91296900	-1.58313300	1.75854400
O	0.72906700	-1.69601200	-0.63454600
O	1.19935100	1.43972300	2.39733600
O	-1.19762400	2.69085400	0.09323300
O	-2.74689400	0.87400700	1.32160300
O	0.45051000	-2.92616100	1.74626200
H	1.38484700	2.52475700	0.62877500
H	0.57630500	3.36069300	1.95245400
H	-1.03772200	0.50944300	2.44856900
H	-1.25688200	-0.14855700	-0.52462900
H	1.07755400	0.03670500	0.34243200
H	2.00361400	-1.63185300	1.78251000
H	0.57508800	-1.04467300	2.64719500
H	2.04994200	1.09190500	2.03293500
H	-3.30909700	3.23846500	-1.07104200
H	-3.10192500	1.16239800	2.16935500
H	-0.51388100	-2.87861500	1.76681600
O	-1.76846200	-1.57886400	0.87839500
H	-2.68204600	-1.28028900	0.97832900
C	5.05174700	-0.01360200	-0.70166300
C	5.71134000	-1.22919500	-0.51374200
C	7.02548400	-1.39496200	-0.93901200
C	7.69494000	-0.34356600	-1.55942100
C	7.04477900	0.87213600	-1.75221100
C	5.73084100	1.03436500	-1.32486700
H	5.18882500	-2.05185400	-0.03494700
H	7.52487800	-2.34530700	-0.79135100
H	8.71675200	-0.47254800	-1.89572400
H	7.55925000	1.69174200	-2.24019100
H	5.22367400	1.98137900	-1.48115200
C	3.64331600	0.17991900	-0.19135000
H	3.09162400	-0.76136200	-0.25086600
H	3.11757600	0.90516300	-0.81775900
N	3.58173800	0.66518900	1.20451800
H	4.11806900	1.52795200	1.27356000
H	0.55724000	-2.59715400	-0.33017200
H	4.06643200	0.00238200	1.80613300
C	-4.73422200	0.22029000	-1.46984500
C	-4.04668900	-0.98032300	-1.30200100
C	-4.70744500	-2.10663900	-0.82067000
C	-6.06142600	-2.03741200	-0.50803800
C	-6.75646700	-0.84480300	-0.68845500
C	-6.09632600	0.27896400	-1.17141800
H	-2.99507600	-1.04403300	-1.55956500
H	-4.16351900	-3.03488400	-0.69257000
H	-6.57633600	-2.91305100	-0.13190800
H	-7.81355100	-0.79154700	-0.45875700
H	-6.64654000	1.20233800	-1.32414900
C	-4.01269400	1.45457700	-1.94067700
H	-4.55150100	1.97023900	-2.73406400

H	-3.00534600	1.22527800	-2.28435600
N	-3.86625800	2.42494100	-0.80331600
H	-3.37267100	1.97449300	-0.00868300
H	-4.77675700	2.75365700	-0.47775000

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C	-3.45874600	-0.81294000	1.22597000
C	-2.22811900	-1.71355200	1.15637000
C	-0.95122700	-0.92393700	1.44715700
C	0.28614300	-1.70773900	1.02541100
C	0.43082300	-1.71496200	-0.49902900
C	0.70198000	-3.04947700	-1.16370200
O	0.41577500	-0.67891200	-1.11918900
O	-3.40794100	-0.04796300	2.42955600
O	-2.15615200	-2.35256900	-0.09988300
O	-0.78895300	-0.68124700	2.83461400
O	1.83494700	-3.59873400	-0.49922700
H	-3.44575500	-0.15026400	0.35619800
H	-4.36607700	-1.42316300	1.19073800
H	-0.95780700	0.02226900	0.89284700
H	0.24178200	-2.73158900	1.41075600
H	-2.29668700	-2.49883000	1.91697000
H	-0.18315100	-3.67569400	-1.02584400
H	0.89270400	-2.89084600	-2.22724300
H	-3.83943300	0.79615500	2.26659500
H	-1.58458000	-0.20647100	3.11362800
H	1.82828600	-4.55613300	-0.58767300
O	1.44090800	-1.04448500	1.52827500
H	1.20119000	-0.68462700	2.39457100
H	3.45907200	-2.57392400	-0.20872300
H	-1.94985100	-1.45057600	-3.10108000
C	-2.69285400	1.40979400	-1.59663400
C	-4.07122700	1.62980700	-1.55027300
C	-4.64445300	2.31200800	-0.48223600
C	-3.84037600	2.79441100	0.54945600
C	-2.46219000	2.60181900	0.49870100
C	-1.89363700	1.91802000	-0.57354500
H	-4.70270400	1.25467400	-2.34996200
H	-5.71584900	2.47089200	-0.45418500
H	-4.28627800	3.32898300	1.38058700
H	-1.83070900	2.97859700	1.29503500
H	-0.82105700	1.75611900	-0.61018800
C	-2.09935800	0.55000200	-2.68388000
H	-1.01263700	0.62375000	-2.65759800
H	-2.44533600	0.89207300	-3.66541000
N	-2.45664100	-0.86461400	-2.44199200
H	-3.44176500	-1.00153400	-2.65655900
H	-2.26419700	-1.69862000	-0.83627600
C	4.02516100	0.73874700	-0.45297300
C	5.30287200	1.29374700	-0.41090500
C	5.49220600	2.57418000	0.09965000
C	4.40436300	3.30268200	0.57011700
C	3.12614100	2.75162500	0.52916900
C	2.93453500	1.47344100	0.01728100
H	6.14946500	0.72643000	-0.78296900
H	6.48686100	3.00217100	0.12701900
H	4.55109300	4.30048500	0.96607700
H	2.27704600	3.32024600	0.88931000
H	1.94182700	1.03575600	-0.01505000
C	3.81322700	-0.65067200	-0.98938700
H	4.61473700	-0.95742600	-1.65863200
H	2.86119800	-0.72805000	-1.51353400

N	3.76439600	-1.65037300	0.13175500
H	3.05391100	-1.36813100	0.83510600
H	4.67015800	-1.73855000	0.59366100

TS4

C	-3.57112800	-1.20989300	1.02958500
C	-2.23475400	-1.85632900	0.70391900
C	-1.06769700	-1.17067200	1.41025100
C	0.14473900	-1.59432800	0.61157900
C	-0.20119600	-1.32894000	-0.86837500
C	0.19963200	-2.44112800	-1.82606400
O	-0.12124500	-0.14136600	-1.28299100
O	-3.66590100	-1.21888800	2.45060900
O	-1.92141500	-1.79003700	-0.68420900
O	-0.89909700	-1.55812100	2.75417200
O	1.62009300	-2.34339300	-1.89060100
H	-3.58118600	-0.18490900	0.65067300
H	-4.39350000	-1.77153100	0.57354100
H	-1.17508200	-0.08096800	1.32111900
H	0.31728600	-2.66558300	0.77558700
H	-2.25381900	-2.90773400	1.01419600
H	-0.11408700	-3.41604300	-1.44655900
H	-0.25765300	-2.25371300	-2.80262600
H	-4.38250000	-0.63501000	2.71334300
H	-1.73252900	-1.35050000	3.19617100
H	1.96300400	-3.09406600	-2.38278900
O	1.30276900	-0.85269500	0.94881500
H	1.37514100	-0.86516400	1.91072500
H	1.51182200	0.27189100	-1.46666900
H	-2.98228700	-0.82549400	-3.21922600
C	-3.22323100	1.69246300	-1.05228100
C	-4.56678900	1.92771900	-0.75223900
C	-4.93664900	2.39806100	0.50313100
C	-3.96195400	2.65188100	1.46626300
C	-2.61939000	2.44753700	1.16284700
C	-2.25101400	1.96910500	-0.09234100
H	-5.32875100	1.73220700	-1.50112900
H	-5.98227300	2.56877000	0.73000900
H	-4.24982900	3.01293300	2.44636100
H	-1.85796400	2.64693000	1.90826300
H	-1.21262400	1.75704400	-0.32286900
C	-2.84328200	1.05139100	-2.36154900
H	-1.76652600	1.10588400	-2.51122200
H	-3.35428800	1.53649300	-3.19611800
N	-3.20036600	-0.39306000	-2.32277600
H	-4.20618100	-0.49952500	-2.19796800
H	-2.53597800	-1.10594800	-1.36963300
C	4.43278500	1.06906400	0.04097400
C	5.46497400	1.89986100	-0.38772700
C	6.77572300	1.65094000	0.01022400
C	7.05962800	0.56624900	0.83283500
C	6.03116800	-0.27003600	1.26144200
C	4.72265900	-0.01747100	0.86973600
H	5.24261900	2.74463300	-1.03067300
H	7.57327800	2.30341500	-0.32394200
H	8.07981100	0.37204600	1.14146700
H	6.24927800	-1.11391500	1.90471200
H	3.91759000	-0.66359500	1.20786500
C	3.01102500	1.31449500	-0.38853700
H	2.90373500	2.26825200	-0.90180500
H	2.32444900	1.27764400	0.45520900
N	2.55173600	0.24591600	-1.32396800

H	2.70565300	-0.68990000	-0.93400000
H	3.03068800	0.29165900	-2.22321300
8			
C	3.62457200	-1.12683000	-0.69606200
C	2.36533600	-1.94662800	-0.49513700
C	1.20408400	-1.46497900	-1.35515100
C	0.01569400	-1.95375900	-0.55392500
C	0.47754900	-1.66825900	0.89042200
C	-0.03706600	-2.66215400	1.91799400
O	0.24173500	-0.34889200	1.26470000
O	3.84409100	-1.09363300	-2.10205600
O	1.89962900	-1.81467700	0.85555800
O	1.19399000	-1.98963100	-2.65952000
O	-1.45006700	-2.58467900	1.91883600
H	3.45062500	-0.12002200	-0.30733800
H	4.47489000	-1.57306100	-0.17096000
H	1.18575700	-0.36806300	-1.36333800
H	-0.08524800	-3.03787400	-0.69738500
H	2.55566900	-3.00330300	-0.71641800
H	0.31089300	-3.66303700	1.64041400
H	0.38480500	-2.39175600	2.89257000
H	4.45211800	-0.37553000	-2.29872400
H	2.01763400	-1.69242600	-3.06707900
H	-1.78556400	-3.14770600	2.62116500
O	-1.19187400	-1.29144400	-0.84764600
H	-1.33876200	-1.37038200	-1.79667000
H	-0.75023700	-0.15272600	1.36585000
H	2.13485300	0.30327400	3.59358000
C	2.67798300	2.12321500	0.82775900
C	4.03795600	2.38102800	0.64603000
C	4.56232600	2.49921400	-0.63674500
C	3.72578300	2.37864200	-1.74408300
C	2.36484100	2.14735800	-1.56616900
C	1.84182600	2.01706700	-0.28281400
H	4.69159200	2.48569000	1.50632400
H	5.61956300	2.69160700	-0.77205300
H	4.13349400	2.47387100	-2.74359300
H	1.71151000	2.05848100	-2.42607100
H	0.79013400	1.79823700	-0.13615700
C	2.13350900	1.88584800	2.20991400
H	1.04671000	1.90802400	2.22293500
H	2.52803700	2.59251700	2.93811700
N	2.52881500	0.51130200	2.67354700
H	3.54375300	0.41594100	2.74176900
H	2.17160100	-0.19968500	2.01243000
C	-4.17952500	1.02259000	-0.11974200
C	-5.12420500	2.01438700	0.13446500
C	-6.44204600	1.86553900	-0.29383200
C	-6.82651800	0.71912200	-0.98018300
C	-5.88868600	-0.27969700	-1.23733200
C	-4.57587400	-0.12689200	-0.80958100
H	-4.82763100	2.91009000	0.67070800
H	-7.16703400	2.64528000	-0.09101800
H	-7.85034500	0.60261500	-1.31504300
H	-6.18182500	-1.17387900	-1.77500700
H	-3.84258100	-0.90388300	-1.00844000
C	-2.74732200	1.15087500	0.34928500
H	-2.57531300	2.14934300	0.75585900
H	-2.07032000	1.01046600	-0.49627100
N	-2.36155800	0.16332900	1.36629500
H	-2.57874000	-0.77826600	1.04599700

H	-2.88217400	0.31328000	2.22529500
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