

## Supporting Information

### Mechanistic insights into iron catalyzed dehydrogenation of formic acid: $\beta$ -hydride elimination vs. direct hydride transfer

Xinzheng Yang\*

State Key Laboratory for Structural Chemistry of Unstable and Stable Species  
Institute of Chemistry, Chinese Academy of Sciences  
Beijing 100190, China  
E-mail: xyang@iccas.ac.cn

#### Solvent corrected absolute free energies (Hartree) and Cartesian coordinates (Å) of all optimized structures

<b>H<sub>2</sub></b>				P	0.05626200	0.70134800	-2.36092900
G <sub>solv</sub> = -1.171383				C	-0.34774400	-0.93289300	-3.15589900
H	0.00000000	0.00000000	0.38461800	C	-0.97384000	-1.89750200	-2.13638700
H	0.00000000	0.00000000	-0.38461800	C	-1.16206400	1.94743200	-2.99943600
<b>HCOOH</b>				C	-2.04621900	2.47115800	-1.84740800
G <sub>solv</sub> = -189.683018				C	1.73880000	1.11661500	-3.00700600
H	-0.09987200	1.50026800	0.00002500	C	2.76163300	0.44381500	-2.07551400
C	-0.12446700	0.40168900	0.00000900	C	1.12542400	-2.87188600	-0.38458400
O	1.10846700	-0.09155100	-0.00001000	C	1.53035200	-3.40456700	0.85138700
O	-1.13617500	-0.26405100	0.00000400	C	2.60053600	-4.29686600	0.92706200
H	1.06833700	-1.06558300	-0.00002700	C	3.28520500	-4.67294900	-0.23174000
<b>HCOO<sup>-</sup></b>				C	2.89415400	-4.14992600	-1.46542700
G <sub>solv</sub> = -189.242247				C	1.82340800	-3.25490800	-1.54178300
H	-0.00009600	1.45754600	0.00000700	C	-1.43752400	-2.38765400	0.71689500
C	-0.00004300	0.33721500	-0.00000300	C	-1.58520500	-1.78544300	1.97514000
O	1.12700600	-0.21753500	0.00000100	C	-2.46606800	-2.31955900	2.91825900
O	-1.12696200	-0.21756900	0.00000100	C	-3.21738000	-3.45362300	2.60179800
<b>CO<sub>2</sub></b>				C	-3.07841300	-4.05929700	1.34891600
G <sub>solv</sub> = -188.520067				C	-2.18526800	-3.53509100	0.41191300
C	0.18315000	-0.07326000	0.00000000	C	-3.55323600	0.29353200	-0.63471700
O	1.34772800	-0.07326000	0.00000000	C	-4.22667400	-0.25120200	0.47192800
O	-0.98142800	-0.07326000	0.00000000	C	-5.30529100	-1.11861200	0.29402400
<b>1</b>				C	-5.72664000	-1.45918200	-0.99452300
G <sub>solv</sub> = -4252.922621				C	-5.07046100	-0.91932700	-2.10259800
Fe	0.03762200	0.58641100	-0.22268900	C	-3.99195900	-0.04862000	-1.92429200
P	-0.24219900	-1.63737000	-0.44637800	C	-2.56089200	2.37590600	1.02241600
P	-2.04719100	1.32047800	-0.37996400	C	-3.69855900	3.19542200	0.94993300
P	2.25280300	0.78165800	-0.31718300	C	-4.06076600	3.99331100	2.03606200
				C	-3.29815000	3.96922700	3.20770700
				C	-2.17045700	3.15008400	3.29191600
				C	-1.80072400	2.35938700	2.20097100
				C	3.00855700	2.44887600	-0.04741600

C	4.26058400	2.60052700	0.57195900	<b>2</b>			
C	4.84239800	3.86415100	0.70569300	G <sub>solv</sub> = -4442.610332			
C	4.19079400	4.99426900	0.20985800	Fe	-0.03846900	0.55859000	0.25241700
C	2.94948000	4.85688700	-0.41562800	P	0.36422400	-1.69161600	0.36847800
C	2.36030100	3.59725900	-0.53587600	P	2.08680700	1.31557100	0.48727900
C	3.29913400	-0.27872500	0.73623400	P	-2.30077800	0.58790500	0.47542300
C	4.44784900	-0.94329200	0.28565400	P	-0.00317800	0.54462300	2.42261200
C	5.20528200	-1.71527900	1.17168100	C	0.45373500	-1.11563100	3.12050300
C	4.83189900	-1.81414000	2.51383500	C	1.10670100	-1.99563700	2.04749500
C	3.68905400	-1.15176100	2.97194600	C	1.18006400	1.79302200	3.11309000
C	2.92225400	-0.39590000	2.08523400	C	1.99773800	2.43106200	1.97222300
H	0.59541700	-1.33490600	-3.55134400	C	-1.66431000	0.87457100	3.15547900
H	-1.01471400	-0.77635400	-4.01390800	C	-2.69689600	0.18933900	2.25176400
H	-0.87321900	-2.94166500	-2.45985600	C	-0.99348300	-2.93509500	0.26905600
H	-2.04690200	-1.68469100	-2.02755500	C	-1.49730900	-3.27803200	-0.99792100
H	-0.60705500	2.77221100	-3.46492800	C	-2.51716200	-4.21996800	-1.12828400
H	-1.76544800	1.47876900	-3.78709900	C	-3.06136900	-4.82647900	0.00817000
H	-1.63102900	3.40949300	-1.45645400	C	-2.58064300	-4.48290600	1.27221200
H	-3.06939600	2.67606800	-2.18652200	C	-1.55186400	-3.54418900	1.40288200
H	1.85877200	0.78582500	-4.04641000	C	1.57661600	-2.49343100	-0.76026200
H	1.85124700	2.20927600	-2.98564000	C	1.74772400	-1.98968300	-2.05843100
H	3.78127000	0.80131700	-2.26956500	C	2.65264000	-2.58765100	-2.93951000
H	2.74641500	-0.64807400	-2.21385900	C	3.39708300	-3.69590300	-2.53181400
H	1.00540500	-3.12107300	1.76245500	C	3.22477900	-4.21357700	-1.24454800
H	2.90014300	-4.69683300	1.89218800	C	2.31613300	-3.62097700	-0.36597100
H	4.11694000	-5.36906600	-0.17237300	C	3.56916400	0.27019700	0.84794200
H	3.41766100	-4.43962500	-2.37233100	C	4.18921100	-0.46376800	-0.17843300
H	1.53480300	-2.86612700	-2.51528300	C	5.25934900	-1.31646900	0.09611700
H	-1.01086800	-0.88669200	2.20686100	C	5.72484400	-1.46224200	1.40520800
H	-2.57287100	-1.84699400	3.89062300	C	5.12318100	-0.73623800	2.43398200
H	-3.91048100	-3.86637900	3.32924700	C	4.05811300	0.12513900	2.15786500
H	-3.66252400	-4.94191800	1.10388000	C	2.69946100	2.39701200	-0.86454700
H	-2.07168000	-4.02103400	-0.55556600	C	3.04909900	3.74024400	-0.65091900
H	-3.90451700	0.00229700	1.48017000	C	3.44465500	4.54993700	-1.71948100
H	-5.81532900	-1.52861900	1.16179000	C	3.50458000	4.02981400	-3.01327700
H	-6.56539100	-2.13519000	-1.13327200	C	3.17213700	2.69115200	-3.23670600
H	-5.39773700	-1.17165900	-3.10733700	C	2.76807400	1.88328000	-2.17272400
H	-3.49270800	0.35705700	-2.80228300	C	-3.14196900	2.23403700	0.30214200
H	-4.30417800	3.20774600	0.04507300	C	-4.38858500	2.36789400	-0.33270500
H	-4.93817500	4.63041400	1.97042200	C	-5.02563900	3.61018900	-0.40673800
H	-3.58394100	4.58824800	4.05327100	C	-4.43690600	4.73871700	0.16357200
H	-1.57791400	3.12917700	4.20207100	C	-3.20231700	4.62000900	0.80654200
H	-0.91355800	1.72728200	2.26219400	C	-2.55908400	3.38304500	0.86896900
H	4.78766000	1.73175700	0.95912000	C	-3.43663000	-0.47968300	-0.48610200
H	5.80642200	3.96135200	1.19717700	C	-4.47550400	-1.21271900	0.10696200
H	4.64468900	5.97565000	0.31278800	C	-5.35885100	-1.95355000	-0.68348800
H	2.43376100	5.73105100	-0.80329700	C	-5.22505800	-1.95837100	-2.07308800
H	1.37930800	3.50739100	-0.99958400	C	-4.19564900	-1.22918100	-2.67401200
H	4.75973100	-0.85967400	-0.75331500	C	-3.30463800	-0.50193100	-1.88526600
H	6.09012800	-2.23386900	0.81305900	H	-0.47634200	-1.57173300	3.48789900
H	5.42673500	-2.40922300	3.20079300	H	1.11567100	-0.99118500	3.98784500
H	3.39265900	-1.23159300	4.01394000	H	1.05357600	-3.05701800	2.32153600
H	2.02207700	0.11061800	2.43790500	H	2.17028800	-1.73650800	1.94403300
H	0.08370700	2.12194900	-0.12965400	H	0.60503200	2.56161400	3.64547300
				H	1.82426900	1.30391900	3.85374600
				H	1.47380100	3.32900300	1.62181700

H	2.99659400	2.73718000	2.30834100	C	-1.60741500	-3.22748000	-0.92953400
H	-1.71914200	0.50360800	4.18698800	C	-2.66872400	-4.12752900	-1.01677600
H	-1.82141800	1.96100900	3.18097300	C	-3.23949400	-4.65362200	0.14615100
H	-3.72052600	0.49692800	2.50126400	C	-2.74375200	-4.27429100	1.39417900
H	-2.63145200	-0.90422400	2.36092800	C	-1.67450200	-3.37735400	1.48248200
H	-1.08334900	-2.80873500	-1.89012500	C	1.48470000	-2.52379100	-0.75414000
H	-2.89167600	-4.47608200	-2.11584300	C	1.71965300	-2.02288500	-2.04241300
H	-3.85564900	-5.56058700	-0.09306200	C	2.60920200	-2.67099600	-2.90406000
H	-2.99772600	-4.94913100	2.16058100	C	3.27096400	-3.82689400	-2.48703700
H	-1.18759800	-3.30186000	2.39821500	C	3.02872200	-4.34468700	-1.21104900
H	1.17524600	-1.12059800	-2.37480700	C	2.13576100	-3.70273500	-0.35213500
H	2.77850600	-2.18352700	-3.94031700	C	3.56977000	0.19491700	0.89684200
H	4.10568900	-4.15804500	-3.21321200	C	4.17700400	-0.61418800	-0.07889200
H	3.79764000	-5.07944800	-0.92427000	C	5.20178400	-1.49702300	0.26375500
H	2.19074300	-4.04145600	0.62959100	C	5.63554500	-1.59001300	1.58876500
H	3.83405600	-0.38512100	-1.20260700	C	5.04975000	-0.78267100	2.56499400
H	5.72491500	-1.87018800	-0.71482500	C	4.02677500	0.10515000	2.22523000
H	6.55349000	-2.13074200	1.61961700	C	2.85474800	2.27685800	-0.92410500
H	5.48258900	-0.83342900	3.45454300	C	3.37875000	3.56291100	-0.71654000
H	3.61344100	0.67685300	2.98075100	C	3.89239400	4.29881800	-1.78782800
H	3.02026800	4.16892100	0.34666900	C	3.89665500	3.75883900	-3.07509700
H	3.70932800	5.58737300	-1.53591000	C	3.38627500	2.47631900	-3.29108200
H	3.81103400	4.66145600	-3.84178300	C	2.86488800	1.74229100	-2.22463900
H	3.21986500	2.27589600	-4.23953800	C	-3.12604900	2.28059500	0.28415900
H	2.48551300	0.85109200	-2.36968400	C	-4.37122400	2.43780000	-0.34838600
H	-4.87284500	1.50328900	-0.77925500	C	-4.99059200	3.68941000	-0.41039800
H	-5.98463800	3.69005400	-0.91093700	C	-4.38413800	4.80468000	0.16693200
H	-4.93320000	5.70310800	0.10685500	C	-3.14894200	4.66354600	0.80383700
H	-2.73381200	5.49179600	1.25486900	C	-2.52369500	3.41723500	0.85606400
H	-1.58454100	3.31808300	1.34911200	C	-3.46570200	-0.42339600	-0.53143400
H	-4.61077800	-1.20838400	1.18556600	C	-4.53746300	-1.11292700	0.05507300
H	-6.15533700	-2.52137000	-0.21050800	C	-5.44302000	-1.81870000	-0.74162400
H	-5.91855500	-2.52814300	-2.68483200	C	-5.29559500	-1.83339700	-2.12987800
H	-4.08405500	-1.23027500	-3.75455900	C	-4.23178900	-1.14888900	-2.72327500
H	-2.50526900	0.06050400	-2.36194900	C	-3.32043400	-0.45358700	-1.92885800
H	-0.18847800	2.10609500	0.39590400	H	-0.41312800	-1.44225600	3.55672500
H	-0.32183400	1.66003200	-3.56359700	H	1.21042000	-0.85367600	3.92536200
C	-0.29717800	1.66278800	-2.46831200	H	0.97201700	-3.00101800	2.34951800
O	-0.51120700	2.83497000	-1.93638900	H	2.14741800	-1.75472600	1.91288300
O	-0.09647000	0.63535700	-1.82241800	H	0.57368700	2.72496800	3.46304200
H	-0.43208300	2.69794000	-0.93859200	H	1.77755200	1.48697500	3.82515500
				H	1.55984800	3.36036300	1.45338800
				H	3.03446000	2.75631900	2.22324600
				H	-1.71034700	0.56592900	4.14328300
				H	-1.84586100	2.01217500	3.12767000
				H	-3.71354700	0.50147600	2.47382100
				H	-2.59436200	-0.87669700	2.32756200
				H	-1.17210000	-2.82017300	-1.84174400
				H	-3.05569900	-4.41192900	-1.99160900
				H	-4.06679600	-5.35423900	0.07775400
				H	-3.18122500	-4.67957300	2.30226100
				H	-1.29826900	-3.10494300	2.46551900
				H	1.20796400	-1.11951300	-2.36513800
				H	2.78703500	-2.26815700	-3.89743000
				H	3.96801100	-4.32710900	-3.15321500
				H	3.53415800	-5.24936000	-0.88493700
<b>TS<sub>2,3</sub></b>							
G <sub>solv</sub>	= -4442.609208						
Fe	-0.03450400	0.59090000	0.19136800				
P	0.31521500	-1.66351300	0.37305500				
P	2.14980800	1.27730100	0.44153900				
P	-2.31700600	0.61843500	0.43594800				
P	0.00326500	0.62539400	2.38063800				
C	0.49389700	-1.01268800	3.10880500				
C	1.07465400	-1.95200500	2.04514900				
C	1.16796000	1.91542400	3.02028800				
C	2.03803100	2.46373800	1.86909800				
C	-1.66450700	0.92986600	3.10913600				
C	-2.68638800	0.21466200	2.21505100				
C	-1.09149600	-2.84812500	0.32158000				

H	1.95275800	-4.12569800	0.63338700	C	5.69831500	-1.65479500	1.29224000
H	3.84619700	-0.56828800	-1.11371000	C	5.07218100	-1.00875400	2.35945200
H	5.65636200	-2.11473700	-0.50607600	C	4.02756600	-0.11188300	2.12271400
H	6.42939000	-2.28120200	1.85608000	C	2.82021100	2.35129200	-0.82709600
H	5.38787000	-0.83847400	3.59575600	C	3.44088200	3.57650100	-0.53383000
H	3.58752700	0.71832900	3.00413300	C	3.94603100	4.37574800	-1.56239600
H	3.39544200	4.00079600	0.27752900	C	3.84721300	3.95825000	-2.89094400
H	4.29224800	5.29334200	-1.61206800	C	3.24206600	2.73575700	-3.19184100
H	4.29656300	4.33314900	-3.90551900	C	2.72887900	1.93851700	-2.16774400
H	3.38838400	2.04802200	-4.28942400	C	-3.12737100	2.27268400	0.29688000
H	2.44960800	0.75399200	-2.41019400	C	-4.24953900	2.45808400	-0.52828000
H	-4.86842700	1.58433900	-0.80185400	C	-4.80930000	3.72714400	-0.70190800
H	-5.94972200	3.78665100	-0.91112000	C	-4.26625600	4.83248500	-0.04815000
H	-4.86677300	5.77639500	0.11951400	C	-3.15556000	4.66314900	0.78176600
H	-2.66523700	5.52513000	1.25544200	C	-2.58820400	3.39950300	0.94702100
H	-1.54919600	3.34180000	1.33398400	C	-3.51598400	-0.45272500	-0.40674900
H	-4.68041000	-1.10031700	1.13265300	C	-4.64299300	-1.04101500	0.18714500
H	-6.26607600	-2.35267900	-0.27485500	C	-5.57441800	-1.72704100	-0.59675200
H	-6.00577300	-2.37644500	-2.74672000	C	-5.39443600	-1.82445700	-1.97813700
H	-4.11010100	-1.15858500	-3.80261600	C	-4.27117900	-1.24807900	-2.57602700
H	-2.49468000	0.07560700	-2.39841100	C	-3.33439700	-0.57206300	-1.79465900
H	-0.16938000	2.18619100	0.31122100	H	-0.54463100	-1.55338900	3.48648000
H	-0.31935200	1.67669000	-3.54541100	H	1.05762400	-1.02372700	4.00296500
C	-0.28219900	1.66064200	-2.44655000	H	0.93621200	-3.07074700	2.31216600
O	-0.44895300	2.76767400	-1.84134200	H	2.11157500	-1.79102100	1.97719400
O	-0.08737400	0.57060600	-1.86411600	H	0.70152200	2.55628700	3.65987400
H	-0.30453800	2.41430600	-0.64921700	H	1.85893100	1.24394200	3.88417300
				H	1.62975700	3.28329000	1.64852500
<b>3</b>				H	3.10209700	2.59630500	2.34465300
$G_{\text{solv}} = -4442.622220$				H	-1.69923800	0.53153100	4.23943100
Fe	-0.06422600	0.60751400	0.25783800	H	-1.78939700	2.00209700	3.25926000
P	0.32988900	-1.66168900	0.37783900	H	-3.72479300	0.60416300	2.59140900
P	2.16282200	1.25847600	0.48690600	H	-2.69551300	-0.83800000	2.44987200
P	-2.36180700	0.60250600	0.53171200	H	-1.03721600	-2.78408400	-1.93524700
P	-0.00300000	0.55983400	2.46795700	H	-2.88580900	-4.39893900	-2.20533800
C	0.40044400	-1.12231500	3.12916900	H	-3.98070200	-5.39597900	-0.20593200
C	1.03734000	-2.00880200	2.05668500	H	-3.21111400	-4.75461100	2.07131600
C	1.23972900	1.75509500	3.13726800	H	-1.36520900	-3.15868900	2.35570700
C	2.09186800	2.34856800	1.99523300	H	1.20418400	-1.05014500	-2.36446600
C	-1.65232500	0.91484700	3.21216700	H	2.80973500	-2.14645100	-3.90966400
C	-2.71930000	0.25523600	2.32478500	H	4.07016500	-4.16023100	-3.17313200
C	-1.06007600	-2.85297500	0.22816900	H	3.70311300	-5.08180100	-0.89228700
C	-1.50896000	-3.21431400	-1.05293600	H	2.10036700	-4.01140400	0.63830800
C	-2.55208500	-4.12673600	-1.20776400	H	3.91797900	-0.32371200	-1.27809800
C	-3.16898900	-4.68450500	-0.08457900	H	5.76763900	-1.88560700	-0.85336400
C	-2.73813300	-4.32411200	1.19325400	H	6.51049700	-2.35159600	1.47711100
C	-1.68878400	-3.41444000	1.35018600	H	5.39629400	-1.19677700	3.37890600
C	1.54796700	-2.43966400	-0.75430400	H	3.55824400	0.37687100	2.97217300
C	1.75332500	-1.93257700	-2.04568700	H	3.53983300	3.91655100	0.49328700
C	2.65711200	-2.55179100	-2.91318800	H	4.42032800	5.32276400	-1.32176000
C	3.36439200	-3.68172200	-2.50022300	H	4.24137000	4.58158100	-3.68807300
C	3.15897600	-4.19986000	-1.21820700	H	3.16478400	2.40310800	-4.22307800
C	2.25260700	-3.58760800	-0.35169600	H	2.24526300	0.99539500	-2.41291100
C	3.59014900	0.14642600	0.81289400	H	-4.69610000	1.61447200	-1.04746700
C	4.23461400	-0.50277600	-0.25353000	H	-5.67286100	3.84512300	-1.35014600
C	5.28179700	-1.39325000	-0.01540800	H	-4.70194100	5.81788200	-0.18348000

H	-2.72320300	5.51567200	1.29769900	C	-3.18747900	3.35163600	1.08884800
H	-1.70989700	3.31142400	1.58318500	C	-3.60675300	-0.46279400	-0.10821000
H	-4.81237400	-0.95719000	1.25765500	C	-4.86567000	-0.68006100	0.47471800
H	-6.44338200	-2.17831100	-0.12643700	C	-5.81889600	-1.45855000	-0.18354200
H	-6.12540800	-2.34997700	-2.58569600	C	-5.52905600	-2.01289300	-1.43327500
H	-4.12188600	-1.32819400	-3.64894400	C	-4.28296600	-1.79082700	-2.02286600
H	-2.45808900	-0.13017000	-2.26298100	C	-3.32251700	-1.02156000	-1.36209000
H	-0.22674700	2.20806800	0.58368400	H	-0.75113400	-1.60386500	3.44496900
H	-0.44200900	1.24892700	-3.59558800	H	0.84951300	-1.22706200	4.08360900
C	-0.43684400	1.49940000	-2.51419100	H	0.70224200	-3.18218700	2.29108200
O	-0.69911800	2.66176900	-2.16376500	H	1.97069400	-1.96334800	2.07761800
O	-0.15218800	0.51144700	-1.76055800	H	1.00670100	2.29711400	3.85608900
H	-0.28940100	2.19475500	-0.24116900	H	2.04341300	0.87386000	3.85702500
<b>TS<sub>3,4</sub></b>				H	1.82890600	3.12548500	1.83237400
$G_{\text{solv}} = -4442.605177$				H	3.29338700	2.29964700	2.38817000
Fe	-0.08595500	0.55233400	0.33337900	H	-1.59165400	0.75081800	4.36113900
P	0.27568000	-1.67182900	0.39230100	H	-1.50697500	2.17495400	3.31010100
P	2.19352900	1.16217200	0.49558800	H	-3.64797100	1.06134000	2.76196000
P	-2.38887400	0.65226300	0.67182900	H	-2.87612900	-0.52805000	2.71699100
P	0.03097400	0.49168600	2.53908700	H	-0.43992500	-3.45705900	-1.87756600
C	0.24511500	-1.23391400	3.16727700	H	-2.22854800	-5.12041800	-2.19661500
C	0.88440900	-2.11885600	2.09176200	H	-3.89763600	-5.53125100	-0.39781800
C	1.42476600	1.51123200	3.21372700	H	-3.75470500	-4.25217300	1.73229800
C	2.25134900	2.14347500	2.07700100	H	-1.97303800	-2.58966000	2.06515500
C	-1.53390600	1.07702500	3.31445600	H	1.03648000	-0.93853800	-2.31326000
C	-2.71986900	0.53830100	2.49938900	H	2.65322800	-1.89235300	-3.94227200
C	-1.06943300	-2.89682700	0.11747200	H	4.08687000	-3.81810100	-3.28992900
C	-1.16167400	-3.62189400	-1.08101400	H	3.89648600	-4.78497600	-1.00756200
C	-2.17418900	-4.56578200	-1.26411900	H	2.27976400	-3.86081400	0.60559200
C	-3.11074000	-4.79626300	-0.25526300	H	4.15757600	0.01203400	-1.42891700
C	-3.03061000	-4.07871300	0.94099400	H	6.03480200	-1.54819000	-1.17514700
C	-2.01900200	-3.13530100	1.12525000	H	6.62077600	-2.46269900	1.06570000
C	1.55762600	-2.31847700	-0.74003100	H	5.29506100	-1.77419100	3.05783500
C	1.66883300	-1.77862900	-2.03042100	H	3.41760100	-0.21653400	2.82169000
C	2.57557800	-2.31821600	-2.94564100	H	3.42434700	3.90247800	0.55645600
C	3.37994400	-3.39923100	-2.57957500	H	4.16121300	5.41323700	-1.23602600
C	3.27350400	-3.94314700	-1.29643600	H	3.98850300	4.72105500	-3.61775300
C	2.36246700	-3.41170200	-0.38163100	H	3.06052200	2.48350600	-4.18963100
C	3.63091200	0.01758600	0.67319800	H	2.26816700	0.97619800	-2.40420100
C	4.39189300	-0.37311900	-0.44046800	H	-3.52457000	1.64839700	-1.84360200
C	5.46095800	-1.25902000	-0.29892800	H	-4.41432400	3.83127900	-2.55727000
C	5.78929700	-1.77262900	0.95720900	H	-4.51777700	5.73109900	-0.95228400
C	5.04517300	-1.38829800	2.07373900	H	-3.74416100	5.40773600	1.39051000
C	3.97697500	-0.49941900	1.93388000	H	-2.84845400	3.23893900	2.11513700
C	2.79042500	2.32217200	-0.78963900	H	-5.11096800	-0.24028000	1.43887700
C	3.32732700	3.58064300	-0.47653200	H	-6.78842300	-1.62692500	0.27646100
C	3.75188900	4.44061100	-1.49325400	H	-6.27333800	-2.61561000	-1.94568100
C	3.65710200	4.05087600	-2.83011400	H	-4.05260900	-2.22423600	-2.99229000
C	3.13624700	2.79483300	-3.15160100	H	-2.34736800	-0.85456100	-1.81743800
C	2.69969600	1.93970700	-2.13970800	H	-0.32130700	3.09999000	1.16226800
C	-3.11173300	2.27750400	0.18913800	H	-0.57019600	1.60618600	-3.41188000
C	-3.56471700	2.46709000	-1.12767400	C	-0.43259300	1.78260300	-2.32221900
C	-4.06773700	3.70304900	-1.53576400	O	-0.42120600	2.95004400	-1.90250500
C	-4.12711600	4.76884800	-0.63459700	O	-0.30160500	0.70562200	-1.65137800
C	-3.69096600	4.58826600	0.67940900	H	-0.27545900	3.20618800	0.41862300

4

$G_{\text{solv}} = -4441.460976$

Fe	0.03628900	0.60872900	-0.11456800
P	-0.16488500	-1.62644300	-0.40023500
P	-2.22894700	1.14919500	-0.36864600
P	2.31018800	0.73115700	-0.37261800
P	-0.00759900	0.72580200	-2.31181700
C	-0.46517200	-0.90201800	-3.08932200
C	-0.97425300	-1.90653300	-2.04694300
C	-1.22376000	1.99679000	-2.88537400
C	-2.11231600	2.43860900	-1.70270100
C	1.65110500	1.09107700	-3.03706000
C	2.69772900	0.38870100	-2.15835600
C	1.26973000	-2.77996500	-0.43424300
C	1.79895600	-3.25582500	0.77747500
C	2.87337000	-4.14510100	0.78319400
C	3.44185400	-4.56748800	-0.42183400
C	2.93102400	-4.09454000	-1.63135700
C	1.85034600	-3.20798600	-1.63834000
C	-1.25075000	-2.49230100	0.79286000
C	-1.38088300	-1.98958000	2.09548000
C	-2.20450600	-2.63411900	3.02240000
C	-2.90056900	-3.78735700	2.65524400
C	-2.75853800	-4.30703600	1.36487300
C	-1.93326700	-3.66737100	0.43900800
C	-3.57281800	0.03332000	-0.94246700
C	-4.09464300	-0.92909300	-0.06023600
C	-5.07742100	-1.82343700	-0.48483500
C	-5.55008600	-1.77624600	-1.79901800
C	-5.04501800	-0.82030800	-2.68147400
C	-4.06648600	0.08186700	-2.25634600
C	-3.03784300	2.02099800	1.02947100
C	-3.66499300	3.26641200	0.86341800
C	-4.26528200	3.90657200	1.95035400
C	-4.25167200	3.31104600	3.21314100
C	-3.63548100	2.06960300	3.38781000
C	-3.02849800	1.43055600	2.30493600
C	3.05351800	2.40717800	-0.15778400
C	4.26887100	2.59888000	0.51990600
C	4.84014300	3.87137100	0.61339700
C	4.21123400	4.96916800	0.02624600
C	3.00040600	4.79288200	-0.64855600
C	2.42284900	3.52600900	-0.73381700
C	3.44674400	-0.31146300	0.59899000
C	4.59188300	-0.90380500	0.04723000
C	5.47331700	-1.62013900	0.86117900
C	5.22739600	-1.73657500	2.23110600
C	4.08921000	-1.14747500	2.78798600
C	3.19915600	-0.44430000	1.97571400
H	0.43994000	-1.27812600	-3.58577600
H	-1.21460600	-0.73519500	-3.87386300
H	-0.82709200	-2.93936100	-2.38622000
H	-2.05019200	-1.76830200	-1.87894800
H	-0.66768500	2.85672400	-3.27994300
H	-1.81607100	1.58733100	-3.71270200
H	-1.65234200	3.30566900	-1.21177100

H	-3.10805500	2.74417000	-2.04739900
H	1.70433200	0.74680700	-4.07746800
H	1.80246100	2.17786600	-3.03763200
H	3.71394900	0.71925000	-2.40769200
H	2.64707000	-0.70149900	-2.29881300
H	1.36618500	-2.93457800	1.72368900
H	3.26816000	-4.50584000	1.72915200
H	4.27694800	-5.26200400	-0.41651100
H	3.36451700	-4.41980100	-2.57282500
H	1.46239200	-2.86368400	-2.59373800
H	-0.84244200	-1.08728300	2.37892200
H	-2.30427800	-2.23189400	4.02683700
H	-3.54678200	-4.28492000	3.37259700
H	-3.29193300	-5.20927100	1.07920700
H	-1.82850700	-4.08402300	-0.56087500
H	-3.72297700	-0.99638600	0.96029700
H	-5.46727700	-2.56134800	0.21100900
H	-6.31054700	-2.47709200	-2.13039800
H	-5.41295600	-0.77020400	-3.70220000
H	-3.69214500	0.81662100	-2.96307400
H	-3.69315600	3.74750500	-0.11012400
H	-4.74461100	4.87069500	1.80700100
H	-4.71853600	3.81124100	4.05650900
H	-3.62076400	1.59955600	4.36696100
H	-2.53563400	0.47285100	2.45799200
H	4.77994000	1.75663400	0.97950400
H	5.77909900	3.99879300	1.14461100
H	4.65709800	5.95691600	0.09785600
H	2.49805600	5.64363900	-1.10006900
H	1.45970900	3.41601600	-1.22576400
H	4.80711300	-0.80723300	-1.01446200
H	6.35471700	-2.08122800	0.42427800
H	5.91931900	-2.28701400	2.86207400
H	3.89185500	-1.24096100	3.85207800
H	2.30722400	0.00770600	2.40756800
C	0.09397300	2.12076100	1.77897600
H	0.11893700	2.81893900	2.63094200
O	0.14258600	0.87558700	1.96797100
O	0.01283500	2.56432000	0.59899000

**TS<sub>4,5</sub>**

$G_{\text{solv}} = -4441.447736$

Fe	0.01336300	0.52318400	-0.25826500
P	-0.11816900	-1.69691900	-0.37023400
P	-2.26756200	0.98459000	-0.45671700
P	2.26163900	0.70766300	-0.53715000
P	-0.08275800	0.43387400	-2.43293000
C	-0.53956700	-1.25005200	-3.08066700
C	-0.97806600	-2.18147400	-1.93986200
C	-1.33786200	1.65146000	-3.04538900
C	-2.18462000	2.18469800	-1.87080000
C	1.54732100	0.82105700	-3.21053900
C	2.65401200	0.27189600	-2.29889100
C	1.35793500	-2.79175700	-0.33423900
C	1.90842100	-3.17814900	0.89921300
C	3.02111600	-4.01840900	0.94789500

C	3.60524000	-4.47974900	-0.23455100	H	-5.39206300	-2.71577300	0.51409200
C	3.07187800	-4.09614700	-1.46625800	H	-6.28864600	-2.86511300	-1.80370000
C	1.95489200	-3.25855500	-1.51652500	H	-5.47814100	-1.28523800	-3.54477200
C	-1.10615800	-2.37078000	1.00501700	H	-3.77810000	0.40311200	-2.99733900
C	-1.12731100	-1.65720100	2.21166700	H	-4.46830900	2.96085600	-0.43044900
C	-1.87523200	-2.12315100	3.29481100	H	-5.61617700	4.15950300	1.39314200
C	-2.60127000	-3.31079000	3.17696100	H	-4.94046700	3.79016900	3.75712800
C	-2.56751400	-4.03825000	1.98302600	H	-3.09145400	2.21178200	4.28412600
C	-1.81914600	-3.57388500	0.89992500	H	-1.90639300	1.03552600	2.45651500
C	-3.58716800	-0.20009800	-0.92148000	H	4.59541400	2.04531800	0.77127400
C	-4.06612300	-1.08464800	0.06082500	H	5.28628300	4.40480700	0.93148000
C	-5.03454800	-2.03710100	-0.25546700	H	3.93638000	6.18652200	-0.15956300
C	-5.53807500	-2.12012200	-1.55672600	H	1.87144200	5.57913200	-1.40861900
C	-5.08099600	-1.23572100	-2.53504800	H	1.13472100	3.23573100	-1.52438500
C	-4.11404200	-0.27718000	-2.22002000	H	4.86084900	-0.67417600	-1.10832100
C	-3.09574000	1.91766900	0.88576000	H	6.48482600	-1.77971300	0.38464100
C	-4.14978400	2.79986200	0.59721900	H	6.05967800	-1.90259500	2.82957200
C	-4.80621400	3.47499900	1.62812200	H	3.97304300	-0.93586200	3.77623900
C	-4.42669200	3.26636400	2.95636600	H	2.31801000	0.15271200	2.28066900
C	-3.38813800	2.38095300	3.25291300	C	0.59276800	2.66445600	1.83361500
C	-2.72338400	1.71289800	2.22227300	H	0.71485200	3.76477000	1.74230900
C	2.82827400	2.45481100	-0.41261900	O	0.99222100	2.09180200	2.85575500
C	3.99258400	2.80985700	0.28718100	O	0.00342900	2.11527700	0.84416400
C	4.38617500	4.14792600	0.38047100				
C	3.62882600	5.14744200	-0.23163700	<b>5</b>			
C	2.46986100	4.80620900	-0.93485900	G <sub>solv</sub> = -4441.452193			
C	2.06741900	3.47311800	-1.01687600	Fe	0.05016000	0.46062300	-0.28850100
C	3.47301000	-0.18820700	0.48536100	P	-0.23826100	-1.73691300	-0.39382600
C	4.65235100	-0.73315700	-0.04272700	P	-2.17218500	1.11643400	-0.51603100
C	5.57602800	-1.35502400	0.80161800	P	2.31786100	0.61795700	-0.57932300
C	5.33618600	-1.42392800	2.17593400	P	0.00156700	0.42052600	-2.49773500
C	4.16438100	-0.87976800	2.70847600	C	-0.34496700	-1.27945100	-3.14889100
C	3.23312800	-0.27136300	1.86681100	C	-0.94597600	-2.16637000	-2.05102700
H	0.34876300	-1.64321500	-3.59337800	C	-1.26712300	1.58666700	-3.17073600
H	-1.32979700	-1.15044400	-3.83547600	C	-2.08507600	2.20594300	-2.01988600
H	-0.79269000	-3.23456300	-2.18337300	C	1.63895100	0.86276300	-3.22816100
H	-2.05410400	-2.06934600	-1.75073800	C	2.73293100	0.24483400	-2.34585700
H	-0.80918700	2.47799200	-3.53630500	C	1.24975700	-2.79003700	-0.20969900
H	-1.95835800	1.16737300	-3.80937200	C	1.79600100	-2.95986500	1.07478200
H	-1.70515800	3.07654600	-1.44339800	C	2.92382700	-3.75680100	1.26466600
H	-3.18453300	2.48282500	-2.20978600	C	3.53113800	-4.38345500	0.17260800
H	1.60564900	0.39059100	-4.21795200	C	3.00445900	-4.21109100	-1.10825700
H	1.62751300	1.91111400	-3.30941500	C	1.86802000	-3.41981600	-1.30029500
H	3.63635700	0.66546200	-2.58904700	C	-1.38170700	-2.50610800	0.80943400
H	2.69259500	-0.82545800	-2.35812800	C	-1.54453600	-1.93255200	2.07929600
H	1.46292800	-2.82895700	1.82879200	C	-2.39875400	-2.52125000	3.01450200
H	3.43187100	-4.31099700	1.91026800	C	-3.09630500	-3.68607200	2.68930600
H	4.46978300	-5.13597100	-0.19522800	C	-2.92985800	-4.26999700	1.43009100
H	3.51687200	-4.45354800	-2.39041500	C	-2.07349900	-3.68734000	0.49442200
H	1.55019200	-2.98492200	-2.48734700	C	-3.57706600	-0.02028700	-0.84735700
H	-0.55610400	-0.73158700	2.29738900	C	-4.16955200	-0.72317400	0.21547500
H	-1.89293600	-1.55972100	4.22360900	C	-5.19264600	-1.64116600	-0.02241900
H	-3.18894500	-3.67317100	4.01535500	C	-5.63573100	-1.87736100	-1.32628300
H	-3.12707000	-4.96511200	1.89470900	C	-5.06181800	-1.17766000	-2.38869500
H	-1.80030500	-4.14418700	-0.02711700	C	-4.04174800	-0.25257000	-2.15228600
H	-3.67389500	-1.03576700	1.07562100	C	-2.83683500	2.21176200	0.79377200

C	-3.40809200	3.46160500	0.50267000	H	6.34897400	-1.73153800	2.71279600
C	-3.90245300	4.26927600	1.52993900	H	4.43658100	-0.50383200	3.72494200
C	-3.83913600	3.83805000	2.85632800	H	2.68586400	0.47825500	2.27721700
C	-3.27930200	2.59381200	3.15598400	C	0.31682000	1.83724000	2.24841100
C	-2.77708600	1.78782600	2.13332000	H	0.19781900	2.72124200	1.58129100
C	2.73702300	2.40544500	-0.44471000	O	0.52823700	2.02316500	3.45718300
C	4.04902800	2.82142000	-0.16281200	O	0.23016600	0.69330000	1.68918100
C	4.36315900	4.17968600	-0.09020400				
C	3.37205100	5.14181200	-0.29728500				
C	2.06486100	4.74253200	-0.58305300	<b>TS<sub>5,6</sub></b>			
C	1.74898800	3.38411000	-0.65687600	G <sub>solv</sub> = -4441.441405			
C	3.60561000	-0.17875900	0.43174400	Fe	0.02755600	0.50978800	-0.19353100
C	4.68536900	-0.87305800	-0.13241200	P	-0.22822400	-1.70742700	-0.36536200
C	5.66720000	-1.43261000	0.69027700	P	-2.22470200	1.12772300	-0.43769400
C	5.58217600	-1.29882800	2.07685900	P	2.30328200	0.61942800	-0.50022800
C	4.50810300	-0.60805900	2.64620800	P	-0.03775100	0.53470500	-2.40126100
C	3.52368000	-0.05377500	1.83010400	C	-0.48211200	-1.13225600	-3.08814400
H	0.61288400	-1.68284400	-3.50471900	C	-1.02771000	-2.06365300	-1.99823500
H	-1.01286000	-1.21813000	-4.01740800	C	-1.27451800	1.76206800	-3.02326300
H	-0.81425000	-3.23125600	-2.27921400	C	-2.06876300	2.33850300	-1.83508700
H	-2.02645500	-1.97971400	-1.96510900	C	1.61048900	0.89097500	-3.15538200
H	-0.75288500	2.37602700	-3.73366800	C	2.67766400	0.22488700	-2.27369600
H	-1.90316400	1.04900200	-3.88380100	C	1.23147500	-2.81674600	-0.31669600
H	-1.58240000	3.12045500	-1.67534000	C	1.78835500	-3.14514800	0.93124700
H	-3.08960700	2.49318100	-2.35651100	C	2.88541600	-4.00165700	1.01323400
H	1.70897300	0.51089700	-4.26516900	C	3.45073800	-4.53026500	-0.15088600
H	1.71816100	1.95838700	-3.23740900	C	2.91310400	-4.20039600	-1.39583800
H	3.72586300	0.63486900	-2.60402000	C	1.80702400	-3.34977600	-1.48009500
H	2.75189600	-0.84938000	-2.46206700	C	-1.31326700	-2.50725100	0.87045900
H	1.33421100	-2.47210500	1.93224300	C	-1.43442200	-1.95444100	2.15363900
H	3.33319400	-3.88172100	2.26325800	C	-2.25970700	-2.55730700	3.10630500
H	4.41175700	-5.00187200	0.32085700	C	-2.96576000	-3.71815100	2.78551500
H	3.47028800	-4.69709300	-1.96073000	C	-2.83249500	-4.28701500	1.51540400
H	1.46965100	-3.31032600	-2.30553500	C	-2.00642200	-3.68922100	0.56264200
H	-1.00457600	-1.02030600	2.32696800	C	-3.61780400	0.03401800	-0.91511200
H	-2.52202900	-2.06582800	3.99319200	C	-4.11306700	-0.90506500	0.00656000
H	-3.76512200	-4.14104900	3.41417400	C	-5.13832400	-1.77963500	-0.35417300
H	-3.46696000	-5.17915200	1.17533600	C	-5.67789800	-1.73731100	-1.64226900
H	-1.95144000	-4.15739700	-0.47896400	C	-5.19959600	-0.80325600	-2.56215500
H	-3.83095400	-0.56321900	1.23616000	C	-4.18049800	0.08131600	-2.20092200
H	-5.63946100	-2.17368400	0.81257600	C	-2.90419300	2.11816200	0.94739500
H	-6.42842400	-2.59618100	-1.51123700	C	-3.32093600	3.44820300	0.77666100
H	-5.40785300	-1.34517000	-3.40451100	C	-3.78027900	4.18992000	1.86819900
H	-3.61606000	0.27955900	-2.99785000	C	-3.83483900	3.61289500	3.13806000
H	-3.47742600	3.81460900	-0.52236200	C	-3.43048900	2.28732500	3.31662100
H	-4.33977100	5.23407800	1.28999200	C	-2.96303800	1.54639000	2.23116900
H	-4.22350200	4.46824000	3.65283100	C	2.91651200	2.35735600	-0.37203800
H	-3.22450000	2.25213900	4.18571000	C	4.18259800	2.64775100	0.16343100
H	-2.32262900	0.83108700	2.38284900	C	4.64726500	3.96400700	0.22087200
H	4.82964900	2.08197800	0.00364700	C	3.85902400	5.01012100	-0.26001500
H	5.38204300	4.48491600	0.12960200	C	2.60053600	4.73562400	-0.79975600
H	3.61720500	6.19798400	-0.23637600	C	2.13110100	3.42231000	-0.85195200
H	1.28944900	5.48511900	-0.74760400	C	3.51181200	-0.29128000	0.50898200
H	0.72037200	3.10001500	-0.88344800	C	4.61328600	-0.95920800	-0.04362700
H	4.77342400	-0.98121100	-1.21048000	C	5.54838100	-1.57727700	0.79120500
H	6.49867000	-1.97063900	0.24374700	C	5.39508900	-1.52494300	2.17792900
				C	4.29836300	-0.86062600	2.73500500



C	3.35874900	-0.24952800	1.90587700	C	1.04090400	-2.03801600	2.01261900
H	0.43332100	-1.54348300	-3.53510200	C	1.15742500	1.81492800	3.02905700
H	-1.20879800	-1.01113200	-3.90153000	C	2.00249900	2.37033700	1.86541600
H	-0.90488800	-3.11753400	-2.27652800	C	-1.69480600	0.83533300	3.11204100
H	-2.10206700	-1.88564800	-1.85028700	C	-2.71879500	0.13542200	2.20571800
H	-0.74338700	2.56638300	-3.54753700	C	-1.17150700	-2.86746000	0.31151700
H	-1.92769200	1.27344000	-3.75584000	C	-1.69508100	-3.23847200	-0.93874400
H	-1.50869200	3.18359900	-1.41035900	C	-2.76557600	-4.12798200	-1.02257600
H	-3.04773100	2.72088500	-2.15119000	C	-3.33578200	-4.65087100	0.14171500
H	1.65281200	0.52085700	-4.18725600	C	-2.83097300	-4.27980900	1.38881100
H	1.74885200	1.97955000	-3.18435700	C	-1.75321100	-3.39377700	1.47487400
H	3.68580300	0.56722500	-2.53941400	C	1.37206900	-2.47555800	-0.85453000
H	2.64611700	-0.86872400	-2.38634300	C	1.50024500	-1.90420400	-2.12868800
H	1.35667700	-2.73606900	1.84375900	C	2.35374900	-2.47603200	-3.07563400
H	3.30210000	-4.25194800	1.98488100	C	3.08109900	-3.62437100	-2.75714100
H	4.30591900	-5.19674000	-0.08607400	C	2.94075300	-4.21228900	-1.49635900
H	3.34568500	-4.61008400	-2.30404500	C	2.08617700	-3.64552400	-0.54976800
H	1.39657300	-3.11818800	-2.45950500	C	3.58857800	0.07314800	0.99431600
H	-0.89087900	-1.04590700	2.40198500	C	4.13910300	-0.84069400	0.07877200
H	-2.35317000	-2.11608100	4.09470400	C	5.16311400	-1.70398100	0.46899300
H	-3.61312900	-4.18319000	3.52324100	C	5.64579800	-1.67526800	1.77993300
H	-3.37336800	-5.19524600	1.26551700	C	5.11107000	-0.76693900	2.69457200
H	-1.91085500	-4.14492100	-0.42068700	C	4.09273300	0.10618100	2.30459700
H	-3.69115100	-0.96986600	1.00698100	C	2.90997800	2.14107800	-0.89057600
H	-5.50842700	-2.49878500	0.37132300	C	3.36185300	3.45677300	-0.69835900
H	-6.46972000	-2.42476800	-1.92440700	C	3.85406900	4.19864500	-1.77510200
H	-5.62084200	-0.75528700	-3.56202600	C	3.90751200	3.63567100	-3.05140800
H	-3.83504200	0.80415300	-2.93347700	C	3.47047200	2.32367400	-3.25077800
H	-3.29341000	3.91818700	-0.20211800	C	2.97039300	1.58259300	-2.17987700
H	-4.09704400	5.21841800	1.72176200	C	-3.01775300	2.26542700	0.31021600
H	-4.19027700	4.19247400	3.98483700	C	-4.28267500	2.49720800	-0.25578400
H	-3.46945300	1.83205100	4.30188300	C	-4.81346300	3.78831200	-0.30981400
H	-2.62390500	0.52518300	2.39197500	C	-4.09382000	4.86689300	0.20559300
H	4.81332400	1.84769600	0.54293600	C	-2.83639700	4.65078200	0.77368700
H	5.62687800	4.16791100	0.64331200	C	-2.30018100	3.36319700	0.82144100
H	4.22083400	6.03290900	-0.21304400	C	-3.46407200	-0.40448400	-0.59835300
H	1.97908300	5.54305300	-1.17615900	C	-4.57559000	-1.08431000	-0.08149400
H	1.13860900	3.24045700	-1.26074000	C	-5.45564000	-1.74414200	-0.94349500
H	4.75383900	-0.99830300	-1.12114100	C	-5.23840500	-1.71993300	-2.32263200
H	6.39764000	-2.09599100	0.35550200	C	-4.13173600	-1.04355000	-2.84408700
H	6.12734700	-2.00108400	2.82347700	C	-3.24513000	-0.39257500	-1.98689400
H	4.17514200	-0.82002500	3.81334400	H	-0.42410900	-1.53451200	3.55156600
H	2.50539000	0.26896800	2.34094100	H	1.20590000	-0.95035800	3.89597200
C	0.19936400	2.04954000	1.59942200	H	0.92887500	-3.09106300	2.29868400
H	0.08284100	2.33170500	0.47844100	H	2.11382100	-1.84889100	1.87228700
O	0.37253100	3.00252300	2.35482600	H	0.58133500	2.62384300	3.49542200
O	0.12526200	0.81037800	1.82759700	H	1.77966000	1.36708300	3.81289600
<b>6</b>				H	1.47159900	3.22064500	1.41449600
G <sub>solv</sub> = -4441.443240				H	2.97431900	2.74090500	2.21546200
Fe	-0.04416300	0.51065000	0.18017100	H	-1.74288800	0.45681000	4.14047200
P	0.25100000	-1.70920100	0.36927100	H	-1.87429500	1.91771100	3.14504100
P	2.19671200	1.15088700	0.47785000	H	-3.74417200	0.43599300	2.45517300
P	-2.32562200	0.55828200	0.44318300	H	-2.64585900	-0.95718700	2.30979500
P	-0.02128500	0.54314600	2.38710100	H	-1.25993400	-2.83533800	-1.85197900
C	0.47585700	-1.10430800	3.09104400	H	-3.15881900	-4.40675600	-1.99634400
				H	-4.16933700	-5.34406600	0.07556100



H	2.54611000	0.68912800	-2.38673500	C	-4.08915200	5.00253100	-0.14791300
H	-4.79664300	1.68309800	-0.80245300	C	-2.79624000	4.85477200	0.35543000
H	-5.80151400	3.92344300	-0.93635800	C	-2.24468200	3.58137600	0.51415000
H	-4.64950300	5.88335400	0.07424200	C	-3.46853700	-0.28625300	-0.45117400
H	-2.45818700	5.56970300	1.21290700	C	-4.49836100	-1.03267800	0.13855000
H	-1.41400800	3.34184700	1.30665700	C	-5.40765300	-1.73506600	-0.65884000
H	-4.73731400	-0.95096300	1.05417700	C	-5.30371000	-1.69149100	-2.04986100
H	-6.27986800	-2.19991000	-0.40778000	C	-4.27856200	-0.95205100	-2.64756700
H	-5.88139400	-2.30216600	-2.85883200	C	-3.36472200	-0.26135600	-1.85345400
H	-3.89136500	-1.17507100	-3.83766200	H	-0.97992400	-1.70408700	3.27353700
H	-2.31385900	0.04543700	-2.37785600	H	0.47875700	-1.29609800	4.19116200
H	-0.09347100	2.09871900	0.29029200	H	0.87844700	-3.17951900	2.44217400
C	-0.19876200	2.02745700	-1.69062200	H	1.92476000	-1.76145700	2.22802600
O	-0.09284200	0.85884200	-1.91282300	H	0.95253100	1.98569700	4.11417300
O	-0.32270000	3.17882400	-1.88412000	H	1.96324400	0.56885200	3.79601300
<b>7</b>				H	1.61458200	3.08104300	2.07685800
$G_{\text{solv}} = -4441.433754$				H	3.13650200	2.30675800	2.54719800
Fe	-0.03891500	0.48319700	0.37088800	H	-1.82373600	0.77393800	4.23391100
P	0.28528300	-1.78312000	0.46702900	H	-1.65271200	2.16217200	3.13423500
P	2.03124000	1.26376000	0.59354500	H	-3.75671500	0.95345400	2.47322800
P	-2.27971600	0.73333200	0.50124300	H	-2.87611300	-0.59071200	2.44953700
P	-0.08465500	0.42332500	2.52843200	H	-1.31526200	-2.52361800	-1.84302600
C	0.03703000	-1.29803600	3.18630000	H	-3.14035200	-4.13333900	-2.22795800
C	0.87921600	-2.11008700	2.19686700	H	-4.04103400	-5.48487100	-0.34084400
C	1.32495700	1.32572500	3.32034100	H	-3.07952600	-5.21121100	1.93757800
C	2.09703900	2.10934700	2.25267800	H	-1.22573400	-3.64968600	2.32627400
C	-1.68006100	1.06459800	3.18526100	H	0.87106400	-1.68141800	-2.38679300
C	-2.77972800	0.49210700	2.27961400	H	2.43226400	-2.89813400	-3.86132700
C	-1.12188800	-2.96645700	0.26922300	H	4.00240200	-4.57618700	-2.90458600
C	-1.68837300	-3.11699300	-1.00936800	H	3.98811000	-5.02304700	-0.45814600
C	-2.72320000	-4.02459200	-1.23043800	H	2.42022800	-3.83354900	1.01652100
C	-3.23069200	-4.78185500	-0.17032700	H	3.47169400	0.05066800	-1.62214100
C	-2.69208800	-4.62764100	1.10698300	H	5.41104600	-1.47123400	-1.77007500
C	-1.63997300	-3.73143200	1.32525300	H	6.55844000	-2.24356200	0.29904600
C	1.52709700	-2.66131000	-0.57531000	H	5.75586700	-1.46252500	2.52008900
C	1.55129600	-2.41299500	-1.95786800	H	3.85040400	0.08838800	2.67944300
C	2.43172600	-3.10096600	-2.79398400	H	4.66126700	2.44723300	-0.10009000
C	3.31234800	-4.04294200	-2.25706700	H	5.32058200	4.41195600	-1.43940800
C	3.30361000	-4.29412700	-0.88347800	H	3.59592100	5.76548300	-2.61366400
C	2.41343300	-3.61401500	-0.04801600	H	1.19334600	5.15001300	-2.40740000
C	3.52023500	0.18988500	0.53903100	H	0.52256600	3.20078700	-1.04183000
C	3.97213200	-0.27395100	-0.70960400	H	-4.88443400	1.72610800	-0.57193500
C	5.06539000	-1.13437800	-0.79649100	H	-5.84045600	3.96919100	-0.86852500
C	5.71000400	-1.56860800	0.36641600	H	-4.51596400	5.99263200	-0.27922400
C	5.25924700	-1.13113400	1.61241900	H	-2.21081800	5.73002700	0.62327400
C	4.17437600	-0.25205100	1.69860300	H	-1.23256000	3.48571800	0.90098900
C	2.54363500	2.66351500	-0.49386700	H	-4.61212800	-1.06301100	1.21912100
C	3.89574900	3.03102000	-0.60682300	H	-6.20108400	-2.30999400	-0.18918600
C	4.27105300	4.14192500	-1.36409700	H	-6.01690000	-2.23090300	-2.66656200
C	3.30192200	4.90431700	-2.02079000	H	-4.19178400	-0.91492500	-3.72987000
C	1.95441100	4.55816500	-1.90651000	H	-2.57410500	0.32007000	-2.32574400
C	1.57769900	3.44885000	-1.14458400	H	-0.13139600	1.99505200	0.54107600
C	-2.97462000	2.42807700	0.17861400	C	0.40850900	1.00694500	-2.81999600
C	-4.28301700	2.59386300	-0.31270700	O	0.81719700	1.31022500	-3.86494500
C	-4.83106000	3.86742600	-0.47975200	O	-0.01552000	0.68770000	-1.78343500

**8**

$G_{\text{solv}} = -4442.174822$

Fe	0.04963700	0.53373400	-0.34871800
P	-0.33750000	-1.70528500	-0.40237100
P	-2.05374400	1.28754100	-0.57266600
P	2.29606000	0.64452000	-0.54751700
P	0.03855200	0.45951600	-2.50617800
C	-0.24174200	-1.25316700	-3.17040100
C	-0.95954800	-2.10026200	-2.11285800
C	-1.24690400	1.55392900	-3.27340900
C	-2.05744900	2.25538800	-2.16831800
C	1.67521500	0.94002400	-3.21271800
C	2.73956000	0.28804900	-2.32113800
C	0.98114300	-2.97107700	-0.13571300
C	1.41815100	-3.21951800	1.17794800
C	2.40475500	-4.17124000	1.43375600
C	2.98184000	-4.88501000	0.37851700
C	2.57182700	-4.63333600	-0.93111800
C	1.57835500	-3.68218400	-1.18783500
C	-1.64720700	-2.42137000	0.67835200
C	-1.83432200	-1.87956300	1.96030100
C	-2.79666600	-2.41045200	2.82263600
C	-3.59383800	-3.47957400	2.40848700
C	-3.41876900	-4.02365800	1.13282700
C	-2.44473000	-3.50544000	0.27585600
C	-3.57691800	0.24330700	-0.75206300
C	-4.31755400	-0.16033000	0.37209900
C	-5.41476400	-1.01344600	0.24162000
C	-5.79587000	-1.48247000	-1.01781600
C	-5.07323300	-1.08842200	-2.14529800
C	-3.97506700	-0.23420700	-2.01318500
C	-2.63966000	2.51558000	0.66585800
C	-3.16238300	3.76696600	0.29943200
C	-3.59077500	4.67298500	1.27399300
C	-3.51313300	4.34052600	2.62755300
C	-3.00709800	3.09442400	3.00505700
C	-2.57153400	2.19202900	2.03312500
C	3.15257300	2.28147100	-0.32261000
C	4.55845400	2.32633900	-0.25688300
C	5.23291100	3.54264500	-0.14886400
C	4.51599300	4.74169500	-0.10422700
C	3.12318300	4.71391100	-0.17386000
C	2.44880500	3.49350500	-0.28315400
C	3.44445300	-0.41594700	0.42033800
C	4.36153000	-1.29858100	-0.16887400
C	5.23838000	-2.04533600	0.62425500
C	5.21562500	-1.91504600	2.01342300
C	4.30534000	-1.03899700	2.61173500
C	3.42611100	-0.29854400	1.82219700
H	0.74467700	-1.67665300	-3.40797500
H	-0.81291900	-1.21587200	-4.10771200
H	-0.88271400	-3.17208300	-2.33626300
H	-2.02864000	-1.84812300	-2.09489000
H	-0.75309400	2.29200000	-3.91874900
H	-1.88913200	0.94355900	-3.92053300
H	-1.57438000	3.20973700	-1.92163000

H	-3.08245400	2.47148800	-2.49640600
H	1.77006900	0.62793600	-4.26102800
H	1.74805500	2.03685400	-3.17284600
H	3.75170900	0.64145200	-2.55644000
H	2.72327500	-0.80397600	-2.45526300
H	0.97970400	-2.66532900	2.00761700
H	2.72875900	-4.35069400	2.45563200
H	3.74937300	-5.62751200	0.57783400
H	3.01819500	-5.17959300	-1.75766800
H	1.27116000	-3.50995400	-2.21650000
H	-1.22642400	-1.03128800	2.27263200
H	-2.93030200	-1.98151600	3.81222400
H	-4.34944000	-3.88720600	3.07421400
H	-4.03734300	-4.85493600	0.80540000
H	-2.31254700	-3.95071800	-0.70808100
H	-4.03985800	0.19026100	1.36317100
H	-5.96915900	-1.31298100	1.12728900
H	-6.64986700	-2.14589100	-1.11950400
H	-5.36277100	-1.44135600	-3.13131700
H	-3.42860300	0.05235200	-2.90847200
H	-3.24578700	4.04707500	-0.74694800
H	-3.98917100	5.63737900	0.97129600
H	-3.84643000	5.04616300	3.38299300
H	-2.94499300	2.82437200	4.05587300
H	-2.16336500	1.23153900	2.34099900
H	5.13354000	1.40292900	-0.28865500
H	6.31816500	3.55354400	-0.09784800
H	5.04096400	5.68858400	-0.01613000
H	2.55590100	5.64022100	-0.14221800
H	1.36265300	3.47906700	-0.33777600
H	4.40956000	-1.40790700	-1.24923800
H	5.94169500	-2.72582800	0.15150600
H	5.90147600	-2.49232800	2.62694800
H	4.28015400	-0.93237700	3.69267800
H	2.72138500	0.38140400	2.29735800
H	0.13758200	2.06685500	-0.49823000
C	0.45325900	1.71991300	2.34631100
H	0.53069300	2.65210600	1.74182200
O	0.62219300	1.79234700	3.58012500
O	0.19902800	0.65674400	1.70193500

**9**

$G_{\text{solv}} = -4442.158721$

Fe	-0.00006100	0.53987000	0.31248500
P	0.41499200	-1.71405500	0.43888500
P	2.07074200	1.35464100	0.49808700
P	-2.27054900	0.69250900	0.51117100
P	0.00141500	0.52215500	2.47762800
C	0.17411600	-1.18609500	3.16148300
C	1.01292100	-2.00448400	2.17637500
C	1.38335300	1.49089500	3.23491800
C	2.13790700	2.24634400	2.13614300
C	-1.59493300	1.12906400	3.15577600
C	-2.68135300	0.45332600	2.31411900
C	-0.93008400	-2.96459300	0.22979600
C	-1.47692000	-3.13149700	-1.05642400

C	-2.44577300	-4.10513800	-1.29662400	H	3.66642500	0.22689400	-1.66193400
C	-2.90056600	-4.91680500	-0.25247700	H	5.63034100	-1.27040200	-1.73442200
C	-2.38372500	-4.74395700	1.03155500	H	6.66456700	-2.08214300	0.37873800
C	-1.40097200	-3.77699300	1.27203500	H	5.72815600	-1.36008900	2.56765000
C	1.71047900	-2.55811100	-0.56957300	H	3.78945900	0.15334700	2.65203800
C	1.87489500	-2.19877100	-1.91630600	H	4.63612600	2.76608600	0.15711200
C	2.79184100	-2.87295900	-2.72589700	H	5.33188800	4.69117500	-1.22414700
C	3.56938300	-3.90461300	-2.19632300	H	3.72193300	5.75258900	-2.79476000
C	3.42215900	-4.26368800	-0.85422600	H	1.39774900	4.88032700	-2.95767800
C	2.49383400	-3.60089600	-0.04726500	H	0.68923100	2.96112400	-1.56898900
C	3.57935800	0.30160800	0.49883100	H	-5.07562900	1.54160800	0.52466000
C	4.11623100	-0.11679700	-0.73097900	H	-6.21551700	3.70848500	0.27146800
C	5.22444300	-0.96200200	-0.77466200	H	-4.90179800	5.77353900	-0.18382500
C	5.80480300	-1.41907700	0.41257000	H	-2.42421400	5.63816400	-0.36980600
C	5.27827600	-1.01562100	1.64063900	H	-1.27370300	3.46728300	-0.09951200
C	4.17525600	-0.15677100	1.68377100	H	-4.17853200	-1.48181800	1.41154900
C	2.61055900	2.72154500	-0.61063200	H	-5.83527300	-2.82044000	0.19450300
C	3.92068500	3.22567300	-0.52238300	H	-6.15367300	-2.51367500	-2.25397500
C	4.31692300	4.31179700	-1.30312600	H	-4.77343300	-0.83909100	-3.47475300
C	3.41096400	4.90950600	-2.18447400	H	-3.10697700	0.51757800	-2.26453600
C	2.10760100	4.42035500	-2.27549300	H	-0.13423000	2.06096600	0.43732500
C	1.70742600	3.33454400	-1.48979700	H	0.21865100	0.68388800	-1.48490000
C	-3.08180500	2.34244800	0.23240000	C	-0.50894700	0.70121100	-2.40613800
C	-4.48335800	2.43480900	0.33393500	O	-0.59955600	-0.38496400	-3.00180700
C	-5.13334500	3.65994500	0.18817800	O	-0.99109100	1.81351900	-2.67967900
C	-4.39558300	4.81968700	-0.06629500				
C	-3.00723000	4.74343200	-0.16968800				
C	-2.35657400	3.51476200	-0.01869000	<b>TS<sub>9,10</sub></b>			
C	-3.50675100	-0.38219700	-0.33499600	G <sub>solv</sub> = -4442.138536			
C	-4.28974100	-1.32949700	0.34159500	Fe	-0.01752200	0.49314400	0.39293500
C	-5.23728500	-2.09276800	-0.34771100	P	0.27043900	-1.74018800	0.43105400
C	-5.41559700	-1.92157300	-1.72055200	P	2.06012300	1.20576300	0.60574700
C	-4.63942200	-0.98231400	-2.40607500	P	-2.22821700	0.71900400	0.55831900
C	-3.69577900	-0.21894200	-1.71963200	P	-0.02753000	0.38380600	2.55431100
H	-0.83142200	-1.61541500	3.27177100	C	0.09531500	-1.35630800	3.18236500
H	0.63165600	-1.15559000	4.15895800	C	0.87284100	-2.17138700	2.14297700
H	1.01945600	-3.06861600	2.44219500	C	1.38191500	1.28150400	3.36150800
H	2.05786200	-1.65623300	2.19161200	C	2.17995300	2.02971800	2.28625000
H	0.98256100	2.17703100	3.99199300	C	-1.62123700	1.00247800	3.24700500
H	2.03777600	0.77878900	3.75481500	C	-2.71753600	0.42798600	2.33963300
H	1.64811700	3.20928900	1.93706900	C	-1.13452700	-2.92765200	0.19235200
H	3.17850100	2.45711600	2.41596000	C	-1.67540800	-3.07182300	-1.09831600
H	-1.69232400	0.88934100	4.22256200	C	-2.70154300	-3.98248400	-1.34762800
H	-1.62105100	2.22236800	3.04203300	C	-3.22269700	-4.75618000	-0.30581500
H	-3.68347400	0.84026300	2.53622600	C	-2.71031200	-4.60947100	0.98302300
H	-2.68502000	-0.62654400	2.51834700	C	-1.67127900	-3.70501400	1.23016500
H	-1.13973400	-2.49368600	-1.87339500	C	1.48976300	-2.60662800	-0.65253500
H	-2.85212400	-4.22480800	-2.29757600	C	1.57252200	-2.22852400	-2.00153000
H	-3.65630300	-5.67439800	-0.43972000	C	2.42201700	-2.89956900	-2.88291200
H	-2.73491600	-5.36621600	1.85018800	C	3.21455500	-3.95362300	-2.42230600
H	-1.00518900	-3.67438600	2.27921100	C	3.14857600	-4.33389100	-1.07952000
H	1.27162700	-1.39439100	-2.33437000	C	2.28615000	-3.67158700	-0.20139100
H	2.90423500	-2.58537800	-3.76788400	C	3.52011100	0.07964900	0.57015000
H	4.28739400	-4.42532100	-2.82370900	C	4.01578600	-0.35779400	-0.67121700
H	4.02584000	-5.06345500	-0.43380100	C	5.08030700	-1.25568700	-0.73968200
H	2.38672700	-3.90774500	0.99032100	C	5.65673300	-1.75200400	0.43405900
				C	5.16777800	-1.33586900	1.67302400

C	4.11039100	-0.42214500	1.74009500	H	-4.49550500	-1.17986200	1.29462500
C	2.70688000	2.60831800	-0.41229600	H	-6.14328500	-2.36878400	-0.09140100
C	4.06898600	2.95450300	-0.38009100	H	-6.11070800	-2.13526700	-2.56689600
C	4.54007600	4.06382500	-1.08503800	H	-4.38035700	-0.70900200	-3.64898500
C	3.65729500	4.84928200	-1.83097000	H	-2.70141500	0.47003900	-2.26659300
C	2.29991400	4.52450400	-1.86079700	H	-0.09440300	2.02117800	0.56916700
C	1.83141400	3.41399600	-1.15338000	H	-0.07003800	0.64807400	-1.23595100
C	-2.99472600	2.39301300	0.27557300	C	0.07674800	1.30916400	-2.87538200
C	-4.37843400	2.56042100	0.47408800	O	1.09321300	0.82631000	-3.24583200
C	-4.98679800	3.79979600	0.27575900	O	-0.90352500	1.96973700	-2.96039300
C	-4.22523800	4.89768900	-0.13608300				
C	-2.85494000	4.74567600	-0.34417300				
C	-2.24660400	3.50310500	-0.13612000				
C	-3.46954200	-0.26892900	-0.38461300				
C	-4.44927600	-1.07407400	0.21365300				
C	-5.39192700	-1.74694000	-0.57106400				
C	-5.37365400	-1.61680800	-1.96018600				
C	-4.40154400	-0.81580900	-2.56775700				
C	-3.45598900	-0.15245100	-1.78635400				
H	-0.92653300	-1.74267900	3.30469400				
H	0.57904600	-1.38470600	4.16761800				
H	0.82133300	-3.24841000	2.34721500				
H	1.93540600	-1.88190600	2.16210400				
H	1.00293200	1.96715100	4.13062600				
H	2.00288200	0.53176400	3.87039700				
H	1.74407100	3.02486900	2.12127800				
H	3.23100500	2.17538400	2.57077300				
H	-1.75827000	0.70295300	4.29438000				
H	-1.60533100	2.10146700	3.19963500				
H	-3.70316500	0.85433700	2.56411600				
H	-2.78253600	-0.66091200	2.48566300				
H	-1.28617600	-2.47089800	-1.91939900				
H	-3.10262000	-4.07966800	-2.35324300				
H	-4.02388900	-5.46391100	-0.49923600				
H	-3.10936700	-5.20358300	1.80076800				
H	-1.28233000	-3.62455800	2.24163400				
H	0.97415500	-1.39363000	-2.35975200				
H	2.47080300	-2.59312300	-3.92460200				
H	3.88199600	-4.47378300	-3.10366400				
H	3.76511800	-5.15070800	-0.71364500				
H	2.24162700	-3.99362900	0.83638900				
H	3.56953400	0.01372100	-1.59323700				
H	5.45665100	-1.57350300	-1.70852200				
H	6.48254100	-2.45586700	0.38091400				
H	5.61249300	-1.71222300	2.59027800				
H	3.75483900	-0.10244500	2.71705100				
H	4.76904900	2.35277400	0.19614800				
H	5.59675900	4.31450400	-1.05084600				
H	4.02556600	5.70984300	-2.38206100				
H	1.60382000	5.13258900	-2.43233600				
H	0.77281100	3.16862500	-1.17128400				
H	-4.99303200	1.71462700	0.77740000				
H	-6.05569100	3.90756800	0.43848700				
H	-4.69970900	5.86180900	-0.29522900				
H	-2.25394600	5.59075800	-0.66893700				
H	-1.17715600	3.39126700	-0.29063100				
				<b>10</b>			
				$G_{\text{solv}} = -4442.154558$			
				Fe	0.04342400	0.43448200	-0.52075700
				P	-0.22130300	-1.77812600	-0.43777400
				P	-2.01143000	1.14110200	-0.76770000
				P	2.22695700	0.69740900	-0.65739800
				P	0.06951700	0.21661900	-2.66548500
				C	-0.06065200	-1.55455300	-3.21268900
				C	-0.80862500	-2.33187400	-2.12199100
				C	-1.32585400	1.09621400	-3.52313400
				C	-2.13268300	1.89127700	-2.48513500
				C	1.67474400	0.79699400	-3.37442400
				C	2.76475100	0.31243800	-2.40672300
				C	1.19339000	-2.93268400	-0.10847900
				C	1.70519400	-3.01192800	1.19989100
				C	2.75438200	-3.87718400	1.50822900
				C	3.32843200	-4.66979300	0.50929600
				C	2.84449200	-4.58829000	-0.79632900
				C	1.78291300	-3.72941800	-1.10249700
				C	-1.45029900	-2.56739800	0.69562500
				C	-1.57869700	-2.05810800	1.99709300
				C	-2.45221400	-2.64235400	2.91530400
				C	-3.22635900	-3.74213400	2.53758800
				C	-3.11359700	-4.25638900	1.24317400
				C	-2.22534900	-3.68005900	0.33015700
				C	-3.49352300	0.04251900	-0.68336900
				C	-4.03197600	-0.28348400	0.57392400
				C	-5.09834400	-1.17532700	0.68632500
				C	-5.63985500	-1.76912000	-0.45848100
				C	-5.11226400	-1.45895200	-1.71298700
				C	-4.04832400	-0.55744500	-1.82438200
				C	-2.64198100	2.56656000	0.22614200
				C	-3.92690800	3.08856600	-0.00603100
				C	-4.38973600	4.18936200	0.71656100
				C	-3.57808200	4.78460200	1.68739500
				C	-2.30070300	4.27588400	1.92772100
				C	-1.83865000	3.17639100	1.19765400
				C	2.92549900	2.40408700	-0.41174100
				C	4.23838400	2.70378000	-0.81790000
				C	4.78667300	3.96762700	-0.59309800
				C	4.03898800	4.95116600	0.06041500
				C	2.74217500	4.66184700	0.48671300
				C	2.19096100	3.39928300	0.24811400
				C	3.47191700	-0.19163500	0.37800800
				C	4.50358600	-0.98835300	-0.13838600

C	5.43346700	-1.58825200	0.71806400	P	2.03900600	1.27429100	0.42884800
C	5.35230000	-1.38921200	2.09691200	P	-2.20555100	0.81497500	0.42239800
C	4.32877300	-0.59408500	2.62283300	P	-0.01341200	0.50661100	2.42302500
C	3.39503000	-0.00651000	1.77042100	C	0.13681800	-1.21640900	3.10308600
H	0.96076800	-1.94059700	-3.34138800	C	0.86342400	-2.07657200	2.06080200
H	-0.56615800	-1.63102600	-4.18446100	C	1.38426900	1.46569900	3.18468100
H	-0.72298800	-3.41729800	-2.26219600	C	2.17735100	2.17115900	2.07316000
H	-1.87989300	-2.07957900	-2.15339300	C	-1.60859900	1.13550400	3.11190200
H	-0.93356300	1.75164400	-4.31194500	C	-2.71226300	0.57174100	2.20573200
H	-1.94897400	0.33529000	-4.01286100	C	-1.16343900	-2.82938000	0.12002200
H	-1.70228400	2.89537600	-2.36575600	C	-1.69846800	-2.98843000	-1.17140900
H	-3.18094700	2.01567700	-2.78786900	C	-2.74888300	-3.87458300	-1.40741200
H	1.83876500	0.42218600	-4.39347200	C	-3.29945800	-4.60800500	-0.35152100
H	1.64464900	1.89649000	-3.41077400	C	-2.79190600	-4.44640000	0.93777200
H	3.74518500	0.73775500	-2.65270600	C	-1.72926100	-3.56636700	1.17175200
H	2.85582900	-0.78268100	-2.47149600	C	1.46917500	-2.52881300	-0.73667100
H	1.27574500	-2.39459100	1.98807100	C	1.66249300	-2.08099600	-2.05260600
H	3.13022800	-3.92643900	2.52700100	C	2.52749000	-2.75414500	-2.91836200
H	4.14738500	-5.34221700	0.74891400	C	3.22648900	-3.87839100	-2.47405000
H	3.28406600	-5.19818600	-1.58105700	C	3.05104000	-4.32981900	-1.16330400
H	1.41821200	-3.69813800	-2.12579600	C	2.17253500	-3.66549300	-0.30368600
H	-0.99352600	-1.18654500	2.28405100	C	3.52871300	0.17914200	0.43740000
H	-2.53506100	-2.23146400	3.91860900	C	4.08763000	-0.23139100	-0.78533000
H	-3.91542900	-4.19475900	3.24517100	C	5.15480500	-1.12949000	-0.81994800
H	-3.71513900	-5.11007600	0.94235200	C	5.68182200	-1.63873000	0.37095400
H	-2.14415300	-4.10456700	-0.66804900	C	5.13711300	-1.24010000	1.59313700
H	-3.61256600	0.16697400	1.47353400	C	4.06943500	-0.33743000	1.62572400
H	-5.50146600	-1.41360400	1.66741900	C	2.65026300	2.59210900	-0.71359600
H	-6.46836200	-2.46645900	-0.37143200	C	3.83592000	3.29338400	-0.42857300
H	-5.53058400	-1.91138200	-2.60812800	C	4.29013000	4.29931900	-1.28242700
H	-3.65600200	-0.32495200	-2.81234200	C	3.57230500	4.61330400	-2.44079500
H	-4.57469900	2.62817900	-0.75021200	C	2.40058300	3.91741300	-2.73945700
H	-5.38472200	4.58144200	0.52438100	C	1.94284200	2.91488500	-1.87898700
H	-3.94133600	5.63898200	2.25142300	C	-2.89902400	2.49777000	0.04063700
H	-1.66096500	4.73106600	2.68014400	C	-4.17516600	2.87372500	0.49588500
H	-0.84326500	2.77854900	1.37976400	C	-4.71545600	4.11796500	0.16518400
H	4.84910600	1.94556000	-1.30441400	C	-3.99857400	5.00102000	-0.64654800
H	5.79964800	4.18173900	-0.92287400	C	-2.74047200	4.63153900	-1.12469100
H	4.46753200	5.93330700	0.23869800	C	-2.19472000	3.39209000	-0.77869300
H	2.15504700	5.41679700	1.00280900	C	-3.47363700	-0.15441300	-0.51021500
H	1.17568800	3.18197300	0.56976600	C	-4.49912700	-0.89508600	0.09522500
H	4.59605800	-1.14744100	-1.21010400	C	-5.44872100	-1.56266700	-0.68600100
H	6.22403800	-2.20754400	0.30225100	C	-5.39299800	-1.48911600	-2.07841700
H	6.07969600	-1.85071900	2.75880300	C	-4.37578600	-0.75202400	-2.69305300
H	4.25768100	-0.43524900	3.69553000	C	-3.42282300	-0.09651600	-1.91476800
H	2.59590700	0.60766500	2.18650700	H	-0.88039200	-1.59273800	3.28471600
H	0.10835600	1.96022700	-0.75590000	H	0.66398500	-1.21608800	4.06652100
H	0.06379600	0.66395400	1.05679800	H	0.77881000	-3.14719400	2.28766300
C	-0.41845200	1.50094700	3.72777700	H	1.93546000	-1.82552800	2.05239200
O	-1.36789900	0.83747800	3.85260500	H	0.99369800	2.18728800	3.91438400
O	0.52740000	2.17290600	3.61993300	H	2.01701300	0.75697300	3.73612200
<b>11</b>				H	1.74460500	3.16163800	1.87543400
$G_{\text{solv}} = -4253.640344$				H	3.22691900	2.31961200	2.35882800
Fe	-0.02298800	0.55157200	0.26884100	H	-1.75301400	0.84316400	4.16048800
P	0.25084400	-1.65315700	0.34606000	H	-1.58267800	2.23444500	3.05964000
				H	-3.69104500	1.00865400	2.43692500

H	-2.79529600	-0.51532300	2.35853900	C	3.29344200	-3.71877500	-2.47310300
H	-1.28768300	-2.41392700	-2.00116200	C	3.06932400	-4.23824100	-1.19525700
H	-3.14467400	-3.98592900	-2.41369600	C	2.16664200	-3.61352000	-0.33245300
H	-4.11963200	-5.29664400	-0.53443700	C	3.52612400	0.18323200	0.54227100
H	-3.21436300	-5.00956200	1.76567900	C	4.18730700	-0.22656600	-0.62756000
H	-1.34489500	-3.47010000	2.18394100	C	5.26038900	-1.11638800	-0.56495000
H	1.13804300	-1.18957600	-2.39461700	C	5.69041700	-1.61180500	0.66922300
H	2.66372900	-2.39322700	-3.93434700	C	5.04418000	-1.20955200	1.83964800
H	3.90617600	-4.39863600	-3.14315100	C	3.96959300	-0.31820700	1.77656900
H	3.59371400	-5.20257600	-0.80998500	C	2.66108700	2.51229200	-0.79963300
H	2.03783900	-4.04255700	0.70783300	C	3.76910300	3.32027900	-0.48644000
H	3.67934400	0.15168600	-1.72013600	C	4.25014000	4.25339200	-1.40482200
H	5.57094500	-1.43594500	-1.77633000	C	3.64066700	4.38422200	-2.65599700
H	6.51238500	-2.33853000	0.34532200	C	2.55143000	3.57702900	-2.98409000
H	5.54424300	-1.62608000	2.52388200	C	2.06343100	2.64822800	-2.05999200
H	3.66196200	-0.03931600	2.58942700	C	-2.96776300	2.47027000	0.08011400
H	4.41255100	3.05092400	0.46246900	C	-4.25819600	2.80998000	0.52348000
H	5.20524400	4.83560800	-1.04638600	C	-4.81158700	4.05428100	0.21862700
H	3.92824800	5.39504600	-3.10595800	C	-4.09231900	4.97237700	-0.55115700
H	1.84039600	4.15305700	-3.64024500	C	-2.81883200	4.63919500	-1.01420400
H	1.02914400	2.36946500	-2.10748800	C	-2.25904700	3.39845700	-0.69669100
H	-4.76494500	2.19190700	1.10535800	C	-3.46607600	-0.19613000	-0.56680100
H	-5.69883200	4.39380900	0.53615100	C	-4.52884300	-0.92597800	-0.01616900
H	-4.42101500	5.96726300	-0.90741900	C	-5.41819800	-1.61141300	-0.85029000
H	-2.17970800	5.30728100	-1.76492800	C	-5.26472400	-1.56093600	-2.23668800
H	-1.20859700	3.11309100	-1.14196700	C	-4.21167700	-0.82923500	-2.79417700
H	-4.57285200	-0.95631400	1.17821900	C	-3.31571000	-0.15692200	-1.96430700
H	-6.23426200	-2.13671200	-0.20145300	H	-0.81676500	-1.52557000	3.37349500
H	-6.13512800	-2.00362800	-2.68237200	H	0.75770600	-1.09780800	4.05183500
H	-4.32355200	-0.69237000	-3.77681200	H	0.75409000	-3.09521700	2.32291100
H	-2.62747800	0.46981900	-2.39966200	H	1.94593000	-1.81437600	2.05215100
H	-0.08871800	2.09441300	0.38297500	H	0.85141900	2.38531400	3.78589200
H	-0.08448100	0.65966600	-1.32043600	H	1.92411100	0.98431900	3.78276900

## 12

$$G_{\text{solv}} = -4254.109127$$

Fe	-0.05719400	0.57370900	0.25195400	H	-1.79257100	0.83992300	4.14148000
P	0.24827900	-1.64731800	0.36819100	H	-1.69936200	2.22150200	3.02164500
P	2.05336000	1.28325500	0.42687800	H	-3.74661600	0.87842400	2.43985200
P	-2.27905600	0.78844900	0.42843000	H	-2.77270500	-0.59756600	2.34314600
P	-0.04445300	0.56426500	2.42638700	H	-1.12986200	-2.59785000	-2.01293400
C	0.18060800	-1.14098700	3.11897300	H	-2.98365600	-4.18224300	-2.40192000
C	0.86887100	-2.03171300	2.07882200	H	-4.08985000	-5.31291800	-0.48049400
C	1.29907000	1.61826200	3.14122200	H	-3.32531200	-4.83487300	1.83804900
C	2.12338700	2.26265700	2.01523300	H	-1.46876900	-3.27531600	2.23886600
C	-1.66974900	1.12412200	3.08871100	H	1.23318600	-1.01632100	-2.33051800
C	-2.74951800	0.49313600	2.19821000	H	2.79610900	-2.15141000	-3.86964100
C	-1.15339100	-2.82251300	0.14040600	H	3.99110300	-4.20957500	-3.14556800
C	-1.60458200	-3.08891100	-1.16404800	H	3.59200200	-5.13382800	-0.87123800
C	-2.65157600	-3.98279900	-1.38660000	H	1.99021200	-4.04405600	0.65092900
C	-3.27472200	-4.61619600	-0.30695900	H	3.86221200	0.15236300	-1.59506100
C	-2.84628000	-4.34766200	0.99333400	H	5.76099500	-1.42168200	-1.47990000
C	-1.79094500	-3.45757700	1.21692900	H	6.52674800	-2.30313900	0.71777900
C	1.48944400	-2.44806400	-0.72977500	H	5.37644900	-1.58409600	2.80378900
C	1.73253900	-1.92992800	-2.01015100	H	3.47951400	-0.01878700	2.70057700
C	2.62138800	-2.56520500	-2.88043900	H	4.26643500	3.21872900	0.47613600
				H	5.10249700	4.87488600	-1.14552900



H	4.01706500	5.10950200	-3.37145600	C	4.89428400	3.97910300	0.21802700
H	2.07788000	3.66717500	-3.95752000	C	4.14319600	5.09758200	-0.14878800
H	1.21653800	2.02381500	-2.33190400	C	2.81496400	4.93583800	-0.54576300
H	-4.84605100	2.10010400	1.10200100	C	2.23717400	3.66421400	-0.56418600
H	-5.80612500	4.30350700	0.57762400	C	3.41517400	-0.14040000	0.67860100
H	-4.52516200	5.93920800	-0.79108300	C	4.40746100	-0.97809800	0.15091500
H	-2.25599100	5.34417500	-1.61958600	C	5.26834400	-1.67490400	1.00463200
H	-1.25995000	3.15427300	-1.04984600	C	5.15082300	-1.53783200	2.38870100
H	-4.67322700	-0.96792300	1.06091500	C	4.16828700	-0.69892600	2.92398900
H	-6.23342300	-2.18097400	-0.41245600	C	3.30757900	-0.00633400	2.07365200
H	-5.96084300	-2.09029800	-2.88090900	H	0.65394600	-1.38274900	-3.46146300
H	-4.08633500	-0.78797800	-3.87249400	H	-0.95053400	-0.87625400	-4.00343600
H	-2.49208800	0.40672200	-2.40261800	H	-0.83759700	-2.98774600	-2.39112200
H	-0.14044600	2.09277900	0.43328800	H	-2.02751000	-1.73409700	-2.00927200
H	-0.20922200	1.11567400	-1.25782700	H	-0.68965500	2.68530100	-3.52708200
H	-0.07998700	0.28238100	-1.34862900	H	-1.83606800	1.36555100	-3.77193700
<b>TS<sub>12,1</sub></b>				H	-1.66024000	3.37163400	-1.49888600
<b>G<sub>solv</sub> = -4254.083069</b>				H	-3.11373300	2.63619600	-2.19945000
Fe	0.01650400	0.59531300	-0.20636600	H	1.79543900	0.79466200	-4.06572800
P	-0.26933500	-1.63618700	-0.38785100	H	1.78847300	2.21149200	-2.99381500
P	-2.08292100	1.30250700	-0.38326200	H	3.74196100	0.78991500	-2.32008300
P	2.25110100	0.83056400	-0.34579800	H	2.69121500	-0.64595600	-2.22986000
P	0.02574100	0.67178100	-2.35470100	H	1.09922600	-2.73143900	1.92858600
C	-0.31340700	-0.99097800	-3.11661900	H	2.97041400	-4.31822800	2.22299000
C	-0.95037600	-1.93789100	-2.09143100	H	4.07295300	-5.33708900	0.23776000
C	-1.22321200	1.87314700	-3.01645700	H	3.29384700	-4.74091600	-2.04759200
C	-2.08865900	2.43001300	-1.86698500	H	1.42380900	-3.17058400	-2.35577100
C	1.68776800	1.11776600	-3.02252300	H	-1.33009900	-0.87114100	2.19020400
C	2.72115200	0.44731100	-2.10561300	H	-2.90982600	-1.93808300	3.78398300
C	1.11731200	-2.83750200	-0.23470700	H	-4.02322300	-4.07859900	3.17975200
C	1.57665300	-3.17064500	1.05239200	H	-3.53088500	-5.15882600	0.99647600
C	2.63101800	-4.06714200	1.22160800	H	-1.90508600	-4.13626300	-0.56105400
C	3.25203900	-4.63798300	0.10607300	H	-3.97350000	0.00383800	1.46300600
C	2.81543600	-4.30279900	-1.17601700	H	-5.83319400	-1.58447000	1.13516300
C	1.75337100	-3.40847200	-1.34703900	H	-6.51511800	-2.25824800	-1.16303500
C	-1.50024500	-2.43216600	0.71487700	H	-5.32487000	-1.30762800	-3.13034400
C	-1.79517800	-1.82460400	1.94238800	H	-3.45788300	0.26267700	-2.81500700
C	-2.69185600	-2.41836300	2.83405200	H	-4.35218800	3.19560300	-0.00883100
C	-3.31877300	-3.61799800	2.49303400	H	-5.02463900	4.61449500	1.90543700
C	-3.04192400	-4.22636900	1.26433200	H	-3.71378100	4.56966700	4.01531500
C	-2.12967600	-3.64306300	0.38307500	H	-1.70957900	3.11082900	4.20279600
C	-3.56881400	0.24787100	-0.64789900	H	-1.00861300	1.71121400	2.27449400
C	-4.26138700	-0.28255800	0.45353200	H	4.92507900	1.84768800	0.47133700
C	-5.31387000	-1.18042100	0.27003300	H	5.92967900	4.09400100	0.52636600
C	-5.69627300	-1.55916900	-1.01980100	H	4.59037000	6.08716000	-0.12566700
C	-5.02689500	-1.02734200	-2.12391700	H	2.22316400	5.79899000	-0.83766200
C	-3.97045400	-0.13140900	-1.93957500	H	1.19647200	3.55263200	-0.86279000
C	-2.62742800	2.36354200	1.00207400	H	4.52186700	-1.09283500	-0.92422800
C	-3.76391100	3.18242500	0.90726500	H	6.03140400	-2.32419100	0.58397900
C	-4.14813900	3.97808400	1.98758000	H	5.82280500	-2.07900300	3.04848800
C	-3.40979000	3.95246200	3.17480700	H	4.07681000	-0.58176600	4.00024200
C	-2.28373800	3.13371400	3.28076800	H	2.55435400	0.65998800	2.49224000
C	-1.89215400	2.34538300	2.19600100	H	0.04296100	2.13001000	-0.13705000
C	2.97873600	2.52998500	-0.19402700	H	0.52975600	-0.12542800	3.09039400
C	4.32019100	2.70646400	0.18938800	H	0.31685400	0.16233300	3.74508900