

Supporting Information

INVESTIGATION OF IRON RELEASE FROM THE N- AND C- LOBES OF HUMAN SERUM TRANSFERRIN BY QUANTUM CHEMICAL CALCULATIONS

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1. The physiological pH models of the N- and C-lobe of hTf

To find out the optimum physiological model, the size of the cluster model is enlarged step by step starting from a basic model. This model (Model 1, Figure S1) includes iron and the first shell residues only and consists of 56 atoms. The all-atom RMSD value with respect to the crystal structure is calculated as 1.057 Å (Table S1). In Model 2, some of the second shell residues (Thr 120, Arg 124, Lys 206, Lys 296 and a water molecule bridging between Asp 63 and Tyr 95) are included and the RMSD value decreased to 0.877 Å. Next, all the residues within 6 Å around iron are included in Model 3 and the RMSD value drastically decreased (0.041 Å) that might point out to the suitability of the cluster size. To further confirm the convergence of the size of the cluster, a larger model (Model 4) consisting of 194 atoms is optimized and the RMSD value is calculated as 0.014 Å. Ultimately, Model 3 is chosen as the model for the iron-binding site at the physiological pH that compromise between the size and the efficiency. The corresponding model for C-lobe is constructed with a cluster size of 146 atoms (TfC^{Phys} , Fig. 1). The RMSD value is calculated as low as 0.002 Å with respect to the C-lobe of the crystal structure. Thus, TfN^{Phys} and TfC^{Phys} are chosen to further assess the release of iron in hTf.

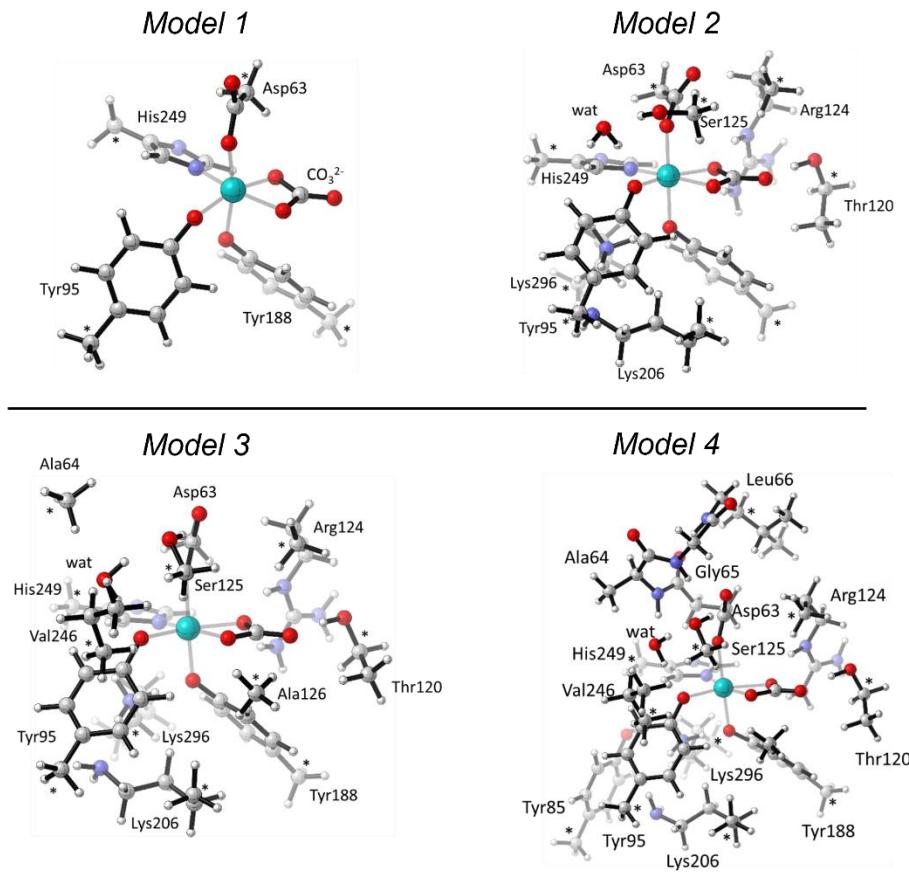


Figure S1. Optimized geometries of the physiological pH model with different cluster size.

Table S1. RMSD Values for different sizes of N-Lobe in physiologic environment.

	Model 1	Model 2	Model 3	Model 4
Atom #	56	124	144	194
RMSD (Å)	1.057	0.877	0.041	0.014

2. The structural changes upon the protonation of the first coordination shell residues

In this part of study, we have considered the protonation of each residue of the first coordination shell (His249, Tyr95, Tyr188 and the synergistic anion) individually in the iron binding site of

the N-lobe of hTf to see how the protonation of each residue affects the coordination mode of iron (Scheme 2). Starting from a smaller model ($s\text{TfN}^{\text{Phys}}$) similar to Model 2 of the physiological pH model of the N-lobe (Fig. S1), each coordinating residue is protonated, and the geometries optimized at B3LYP/6-311+G(d) level of theory (SDD for Fe atom) are depicted in Fig. S2.

The protonation of His249-N δ 1 ($s\text{TfN}_{\text{H249H}}$) and Tyr95 ($s\text{TfN}_{\text{Y95H}}$) resulted in the elongation of the iron-protonated residue distance: the HisN ϵ 2–iron distance elongates from 2.11 Å in $s\text{TfN}^{\text{Phys}}$ to 2.22 Å and the Tyr95–O–iron distance elongates from 1.96 Å in $s\text{TfN}^{\text{Phys}}$ to 2.17 Å in $s\text{TfN}_{\text{Y95H}}$. This elongation results in a weaker coordination of His249 and Tyr95 residues to iron in $s\text{TfN}_{\text{H249H}}$ and $s\text{TfN}_{\text{Y95H}}$ but still, does not affect the octahedral arrangement around iron in both complexes. However, the octahedral coordination is disrupted via the protonation of Tyr188 or the synergistic anion. The former leads to the detachment of this residue from the first coordination shell, adopting a square pyramidal coordination. The protonated Tyr188 forms hydrogen bond with O¹ of carbonate ($s\text{TfN}_{\text{Y188H}}$). The coordination of the synergistic anion changes from bidentate to monodentate as the anion is protonated ($s\text{TfN}_{\text{HCO}_3}$, Fig. S2).

The distance between iron and the second coordinating oxygen (O²) of bicarbonate increases to 3.21 Å, resulting in the weakening of this coordination. The loss of the coordination of one of the oxygens of bicarbonate in the equatorial plane results in a trigonal bipyramidal coordination around iron, consistent with the previously reported studies.^{1,2}

The protonation of His249 ($s\text{TfN}_{\text{H249H}}$) leads to the thermodynamically stable complex with the octahedral coordination around iron. This complex is energetically followed by the complexes formed through the protonation of the synergistic carbonate ion ($s\text{TfN}_{\text{HCO}_3}$), the protonation of Tyr95 ($s\text{TfN}_{\text{Y95H}}$) and the protonation of Tyr188 ($s\text{TfN}_{\text{Y188H}}$), respectively.

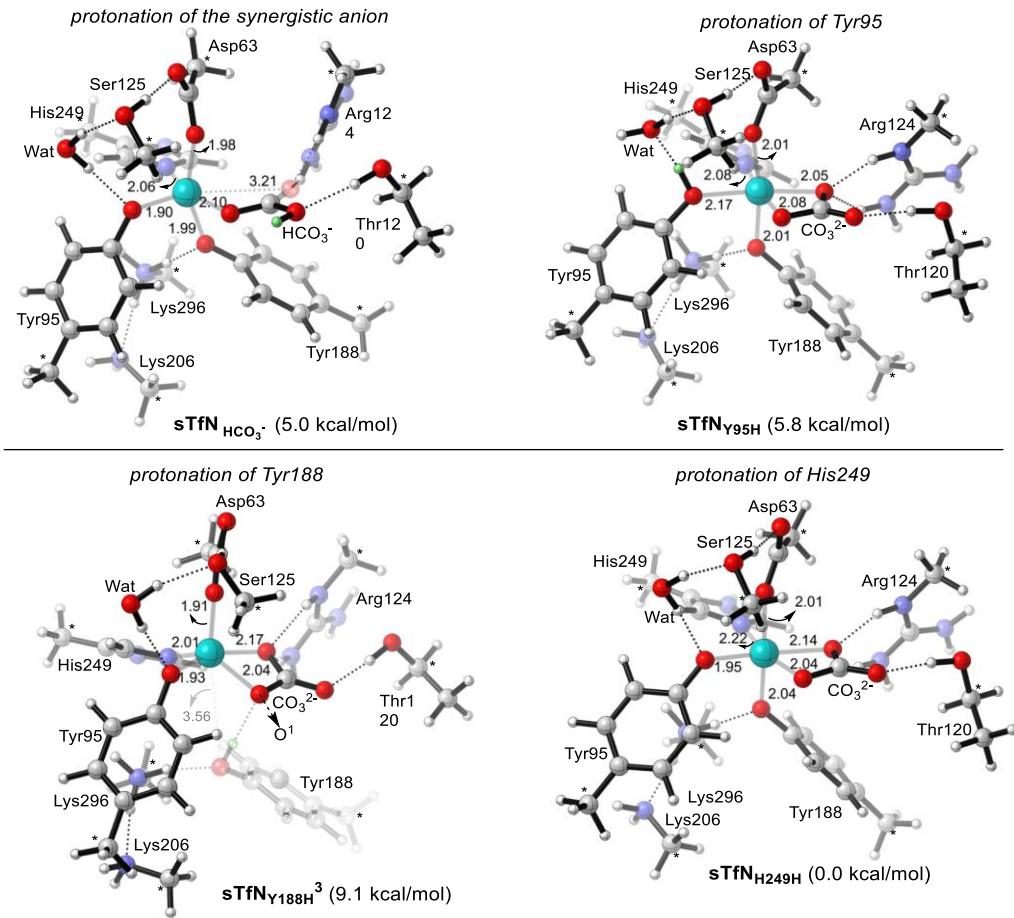
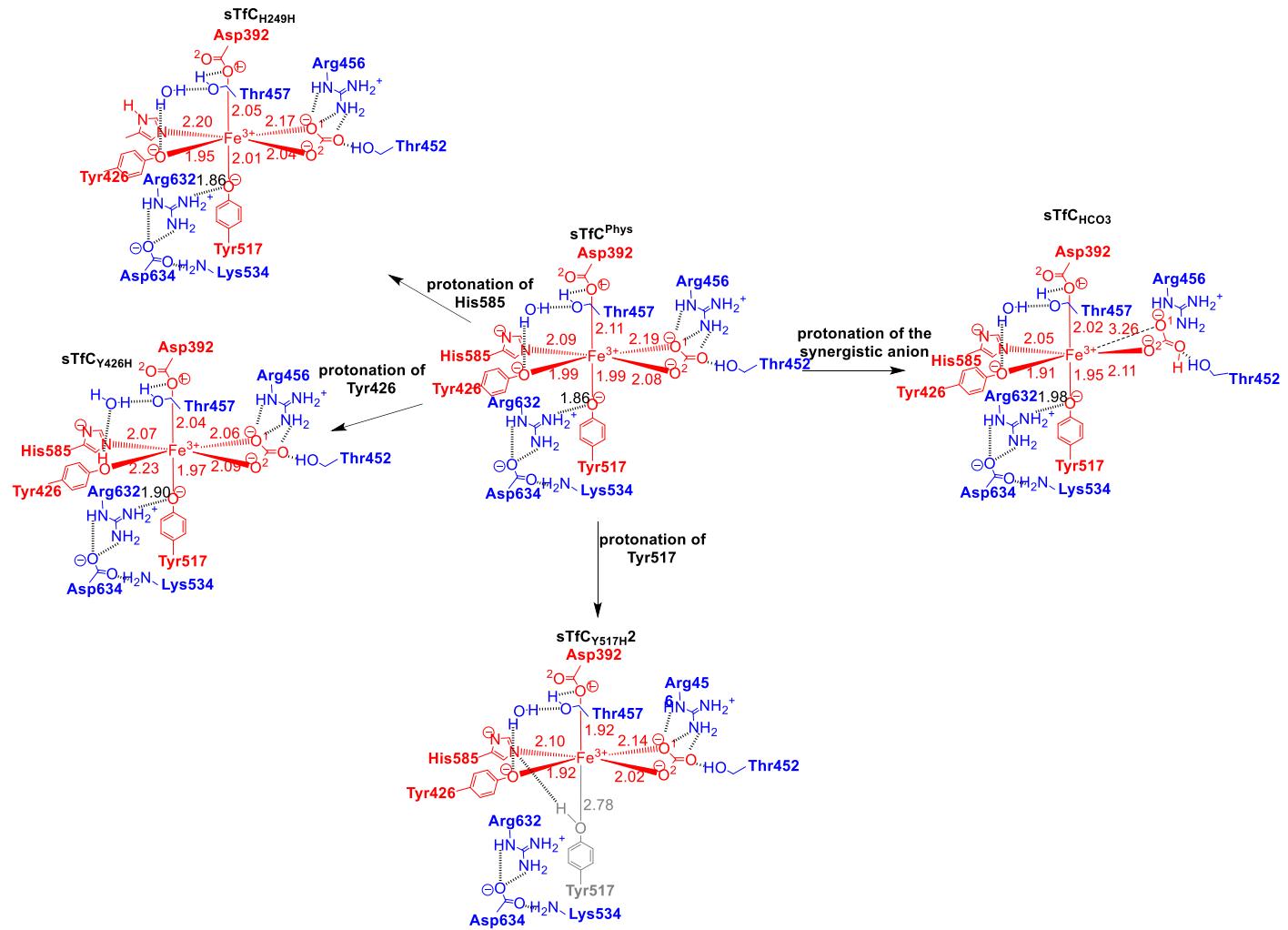


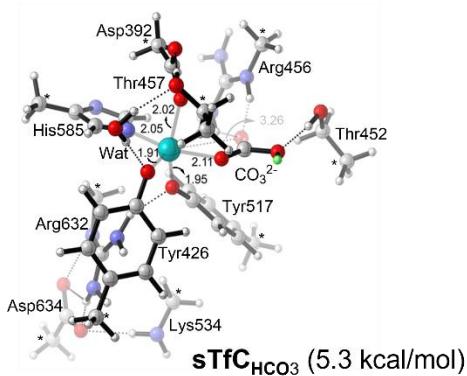
Figure S2. The complexes associated with the protonation of each residue in $\text{TfN}_3^{\text{Phys}}$ and their relative free energies in parentheses. Hydrogen atom of the protonated residue is shown in green. Distances are given in Å. Atoms with asterisks (*) are kept fixed.

For the release of iron in the C-lobe of hTf, the protonation of each residue (His585, Tyr426, Tyr517 and the synergistic anion) is also modelled individually in the iron binding site of the C-lobe of hTf (Scheme S1). Similar geometry changes in the protonated complexes of the C-lobe of hTf have been observed as in the case of the protonated complexes of the N-lobe of hTF: The octahedral arrangement is conserved for the protonation of His585 and Tyr426, and a disruption of the octahedral geometry is observed upon protonating Tyr517 and the synergistic anion (Fig. S3).

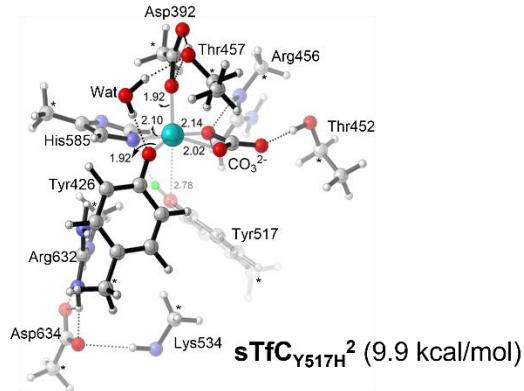
Scheme S1. The protonation of His585, Tyr426, Tyr517 and the synergistic anion in the physiological pH model of the C-lobe of hTf (sTfC^{Phys}). The first and the second coordination shells are represented in red and blue respectively. The gray color of residues implies the departure of a residue from the first coordination shell. Distances are given in Å.



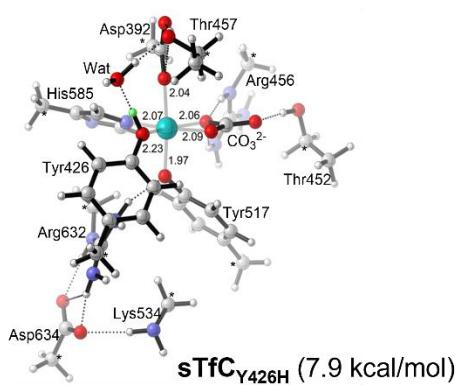
protonation of the synergistic anion



protonation of Tyr517



protonation of Tyr426



protonation of His585

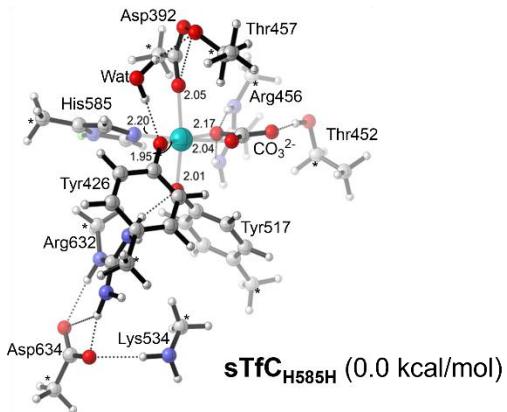


Figure S3. The complexes associated with the protonation of each residue in the physiological pH model of the C-lobe of hTf (sTfC^{Phys}) and their relative free energies in parentheses. Hydrogen atom of the protonated residue is shown in green. Distances are given in Å. Atoms with asterisks (*) are kept fixed.

3. Coordinates

3.1 N-Lobe

TfN ^{Phys}	TfN ^{Acid}
C 0 -1.05802500 3.59963700 1.79374900	C 0 -1.36617600 3.54384200 1.78398500
O -1 -0.34050600 2.89184800 0.97919700	O -1 -0.62614500 2.87594800 0.94695800
O 0 -1.21806300 4.81751800 1.62123600	O 0 -1.55851100 4.75624900 1.63647200
C 0 5.12218300 -1.24246600 -1.21033300	C 0 5.13305200 -0.89196100 -1.15409300
C 0 4.04041200 -0.92875600 -2.04734900	C 0 4.04288300 -0.63920200 -2.01306400
C 0 5.09961800 -0.73342200 0.09581800	C 0 5.04120000 -0.40354200 0.16189200
C 0 2.97148500 -0.15077000 -1.61008900	C 0 2.92792500 0.07919900 -1.59702300
C 0 4.05172800 0.06891700 0.54279400	C 0 3.93352300 0.33456000 0.59028000
C 0 2.97130500 0.38709300 -0.30850500	C 0 2.86427700 0.62635600 -0.29113700
O -1 2.02689700 1.22911100 0.10712800	O -1 1.87973000 1.41771900 0.09611700
C 0 -5.23429000 -0.22158900 -4.000095800	C 0 -5.29531500 -0.64177400 -4.02461900
O 0 -5.43545500 1.04352600 -1.90864900	O 0 -5.53631800 0.53575500 -1.88756900
C 0 -4.84798100 3.59677600 0.90138500	C 0 -5.15921400 3.16888600 0.86486600
C 0 -5.53028000 2.23429000 1.04860800	C 0 -5.71852900 1.75287600 1.02920400
N 0 -4.54902300 1.15024300 0.96308200	N 0 -4.64820900 0.75451200 0.95123900
C 0 -4.88873900 -0.12061300 0.73627700	C 0 -4.87675600 -0.54685500 0.76765900
N 0 -3.93771800 -0.98364300 0.37353400	N 0 -3.84644400 -1.34506400 0.45570300
N 0 -6.15077800 -0.55417600 0.96552000	N 0 -6.09888100 -1.07383400 0.99675800
O 0 1.07837000 5.28667500 -0.28600800	O 0 0.65438100 5.36827300 -0.33823000
C 0 -2.59726400 -3.98408900 -1.76518400	C 0 -2.24165700 -4.21681000 -1.72033000
C 0 -2.08754600 -2.93790700 -2.56123100	C 0 -1.87371500 -3.10692100 -2.50883100
C 0 -2.27385900 -3.92390900 -0.39839500	C 0 -1.86085800 -4.15724200 -0.36935300
C 0 -1.26172200 -1.92946500 -2.04644000	C 0 -1.12767400 -2.03140700 -2.00376600
C 0 -1.46187600 -2.91469000 0.13259200	C 0 -1.13037700 -3.08356800 0.15124100
C 0 -0.88965300 -1.90848300 -0.68171500	C 0 -0.70458500 -2.00345500 -0.65545700
O 0 -0.00263100 -1.03211900 -0.17876600	O 0 0.09450600 -1.03703100 -0.15205900
C 0 1.46890500 -4.36681100 -2.96486400	C 0 1.81649000 -4.12950200 -2.79728000

C	0	1.86700300	-4.17636300	-1.49478800	C	0	2.42212800	-3.88364200	-1.40550700
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N	0	3.72501000	-3.91805300	0.14000600	N	0	4.57573900	-3.72848800	-0.11690600
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C	0	4.80409700	2.73642700	-2.27929200	C	0	4.45599800	3.14720800	-2.31165500
C	0	0.95107400	-0.24715600	4.61748900	C	0	0.92737400	-0.10273600	4.62657800
C	0	1.10484700	0.10280400	3.28050900	C	0	1.02367900	0.34096100	3.30960700
N	0	-0.36535300	-0.57728900	4.84124300	N	0	-0.30549700	-0.67646200	4.81200900
C	0	-0.95016000	-0.41347800	3.63790600	C	0	-0.90489700	-0.56396400	3.60845500
N	-1	-0.11942300	-0.02064900	2.65224400	N	-1	-0.15286300	0.01372900	2.65409800
C	0	-0.26942600	-4.73497900	3.78907900	C	0	0.18464500	-4.77717300	3.59248600
C	0	0.36292500	-3.42610900	3.30098600	C	0	0.67576700	-3.36675800	3.25694200
C	0	1.26529900	-3.62931900	2.09210400	C	0	1.72298300	-3.30586600	2.14307000
N	0	1.73572000	-2.34338900	1.48934000	N	0	1.84062300	-1.90333600	1.63285400
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O	0	-2.09729800	0.91537200	-0.27358400	O	0	-2.18931500	0.71483300	-0.29058300
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O	-1	-2.77767700	1.30406400	-2.42188700	O	-1	-2.90841000	1.04076300	-2.43711800
Fe	0	-0.02239900	0.98909300	0.26365400	Fe	0	-0.18598200	1.02719100	0.25541100
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H	0	-2.66047700	-4.68719700	0.27563400	H	0	-2.14099700	-4.96735500	0.30201300
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C	-1	-3.41522000	-5.14682900	-2.34616000	C	-1	-2.97664100	-5.43990600	-2.28636500
H	0	-2.75793600	-5.93850600	-2.72610300	H	0	-2.26729100	-6.17192100	-2.69102000
H	0	-4.06273600	-5.59205000	-1.58445700	H	0	-3.56173000	-5.94054000	-1.50919100
H	0	-4.04212100	-4.81373200	-3.17954000	H	0	-3.65294300	-5.15529700	-3.09831900
C	-1	-5.75803700	-0.16794800	-2.56610300	C	-1	-5.74758700	-0.68912100	-2.56622100
H	0	-5.36003300	-1.03770800	-2.01221300	H	0	-5.22582900	-1.51874900	-2.05512100
H	0	-6.85283200	-0.25632500	-2.55499700	H	0	-6.82247500	-0.90464900	-2.50651100
C	-1	2.02497400	-3.26974100	-3.88338500	C	-1	2.28017000	-3.10982400	-3.84142600
H	0	3.11507600	-3.31357500	-3.96724800	H	0	3.36377000	-3.12222100	-3.99688500
H	0	1.61636800	-3.36069500	-4.89554400	H	0	1.81525000	-3.31584000	-4.81029300
H	0	1.75715800	-2.27955100	-3.50025200	H	0	1.99004900	-2.09820000	-3.54280400
C	-1	1.12972000	4.57789600	-1.52466500	C	-1	0.69456600	4.65554800	-1.57541700
H	0	0.29110900	4.84783300	-2.18265400	H	0	-0.15733400	4.91380800	-2.22063000
H	0	2.06472400	4.85784800	-2.01782200	H	0	1.61777500	4.94516400	-2.08443400
H	0	1.11667800	3.49122400	-1.38047900	H	0	0.69632300	3.56931300	-1.42719500
C	-1	2.00544200	-0.31130500	5.68737300	C	-1	1.98402200	-0.05383800	5.69395100
H	0	1.72397600	0.27780900	6.56876400	H	0	1.62544100	0.45739700	6.59498300
H	0	2.17454400	-1.33991100	6.03522800	H	0	2.29290600	-1.06112600	6.00296300
H	0	2.95897600	0.07674900	5.31431400	H	0	2.87104700	0.47825100	5.33615900
C	-1	0.74673900	-5.77827000	4.26986200	C	-1	1.21313000	-5.62634900	4.33954800

H	0	0.24469100	-6.65833300	4.68497600	H	0	0.81003800	-6.61222500	4.59175500
H	0	1.39261000	-6.12588000	3.45599800	H	0	2.12001100	-5.78721600	3.74381000
H	0	1.39238200	-5.36132300	5.05155500	H	0	1.51349700	-5.13773300	5.27289200
C	-1	-4.19199000	3.80396400	-0.46835500	C	-1	-4.54035200	3.42911300	-0.51395300
H	0	-3.81575100	4.82727100	-0.55736000	H	0	-4.26007000	4.48210100	-0.60971700
H	0	-3.34131500	3.13819900	-0.61818300	H	0	-3.63611600	2.84085800	-0.67247600
H	0	-4.90090800	3.61294400	-1.27977900	H	0	-5.24039600	3.17427100	-1.31566600
C	-1	-1.66432000	2.87976500	2.99065200	C	-1	-1.94727100	2.77083100	2.95743000
H	0	-0.86258100	2.46456000	3.60608600	H	0	-1.12966800	2.39481700	3.57832500
H	0	-2.27691900	3.56548300	3.57892000	H	0	-2.60579400	3.41096200	3.54662800
H	0	-2.26179200	2.03002100	2.65111500	H	0	-2.48864100	1.89279800	2.59691800
C	-1	0.03258500	0.98428700	-4.78108200	C	-1	-0.07678800	0.94189400	-4.79032700
H	0	0.66886700	1.82113600	-4.48703600	H	0	0.53288500	1.79321000	-4.48133600
H	0	0.51278000	0.05146900	-4.47112100	H	0	0.41480000	0.01869300	-4.46894000
H	0	-0.92767900	1.07766900	-4.27189300	H	0	-1.05098300	1.01455600	-4.30550300
H	0	-0.09865800	0.97940700	-5.86737200	H	0	-0.18214300	0.93462000	-5.87899700
C	-1	5.18831900	4.20705800	-2.09896900	C	-1	4.77107600	4.63626200	-2.14240300
H	0	6.26045700	4.28659300	-1.87066300	H	0	5.83965500	4.76582900	-1.92195200
H	0	4.64984200	4.58324700	-1.22182200	H	0	4.22221100	4.99222600	-1.26337800
C	-1	3.29369400	5.68502800	3.37753300	C	-1	2.74432000	6.00533800	3.31505200
H	0	4.20299100	6.29227700	3.34688200	H	0	3.32618200	6.90116800	3.08082000
H	0	3.36138400	4.87476300	2.64867100	H	0	2.97694900	5.21348300	2.60056300
H	0	3.16715100	5.27580100	4.38396000	H	0	2.97803800	5.67957600	4.33279400
H	0	2.43250500	6.31320100	3.13511500	H	0	1.67888600	6.24163600	3.24845800
					H	0	4.61307000	-2.68481200	-0.13027700

TS1

C	0	-1.44503100	3.52265400	1.76318300
O	-1	-0.67153300	2.86798800	0.93924100
O	0	-1.67989800	4.72192200	1.59019300
C	0	5.15180300	-0.81767100	-1.12974200

TfN^{Acid}_{Y188H¹}

C	0	-1.41214700	3.52772700	1.79429300
O	-1	-0.64579500	2.86891600	0.95873600
O	0	-1.63946700	4.72582100	1.62148500
C	0	5.13533300	-0.83902900	-1.18254200

C	0	4.05623100	-0.59658000	-1.98931800	C	0	4.02470400	-0.62736000	-2.02427400
C	0	5.05592800	-0.30990400	0.17927300	C	0	5.07068000	-0.30632300	0.11866800
C	0	2.92934500	0.10860100	-1.58001300	C	0	2.90684400	0.08408200	-1.60186500
C	0	3.93882300	0.41624800	0.59865300	C	0	3.96356500	0.42636500	0.54992400
C	0	2.86114000	0.66959200	-0.28218900	C	0	2.86553400	0.65440900	-0.30906000
O	-1	1.85888800	1.44515700	0.10187700	O	-1	1.86407400	1.42790700	0.09043700
C	0	-5.42016800	-0.60302200	-4.08537800	C	0	-5.45832400	-0.54713000	-4.04200200
O	0	-5.52884900	0.42763200	-1.86618500	O	0	-5.55406000	0.49477100	-1.82704700
C	0	-5.18215000	3.10721700	0.84719500	C	0	-5.15377200	3.12738800	0.90547700
C	0	-5.71808900	1.68472400	1.03242600	C	0	-5.69107500	1.70309000	1.07686900
N	0	-4.63611900	0.69852600	0.95367900	N	0	-4.61225100	0.71415800	0.98507100
C	0	-4.85262300	-0.60802700	0.79112500	C	0	-4.83192700	-0.59293400	0.83460200
N	0	-3.81943200	-1.39999000	0.47286700	N	0	-3.80132500	-1.39161400	0.51553300
N	0	-6.06436300	-1.14488700	1.04763300	N	0	-6.04248400	-1.12467800	1.09991300
O	0	0.56604700	5.37794000	-0.34165500	O	0	0.60738700	5.37423200	-0.31880000
C	0	-2.16931900	-4.25952700	-1.72140000	C	0	-2.21595800	-4.24463700	-1.73517100
C	0	-1.80352700	-3.14430500	-2.50146700	C	0	-1.94941900	-3.08419800	-2.48573700
C	0	-1.80232700	-4.21166100	-0.36689300	C	0	-1.71337300	-4.27557500	-0.42532300
C	0	-1.06169300	-2.07263100	-1.98325200	C	0	-1.17337200	-2.03130400	-1.98272100
C	0	-1.07886400	-3.14106100	0.16793800	C	0	-0.95481500	-3.22611400	0.09873600
C	0	-0.65305300	-2.06568400	-0.63617700	C	0	-0.64784300	-2.10675300	-0.68677100
O	0	0.14986100	-1.08856800	-0.12622900	O	0	0.17412600	-1.10937800	-0.20561600
C	0	1.89294800	-4.12275800	-2.80693500	C	0	1.77720000	-4.08443500	-2.82995600
C	0	2.48341400	-3.88253300	-1.40849700	C	0	2.36507600	-3.83858900	-1.43141800
C	0	3.97501800	-4.19657800	-1.37966300	C	0	3.83685700	-4.23385400	-1.37496800
N	0	4.62580900	-3.68349700	-0.11357800	N	0	4.50631500	-3.69047300	-0.13145700
C	0	4.34566800	5.53169200	-3.35841900	C	0	4.35195400	5.51011900	-3.36834000
C	0	4.41223100	3.21217600	-2.29638000	C	0	4.41925400	3.18396400	-2.32114100
C	0	0.90356100	-0.08252200	4.62776700	C	0	0.93303600	-0.11004000	4.61587900
C	0	1.00224600	0.35426000	3.31102500	C	0	1.02524400	0.32581600	3.30010500
N	0	-0.32878800	-0.66384900	4.80998200	N	0	-0.30677600	-0.67730000	4.80761400

C	0	-0.92219800	-0.56415800	3.60420100	C	0	-0.90838700	-0.57157400	3.60824400
N	-1	-0.16608600	0.01378300	2.65022800	N	-1	-0.15135100	0.00017600	2.64889200
C	0	0.23868300	-4.74732900	3.61237000	C	0	0.23492900	-4.74169800	3.59629700
C	0	0.73557900	-3.34511500	3.24851300	C	0	0.78490400	-3.35867700	3.24612000
C	0	1.75914400	-3.29517500	2.11004000	C	0	1.89114300	-3.34966400	2.18339800
N	0	1.83110600	-1.91513800	1.55034000	N	0	1.95921100	-2.01252800	1.55538900
C	0	-1.98977300	1.02444300	-1.58943100	C	0	-2.00371400	1.04799700	-1.56633700
O	0	-2.18020200	0.65967500	-0.30873900	O	0	-2.17360900	0.66864900	-0.28669000
O	-1	-0.73030500	1.39090400	-1.74947300	O	-1	-0.74440800	1.40636000	-1.73708500
O	-1	-2.91053100	0.99905600	-2.45564200	O	-1	-2.93200800	1.04000100	-2.42602000
Fe	0	-0.19596400	1.06161400	0.26605100	Fe	0	-0.17913400	1.11655900	0.27555500
O	0	2.81244000	4.03065700	0.68446800	O	0	2.85031800	3.99978200	0.67940400
H	0	4.10660600	-0.96571600	-3.00935900	H	0	4.05504600	-1.01041000	-3.03976600
H	0	5.88722400	-0.44918000	0.86808400	H	0	5.91589700	-0.43714700	0.79155200
H	0	2.09541300	0.28288200	-2.25203500	H	0	2.05979100	0.25113700	-2.25911600
H	0	3.89716100	0.83642400	1.59843300	H	0	3.93979300	0.86063300	1.54402700
H	0	-4.37292100	-0.31583000	-4.21962400	H	0	-4.40808500	-0.27227100	-4.17915000
H	0	-6.04818600	0.18365900	-4.51588900	H	0	-6.07775100	0.24440800	-4.47591700
H	0	-5.60138200	-1.53489200	-4.63377000	H	0	-5.65076400	-1.47953100	-4.58565500
H	0	-4.58706800	0.68814300	-1.99609400	H	0	-4.61095200	0.74631100	-1.96092400
H	0	-6.02330700	3.78748200	1.02265900	H	0	-5.99288300	3.80551200	1.09817900
H	0	-4.43873400	3.32765000	1.62155700	H	0	-4.40468100	3.33595000	1.67758400
H	0	-6.44623000	1.47317900	0.23851200	H	0	-6.42230900	1.50030600	0.28379200
H	0	-6.21264900	1.59567200	2.00742100	H	0	-6.18125700	1.60567100	2.05324800
H	0	-3.73138000	0.99548200	0.56808600	H	0	-3.71056300	1.00775300	0.58951600
H	0	-2.98780300	-0.92958400	0.10240900	H	0	-2.97418500	-0.92277400	0.13402400
H	0	-3.94866200	-2.37750400	0.26360600	H	0	-3.94517700	-2.36382700	0.29109100
H	0	-6.86319700	-0.53256300	1.10171300	H	0	-6.84206000	-0.51439200	1.16148200
H	0	-6.25618800	-2.08199900	0.72878800	H	0	-6.23356400	-2.07390300	0.81964100
H	0	-0.20244000	5.05026600	0.16586800	H	0	-0.16434200	5.05976600	0.19087700
H	0	-2.09108200	-3.11141000	-3.54997900	H	0	-2.33888200	-3.00103600	-3.49734500

H	0	-2.08577800	-5.02835800	0.29436000	H	0	-1.91420200	-5.13844500	0.20581600
H	0	-0.78828800	-1.23326200	-2.61419600	H	0	-0.96354800	-1.15664500	-2.58817900
H	0	-0.85544100	-3.12755400	1.22539200	H	0	-0.60592000	-3.27259800	1.11956400
H	0	2.15421600	-5.13298300	-3.14840400	H	0	2.00438200	-5.10965600	-3.15093600
H	0	0.80341900	-4.09188000	-2.71811200	H	0	0.68862700	-4.01549000	-2.75172300
H	0	1.96591000	-4.51440700	-0.67948000	H	0	1.80471200	-4.41627200	-0.68994100
H	0	2.30875000	-2.83656200	-1.12890500	H	0	2.24725900	-2.77950900	-1.17598400
H	0	4.51130000	-3.71125200	-2.19448500	H	0	4.40499400	-3.82569200	-2.21080000
H	0	4.16548900	-5.27008300	-1.42471100	H	0	3.96754400	-5.31726900	-1.36108900
H	0	4.13121300	-4.00208300	0.72419100	H	0	3.98435000	-3.93325100	0.71547800
H	0	5.59610700	-3.99951300	-0.03530000	H	0	5.45568600	-4.05620600	-0.02242600
H	0	3.28051900	5.42832000	-3.59746300	H	0	3.28450000	5.41154100	-3.59916500
H	0	4.54919800	6.59761700	-3.20784400	H	0	4.56010900	6.57445100	-3.21296500
H	0	4.91035200	5.20385800	-4.24025300	H	0	4.90806000	5.18594100	-4.25691800
H	0	3.34000000	3.04924800	-2.45202700	H	0	3.34458300	3.02577900	-2.46469200
H	0	4.94323300	2.78646800	-3.15752200	H	0	4.93798900	2.76284400	-3.19194000
H	0	4.69370100	2.64211700	-1.40676200	H	0	4.70984300	2.60636600	-1.43936300
H	0	1.77075100	0.93842400	2.81906900	H	0	1.80566900	0.88317300	2.79666600
H	0	-1.92091700	-0.93474100	3.39857600	H	0	-1.91342100	-0.92858700	3.41020900
H	0	-0.64544800	-4.63307200	4.24994900	H	0	-0.63956400	-4.60737100	4.24356700
H	0	-0.10309600	-5.26177300	2.70280000	H	0	-0.12978900	-5.23380200	2.68277800
H	0	1.14603400	-2.84509600	4.13164300	H	0	1.14283800	-2.85348800	4.14864200
H	0	-0.11641100	-2.72815900	2.95896600	H	0	-0.02938600	-2.72585500	2.88656000
H	0	1.46166500	-3.97403700	1.30677300	H	0	1.65770900	-4.09288100	1.41006200
H	0	2.74909200	-3.60164800	2.47331500	H	0	2.85012500	-3.63951400	2.64236200
H	0	0.93910900	-1.55213200	0.73539700	H	0	0.81365300	-1.49466100	0.51069500
H	0	1.72626700	-1.22770300	2.31652800	H	0	1.82458400	-1.29996000	2.28247600
H	0	2.72764500	-1.69535400	1.11795900	H	0	2.86829300	-1.80024800	1.15282900
H	0	2.47020600	3.13747900	0.49977300	H	0	2.49815800	3.11088400	0.49420900
H	0	2.05697800	4.60778100	0.45574000	H	0	2.09933400	4.58591000	0.45993600
C	-1	6.43199000	-1.45511300	-1.63274500	C	-1	6.39463100	-1.50348800	-1.70127600

H	0	6.99737700	-1.93596700	-0.82656600	H	0	7.01444900	-1.89708400	-0.88825300
H	0	6.24635300	-2.19570400	-2.41803400	H	0	6.17778100	-2.31969400	-2.39931900
H	0	7.09590700	-0.69961100	-2.06898900	H	0	7.01587700	-0.78504200	-2.24896300
C	-1	-2.88782200	-5.48125600	-2.30156400	C	-1	-2.96689300	-5.44166600	-2.30916400
H	0	-2.16698900	-6.20910000	-2.69299100	H	0	-2.27291800	-6.14161700	-2.78970000
H	0	-3.48538500	-5.98645800	-1.53701200	H	0	-3.49696200	-5.98967400	-1.52468200
H	0	-3.54945800	-5.19902300	-3.12619200	H	0	-3.69434700	-5.13170800	-3.06547000
C	-1	-5.72409500	-0.77010800	-2.59758000	C	-1	-5.76292000	-0.70362600	-2.55317500
H	0	-5.10158800	-1.58635000	-2.18865500	H	0	-5.14941300	-1.52527000	-2.14117900
H	0	-6.77177100	-1.06399200	-2.45235900	H	0	-6.81345500	-0.98546400	-2.40573600
C	-1	2.34325900	-3.07795000	-3.83151100	C	-1	2.27186800	-3.07682700	-3.87238700
H	0	3.42787900	-3.06596400	-3.97888900	H	0	3.35877100	-3.09892000	-4.00147900
H	0	1.89032800	-3.27775700	-4.80741300	H	0	1.82893400	-3.28652100	-4.85085100
H	0	2.03056100	-2.07714900	-3.51968200	H	0	1.98386200	-2.06028000	-3.58872200
C	-1	0.63693600	4.66527000	-1.57731900	C	-1	0.65599900	4.66842400	-1.55934600
H	0	-0.21680700	4.89729600	-2.22971600	H	0	-0.20384800	4.91166800	-2.19927600
H	0	1.55548200	4.98116800	-2.07879700	H	0	1.57088200	4.97899500	-2.07042700
H	0	0.67052800	3.57965500	-1.42821300	H	0	0.68253600	3.58152200	-1.41791400
C	-1	1.95634800	-0.02227700	5.70071100	C	-1	1.99775700	-0.07244100	5.68004400
H	0	1.58868400	0.48125500	6.60258300	H	0	1.64365400	0.42018900	6.59341200
H	0	2.27898100	-1.02624500	6.00698700	H	0	2.31684800	-1.08328300	5.96734900
H	0	2.83714400	0.52257500	5.34654600	H	0	2.87889400	0.47091300	5.32421200
C	-1	1.27097100	-5.60569600	4.34531400	C	-1	1.24972300	-5.64154100	4.29924500
H	0	0.85987100	-6.58406700	4.61387400	H	0	0.81354100	-6.60909700	4.56851100
H	0	2.16286000	-5.78220800	3.73168100	H	0	2.12118800	-5.84018900	3.66390100
H	0	1.59769200	-5.11376300	5.26814900	H	0	1.61384800	-5.17039300	5.21926400
C	-1	-4.58542300	3.36550300	-0.54142200	C	-1	-4.56847400	3.40986900	-0.48396100
H	0	-4.32674600	4.42256400	-0.65121200	H	0	-4.30902700	4.46830900	-0.57666400
H	0	-3.67175800	2.79315600	-0.70606700	H	0	-3.65744800	2.83850300	-0.66749500
H	0	-5.28955800	3.08867400	-1.33223800	H	0	-5.28040500	3.14867800	-1.27307900
C	-1	-2.00063600	2.74546000	2.94320600	C	-1	-1.95849700	2.74655400	2.97377200

H	0	-1.17101200	2.39252400	3.56171600	H	0	-1.12366700	2.38256300	3.57873000
H	0	-2.67118300	3.37473100	3.53020100	H	0	-2.61714500	3.37727000	3.57216400
H	0	-2.52278800	1.85209100	2.59245800	H	0	-2.49059000	1.85947200	2.62213300
C	-1	-0.06692700	0.93931100	-4.79342600	C	-1	-0.10917100	0.96787200	-4.79079400
H	0	0.50535900	1.81294200	-4.47551500	H	0	0.50314800	1.81605600	-4.47859100
H	0	0.45286400	0.03538100	-4.46163000	H	0	0.37112600	0.04274700	-4.45786800
H	0	-1.05151100	0.97728200	-4.32575400	H	0	-1.08920000	1.05033200	-4.31930200
H	0	-0.15350000	0.92627100	-5.88363500	H	0	-0.20107500	0.95530000	-5.88048900
C	-1	4.71606100	4.70327300	-2.12403600	C	-1	4.73025200	4.67282000	-2.14233700
H	0	5.78309100	4.84002300	-1.90062000	H	0	5.79974700	4.80421300	-1.92789300
H	0	4.16259000	5.05437800	-1.24579200	H	0	4.18619300	5.02084700	-1.25706000
C	-1	2.64294800	6.04593500	3.32252300	C	-1	2.71804800	6.00294500	3.33014500
H	0	3.26835900	6.92437900	3.14033800	H	0	3.39771700	6.84711700	3.18383000
H	0	2.89255300	5.25654800	2.61120000	H	0	2.94488700	5.21264200	2.61229400
H	0	2.80106400	5.69718200	4.34712600	H	0	2.82424500	5.62772000	4.35204400
H	0	1.59235200	6.32029300	3.19437700	H	0	1.68914900	6.33932900	3.17634100
H	0	4.64474000	-2.64064400	-0.12908700	H	0	4.58088900	-2.65278900	-0.19869300

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C	0	-1.17761200	3.44591300	1.99059000
O	-1	-0.44502000	2.80133900	1.10828000
O	0	-1.40126900	4.64697100	1.85397500
C	0	5.11205900	-0.90857800	-1.55533400
C	0	3.94061500	-0.68407000	-2.30111300
C	0	5.18404600	-0.33826200	-0.27086000
C	0	2.86068200	0.02651700	-1.77758500
C	0	4.12256000	0.38812700	0.25857600
C	0	2.93332000	0.56817100	-0.48004200
O	-1	1.94392500	1.28051400	0.05457500
C	0	-5.61239100	-0.08735900	-3.85074700
O	0	-5.59852300	0.85794100	-1.58819100

TS2

C	0	1.15115200	-3.45440500	1.98723100
O	-1	0.42194100	-2.80378400	1.10660900
O	0	1.36683200	-4.65668400	1.84905900
C	0	-5.11360500	0.94547000	-1.54833600
C	0	-3.94622400	0.71039700	-2.29671300
C	0	-5.18693300	0.37824600	-0.26347900
C	0	-2.87044000	-0.00701200	-1.77499600
C	0	-4.12902200	-0.35567300	0.26523900
C	0	-2.94358300	-0.54532700	-0.47625900
O	-1	-1.95700000	-1.26471300	0.05677000
C	0	5.60625500	0.05109900	-3.85578000
O	0	5.58680600	-0.89591900	-1.59395900

C	0	-4.97679000	3.38710500	1.26396000	C	0	4.95305500	-3.42666400	1.25600200
C	0	-5.61447600	2.00474200	1.41784900	C	0	5.60210600	-2.04986500	1.41120700
N	0	-4.61430300	0.94700800	1.23624800	N	0	4.60974600	-0.98431000	1.23234600
C	0	-4.94307000	-0.32065300	0.97603200	C	0	4.94797500	0.28057400	0.97075200
N	0	-3.99394200	-1.14786100	0.52029800	N	0	4.00376100	1.11521800	0.51854600
N	0	-6.17173400	-0.79054100	1.26424300	N	0	6.18120800	0.74082700	1.25523600
O	0	0.83906600	5.30807700	-0.08879400	O	0	-0.88251800	-5.29863600	-0.09047400
C	0	-2.60841400	-4.05095000	-1.77292600	C	0	2.63588100	4.03301000	-1.77084600
C	0	-2.13806000	-2.91202900	-2.45284500	C	0	2.14714500	2.90310200	-2.45293000
C	0	-2.31200500	-4.12280500	-0.40025600	C	0	2.35456100	4.09920200	-0.39490500
C	0	-1.35121500	-1.93765100	-1.82600300	C	0	1.35613200	1.93331800	-1.82433700
C	0	-1.53997900	-3.14935700	0.24934100	C	0	1.57839100	3.13008200	0.25599300
C	0	-1.02027700	-2.06783000	-0.47331400	C	0	1.03883400	2.05949800	-0.46814500
O	0	-0.14484300	-1.15861900	0.09587900	O	0	0.15654800	1.15833600	0.10431800
C	0	1.26242200	-3.93542700	-3.13856500	C	0	-1.24250900	3.95346400	-3.13540400
C	0	1.63809500	-3.61478200	-1.67858800	C	0	-1.60843700	3.63035800	-1.67344900
C	0	2.98719200	-4.22317500	-1.27438600	C	0	-2.95025700	4.24335600	-1.25015500
N	0	3.75250200	-3.33906400	-0.33870900	N	0	-3.69629500	3.36886300	-0.29703500
C	0	4.52708300	5.61340400	-3.09929800	C	0	-4.57594100	-5.57690500	-3.09726300
C	0	4.52879300	3.09958300	-2.65749500	C	0	-4.55571500	-3.06340200	-2.65425500
C	0	1.15132900	-0.53079900	4.49016600	C	0	-1.15054900	0.54331100	4.48928500
C	0	1.16574000	0.08176900	3.24613200	C	0	-1.17026800	-0.06865700	3.24473100
N	0	-0.05229700	-1.18610200	4.65362500	N	0	0.05902900	1.18666100	4.65420000
C	0	-0.71854300	-0.93867900	3.51888300	C	0	0.72446200	0.93195200	3.52073000
N	-1	-0.04102200	-0.17967800	2.61849500	N	-1	0.04128900	0.17881600	2.61976200
C	0	0.90667700	-5.44253600	2.48009600	C	0	-0.88063700	5.46401700	2.47924900
C	0	1.16492000	-3.93823600	2.35528700	C	0	-1.10761100	3.95504200	2.34343100
C	0	2.56786000	-3.51525400	2.80579000	C	0	-2.50006900	3.49885000	2.79518800
N	0	2.99418200	-2.33942300	2.01795200	N	0	-2.92783500	2.34965900	1.95973400
C	0	-2.02404600	1.21850000	-1.43391400	C	0	2.01055500	-1.23071300	-1.43538800
O	0	-2.17262500	0.83955100	-0.16606600	O	0	2.16337500	-0.85607800	-0.16727800

O	-1	-0.73423700	1.49953500	-1.65526300	O	-1	0.71765200	-1.50178000	-1.65615300
O	-1	-2.96498900	1.28636000	-2.26671300	O	-1	2.94923700	-1.30433500	-2.26984000
Fe	0	-0.06542700	1.18288800	0.21435300	Fe	0	0.05049000	-1.18662600	0.20860800
O	0	3.02838100	3.77799600	0.77900200	O	0	-3.05836400	-3.75248500	0.78316900
H	0	3.86656300	-1.09297200	-3.30375200	H	0	-3.87061600	1.11847700	-3.29954200
H	0	6.08112300	-0.48339000	0.32677100	H	0	-6.08192900	0.53010500	0.33567900
H	0	1.95639800	0.18582200	-2.35711800	H	0	-1.96861200	-0.17397700	-2.35624200
H	0	4.18399500	0.83127100	1.24732500	H	0	-4.19329900	-0.80080400	1.25313800
H	0	-4.55054900	0.12652600	-4.00556700	H	0	4.54305600	-0.15592300	-4.01058400
H	0	-6.19111900	0.75995300	-4.23205400	H	0	6.17955200	-0.79953200	-4.23790300
H	0	-5.87743900	-0.98024100	-4.42886600	H	0	5.87679200	0.94275900	-4.43321200
H	0	-4.65112300	1.07145600	-1.74760100	H	0	4.63788200	-1.10276200	-1.75296500
H	0	-5.75980100	4.12448800	1.47304700	H	0	5.73070600	-4.17100400	1.46027400
H	0	-4.20394700	3.52909400	2.02810500	H	0	4.18159200	-3.56437300	2.02234700
H	0	-6.39299300	1.88531200	0.65331900	H	0	6.38030000	-1.93547500	0.64555800
H	0	-6.06821000	1.90662500	2.41162600	H	0	6.05815000	-1.95652900	2.40438000
H	0	-3.70778000	1.20689200	0.83441800	H	0	3.70060300	-1.23726400	0.83220700
H	0	-3.15775300	-0.70201000	0.13436300	H	0	3.16361600	0.67544100	0.13409500
H	0	-4.20405100	-2.09474800	0.24592600	H	0	4.22137300	2.05932200	0.24027400
H	0	-6.91320800	-0.14123100	1.47309000	H	0	6.91888700	0.08505000	1.45741000
H	0	-6.45667000	-1.68450900	0.89637400	H	0	6.47139700	1.63238600	0.88553400
H	0	0.05852400	5.00158000	0.41094000	H	0	-0.09800000	-4.99998300	0.40773700
H	0	-2.36893300	-2.78652300	-3.50760900	H	0	2.36656000	2.78165300	-3.51058900
H	0	-2.67542900	-4.96612700	0.18228700	H	0	2.73342300	4.93447400	0.18938000
H	0	-0.97981700	-1.08206500	-2.37989000	H	0	0.97041600	1.08483000	-2.37939600
H	0	-1.33571800	-3.23695500	1.31067300	H	0	1.38807700	3.21226900	1.32023200
H	0	1.50499200	-4.98376700	-3.35944400	H	0	-1.48844700	5.00175500	-3.35329100
H	0	0.17898200	-3.84486400	-3.24229700	H	0	-0.15966300	3.86464400	-3.24902600
H	0	0.86196700	-3.98564400	-1.00493900	H	0	-0.82176200	3.99178300	-1.00642400
H	0	1.66609400	-2.52791600	-1.54332600	H	0	-1.64347300	2.54307000	-1.54267300
H	0	3.62833400	-4.37778500	-2.14777600	H	0	-3.59488000	4.40379400	-2.12179400

H	0	2.85637600	-5.18985000	-0.78259200	H	0	-2.80317700	5.21400200	-0.76922200
H	0	4.61011400	-3.80146600	-0.03281300	H	0	-4.55013100	3.83872600	0.00675500
H	0	4.04617600	-2.48530800	-0.83596000	H	0	-4.00534500	2.52778500	-0.79752200
H	0	3.45524600	5.60406400	-3.33087000	H	0	-3.50420500	-5.57658800	-3.32951900
H	0	4.76815500	6.59997500	-2.68865400	H	0	-4.82515900	-6.56156500	-2.68688400
H	0	5.06541800	5.50435600	-4.04910600	H	0	-5.11390800	-5.46282700	-4.04667200
H	0	3.44733400	3.01403200	-2.81713800	H	0	-3.47356300	-2.98686100	-2.81372300
H	0	5.02340300	2.89186800	-3.61498500	H	0	-5.04833900	-2.85137900	-3.61180300
H	0	4.81255400	2.31362500	-1.95126700	H	0	-4.83318400	-2.27515900	-1.94813300
H	0	1.91138300	0.71203100	2.77776300	H	0	-1.91940200	-0.69576200	2.77745100
H	0	-1.71757000	-1.31014200	3.31503300	H	0	1.72730700	1.29361300	3.31815300
H	0	-0.11657100	-5.65736500	2.14761700	H	0	0.13154300	5.70115000	2.12922900
H	0	1.57299200	-5.97781200	1.78806200	H	0	-1.57037100	5.99018300	1.80381800
H	0	0.42820600	-3.37151700	2.93730500	H	0	-0.35831800	3.39938500	2.91951400
H	0	1.03506600	-3.63961200	1.30835500	H	0	-0.97326200	3.67085900	1.29352200
H	0	3.29041400	-4.31949200	2.61110100	H	0	-3.23865000	4.29591300	2.64471700
H	0	2.58517900	-3.31511300	3.88302000	H	0	-2.50515900	3.23288700	3.85580300
H	0	-0.16422200	-1.12364500	1.10077100	H	0	0.19137200	1.10930100	1.10885900
H	0	2.30933000	-1.58646800	2.13267900	H	0	-2.23004300	1.60004700	2.01430800
H	0	3.86837200	-1.95789500	2.37782200	H	0	-3.79102200	1.93609500	2.31258600
H	0	2.62744900	2.92074500	0.55239300	H	0	-2.65212700	-2.89856100	0.55352600
H	0	2.30402200	4.41510400	0.62033200	H	0	-2.33943300	-4.39506900	0.62189700
C	-1	6.22921400	-1.78079300	-2.08828600	C	-1	-6.22218900	1.82952900	-2.07887600
H	0	6.77381500	-2.27410900	-1.27684200	H	0	-6.77613600	2.30721100	-1.26466200
H	0	5.84533500	-2.55342800	-2.76301000	H	0	-5.82722500	2.61577300	-2.73098400
H	0	6.96361700	-1.19754200	-2.65720000	H	0	-6.94883300	1.25925400	-2.67059100
C	-1	-3.35192500	-5.17940400	-2.49646300	C	-1	3.38299900	5.15863300	-2.49458300
H	0	-2.64004500	-5.90677000	-2.90338600	H	0	2.67376400	5.89350200	-2.89251300
H	0	-4.02041100	-5.71363000	-1.81541500	H	0	4.06097700	5.68419800	-1.81618300
H	0	-3.94250900	-4.79127900	-3.33130800	H	0	3.96396700	4.76988900	-3.33588200
C	-1	-5.89017000	-0.29372100	-2.36301700	C	-1	5.88574200	0.25448700	-2.36798800

H	0	-5.31354600	-1.16470500	-2.00262400	H	0	5.31500200	1.12893400	-2.00672100
H	0	-6.95105900	-0.52312900	-2.20066300	H	0	6.94816300	0.47676600	-2.20573200
C	-1	1.94101400	-3.01051700	-4.15826000	C	-1	-1.92738100	3.02975000	-4.15246300
H	0	3.03348200	-3.07342900	-4.09999700	H	0	-3.01930000	3.09194600	-4.08543500
H	0	1.65197600	-3.27171900	-5.18092000	H	0	-1.64585300	3.29208800	-5.17706300
H	0	1.65435100	-1.96847600	-3.98149200	H	0	-1.63948600	1.98736100	-3.97898900
C	-1	0.84995300	4.66759100	-1.36416000	C	-1	-0.88925100	-4.65846200	-1.36599200
H	0	-0.05116800	4.90279100	-1.94647500	H	0	0.00680800	-4.90552800	-1.95122600
H	0	1.72434700	5.04024200	-1.90320500	H	0	-1.77021000	-5.01977900	-1.90204200
H	0	0.93071100	3.57660200	-1.28378100	H	0	-0.95558500	-3.56656900	-1.28580500
C	-1	2.22298200	-0.53530900	5.54457100	C	-1	-2.21691100	0.54844300	5.54858700
H	0	1.87677500	-0.06896500	6.47468000	H	0	-1.86977100	0.06929200	6.47174800
H	0	2.53511500	-1.55653500	5.79743000	H	0	-2.51788100	1.56967200	5.81485600
H	0	3.10533200	0.01469500	5.20242000	H	0	-3.10645400	0.00991000	5.20670000
C	-1	1.11346500	-5.97125800	3.90082800	C	-1	-1.06961000	5.97756000	3.90820500
H	0	0.88178500	-7.03923900	3.96735300	H	0	-0.86481600	7.05073700	3.97629900
H	0	2.14842600	-5.83772900	4.23286700	H	0	-2.09329400	5.81500100	4.26234500
H	0	0.46923600	-5.44176000	4.61188500	H	0	-0.39610400	5.46075700	4.60114900
C	-1	-4.38765600	3.62827200	-0.13025000	C	-1	4.35711400	-3.65835200	-0.13688600
H	0	-4.07248300	4.67034800	-0.23450000	H	0	4.03343900	-4.69760200	-0.24365500
H	0	-3.50817900	3.01024200	-0.31382900	H	0	3.48163400	-3.03307900	-0.31498800
H	0	-5.11793000	3.40032700	-0.91261400	H	0	5.08625400	-3.43341500	-0.92114200
C	-1	-1.67926300	2.63559100	3.16929200	C	-1	1.65957800	-2.64877300	3.16642000
H	0	-0.82290000	2.22930000	3.71445000	H	0	0.80691800	-2.23491300	3.71156300
H	0	-2.28974500	3.26008100	3.82215400	H	0	2.26458900	-3.27868200	3.81917400
H	0	-2.25060900	1.77518700	2.81207700	H	0	2.23884700	-1.79368000	2.80911700
C	-1	-0.24912400	1.19965300	-4.75308600	C	-1	0.23139800	-1.19574900	-4.75319500
H	0	0.41496200	2.01147400	-4.44956000	H	0	-0.43655900	-2.00493100	-4.45107800
H	0	0.20592500	0.24562300	-4.46959600	H	0	-0.21916100	-0.24002900	-4.46821400
H	0	-1.20018200	1.30845700	-4.23054400	H	0	1.18199300	-1.30980300	-4.23092200
H	0	-0.39439100	1.22326100	-5.83659100	H	0	0.37652900	-1.21829000	-5.83673700

C	-1	4.89105500	4.48967000	-2.12388300	C	-1	-4.92976700	-4.45047900	-2.12118600
H	0	5.96750800	4.53105100	-1.90805900	H	0	-6.00645300	-4.48266600	-1.90497400
H	0	4.37378800	4.62967100	-1.16729800	H	0	-4.41348100	-4.59574300	-1.16484900
C	-1	3.18019900	5.61565700	3.49496800	C	-1	-3.22110200	-5.59365200	3.49486100
H	0	4.09072800	6.22129500	3.48005600	H	0	-4.13483700	-6.19430200	3.47574200
H	0	3.25318600	4.81520500	2.75730300	H	0	-3.28787600	-4.79075200	2.75928800
H	0	3.04316000	5.19731100	4.49634400	H	0	-3.08450000	-5.17903400	4.49785800
H	0	2.32353700	6.25000500	3.25186700	H	0	-2.36727600	-6.23197800	3.25221800
H	0	3.26771100	-2.93686700	0.58927600	H	0	-3.19200100	2.87693800	0.73013400

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C	0	-1.22145100	3.42450600	2.00212300
O	-1	-0.48582600	2.79249300	1.11407800
O	0	-1.46239100	4.62292600	1.87231000
C	0	5.10139600	-0.84649000	-1.58423800
C	0	3.92731500	-0.62869100	-2.32480800
C	0	5.17028900	-0.29073800	-0.29527700
C	0	2.84347800	0.06790300	-1.79580400
C	0	4.10088200	0.42105800	0.24447500
C	0	2.91328000	0.59943100	-0.49475000
O	-1	1.91710800	1.30755600	0.04120500
C	0	-5.63556900	-0.15596300	-3.82217900
O	0	-5.62860700	0.78844600	-1.55894800
C	0	-5.01520100	3.30615000	1.30076100
C	0	-5.63354800	1.91434900	1.44952300
N	0	-4.62186200	0.87046100	1.25244000
C	0	-4.93626400	-0.39919000	0.98488100
N	0	-3.97731700	-1.21377800	0.52483700
N	0	-6.15875400	-0.88562600	1.27281100
O	0	0.76480000	5.31566900	-0.08040900
C	0	-2.55857900	-4.08365900	-1.78483000

C	0	-2.09568000	-2.94531600	-2.47123300
C	0	-2.25299700	-4.15172900	-0.41439500
C	0	-1.31405800	-1.96277300	-1.85064400
C	0	-1.48420100	-3.17136100	0.22797900
C	0	-0.98001600	-2.08583600	-0.49864500
O	0	-0.12235000	-1.15856700	0.07257500
C	0	1.35433300	-3.93295400	-3.14599000
C	0	1.77049900	-3.60122600	-1.70085400
C	0	3.15474500	-4.14962900	-1.33921300
N	0	3.77866100	-3.38977500	-0.22919100
C	0	4.41908500	5.65838500	-3.14323200
C	0	4.47582400	3.15513100	-2.65025100
C	0	1.18505200	-0.54116000	4.46940400
C	0	1.17897300	0.08763100	3.22833400
N	0	0.00163100	-1.22495800	4.63213300
C	0	-0.68154900	-0.97198400	3.50580800
N	-1	-0.03219800	-0.18742300	2.61233600
C	0	1.02985300	-5.40364100	2.45681500
C	0	1.23595600	-3.88693600	2.37083300
C	0	2.61456100	-3.44161600	2.86464400
N	0	3.00690200	-2.19011800	2.14299500
C	0	-2.05927300	1.19256700	-1.42373100
O	0	-2.19179000	0.80370800	-0.15831900
O	-1	-0.77407500	1.49544600	-1.65179700
O	-1	-3.00539000	1.25384300	-2.25048600
Fe	0	-0.07911100	1.19369400	0.19403700
O	0	2.98328200	3.81271000	0.76908800
H	0	3.85426000	-1.03187100	-3.32949800
H	0	6.07224300	-0.42877000	0.29714700
H	0	1.93676200	0.22346600	-2.37253100
H	0	4.16441900	0.86762200	1.23224300

H	0	-4.57602600	0.06782700	-3.97855700
H	0	-6.22286100	0.68595600	-4.20232100
H	0	-5.89305100	-1.05114400	-4.40008900
H	0	-4.68541000	1.01555900	-1.72403600
H	0	-5.80509400	4.03116400	1.52665500
H	0	-4.23509700	3.45137100	2.05684100
H	0	-6.41647200	1.79128300	0.69009200
H	0	-6.07837100	1.80279000	2.44589700
H	0	-3.72104100	1.14440600	0.84640300
H	0	-3.14957400	-0.75434800	0.13597600
H	0	-4.18317700	-2.15584400	0.23070400
H	0	-6.90941800	-0.24450700	1.47463200
H	0	-6.43191300	-1.78141100	0.90012000
H	0	-0.00769700	4.99799500	0.42460100
H	0	-2.33103400	-2.82537100	-3.52558500
H	0	-2.60763500	-4.99607400	0.17207300
H	0	-0.95299000	-1.10461600	-2.40739100
H	0	-1.27668300	-3.25453900	1.28921200
H	0	1.64522400	-4.96545400	-3.38524700
H	0	0.26406000	-3.89909700	-3.21616200
H	0	1.03263800	-4.00152200	-0.99804200
H	0	1.76459500	-2.51436600	-1.56203600
H	0	3.80783300	-4.13357500	-2.22397900
H	0	3.06917200	-5.19797600	-1.03362100
H	0	4.58528200	-3.90762400	0.11742100
H	0	4.16434500	-2.53384100	-0.62798500
H	0	3.34783800	5.62009900	-3.37482300
H	0	4.63783800	6.65848100	-2.75325000
H	0	4.96029100	5.54158200	-4.09045100
H	0	3.39657700	3.04244800	-2.80760300
H	0	4.97459100	2.93955000	-3.60378200

H	0	4.77678000	2.38906100	-1.92955300
H	0	1.88701200	0.77538600	2.78121900
H	0	-1.67224100	-1.36649600	3.30546300
H	0	0.02409000	-5.63661300	2.08756500
H	0	1.73151400	-5.89552200	1.76943000
H	0	0.47438400	-3.35702500	2.95387900
H	0	1.12163400	-3.57804600	1.32597200
H	0	3.38281500	-4.18272300	2.62861700
H	0	2.62749000	-3.24564300	3.93710400
H	0	-0.15950400	-1.12438300	1.07268200
H	0	2.30159800	-1.44165500	2.29079700
H	0	3.89788900	-1.81342600	2.47072400
H	0	2.59656600	2.95364400	0.52558600
H	0	2.25076400	4.44146400	0.61425700
C	-1	6.23049700	-1.68849400	-2.13711300
H	0	6.79444900	-2.17520600	-1.33527500
H	0	5.85293700	-2.46726300	-2.80753100
H	0	6.94246400	-1.08440900	-2.71311400
C	-1	-3.30586500	-5.21584200	-2.49845800
H	0	-2.59590600	-5.94156300	-2.91150700
H	0	-3.96545600	-5.75073000	-1.80930100
H	0	-3.90640400	-4.83126300	-3.32784800
C	-1	-5.90937000	-0.36557000	-2.33420800
H	0	-5.32358600	-1.23095900	-1.97511100
H	0	-6.96763300	-0.60592000	-2.17060400
C	-1	1.94697900	-2.97004500	-4.18518700
H	0	3.04208700	-2.98247200	-4.17316900
H	0	1.62697000	-3.23415300	-5.19849600
H	0	1.62130200	-1.94307300	-3.98667400
C	-1	0.76870700	4.68383800	-1.36013300
H	0	-0.14887700	4.89836300	-1.92409900

H	0	1.62277500	5.08281600	-1.91284100
H	0	0.88028700	3.59475200	-1.28899500
C	-1	2.25410100	-0.52128500	5.52360500
H	0	1.91103900	-0.01120100	6.43142800
H	0	2.54635200	-1.53542000	5.82310700
H	0	3.14654800	0.00222300	5.16630000
C	-1	1.20854700	-5.96669500	3.86930700
H	0	1.00721800	-7.04206500	3.89464000
H	0	2.22928900	-5.81596400	4.23791700
H	0	0.52711700	-5.47853000	4.57506300
C	-1	-4.44676000	3.56956100	-0.09806500
H	0	-4.14632900	4.61662300	-0.19473100
H	0	-3.56227700	2.96454100	-0.30002100
H	0	-5.18416800	3.34080200	-0.87352000
C	-1	-1.70518800	2.60359300	3.18194600
H	0	-0.84023300	2.20937400	3.72216600
H	0	-2.32066200	3.21772800	3.83985600
H	0	-2.26670300	1.73627400	2.82573900
C	-1	-0.30370600	1.21178200	-4.75341700
H	0	0.35306900	2.02938200	-4.44937700
H	0	0.15631000	0.26222000	-4.46336000
H	0	-1.25864000	1.31623000	-4.23698500
H	0	-0.44300800	1.23015500	-5.83780300
C	-1	4.80712700	4.56325200	-2.14475200
H	0	5.88205000	4.63313200	-1.92873000
H	0	4.28520300	4.71145400	-1.19183200
C	-1	3.11522500	5.64845000	3.48783400
H	0	4.01625300	6.26812900	3.47684800
H	0	3.20429300	4.84852700	2.75137000
H	0	2.97933100	5.22946600	4.48913600
H	0	2.25009900	6.26893300	3.23908100

H 0 3.13200400 -2.48256400 1.12243300

3.2 C-Lobe

	TfC ^{Phys}					TfC ^{Acid}			
C	0	5.48867100	-1.26319700	3.16143500	C	0	5.48528700	-1.08017200	3.18203800
O	0	6.61021000	-1.00972200	3.61393900	O	0	6.60391000	-0.77421400	3.60569400
C	0	4.37432100	0.83672200	2.17005400	C	0	4.30849100	0.96524800	2.15058800
C	0	4.65685500	0.28596600	0.75726500	C	0	4.61787700	0.39371900	0.75557700
O	-1	3.69755400	-0.31725600	0.13472100	O	-1	3.67926100	-0.25678100	0.13739000
O	0	5.80636600	0.41666700	0.30593800	O	0	5.76062600	0.54081700	0.30176800
N	0	5.17974600	-2.43873300	2.54317000	N	0	5.20324700	-2.28480700	2.60848400
C	0	-2.16568300	-4.37014300	-1.80319400	C	0	-2.09168900	-4.47930900	-1.70864200
C	0	-1.42970800	-4.67079800	-0.64468400	C	0	-1.36729100	-4.71800300	-0.52866400
C	0	-1.71952100	-3.29985300	-2.59396900	C	0	-1.64723500	-3.43725800	-2.54058400
C	0	-0.29566700	-3.94435100	-0.29669300	C	0	-0.24721300	-3.95982000	-0.19767600
C	0	-0.58950600	-2.55362000	-2.25285700	C	0	-0.53205300	-2.66261400	-2.21851500
C	0	0.15436200	-2.87252900	-1.09867900	C	0	0.20078600	-2.91986100	-1.04118800
O	-1	1.27058600	-2.21295000	-0.78303800	O	-1	1.30214300	-2.23137400	-0.74376400
C	0	5.47754000	3.77566600	-0.16391000	C	0	5.37654900	3.87631400	-0.25565500
C	0	4.39252800	4.84448800	0.01088200	C	0	4.26730100	4.92249600	-0.10629200
N	0	3.06309600	4.23622500	0.06478600	N	0	2.95312500	4.28092900	-0.04619400
C	0	1.91687200	4.90736600	0.08870900	C	0	1.79170300	4.92271500	-0.01100700
N	0	1.90429900	6.26165900	0.06729700	N	0	1.74137900	6.27318900	-0.05074600
N	0	0.75886300	4.23131000	0.15644700	N	0	0.65113200	4.21677600	0.09324700
C	0	3.63927300	-1.91577200	-3.40482200	C	0	3.66437400	-1.88683800	-3.32837100
O	0	4.85523600	-3.54749500	-2.01972800	O	0	4.89915400	-3.51872100	-1.96002200
C	0	-2.65840500	3.88819100	-1.63242300	C	0	-2.76985200	3.75293900	-1.74839900
C	0	-1.89960700	3.08108000	-2.49787500	C	0	-2.00787200	2.92772300	-2.59569300
C	0	-2.65756200	3.54533000	-0.27205600	C	0	-2.73974600	3.46113700	-0.37664700

C	0	-1.22112500	1.94853600	-2.04885100	C	0	-1.30006800	1.82742600	-2.11680600
C	0	-1.96843000	2.42718400	0.19454200	C	0	-2.02422000	2.37057300	0.11996700
C	0	-1.26797500	1.57350200	-0.68765000	C	0	-1.32063100	1.49426400	-0.74128500
O	-1	-0.71402400	0.45914900	-0.21554500	O	-1	-0.74810700	0.40514900	-0.24739700
C	0	-4.36805700	0.70443600	-3.47405800	C	0	-4.39954300	0.44065500	-3.42169000
C	0	-4.81683000	0.57509600	-2.01616700	C	0	-4.67716200	0.34234600	-1.91590400
C	0	-5.77985800	1.66894000	-1.53643700	C	0	-5.54953700	1.48432300	-1.40350500
N	0	-6.23975800	1.53846000	-0.14777800	N	0	-5.68891100	1.44457600	0.09242000
C	0	0.72213500	-1.06432500	3.92091000	C	0	0.71214400	-0.97999600	3.93219800
C	0	0.96742300	-1.34565500	2.58985800	C	0	0.91260800	-1.30374300	2.60331900
N	0	0.35738800	0.26731900	4.03188700	N	0	0.40003800	0.36708200	4.01700500
C	0	0.40135600	0.73305700	2.77770900	C	0	0.43672100	0.80135200	2.75122000
N	-1	0.75648300	-0.19248000	1.85397100	N	-1	0.72885000	-0.16171800	1.84241000
C	0	-3.21966700	1.19721000	3.36811000	C	0	-3.14256700	1.18997400	3.44794800
C	0	-2.93435700	-0.06407800	2.55620500	C	0	-2.78131800	-0.04534700	2.62764200
N	0	-4.09733200	-0.49870900	1.76904200	N	0	-3.91556000	-0.47837100	1.78249800
C	0	-3.97570800	-1.32735300	0.72178500	C	0	-3.74976100	-1.43604800	0.83010300
N	0	-2.79421100	-1.50909400	0.11367500	N	0	-2.59923000	-1.57406900	0.18806600
N	0	-5.05913600	-2.01475100	0.30775400	N	0	-4.81125500	-2.21196300	0.55611100
C	0	-7.75063600	-0.70715200	2.08157300	C	0	-7.85825500	-0.45893000	1.85753900
O	0	-6.79583200	-0.36040800	2.82749100	O	0	-6.84550600	-1.08182700	2.27969700
O	0	-7.63158100	-1.21498000	0.92112000	O	0	-7.85547800	0.38460100	0.89786300
C	0	1.93121600	1.64688600	-1.70982700	C	0	1.85019000	1.62065000	-1.77398400
O	0	1.85142400	1.80442100	-0.37392500	O	0	1.79484300	1.80405500	-0.43798200
O	0	1.60965100	0.42260000	-2.05069900	O	0	1.56772500	0.37559200	-2.07813400
O	0	2.24974300	2.55967400	-2.47680100	O	0	2.12172500	2.52549700	-2.56512000
Fe	0	1.23201900	-0.18081600	-0.17000000	Fe	0	1.31791900	-0.19465000	-0.16417900
O	0	3.51134700	-2.97281200	0.31154100	O	0	3.55758100	-2.93671800	0.38339300
H	0	5.17406600	1.54149700	2.41351700	H	0	5.08222700	1.70282100	2.37851200
H	0	3.41387400	1.36193300	2.17393000	H	0	3.33071400	1.45728400	2.13834700
H	0	4.27966900	-2.53435900	2.08161000	H	0	4.29872600	-2.42147200	2.16863800

H	0	-1.75762600	-5.48583400	-0.00213000	H	0	-1.69000600	-5.51116800	0.14284000
H	0	-2.26370000	-3.04655500	-3.49973500	H	0	-2.17856800	-3.23595600	-3.46681100
H	0	0.26268700	-4.18212200	0.60409100	H	0	0.30156700	-4.15168600	0.71957400
H	0	-0.25904800	-1.72028500	-2.86511800	H	0	-0.19658400	-1.85621400	-2.86278000
H	0	6.44160300	4.25141900	0.05235100	H	0	6.32987900	4.38129500	-0.06062000
H	0	5.34247900	2.99795400	0.59334200	H	0	5.26504800	3.11837600	0.52536600
H	0	4.44035800	5.55711400	-0.82541900	H	0	4.30111800	5.61813600	-0.95733400
H	0	4.56821300	5.40467400	0.93982500	H	0	4.42320100	5.50493600	0.81190800
H	0	2.94601800	3.22138100	-0.07834100	H	0	2.86323500	3.26287200	-0.17705800
H	0	2.76198600	6.76892100	0.21426900	H	0	2.58877400	6.81169900	0.02621300
H	0	1.05678600	6.73931200	0.33172600	H	0	0.88733500	6.73933700	0.21222900
H	0	0.84268700	3.21978400	-0.03074700	H	0	0.76148500	3.20601900	-0.07966700
H	0	-0.10528300	4.67664100	-0.11945300	H	0	-0.21877900	4.63162300	-0.21034700
H	0	2.73434600	-1.99474900	-2.79762600	H	0	2.76939900	-1.95622400	-2.70610000
H	0	3.68260600	-0.89479000	-3.79647100	H	0	3.70483100	-0.86825700	-3.72666300
H	0	3.56057700	-2.61450100	-4.24631300	H	0	3.56632800	-2.58889900	-4.16483400
H	0	4.35412900	-3.48437500	-1.17762600	H	0	4.40396800	-3.45569800	-1.11596900
H	0	-3.21671700	4.15675500	0.43416400	H	0	-3.28653100	4.09800200	0.31814100
H	0	-1.85320100	3.33539300	-3.55507000	H	0	-1.98153300	3.14510000	-3.66160900
H	0	-1.95387700	2.19305200	1.25018000	H	0	-1.97692000	2.18447300	1.18487100
H	0	-0.63684600	1.33561200	-2.72542100	H	0	-0.71209900	1.20385100	-2.78048300
H	0	-5.24367500	0.66957300	-4.13837800	H	0	-5.33527700	0.32574300	-3.98451700
H	0	-3.90173200	1.68579500	-3.61943400	H	0	-4.01630900	1.44345600	-3.64111000
H	0	-3.92858400	0.59088200	-1.37290300	H	0	-3.71704800	0.38180200	-1.39146600
H	0	-5.29695000	-0.40171100	-1.86855300	H	0	-5.14361000	-0.62078600	-1.67577500
H	0	-6.66502800	1.69381000	-2.18809900	H	0	-6.55948500	1.44766000	-1.82151000
H	0	-5.28527200	2.64252600	-1.64481900	H	0	-5.09244500	2.43692700	-1.67309000
H	0	-6.73931000	0.65524800	-0.03230200	H	0	-6.60819500	0.85505600	0.45166300
H	0	-5.42525200	1.45319700	0.45936800	H	0	-4.84323100	1.06192300	0.53507800
H	0	1.30424700	-2.25375600	2.10841800	H	0	1.20548400	-2.23628200	2.14052200
H	0	0.16414400	1.75201100	2.49750900	H	0	0.23800500	1.82325400	2.45124800

H	0	-2.25403700	1.52873400	3.76600300	H	0	-2.22649200	1.48494400	3.97002400
H	0	-3.58729900	1.98195400	2.69516700	H	0	-3.40866200	2.01127800	2.77022800
H	0	-2.61814500	-0.87179600	3.23087500	H	0	-2.48197900	-0.86407000	3.29403800
H	0	-2.09359500	0.12615100	1.88870200	H	0	-1.92708100	0.17023500	1.98699900
H	0	-5.04111300	-0.45591300	2.19690000	H	0	-4.82415300	-0.55401900	2.24567400
H	0	-6.01758000	-1.71454100	0.61631500	H	0	-5.68303200	-2.03599400	1.06390200
H	0	-5.00912100	-2.40606500	-0.62181000	H	0	-4.81275800	-2.79916800	-0.26320700
H	0	-2.01790400	-0.84195600	0.19149300	H	0	-1.85897900	-0.83816900	0.17784700
H	0	-2.73072200	-2.15154300	-0.66476200	H	0	-2.50697100	-2.30100300	-0.51152000
H	0	3.74936000	-2.01528800	0.20511800	H	0	3.78501800	-1.98228400	0.25834200
H	0	2.58416000	-2.92719400	-0.02945000	H	0	2.63426300	-2.91668700	0.03425800
C	-1	4.32762600	-0.26109700	3.26715500	C	-1	4.29458600	-0.11115600	3.26987400
H	0	4.39283000	0.21015900	4.25195100	H	0	4.34606200	0.38316000	4.24389800
H	0	3.36820600	-0.78227600	3.20627200	H	0	3.35026800	-0.66072100	3.22049700
C	-1	6.15935500	-3.45814800	2.17056000	C	-1	6.20672800	-3.28853000	2.25652000
H	0	7.14871100	-3.11069000	2.47261800	H	0	7.19029300	-2.89645600	2.52004700
H	0	5.94551400	-4.41122300	2.66830000	H	0	6.03558500	-4.22474400	2.80031000
H	0	6.13531600	-3.61217000	1.08723900	H	0	6.16344800	-3.49057900	1.18190900
C	-1	0.86806200	-1.98264600	5.10791100	C	-1	0.86936100	-1.87092500	5.13851900
H	0	1.65256500	-1.63216100	5.79094000	H	0	1.70931700	-1.54752400	5.76624000
H	0	-0.05913000	-2.05031000	5.69067400	H	0	-0.02635900	-1.86577200	5.77196800
H	0	1.13666300	-2.99169300	4.77975600	H	0	1.06128400	-2.90301800	4.82936800
C	-1	-4.20451700	0.99211200	4.51818500	C	-1	-4.27024900	0.96656200	4.45949800
H	0	-4.31616500	1.91349500	5.10071100	H	0	-4.44872900	1.87114700	5.04908500
H	0	-5.19707100	0.69746200	4.16573900	H	0	-5.21981900	0.69895000	3.98009800
H	0	-3.84188000	0.21303300	5.19957500	H	0	-4.01364900	0.15973900	5.15489400
C	-1	-9.19980200	-0.48444600	2.58380100	C	-1	-9.22063400	-0.67480700	2.54263600
H	0	-9.63343800	0.36563900	2.04537000	H	0	-9.40877200	0.16616800	3.21900100
H	0	-9.81209200	-1.36300200	2.36141400	H	0	-10.01858700	-0.68681600	1.79677600
H	0	-9.21650300	-0.27114300	3.65452000	H	0	-9.22100600	-1.59920300	3.12244700
C	-1	-3.50190400	5.03522500	-2.14606600	C	-1	-3.63624700	4.86590100	-2.29663400

H	0	-4.48316500	4.68349300	-2.49074500	H	0	-4.57050700	4.47833700	-2.72516400
H	0	-3.68417100	5.78125000	-1.36547200	H	0	-3.91054600	5.58277700	-1.51595900
H	0	-3.02600800	5.53999500	-2.99408900	H	0	-3.12951700	5.41649100	-3.09672500
C	-1	1.34160200	-0.21625400	-5.44444700	C	-1	1.34514200	-0.34481500	-5.45116000
H	0	0.55654000	0.35916500	-5.94387700	H	0	0.47590800	0.08192000	-5.96053000
H	0	2.25886100	-0.17170400	-6.03716300	H	0	2.22798000	-0.23539000	-6.08613500
H	0	1.52606300	0.18540300	-4.44680000	H	0	1.50908000	0.15996000	-4.49713600
H	0	1.02485400	-1.25891100	-5.35350800	H	0	1.17102000	-1.40706400	-5.26024900
C	-1	-3.37401100	-0.39671800	-3.86061600	C	-1	-3.37146400	-0.60057500	-3.88069400
H	0	-3.01252700	-0.28411900	-4.88884600	H	0	-3.13570800	-0.48808100	-4.94344500
H	0	-2.50564200	-0.38435300	-3.19441100	H	0	-2.44196000	-0.50414200	-3.31239900
H	0	-3.84077400	-1.38500900	-3.77529100	H	0	-3.75112300	-1.61630700	-3.72610700
C	-1	-3.37751200	-5.18863300	-2.18448200	C	-1	-3.26764400	-5.35003800	-2.09081400
H	0	-3.09728600	-6.19365300	-2.52529100	H	0	-2.94115900	-6.26196600	-2.60721500
H	0	-4.05885000	-5.31899500	-1.33535100	H	0	-3.83710000	-5.66850600	-1.21055200
H	0	-3.94077000	-4.71537800	-2.99543600	H	0	-3.95286500	-4.82726500	-2.76681400
C	-1	4.87424900	-2.22265300	-2.56149200	C	-1	4.91246900	-2.19693100	-2.50830400
H	0	4.96984800	-1.47612100	-1.76105300	H	0	5.02410000	-1.44533300	-1.71539700
H	0	5.77832500	-2.14993700	-3.18394400	H	0	5.80544200	-2.13093700	-3.14656900
C	-1	1.71581800	-5.06670700	-3.29413200	C	-1	1.82596600	-5.13246400	-3.18444800
H	0	1.06458600	-5.40376200	-2.48480800	H	0	1.18337200	-5.40489700	-2.34432300
H	0	1.91403700	-5.89347600	-3.98266000	H	0	2.06416100	-6.02209200	-3.77476600
H	0	1.21495000	-4.25401400	-3.82286300	H	0	1.29588600	-4.40750600	-3.80507800
H	0	2.65587600	-4.69320400	-2.88079600	H	0	2.74673900	-4.67725700	-2.81082700
C	-1	5.51000500	3.13182400	-1.55481300	C	-1	5.41597000	3.19364200	-1.62728000
H	0	6.20665600	2.29081900	-1.55809100	H	0	6.13812400	2.37461000	-1.61034700
H	0	4.53005400	2.74460700	-1.84545500	H	0	4.44567700	2.76895600	-1.89960000
H	0	5.81931500	3.86033600	-2.31458600	H	0	5.69801600	3.90766700	-2.41061000
					H	0	-5.80888000	2.38786900	0.46181500

TfC _{X517H²}					TfC _{R632H^{Acid}}				
C	0	5.45403500	-1.00349200	3.18088000	C	0	5.47097600	-1.07355300	3.17007300
O	0	6.57689400	-0.67931400	3.57635200	O	0	6.60618000	-0.77734400	3.54876200
C	0	4.30108100	1.01796800	2.10214500	C	0	4.43883200	0.95519000	2.03790800
C	0	4.60068300	0.41566600	0.72375800	C	0	4.67222000	0.31146600	0.66676300
O	-1	3.65038300	-0.25662400	0.11931100	O	-1	3.66138000	-0.32164500	0.09505900
O	0	5.72507100	0.53822500	0.23861600	O	0	5.77417100	0.36521600	0.13498200
N	0	5.17035700	-2.22369100	2.64210800	N	0	5.14892100	-2.28882500	2.64230700
C	0	-2.11727500	-4.52248600	-1.63335600	C	0	-2.24823000	-4.44715600	-1.51234200
C	0	-1.39851300	-4.72850600	-0.44479100	C	0	-1.49965100	-4.67833600	-0.34574900
C	0	-1.67180600	-3.50366900	-2.49024000	C	0	-1.80870000	-3.42719700	-2.37188600
C	0	-0.28124700	-3.96125100	-0.13027100	C	0	-0.36062400	-3.93423200	-0.05604000
C	0	-0.56020600	-2.71631000	-2.18290000	C	0	-0.67575300	-2.65943600	-2.08711500
C	0	0.16321900	-2.94187200	-0.99686200	C	0	0.07493200	-2.91388000	-0.92632600
O	-1	1.26985200	-2.24923600	-0.71063600	O	-1	1.21312600	-2.25658200	-0.66863300
C	0	5.38219900	3.87813700	-0.38713000	C	0	5.56852400	3.71026600	-0.49222400
C	0	4.27442900	4.92915800	-0.24955800	C	0	4.50790600	4.79758500	-0.29310500
N	0	2.96336300	4.29445700	-0.09487400	N	0	3.17619400	4.21221700	-0.11595600
C	0	1.80080700	4.93744000	-0.09114500	C	0	2.04724600	4.91034900	-0.02890400
N	0	1.75002800	6.28003000	-0.22771000	N	0	2.06125200	6.25601400	-0.09037300
N	0	0.66041200	4.24362200	0.08384700	N	0	0.88300100	4.26270100	0.16012800
C	0	3.60946500	-2.00924900	-3.27720000	C	0	3.52773200	-2.09401000	-3.24887200
O	0	4.93624700	-3.59100400	-1.93608700	O	0	4.82209500	-3.75941100	-1.97959200
C	0	-2.78907000	3.72363700	-1.85831700	C	0	-2.68760900	3.81184000	-1.872444000
C	0	-2.01346500	2.88982600	-2.68062400	C	0	-2.01251500	2.88506400	-2.68337000
C	0	-2.79173900	3.45838200	-0.48088600	C	0	-2.60170300	3.64109700	-0.48410800
C	0	-1.32401200	1.79140400	-2.16796200	C	0	-1.33884400	1.79283700	-2.14257300
C	0	-2.09606100	2.36803000	0.04620100	C	0	-1.91789900	2.55732600	0.07758700
C	0	-1.39096300	1.49923000	-0.79861500	C	0	-1.32131200	1.60859500	-0.75720300
O	-1	-0.77587000	0.40270600	-0.28231200	O	-1	-0.74545200	0.46269800	-0.26890500
C	0	-4.41773600	0.35310300	-3.41255300	C	0	-4.45461200	0.48660700	-3.49679700

C	0	-4.69880100	0.23386100	-1.90884000	C	0	-4.88893300	0.45690800	-2.02870600
C	0	-5.51976900	1.40292300	-1.37240700	C	0	-5.83912100	1.59365600	-1.62575700
N	0	-5.64422700	1.36463900	0.12226000	N	0	-6.29146100	1.58151600	-0.22992600
C	0	0.71288600	-0.86608700	3.93621200	C	0	0.80993500	-0.77964800	3.95020100
C	0	0.80339000	-1.24709000	2.61231800	C	0	0.64840000	-1.18284600	2.64177200
N	0	0.54883400	0.50930100	3.99091600	N	0	0.98470400	0.59788000	3.97974100
C	0	0.56423600	0.90326900	2.71306800	C	0	0.94904700	0.97092500	2.70667500
N	-1	0.70022200	-0.11262100	1.82139800	N	-1	0.73510900	-0.05784300	1.82589200
C	0	-3.09897000	1.25576800	3.47506100	C	0	-3.30461200	1.44121400	3.20388900
C	0	-2.77350000	-0.00631100	2.68482800	C	0	-3.04406200	0.10521300	2.50577700
N	0	-3.89560500	-0.40621200	1.81606800	N	0	-4.22278800	-0.40574700	1.79992200
C	0	-3.65713400	-1.38797100	0.85753500	C	0	-4.13773700	-1.32831200	0.83215200
N	0	-2.51039300	-1.43829700	0.25167200	N	0	-2.95754000	-1.62194100	0.25085400
N	0	-4.72280700	-2.20979500	0.62237000	N	0	-5.23979000	-2.00249600	0.47090300
C	0	-7.88555200	-0.40751000	1.85098800	C	0	-7.78644200	-0.48828600	2.14975700
O	0	-6.88584200	-1.03380400	2.28425000	O	0	-6.80703700	-0.12946700	2.85894300
O	0	-7.87633100	0.42151500	0.87471900	O	0	-7.70118700	-1.06179300	1.01631200
C	0	1.79058200	1.63403600	-1.68761100	C	0	1.81472300	1.58823900	-1.70175700
O	0	1.75971700	1.79408000	-0.35002300	O	0	1.80254700	1.72695700	-0.36292900
O	0	1.60034500	0.37350600	-2.00345700	O	0	1.65681600	0.32158100	-2.03261000
O	0	1.97041500	2.56491600	-2.47374900	O	0	1.96328500	2.52643800	-2.48113200
Fe	0	1.54194700	-0.26742900	-0.10305400	Fe	0	1.72202000	-0.35923500	-0.16669400
O	0	3.54847300	-3.02318800	0.39650900	O	0	3.50025400	-3.16030600	0.41300600
H	0	5.09110700	1.74313900	2.31078100	H	0	5.29493200	1.60768800	2.22297300
H	0	3.33418100	1.52983900	2.07485700	H	0	3.52590800	1.55640000	2.00074700
H	0	4.24941300	-2.39048200	2.25356200	H	0	4.20681500	-2.45135200	2.31060400
H	0	-1.72386900	-5.50272700	0.24709800	H	0	-1.81674400	-5.45594800	0.34550000
H	0	-2.20195200	-3.32508000	-3.42176800	H	0	-2.35807600	-3.23256500	-3.28812400
H	0	0.26616600	-4.13183500	0.79182900	H	0	0.22038400	-4.13469300	0.83941000
H	0	-0.22805700	-1.92426100	-2.84638900	H	0	-0.34007800	-1.87637000	-2.75953400
H	0	6.33842900	4.39177000	-0.23490200	H	0	6.54802800	4.19064800	-0.38887000

H	0	5.29273000	3.15216900	0.42693300	H	0	5.49852800	2.98331200	0.32253500
H	0	4.27029100	5.57344300	-1.14049700	H	0	4.50256500	5.46546100	-1.16623600
H	0	4.46779100	5.56370600	0.62559000	H	0	4.75163600	5.39889200	0.59249900
H	0	2.87189000	3.27335700	-0.16655900	H	0	3.03927200	3.20318900	-0.22289000
H	0	2.59697300	6.82439600	-0.21347800	H	0	2.93059100	6.76273500	-0.12075200
H	0	0.89704300	6.76598400	0.00037800	H	0	1.23542900	6.77667800	0.15871300
H	0	0.76487600	3.22373800	-0.03157700	H	0	0.92670400	3.24789700	-0.00654200
H	0	-0.20827000	4.64403400	-0.24206300	H	0	0.01896200	4.72149200	-0.09263600
H	0	2.72641500	-2.10920200	-2.64197600	H	0	2.64837400	-2.18164200	-2.60717300
H	0	3.60700700	-0.99207200	-3.68062500	H	0	3.55300000	-1.06719300	-3.62534500
H	0	3.52691100	-2.72010000	-4.10709600	H	0	3.41133600	-2.77979200	-4.09487800
H	0	4.42173100	-3.56665400	-1.10412000	H	0	4.32467500	-3.74952500	-1.13969200
H	0	-3.35685000	4.10433400	0.18875800	H	0	-3.09540400	4.34987000	0.17621800
H	0	-1.96741000	3.08992900	-3.74835200	H	0	-2.02300400	3.01367900	-3.76243400
H	0	-2.08164600	2.17864700	1.11101100	H	0	-1.85610800	2.44744700	1.15391400
H	0	-0.73136400	1.14433300	-2.80363000	H	0	-0.81044300	1.08283200	-2.76730500
H	0	-5.35296100	0.26010900	-3.98047100	H	0	-5.33639000	0.39155300	-4.14567100
H	0	-4.02149900	1.35441200	-3.61701600	H	0	-4.01056900	1.46388700	-3.71867100
H	0	-3.74122100	0.21206800	-1.38091300	H	0	-3.99529500	0.50953100	-1.39306900
H	0	-5.20570500	-0.71252400	-1.68565700	H	0	-5.37334600	-0.50352900	-1.80797000
H	0	-6.53536300	1.40537800	-1.77982400	H	0	-6.72789700	1.57492000	-2.27167900
H	0	-5.03567000	2.34008300	-1.64862400	H	0	-5.33807400	2.55154800	-1.81761400
H	0	-6.60849700	0.83791100	0.46715500	H	0	-6.80951700	0.72200400	-0.04289700
H	0	-4.83511300	0.91000500	0.58271500	H	0	-5.47772300	1.53110500	0.38115900
H	0	0.94237700	-2.22294200	2.16807300	H	0	0.48242200	-2.16290000	2.21850300
H	0	0.46819000	1.93231000	2.38884600	H	0	1.06666300	1.98994400	2.35822100
H	0	-2.20032000	1.51137200	4.04737100	H	0	-2.32376800	1.84432400	3.48678900
H	0	-3.28852000	2.08512500	2.78106700	H	0	-3.74276400	2.13872200	2.47934200
H	0	-2.52291400	-0.82104000	3.37885300	H	0	-2.68496600	-0.63608200	3.23347500
H	0	-1.89326000	0.15150600	2.06639200	H	0	-2.23635000	0.24746900	1.78886900
H	0	-4.76897800	-0.57418500	2.31439100	H	0	-5.16717100	-0.29476100	2.23378000

H	0	-5.61744400	-1.98152600	1.05646300	H	0	-6.19692700	-1.63939800	0.74738400
H	0	-4.72539900	-2.75347300	-0.22643900	H	0	-5.19632300	-2.50095400	-0.40618000
H	0	-2.45340400	-2.19067100	-0.42806800	H	0	-2.18380800	-0.96821200	0.25590600
H	0	3.83025100	-2.09350900	0.26452000	H	0	-2.92885000	-2.30049000	-0.49863500
H	0	2.62947800	-2.97319200	0.03751500	H	0	3.84206700	-2.25743700	0.27184600
C	-1	4.26616200	-0.03133700	3.24697900	H	0	2.58372200	-3.06980500	0.06466200
H	0	4.31544100	0.48977200	4.20629800	C	-1	4.32050900	-0.05600800	3.21078000
H	0	3.31617000	-0.57258600	3.20606600	H	0	4.37511600	0.48916100	4.15525900
C	-1	6.17283300	-3.23703000	2.31583400	H	0	3.34896800	-0.55604400	3.16459400
H	0	7.15708300	-2.82928900	2.55060200	C	-1	6.11959700	-3.33439900	2.32016900
H	0	6.01352200	-4.15090000	2.89906700	H	0	7.12081500	-2.92055400	2.44849500
H	0	6.11681900	-3.48201600	1.25102500	H	0	6.00453100	-4.20145100	2.98038500
C	-1	0.83807900	-1.73651500	5.16044000	H	0	5.97932400	-3.65523500	1.28464800
H	0	1.73033600	-1.47633100	5.74360800	C	-1	0.86631500	-1.62092300	5.19536300
H	0	-0.02573800	-1.63124600	5.82845000	H	0	1.84863200	-1.54227500	5.67644000
H	0	0.91923800	-2.78938900	4.87368700	H	0	0.11907300	-1.30329200	5.93196600
C	-1	-4.29675100	1.09126100	4.40861500	H	0	0.68777800	-2.67407800	4.95930300
H	0	-4.46939000	1.99840000	4.99725200	C	-1	-4.19085700	1.34502000	4.44660300
H	0	-5.22318500	0.87765800	3.86257000	H	0	-4.28930100	2.32456000	4.92585200
H	0	-4.13323000	0.26619200	5.11156400	H	0	-5.19525100	0.98781200	4.20086400
C	-1	-9.25000100	-0.59055100	2.53477600	H	0	-3.75276500	0.65747600	5.17935200
H	0	-9.45075600	0.28590100	3.16081400	C	-1	-9.21400700	-0.22236200	2.66130700
H	0	-10.04250800	-0.64764300	1.78443600	H	0	-9.72835400	0.44161200	1.95907100
H	0	-9.25402800	-1.48228800	3.16383100	H	0	-9.77291800	-1.16286900	2.68891100
C	-1	-3.65656400	4.81403000	-2.44581000	H	0	-9.20329800	0.23306600	3.65342000
H	0	-4.59898200	4.40289700	-2.83045000	C	-1	-3.52106100	4.91683500	-2.48505100
H	0	-3.91294200	5.57204400	-1.69910900	H	0	-4.49348400	4.53222300	-2.81576100
H	0	-3.16303300	5.31572300	-3.28449300	H	0	-3.71469400	5.71995600	-1.76784800
C	-1	1.31575000	-0.48472800	-5.46507000	H	0	-3.02939500	5.35090800	-3.36184300
H	0	0.41837900	-0.11770000	-5.97159600	C	-1	1.25499500	-0.58508700	-5.45739200
H	0	2.19504800	-0.25892300	-6.07350500	H	0	0.39873600	-0.16372000	-5.99161100

H	0	1.41554300	-0.01087600	-4.48622100	H	0	2.15217900	-0.48865500	-6.07374300
H	0	1.24148300	-1.56643100	-5.32802400	H	0	1.40243700	-0.06100300	-4.51067800
C	-1	-3.40121700	-0.69188500	-3.88837600	H	0	1.07292900	-1.64305400	-5.25225300
H	0	-3.16654300	-0.56842400	-4.95042000	C	-1	-3.44686000	-0.62065100	-3.82411600
H	0	-2.46947400	-0.61475900	-3.32045400	H	0	-3.09216700	-0.56176800	-4.85885300
H	0	-3.78939000	-1.70593800	-3.74476000	H	0	-2.57611000	-0.56357700	-3.16411200
C	-1	-3.30531300	-5.39380000	-1.97670600	H	0	-3.90123700	-1.60777100	-3.68177700
H	0	-2.99089200	-6.37449700	-2.35625700	C	-1	-3.46867000	-5.28646200	-1.82350800
H	0	-3.93444100	-5.57811500	-1.09846500	H	0	-3.18970400	-6.30743600	-2.11130200
H	0	-3.93045000	-4.93308700	-2.74868600	H	0	-4.12985700	-5.36815800	-0.95334200
C	-1	4.88011800	-2.26642800	-2.47551500	H	0	-4.04738100	-4.85982400	-2.64849000
H	0	4.97858500	-1.51197900	-1.68339400	C	-1	4.80011100	-2.41626000	-2.47420000
H	0	5.75893400	-2.16028000	-3.12705100	H	0	4.93672900	-1.69165000	-1.65929100
C	-1	1.78858300	-5.21316000	-3.07569000	H	0	5.67233100	-2.31620300	-3.13433000
H	0	1.13841100	-5.43189200	-2.22602900	C	-1	1.61511800	-5.27957300	-2.98288100
H	0	1.96647600	-6.12474000	-3.65358400	H	0	1.03605600	-5.53255600	-2.09197100
H	0	1.29827800	-4.46629900	-3.70275300	H	0	1.73726300	-6.16743200	-3.60951700
H	0	2.73916800	-4.80962100	-2.71894300	H	0	1.07939100	-4.50644500	-3.53677500
C	-1	5.39283800	3.14420400	-1.73376500	H	0	2.59537500	-4.89583600	-2.69047500
H	0	6.11454100	2.32536300	-1.70531800	C	-1	5.48248000	2.98965600	-1.84251100
H	0	4.41402800	2.71421900	-1.96725800	H	0	6.18899200	2.15741300	-1.87061200
H	0	5.65679200	3.82913600	-2.54818600	H	0	4.48341800	2.58019100	-2.02339300
H	0	-5.69421200	2.31152500	0.49723100	H	0	5.70930800	3.67742700	-2.66529300
H	0	-1.46364200	-0.32685600	0.02478000	H	0	-0.41975000	0.51991500	0.66889100