

Exploring the Decomposition Pathways of Iron Asymmetric Transfer Hydrogenation Catalysts

*Paraskevi O. Lagaditis, Peter E. Sues, Alan J. Lough, and Robert H. Morris**

Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6, Canada

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Table S1. Crystallographic Data Tables for **4**, **5**, and **6**

	4	5	6
empirical formula	C ₁₅ H ₃₂ Br _{0.5} Cl _{1.5} FeN ₂ OP ₂	C ₂₅ H ₄₄ F ₆ FeN ₂ OP ₃ Ru	C ₃₉ H ₅₅ BFeN ₂ OP ₂
FW	467.35	752.45	696.45
lattice type	Monoclinic	Monoclinic	Triclinic
space group	<i>P</i> 2 ₁ /n	<i>P</i> 2 ₁ /c	<i>P</i> ₋₁
<i>T</i> , K	150(1)	150(1)	150(1)
<i>a</i> , Å	13.1588(5)	8.4983(2)	10.3749(4)
<i>b</i> , Å	7.6800(2)	21.6914(8)	11.5650(4)
<i>c</i> , Å	21.6873(7)	17.3708(6)	16.1355(7)
α , deg	90	90	106.437(2)
β , deg	106.382(2)	93.653(1)	101.679(2)
γ , deg	90	90	92.517(2)
<i>V</i> , Å ³	2102.7(1)	3195.6(2)	1807.8(1)
<i>Z</i>	4	4	2
ρ_{calc} /Mg m ⁻³	1.476	1.564	1.279
μ (Mo, K α), mm ⁻¹	2.015	1.134	0.539
<i>F</i> (000)	972	1540	744
cryst size, mm ³	0.30 x 0.14 x 0.12	0.14 x 0.10 x 0.05	0.25 x 0.25 x 0.20
range θ collected, deg	2.83 to 27.45	1.88 to 26.99	1.85 to 26.99
reflns collected/unique	11795/4764	28470/6938	26212/7820
abs cor		Semi-empirical from equivalents	
max and min transmn coeff.	0.744 and 0.679	0.7455 and 0.6959	0.890 and 0.771
goodness of fit	1.047	1.010	1.036
$R_1(I > 2s(I))$	1.019	0.0531	0.0556
wR_2 (all data)	0.1162	0.1391	0.1203
peak and hole, e Å ⁻³	0.714 and -0.525	1.290 and -0.951	0.313 and -0.326

^a Definition of R indices: $R_1 = \sum(F_O - F_C)/\sum(F_O)$; $wR_2 = [\sum[w(F_O^2 - F_C^2)^2]/[\sum[w(F_O^2)^2]]^{1/2}$.

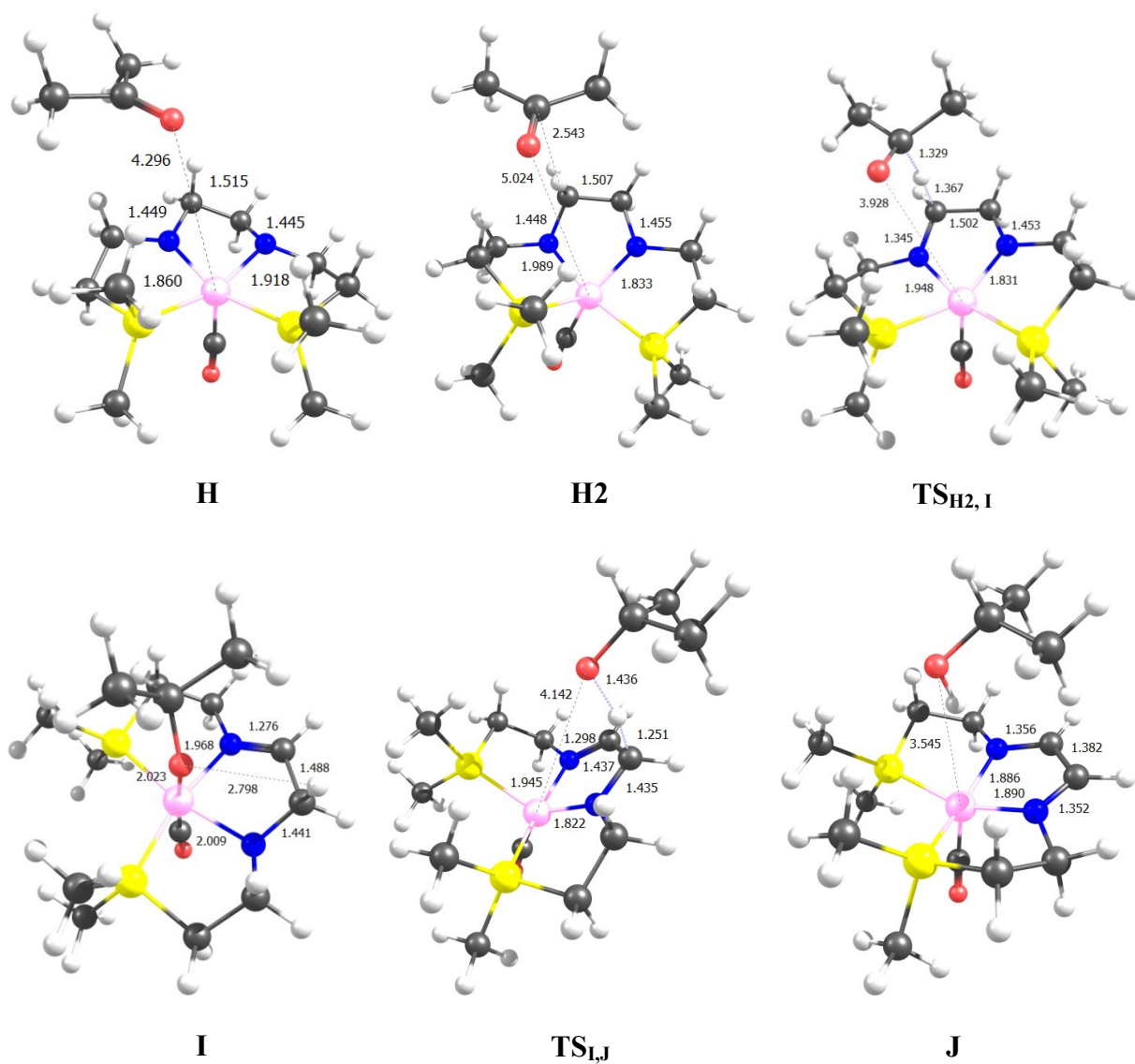


Figure S1. Optimized structures, as well as selected bond lengths and angles for **H**, **H2**, **TS_{H2,I}**, **I**, **TS_{I,J}**, and **J**.

Full Gaussian09 Reference. Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Cartesian Coordinates (Å) and Free Energies (G°_{solv} , kcal/mol) of Optimized Structures

Acetone

G°_{solv}	-192.993877		
C	-0.00003853	0.181890213	-0.000012835
C	-1.272544551	-0.612209784	-0.003100390
H	-2.136658089	0.033938513	-0.176593310
H	-1.234318374	-1.403679246	-0.761515738
H	-1.386011271	-1.112979661	0.967493854
C	1.272576069	-0.612147453	0.003095112
H	2.136669530	0.034076613	0.176422322
H	1.234490029	-1.403459039	0.761685979
H	1.386034894	-1.113075823	-0.967414208
O	-0.000046589	1.402497603	0.000003722

iPrOH

G°_{solv}	-194.168373		
H	0.965992234	1.719869637	0.074787659
H	0.007881553	0.090664015	1.469227521
C	-0.002739674	0.040712764	0.365834970
C	1.155074907	-0.817307440	-0.101901826
H	2.117999670	-0.399902814	0.220228506
H	1.079634790	-1.832309277	0.307700716
H	1.158919422	-0.885604178	-1.197940354
C	-1.335475299	-0.504245725	-0.089890287
H	-2.157781411	0.139615073	0.241884257
H	-1.364836614	-0.563516254	-1.185963411
H	-1.500424452	-1.509722556	0.314207518
O	0.098931901	1.365743592	-0.161048693

A

G°_{solv}	-2561.799638		
Fe	0.020276966	0.336379351	0.100379053
P	1.674883872	-1.112871275	-0.290522178
O	0.150088445	-0.324635549	2.895692890
N	-1.098566476	1.833995807	-0.258576608
N	1.395346905	1.641240655	-0.130284594
C	-2.430570272	1.703071794	-0.448981066
H	-3.005891793	2.613282021	-0.662209155
C	2.697067729	1.298505320	-0.121281538
H	3.440147058	2.106240272	-0.112320888
C	3.082201216	-0.019847621	-0.148861333
H	4.121073122	-0.334640164	-0.227152832
C	0.099099182	-0.075772549	1.752535431
C	1.674227972	-1.770889224	-2.004705985
H	2.650377087	-2.215411951	-2.236597843
H	0.896057503	-2.533835672	-2.124725153
H	1.479408325	-0.949951904	-2.705350030

C	1.983879426	-2.612693449	0.700716124
H	1.147268966	-3.313061019	0.582824614
H	2.906939151	-3.105073484	0.370222859
H	2.081042566	-2.351036736	1.760197886
P	-1.875548281	-0.849737935	-0.144418565
C	-2.510323914	-1.930384242	1.187600374
H	-3.492182861	-2.336059401	0.914188846
H	-1.815886150	-2.761952808	1.361710690
H	-2.608672358	-1.354256922	2.114399582
C	-1.994361819	-1.947870396	-1.608041683
H	-1.646431360	-1.414769494	-2.500258232
H	-1.369193193	-2.837425480	-1.457363690
H	-3.033928958	-2.263893610	-1.761661696
C	0.949633593	3.002800683	0.118983671
H	0.891408929	3.191073011	1.206866109
H	1.641089475	3.744710489	-0.309535066
C	-0.436998806	3.115224644	-0.489296285
H	-0.352175531	3.310147015	-1.573314654
H	-1.000360185	3.952364007	-0.048604391
C	-3.047619837	0.482118177	-0.378031542
H	-4.122902155	0.351677183	-0.484392893

B

G°_{solv}	-2756.060980		
Fe	-0.274489370	0.005383016	-0.397095635
P	0.615895186	2.060659309	-0.011814331
O	-2.223034575	1.086399421	-2.214089156
N	-0.662665671	-1.816777285	-0.983643090
N	1.182072419	-0.168127727	-1.683455035
C	-1.766457984	-2.435008529	-0.523638451
H	-2.049631208	-3.388133120	-0.991413264
C	2.176061262	0.718736451	-1.686135937
H	3.043609452	0.513587935	-2.330790399
C	2.144831412	1.871369935	-0.918005928
H	2.893629861	2.656262622	-1.023149309
C	-1.425124106	0.682445263	-1.466490833
C	0.935140243	2.779053790	1.646196125
H	1.622286791	3.630760989	1.558813229
H	-0.016669940	3.137607529	2.059595605
H	1.360038083	2.046260528	2.336324042
C	-0.269371894	3.487385113	-0.765799501
H	-1.255424688	3.625067857	-0.302313315
H	0.316606582	4.406069362	-0.632559269

H	-0.404603770	3.312634074	-1.839259385	H	-4.498514463	0.405023098	0.782327093
P	-1.929377784	-0.329139110	1.099513285	H	-3.684159636	1.844360569	0.109045894
C	-3.373206226	0.797237530	1.167487738	H	-3.788101314	0.349477432	-0.854666586
H	-4.139451972	0.402598224	1.846711884	C	-2.159938957	0.730883762	2.587827770
H	-3.052278730	1.783073070	1.529889729	H	-1.253933176	0.428472868	3.123328263
H	-3.813695051	0.915218704	0.171351909	H	-2.244065074	1.823664325	2.617373180
C	-1.521900745	-0.462235396	2.882719115	H	-3.036093404	0.296469452	3.086086938
H	-0.710653147	-1.182148334	3.030204852	C	1.063420873	-1.553845260	-2.405456620
H	-1.202926410	0.517965150	3.260647203	H	1.420855408	-1.376910502	-3.432819324
H	-2.404737760	-0.790535770	3.446244085	H	1.604394276	-2.437857926	-2.029182455
C	1.285815216	-1.470266667	-2.322751175	C	-0.439322737	-1.856162312	-2.430557365
H	1.663825025	-1.393176411	-3.355107036	H	-0.638937241	-2.914784362	-2.652760818
H	1.983393700	-2.127221769	-1.770178867	H	-0.922168071	-1.247834000	-3.210744783
C	-0.103033604	-2.095504049	-2.297786693	C	-2.097643274	-1.652771015	0.915261001
H	-0.056972568	-3.177554077	-2.501646762	H	-2.884242177	-2.156111624	1.482659696
H	-0.723587842	-1.637075237	-3.091220677	C	1.283340974	-2.026373778	1.703781897
C	-2.505119276	-1.924880354	0.519177414	H	0.765036274	-2.667240828	2.450412064
H	-3.334293383	-2.473716083	0.964565927	C	2.480935754	-1.401669346	2.399539710
C	2.208658036	-1.532799659	1.717234281	H	3.018873384	-0.731425904	1.712113909
H	2.011497907	-2.360345260	2.418950058	H	2.171575850	-0.821727150	3.278609030
C	2.591887591	-0.304653475	2.499907769	H	3.184009717	-2.174898136	2.738385021
H	2.833372215	0.521237467	1.816741824	C	1.748353756	-2.945377824	0.586290106

TS_{B,C}

G°_{solv} -2756.037262

Fe	-0.199883101	0.168856986	-0.412721005
P	1.202243100	1.811697067	0.251066796
O	-1.391801804	1.949497569	-2.352396769
N	-1.003171799	-1.461997791	-1.151498489
N	1.282943382	-0.399915291	-1.550133844
C	-1.776210848	-2.171886758	-0.399587873
H	-2.089677029	-3.175756224	-0.714726346
C	2.461422570	0.206562662	-1.454039901
H	3.286125966	-0.170902080	-2.076421086
C	2.675999621	1.280739200	-0.603713415
H	3.623968232	1.817259873	-0.579104789
C	-0.897589725	1.230873997	-1.578943036
C	1.558325280	2.101077105	2.025158765
H	2.460183846	2.718836107	2.127729546
H	0.714666676	2.635875926	2.479808881
H	1.706942170	1.157466005	2.556192590
C	0.854942129	3.538593807	-0.273508323
H	-0.080711975	3.893136187	0.179003511
H	1.673329752	4.202355388	0.034193306
H	0.760896489	3.586009861	-1.363963302
P	-2.071997149	0.179970145	0.852282532
C	-3.663875822	0.748697948	0.158963336

H	-4.498514463	0.405023098	0.782327093
H	-3.684159636	1.844360569	0.109045894
H	-3.788101314	0.349477432	-0.854666586
C	-2.159938957	0.730883762	2.587827770
H	-1.253933176	0.428472868	3.123328263
H	-2.244065074	1.823664325	2.617373180
H	-3.036093404	0.296469452	3.086086938
C	1.063420873	-1.553845260	-2.405456620
H	1.420855408	-1.376910502	-3.432819324
H	1.604394276	-2.437857926	-2.029182455
C	-0.439322737	-1.856162312	-2.430557365
H	-0.638937241	-2.914784362	-2.652760818
H	-0.922168071	-1.247834000	-3.210744783
C	-2.097643274	-1.652771015	0.915261001
H	-2.884242177	-2.156111624	1.482659696
C	1.283340974	-2.026373778	1.703781897
H	0.765036274	-2.667240828	2.450412064
C	2.480935754	-1.401669346	2.399539710
H	3.018873384	-0.731425904	1.712113909
H	2.171575850	-0.821727150	3.278609030
H	3.184009717	-2.174898136	2.738385021
C	1.748353756	-2.945377824	0.586290106
H	2.334281450	-3.777579810	0.999239531
H	0.897857425	-3.370416546	0.037155481
H	2.383726989	-2.400014313	-0.123256472
O	0.355223902	-1.044731311	1.301820166
H	-0.861584367	-1.581029143	1.354431053

C

G°_{solv} -2756.072483

Fe	0.236416300	0.024759009	-0.396814585
P	2.102291520	-0.009074141	0.875458871
O	1.731200608	1.457340861	-2.435420547
N	-1.290679508	-0.363315828	-1.580875068
N	0.923295340	-1.667282415	-1.124727110
C	-2.386216683	0.290680251	-1.591681656
H	-3.205265402	-0.007339141	-2.258192895
C	2.053238879	-2.182086363	-0.654399806
H	2.356445060	-3.175308556	-1.017673865
C	2.848805326	-1.505094578	0.256531198
H	3.807359386	-1.898356863	0.593667398
C	1.118578885	0.904875644	-1.612000660
C	1.926741603	-0.146923652	2.695215460
H	2.915481728	-0.247533457	3.161544465
H	1.430336412	0.747742196	3.094293091
H	1.319127760	-1.024463103	2.934237881
C	3.333351802	1.346582407	0.766068445

H	2.912465349	2.265931530	1.195772982	H	1.530357490	1.243831288	2.983900711
H	4.244695489	1.086271133	1.319759788	H	0.854799712	-0.400477448	3.132745592
H	3.602935098	1.537684208	-0.278581972	C	3.526483840	0.961216007	0.793845652
P	-0.946606440	1.851135800	0.154144822	H	3.225900415	2.013869769	0.889079719
C	-0.474084151	3.458838355	-0.582282694	H	4.301830096	0.745760956	1.540186396
H	-1.199608718	4.239637952	-0.323068354	H	3.949831259	0.806939080	-0.204959915
H	0.517425435	3.754465305	-0.216891068	P	-0.598169288	1.942656990	-0.223547457
H	-0.426835209	3.366820972	-1.673564691	C	-0.081780046	3.292089349	-1.344393402
C	-1.404630018	2.350331507	1.850571560	H	-0.745404984	4.160023468	-1.243379466
H	-1.734228184	1.488234944	2.438852520	H	0.944355521	3.599154391	-1.106036416
H	-0.519414829	2.783592458	2.332710444	H	-0.109662378	2.941428119	-2.382692913
H	-2.200935366	3.104776775	1.829402840	C	-0.711503889	2.835168116	1.369723376
C	-0.075185478	-2.451998342	-1.812888356	H	-0.871200703	2.143864965	2.202851099
H	0.369998079	-3.126839444	-2.562237917	H	0.243883210	3.352300486	1.528262794
H	-0.645497425	-3.082094841	-1.107947302	H	-1.513276172	3.584227820	1.350537123
C	-1.025382263	-1.478265900	-2.496775976	C	-0.240379046	-2.718411014	-1.418828040
H	-1.958148198	-1.956410650	-2.825364964	H	0.202831155	-3.465600309	-2.099471126
H	-0.530485687	-1.044581184	-3.378596785	H	-0.861306142	-3.280324083	-0.699528650
C	-1.879696152	-1.188750477	1.507212954	C	-1.110966607	-1.736960617	-2.202866603
H	-2.476883172	-0.276570473	1.278522873	H	-2.106240992	-2.165934164	-2.401453945
C	-1.919490377	-1.361710203	3.025532365	H	-0.636075091	-1.554078251	-3.182691065
H	-1.385825477	-2.281368350	3.309527153	C	-2.252801499	-0.824773464	1.302725043
H	-1.424324218	-0.521300938	3.531748164	C	-3.076263546	0.090164304	2.185000574
H	-2.948019895	-1.433621359	3.407192815	H	-2.941311531	-0.227924540	3.230249336
C	-2.617808698	-2.359834662	0.854681340	H	-2.754012138	1.133055079	2.112713787
H	-3.649561032	-2.442618876	1.227098380	H	-4.146175963	0.028876026	1.953766579
H	-2.661443453	-2.253509850	-0.236392959	C	-2.779096685	-2.242308576	1.234672336
H	-2.098697623	-3.303293482	1.083074526	H	-2.481882574	-2.771754626	2.151974490
O	-0.564214159	-1.071638472	1.089267927	H	-3.872330261	-2.270526640	1.160496735
C	-2.563910376	1.477904515	-0.706789586	H	-2.347373533	-2.783486586	0.385925797
H	-2.903406580	2.340496446	-1.298629449	O	-0.977396565	-0.647076792	1.255813009
H	-3.359865488	1.286175046	0.027329329	C	-2.327567180	1.551441552	-0.801601338
TS_{C,D}				H	-2.510595763	2.125895963	-1.720310569
G°_{solv} -2756.033762				H	-3.081736884	1.861507754	-0.067818647
Fe	0.355506590	-0.062973930	-0.426380349	C	-2.396584895	0.062484815	-1.117330525
P	2.069548280	-0.126427644	1.037367043	H	-3.277571837	-0.241593159	-1.705528246
O	2.145625829	0.853874376	-2.485634731	H	-2.721282890	-0.411333660	0.015934771
N	-1.203779566	-0.466259097	-1.497491137	D			
N	0.777548221	-1.949057865	-0.727646245	G°_{solv} -2756.066459			
C	1.751269930	-2.530263667	-0.034139484	Fe	0.148633654	-0.251061472	0.310878905
H	1.900889045	-3.611979166	-0.168132727	P	2.154992393	0.250646421	-0.672525640
C	2.568921579	-1.823939847	0.834322039	O	1.258966662	-2.761686282	1.168505753
H	3.398942709	-2.292506155	1.361758078	N	-1.446118954	-0.352943686	1.452240889
C	1.427220299	0.490155894	-1.639496593	N	0.908311533	0.666934189	1.855194706
C	1.728161141	0.177495248	2.814615670	C	2.170666020	1.073849787	1.857157710
H	2.597067956	-0.117844915	3.417259137	H	2.559573425	1.539643952	2.774569642

C	2.996128748	0.922009239	0.750927351	O	0.179033131	-0.203012985	2.909871068
H	4.031757433	1.261160620	0.753135745	N	-1.158959348	1.675014002	-0.401499460
C	0.802247357	-1.750997700	0.799366521	N	1.322759752	1.773384808	-0.030370979
C	2.260270598	1.492743534	-2.026610537	C	2.626361224	1.502418407	-0.166398438
H	3.310839200	1.674117099	-2.289656599	H	3.313484060	2.352975869	-0.280657254
H	1.724228290	1.135597977	-2.916244976	C	3.108534701	0.210089626	-0.174864085
H	1.808209259	2.433494161	-1.696949224	H	4.170076317	-0.021566956	-0.247796330
C	3.204942413	-1.076434886	-1.385282928	C	0.131709168	-0.013876348	1.754233423
H	2.768768113	-1.433068718	-2.327837600	C	1.930855935	-1.840017961	-1.886064653
H	4.215840745	-0.699151871	-1.588388760	H	2.953564598	-2.209524431	-2.037169475
H	3.281210365	-1.920212788	-0.690029792	H	1.236474613	-2.687795977	-1.937429856
P	-1.117048081	-1.261214771	-1.223172488	H	1.685133305	-1.132466311	-2.686592898
C	-0.681301759	-2.960604164	-1.744958010	C	2.173860197	-2.371936147	0.886592617
H	-1.403413165	-3.346027587	-2.475442195	H	1.355533932	-3.104300526	0.873992224
H	0.321749942	-2.969028189	-2.189719507	H	3.104547832	-2.875498391	0.595837591
H	-0.675035840	-3.625770885	-0.872951936	H	2.283765512	-1.986344704	1.906344270
C	-1.565187931	-0.471659355	-2.811521793	P	-1.715817272	-1.025863629	-0.191212149
H	-1.913277979	0.554710602	-2.645779198	C	-2.485222328	-1.774278811	1.289002048
H	-0.680281526	-0.437692295	-3.459631004	H	-3.401234485	-2.315266725	1.021180283
H	-2.356111959	-1.039912343	-3.317686531	H	-1.781930645	-2.473392671	1.758510625
C	-0.012428917	0.829711402	2.960274910	H	-2.731429996	-0.988526438	2.013541727
H	0.503205511	0.816636660	3.934942423	C	-1.713564591	-2.414714497	-1.378541903
H	-0.544756651	1.798315788	2.883383646	H	-1.296684892	-2.087583324	-2.337721954
C	-1.031498499	-0.292606282	2.838056016	H	-1.104715590	-3.238950852	-0.987927409
H	-1.890455331	-0.107719093	3.514070527	H	-2.737189636	-2.778531381	-1.537701861
H	-0.565343275	-1.246911031	3.184950954	C	0.783808255	3.069639390	-0.409280505
C	-1.357730584	2.526719735	-0.532117093	H	1.286435195	3.900610721	0.112100585
C	-1.181441973	3.749689713	-1.371689301	H	0.914527900	3.238320067	-1.494362726
H	-1.008955707	4.609828389	-0.710897669	C	-0.697887296	3.022941730	-0.095483288
H	-0.331882961	3.644967118	-2.052367578	H	-1.248949427	3.780782231	-0.679157247
H	-2.097206295	3.965221638	-1.935103106	H	-0.877271139	3.255336799	0.974092811
C	-2.639127106	2.402509087	0.217887661	C	-2.984237357	0.146559619	-0.839548860
H	-3.449134954	2.243283299	-0.508824227	H	-3.999203856	-0.160445478	-0.554845531
H	-2.591974069	1.560917518	0.917131595	H	-2.911883079	0.117955298	-1.936085809
H	-2.867061724	3.347045317	0.727924227	C	-2.604208282	1.526215725	-0.327372113
O	-0.465296984	1.680460183	-0.494676911	H	-2.959795724	1.658892050	0.715355865
C	-2.702433364	-1.459203645	-0.293280640	H	-3.105092651	2.309390444	-0.923329213
H	-3.242334993	-2.362369485	-0.609247948				
H	-3.331486834	-0.587832711	-0.526714562	F			
C	-2.337360732	-1.459427757	1.188130540	G°_{solv}	-2757.275068		
H	-1.890191579	-2.448740578	1.456528744	Fe	-0.601441636	0.022931176	-0.457478346
H	-3.259288176	-1.380296067	1.798732843	P	-0.494437289	2.045394874	0.559311041
				O	-2.946658946	0.840414383	-1.906909765
E				N	0.024220139	-1.593001979	-1.116562328
G°_{solv}	-2563.013930			N	0.810657053	0.737431018	-1.567911559
Fe	0.017575655	0.340741157	0.086853469	C	1.192218207	2.021063987	-1.477049311
P	1.795546953	-0.994554476	-0.259313821	H	1.974438878	2.372682752	-2.163976383

C	0.639236655	2.874943824	-0.548609802	Fe	-0.629369648	-0.073547714	-0.404109257
H	0.945882118	3.915654081	-0.455635575	P	0.533303604	1.872870719	-0.196466331
C	-1.997652132	0.538419631	-1.289553218	O	-2.606699617	1.117422628	-2.118803289
C	0.183874379	2.206904083	2.260064176	N	-0.973740860	-1.900150150	-0.503045602
H	0.406130223	3.261043187	2.471976000	N	0.758194780	-0.503261541	-1.715183254
H	-0.545383165	1.844280595	2.995227607	C	1.817613496	0.225539827	-1.887945290
H	1.105278682	1.620784637	2.350875295	H	2.595233859	-0.124635189	-2.580649761
C	-2.011919719	3.060241546	0.708806191	C	2.059599870	1.415337925	-1.101326315
H	-2.734072649	2.549513918	1.360402358	H	2.564133715	2.231618100	-1.633387014
H	-1.780583841	4.043760543	1.137050129	C	-1.787973759	0.674937778	-1.413342694
H	-2.467262983	3.202445427	-0.277615765	C	1.070398514	2.611221383	1.389141127
P	-1.786011782	-1.219092458	0.952810593	H	1.874445158	3.337737269	1.214536242
C	-3.594821287	-1.341092722	0.726306278	H	0.218948120	3.133024479	1.842914069
H	-4.028508803	-2.063832954	1.428310219	H	1.430890339	1.845549461	2.083388906
H	-4.060008571	-0.360557289	0.886785740	C	-0.117344051	3.347131229	-1.065438790
H	-3.811905955	-1.663239713	-0.299595069	H	-1.071418387	3.656654691	-0.619942466
C	-1.607241827	-1.052340705	2.761904393	H	0.597082517	4.176876027	-0.994337143
H	-0.545121529	-0.975608099	3.023298227	H	-0.283626871	3.110105420	-2.122739706
H	-2.124114673	-0.144110199	3.096341308	P	-2.043915146	-0.076753873	1.319849235
H	-2.044332736	-1.918510732	3.275574198	C	-3.667855039	0.740671943	1.155006198
C	1.488203913	-0.217679438	-2.432364918	H	-4.259983383	0.597532868	2.066997159
H	1.632261227	0.173569226	-3.452017567	H	-3.530856791	1.814490434	0.977861357
H	2.493227404	-0.454811920	-2.034449642	H	-4.212770586	0.312871864	0.304840703
C	0.635967604	-1.477054630	-2.432410825	C	-1.499158908	0.414041019	2.989661059
H	1.248810459	-2.364584118	-2.670808049	H	-0.524258922	-0.034232987	3.212908457
H	-0.146955439	-1.413044365	-3.217014894	H	-1.410165736	1.505032411	3.048017588
C	-1.148373464	-2.899923207	0.539943683	H	-2.229963834	0.076250037	3.735773897
H	-1.899099669	-3.677544037	0.732626163	C	0.703768111	-1.881093852	-2.212963909
H	-0.284354910	-3.080362092	1.196098468	H	0.874664353	-1.923679572	-3.297126249
C	-0.693384966	-2.839056335	-0.910537194	H	1.507969995	-2.452273143	-1.720591181
H	-1.569331997	-2.916348345	-1.589581404	C	-0.642117962	-2.449958998	-1.809750731
H	-0.046357697	-3.702325666	-1.147696144	H	-0.597685986	-3.552460780	-1.783736918
C	3.646443898	-0.766299733	0.624356016	H	-1.418689554	-2.183582580	-2.556333558
H	3.401096777	-1.553325798	-0.111890019	C	-2.414175096	-1.878867651	1.437590136
C	4.276891697	-1.403861669	1.840120679	H	-3.421029286	-2.059486451	1.835682644
H	5.215560711	-1.902851176	1.572448708	H	-1.682183909	-2.307630120	2.137887733
H	4.499093351	-0.639471896	2.597393548	C	-2.201646591	-2.452731517	0.046203542
H	3.607017822	-2.148048418	2.286690936	H	-3.071814335	-2.214134480	-0.602372019
C	4.556660533	0.258009140	-0.021998081	H	-2.144599151	-3.554671662	0.088568543
H	4.062969704	0.746195501	-0.873170063	C	3.487592196	-0.834375248	0.747618363
H	4.827705982	1.035619736	0.705462833	H	3.271081182	-1.180746343	-0.297785272
H	5.479233901	-0.210015981	-0.388119431	C	2.258907914	-1.188070780	1.584771828
O	2.430037967	-0.149146892	1.057878921	H	2.025492988	-2.263338000	1.550810450
H	1.925112494	0.117510563	0.267316272	H	2.422171922	-0.900419643	2.634905748
				H	1.369171327	-0.648393903	1.218551707
				C	4.697257435	-1.630780769	1.222805282
				H	5.575290631	-1.407455015	0.602998153

TS_{F,G}

G°_{solv} -2757.251937

H	4.939697118	-1.361507597	2.261693545	H	0.256359192	4.366477854	-1.732227783
H	4.517378425	-2.714605139	1.184754908	H	0.280978730	3.035476474	-2.914966976
O	3.749162033	0.527619317	0.758120208	H	-1.037806016	3.146342166	-1.725086706
H	2.878105436	1.041530011	-0.217105554	C	2.333375419	2.691572699	-1.086495626
G				H	2.929222842	2.150156988	-0.338120524
G°_{solv} -2757.280887				H	2.663473964	2.358522583	-2.083715271
Fe	-0.091230272	-0.179565803	0.341446649	H	2.570484652	3.761646484	-0.992308722
P	1.434511488	-1.533281289	-0.598607812	O	0.540870082	1.078775363	-1.112160241
O	-0.958792931	-2.307734691	2.116945639	C	2.985804426	-0.856893809	0.185341465
N	-1.053651245	1.273283796	1.289193732	H	3.541040770	-0.278253027	-0.569910424
N	1.406062454	0.405038937	1.482875198	H	3.664600774	-1.653008150	0.521391097
C	2.619549638	0.052709856	1.307222124	TS_{G,H}			
H	3.412620469	0.445414119	1.956992052	G°_{solv} -2757.242395			
C	-0.609974921	-1.432437002	1.423759570	Fe	-0.327636705	-0.028564329	-0.368796688
C	1.806105362	-1.566716565	-2.386160151	P	0.982340721	1.794762029	-0.329348109
H	2.776282335	-2.044950487	-2.571408087	O	-1.976447026	1.085278274	-2.445171315
H	1.027568109	-2.142712470	-2.900790381	N	-1.027628641	-1.860841853	-0.460550142
H	1.815745463	-0.547912807	-2.785961791	N	1.081927508	-0.748162733	-1.518910740
C	1.503849901	-3.312895228	-0.167071009	C	-1.320091349	0.629039023	-1.589619785
H	0.596523066	-3.811629677	-0.531052574	C	1.378275817	2.722995255	1.196480269
H	2.381341431	-3.799863903	-0.610513777	H	2.273813016	3.343115964	1.062219159
H	1.546699166	-3.429511050	0.922265620	H	0.529059468	3.380822452	1.423081598
P	-1.961572885	-0.418145808	-0.834219453	H	1.525055049	2.039846196	2.038290844
C	-2.995785635	-1.915078039	-0.616901846	C	0.659527295	3.165426705	-1.500593159
H	-3.909477451	-1.847779250	-1.220805209	H	-0.276380476	3.671008232	-1.230527391
H	-2.431406594	-2.805383184	-0.923583398	H	1.475614976	3.899147133	-1.487654494
H	-3.279926983	-2.032108477	0.435294199	H	0.557318863	2.764514486	-2.516225182
C	-2.007290048	-0.207542811	-2.647745689	P	-1.938648228	0.300628052	1.133822593
H	-1.379827788	0.637412354	-2.947742659	C	-3.295799289	1.471564474	0.762543670
H	-1.627402591	-1.117855537	-3.127290700	H	-4.030346583	1.488037391	1.577404554
H	-3.038235689	-0.038469918	-2.984423474	H	-2.887503449	2.481576868	0.625554026
C	1.014859457	1.384462872	2.505720913	H	-3.802848743	1.174686877	-0.163299629
H	1.521153684	1.175946557	3.457830982	C	-1.571057835	0.687992591	2.881124916
H	1.345010401	2.373740440	2.157136799	H	-0.779294696	0.029525803	3.252310614
C	-0.500308535	1.351211930	2.621634279	H	-1.232274184	1.727628339	2.966333661
H	-0.844075956	2.254397847	3.163378355	H	-2.472096356	0.555397897	3.493785104
H	-0.796961649	0.485425007	3.262209536	C	0.830851578	-2.122426402	-1.942559102
C	-2.991241103	0.935403408	-0.115665964	H	1.138979055	-2.284479494	-2.989513043
H	-4.062188432	0.696354513	-0.173040341	H	1.418900309	-2.825872445	-1.325712005
H	-2.806899382	1.843067705	-0.708477757	C	-0.650178903	-2.395029876	-1.751071801
C	-2.490984115	1.129685713	1.311697259	H	-0.852913936	-3.482060447	-1.825199633
H	-2.828559300	0.264294334	1.936428335	H	-1.219866295	-1.921855434	-2.587392484
H	-2.974109672	2.020252096	1.761364388	C	-2.747450245	-1.359710405	1.153020926
C	0.839081750	2.419972566	-0.909090456	H	-3.821059145	-1.283627258	1.372818909
H	0.553932245	2.735626584	0.114375021	H	-2.268711462	-1.939401687	1.956027595
C	0.041000507	3.296947196	-1.872113106	C	-2.442462790	-1.997047970	-0.197382018

H	-3.075917861	-1.516236347	-0.983423121	C	0.040451117	-2.545998393	-1.472787656
H	-2.743571455	-3.063250352	-0.186941686	H	0.275004727	-3.621122968	-1.355924322
C	2.184385083	-1.104765745	1.285184431	H	-0.539011638	-2.446310147	-2.420864203
C	2.225909140	-2.621656383	1.347428593	C	-2.477451138	-2.146338212	1.253959449
H	3.163058341	-3.033172785	0.953055131	H	-3.530379045	-2.394103752	1.441703182
H	2.145785503	-2.922164707	2.403939268	H	-1.878364552	-2.525582100	2.093711381
H	1.376445625	-3.051717357	0.808689746	C	-1.938408675	-2.700610078	-0.059199324
C	3.328231579	-0.440302322	2.026414783	H	-2.692592186	-2.556855702	-0.867897314
H	3.352540658	0.641779505	1.857941792	H	-1.784970906	-3.793278292	0.023744919
H	3.184019253	-0.606937533	3.104812706	C	4.036066523	-0.601820257	1.047051902
H	4.298459326	-0.869312742	1.747727872	C	4.734305161	-1.646058761	0.234387160
O	1.028106213	-0.532096678	1.335931508	H	4.678218061	-1.369505323	-0.828154515
C	2.575833819	1.069932044	-0.971853650	H	5.800747974	-1.679874997	0.490189699
H	3.414273704	1.265952045	-0.292378269	H	4.279568482	-2.630194663	0.375994270
H	2.816917343	1.556520177	-1.927193695	C	4.712657784	0.731169841	1.143529746
C	2.357871060	-0.412306030	-1.209237077	H	4.009554383	1.510312372	1.453562372
H	2.621700358	-0.917716881	-0.037209342	H	5.506517433	0.657635889	1.900173698
H	3.157575429	-0.914583104	-1.778867360	H	5.198338611	1.005086722	0.199834899
H				O	2.975802293	-0.827250956	1.619930344
G°_{solv} -2757.275574				C	1.251686532	2.044832898	-1.522597476
Fe	-0.725638642	-0.107584611	-0.439368964	H	1.980447781	2.854429638	-1.380980574
P	0.021344166	1.957870190	-0.158344107	H	0.673990805	2.255009475	-2.435014144
O	-2.716374433	0.696429936	-2.351526950	C	1.895174121	0.666607512	-1.609573112
N	-0.694749571	-2.022619916	-0.343867282	H	2.757320120	0.621871794	-0.909977865
N	0.913796863	-0.345602572	-1.285076580	H	2.324160871	0.505066974	-2.617219576
C	-1.942450933	0.362423406	-1.529691631	H2			
C	0.983617081	2.279598342	1.366028369	G°_{solv} -2757.276525			
H	1.619862868	3.166668922	1.249197018	Fe	-0.860606352	0.082337987	-0.604726710
H	0.297362851	2.443043403	2.205740174	P	-0.092596077	1.649881824	0.716230632
H	1.602384334	1.403768576	1.596605539	O	-2.766356531	1.908374284	-1.815825834
C	-0.994940421	3.464533985	-0.326633704	N	-0.200661567	-1.617196159	-0.794580489
H	-1.714763585	3.509760680	0.500533326	N	0.610179617	0.561392941	-1.854990089
H	-0.376469936	4.370979602	-0.308398126	C	-1.989848662	1.198965730	-1.296004714
H	-1.553330058	3.428903423	-1.269747696	C	0.445108909	1.181038560	2.400724850
P	-2.222857168	-0.315240173	1.183590380	H	1.178321700	1.904343139	2.781774099
C	-3.904387564	0.376284031	0.980709596	H	-0.418962452	1.169537855	3.075728256
H	-4.526346884	0.165130859	1.859609817	H	0.896093391	0.181791790	2.383364703
H	-3.849328407	1.462208736	0.831818496	C	-1.032352003	3.188611485	1.022320200
H	-4.377113518	-0.069472654	0.096723749	H	-2.018355477	2.945748968	1.437329341
C	-1.799913750	0.182898533	2.892136063	H	-0.495894662	3.839100972	1.724462229
H	-0.785901691	-0.159736329	3.132011014	H	-1.176293962	3.726790594	0.077570855
H	-1.831690849	1.276889430	2.972368308	P	-2.396697366	-0.926691727	0.645287543
H	-2.509279149	-0.244280300	3.612886620	C	-3.951575887	-1.344287111	-0.226633545
C	1.303192915	-1.714021636	-1.562216124	H	-4.552892177	-2.056843565	0.352190623
H	1.794554803	-1.815145037	-2.548106942	H	-4.538831212	-0.432064837	-0.387665104
H	2.034461659	-2.070436309	-0.804463927	H	-3.717779806	-1.778020427	-1.206254136

C	-3.009288672	-0.389065367	2.281065274	H	-1.310860635	4.185352727	0.889197164
H	-2.170110849	-0.255396138	2.972992965	H	-1.583961563	3.569782874	-0.764290881
H	-3.541108198	0.564851940	2.182993082	P	-2.174592319	-1.070501592	0.622879167
H	-3.697213777	-1.135494782	2.699104093	C	-3.745109578	-1.386118483	-0.257777767
C	1.621030154	-0.470412951	-1.753227680	H	-4.364391859	-2.102418691	0.295970700
H	2.354770351	-0.421788722	-2.583378198	H	-4.301051020	-0.448219029	-0.374134612
H	2.209095120	-0.403524293	-0.808473757	H	-3.533564660	-1.787552566	-1.256357019
C	0.894332004	-1.790773901	-1.736423312	C	-2.738049427	-0.610118492	2.295879327
H	1.556884785	-2.623640856	-1.441331884	H	-1.873800472	-0.495607135	2.959635568
H	0.507471351	-2.032979508	-2.746077379	H	-3.284158215	0.340171148	2.255532720
C	-1.593854135	-2.551899365	0.957549471	H	-3.402752113	-1.384284439	2.700651095
H	-2.323836089	-3.336685169	1.196085593	C	1.290188009	-1.774312662	-1.581154272
H	-0.939904320	-2.409638528	1.830571591	H	1.969166637	-2.586815226	-1.274757094
C	-0.757063748	-2.858316080	-0.274555491	H	0.981594793	-1.999334810	-2.622159186
H	-1.374894416	-3.361819580	-1.042982799	C	3.378591525	-0.568741064	0.740781165
H	0.052552189	-3.566281869	-0.023794444	H	2.691132053	-0.566435010	-0.396413211
C	4.139463307	-0.625994661	0.832250485	C	3.472246357	-2.065904075	1.001040316
C	3.994151007	-2.071944728	0.472240550	H	2.489603037	-2.473624398	1.271505374
H	3.056722570	-2.478485758	0.866525332	H	3.871948295	-2.622146036	0.143046699
H	4.059621975	-2.231132739	-0.610315780	H	4.150800273	-2.230193274	1.852554852
H	4.830492413	-2.620653566	0.928164126	C	4.674863252	0.030141605	0.210036949
C	5.059548669	0.192701203	-0.016210427	H	5.432854373	0.012040264	1.007855838
H	5.224479713	1.182180408	0.418741417	H	5.071950795	-0.526141776	-0.649555458
H	6.016390931	-0.326947849	-0.151926972	H	4.520360080	1.076490656	-0.083523979
H	4.620770415	0.303867730	-1.018042855	O	2.721430261	0.135894545	1.606014157
O	3.548234914	-0.145119655	1.793576334	C	-1.407014713	-2.733215197	0.813717168
C	1.431107238	2.193677726	-0.165449032	H	-2.163305540	-3.519641017	0.935697075
H	2.266352109	1.593030322	0.223394751	H	-0.795668483	-2.691081215	1.727109126
H	1.655201457	3.251249529	0.036670235	C	1.439050342	1.951902632	-1.447393700
C	1.167675929	1.888639248	-1.645122223	H	2.483818913	2.067519235	-1.775215804
H	2.103348234	2.017829105	-2.222402520	H	0.806576778	2.462602022	-2.194688391
H	0.460417395	2.641383439	-2.035052067	C	1.219395327	2.592603049	-0.079357180
TS_{H2,I}				H	1.996165959	2.251798412	0.619734732
<i>G_{solv}^o</i> -2757.244563				H	1.217221446	3.690888585	-0.112315489
Fe	-0.586032518	0.001726717	-0.507787673	C	-0.509426464	-2.934230319	-0.396305711
P	-0.381343655	1.947400402	0.582831493	H	-1.099065771	-3.296365848	-1.260738210
O	-2.503244422	1.151366168	-2.339393064	H	0.245908343	-3.712304769	-0.191852669
N	0.140259865	-1.667957703	-0.699835107	C	1.965163628	-0.432556909	-1.547163381
N	1.061298110	0.551601172	-1.390360399	H	2.824586200	-0.262734055	-2.214219879
C	-1.725073894	0.724582081	-1.575782626	I			
C	-0.175068632	1.977937628	2.398315167	<i>G_{solv}^o</i> -2757.274039			
H	0.272727544	2.932551843	2.704401803	Fe	-0.186552821	0.187906663	-0.393860327
H	-1.149846821	1.870903529	2.887798503	P	1.276028628	1.545169119	0.643101252
H	0.478128893	1.155443320	2.711508013	O	-1.295451978	2.337024958	-1.994528801
C	-1.578842360	3.300197408	0.298937758	N	-1.171366263	-1.012485176	-1.668856834
H	-2.588104894	2.974384685	0.580602715	N	1.286579877	-0.156304085	-1.652662930

C	-0.826164968	1.505032622	-1.324846033	TS_{I,J}			
C	1.687313578	1.545062510	2.426652138	G°_{soln}	-2757.257107		
H	2.622935060	2.086613035	2.615974448	Fe	0.840521414	-0.028620076	-0.605063457
H	0.872108888	2.049756305	2.961460314	P	1.238799987	-1.490912930	1.009901542
H	1.772823372	0.525508727	2.816301042	O	3.423519991	-0.568845413	-1.829623073
C	1.140300320	3.345559191	0.321008127	N	-0.644287774	0.938115706	-1.029045667
H	0.177243396	3.719605150	0.691213360	N	-0.226537523	-1.484508784	-1.329013934
H	1.952389649	3.895069975	0.813476805	C	2.386042420	-0.387182397	-1.317271115
H	1.189370207	3.535787056	-0.758018574	C	0.466913979	-1.274143942	2.650859522
P	-2.067183377	0.162297864	0.809238842	H	0.487164578	-2.226374001	3.197080501
C	-2.987703008	1.698065994	1.187623160	H	1.007206591	-0.520094400	3.233414303
H	-3.996482165	1.473443302	1.556866650	H	-0.573387897	-0.949857615	2.525611257
H	-2.448106439	2.262379396	1.959629493	C	2.949480779	-1.972593367	1.426538893
H	-3.068931181	2.327054709	0.293645592	H	3.508023089	-1.087170745	1.757186809
C	-2.162612662	-0.723920864	2.404762768	H	2.958866695	-2.723857994	2.225763045
H	-1.862999282	-1.768302447	2.274320137	H	3.443974433	-2.385554248	0.539352222
H	-1.485601895	-0.253678521	3.128953327	P	1.529099053	1.866324468	0.296868957
H	-3.188238896	-0.682839130	2.793327843	C	3.221016167	2.502860133	0.061193189
C	-0.210524162	-1.853551515	-2.336378219	H	3.319602227	3.517685569	0.466182839
H	0.007798495	-2.803532111	-1.793054258	H	3.935262829	1.844396686	0.571170136
H	-0.533099087	-2.179633378	-3.346830741	H	3.463942296	2.515717632	-1.007643246
C	1.523162399	-1.853051401	1.225471002	C	1.227438673	2.153434093	2.076562265
H	2.202593426	-0.990744558	1.404587626	H	0.192437550	1.888011384	2.325058980
C	2.311585069	-2.841582913	0.362146718	H	1.905081256	1.534268205	2.676627654
H	1.705754898	-3.740886373	0.171339873	H	1.401047282	3.208387823	2.324420459
H	2.579908187	-2.402448989	-0.607989225	C	0.423504241	3.065585812	-0.553977247
H	3.241574735	-3.158476841	0.856886411	H	0.891213499	3.289114939	-1.523009334
C	1.267762842	-2.482126662	2.595182550	H	0.325121320	4.003479587	0.007687910
H	2.199817643	-2.794352330	3.088234218	C	-0.900732979	2.349141673	-0.752768522
H	0.749989977	-1.777382441	3.260294523	H	-1.477120438	2.802625683	-1.575878221
H	0.627320959	-3.370625016	2.483594954	H	-1.527308593	2.437955613	0.153023547
O	0.327025173	-1.469833371	0.645758151	C	0.201703568	-2.864213305	-1.130989140
C	-3.168332264	-0.787797913	-0.330710511	H	-0.550609721	-3.570263726	-1.509430376
H	-3.616692818	-0.056512872	-1.021045893	H	1.136884370	-3.025437563	-1.685702810
H	-3.979753438	-1.290798219	0.213023552	C	0.430048575	-3.035805680	0.365956865
C	2.495148502	0.664901175	-1.664989696	H	-0.539809060	-3.116596610	0.877936891
H	3.324831234	0.130614006	-2.149913376	H	1.023365277	-3.925858302	0.611542418
H	2.273902611	1.555189889	-2.273794029	C	-1.803799048	0.202988392	-1.446232817
C	2.847915720	1.096658787	-0.244456523	H	-2.441757613	0.688688370	-2.199604067
H	3.324783412	0.273989353	0.303592253	C	-1.434720677	-1.166559963	-1.679393917
H	3.548511816	1.942231383	-0.251503077	H	-2.153446364	-1.923811707	-2.008488904
C	-2.273729105	-1.750876931	-1.102739123	C	-4.397675700	0.009020911	0.880635002
H	-2.867957711	-2.254050908	-1.892535575	H	-4.815403410	-0.268014988	1.876068769
H	-1.942654905	-2.565821277	-0.417889361	C	-4.980715060	-0.980503539	-0.129028745
C	1.091569197	-1.141283235	-2.439862677	H	-6.079218029	-1.005572126	-0.091966959
H	1.861324801	-1.467275794	-3.151259710	H	-4.688901017	-0.706861613	-1.154538115
				H	-4.609478211	-1.995521818	0.067963267

C	-4.892351884	1.420958962	0.570401607
H	-4.500256922	2.137662161	1.304349025
H	-4.543242439	1.735707695	-0.425568291
H	-5.989960644	1.487865467	0.580478708
O	-3.007889987	-0.050044644	0.925597960
H	-2.487516597	0.090174822	-0.405292938

J
 G°_{solv} -2757.302312

Fe	-0.590591581	0.022164311	-0.546809911
P	-0.984407947	1.818960590	0.693869248
O	-3.117595982	0.147811380	-1.950199596
N	0.430260389	-1.316001894	-1.406202797
N	0.695905019	1.118406993	-1.383580977
C	-2.098119528	0.101544221	-1.361023818
C	-0.892445704	1.899837782	2.522022621
H	-0.879104558	2.945970402	2.855730472
H	-1.769011635	1.404264875	2.956832363
H	0.012225888	1.397034695	2.881366824
C	-2.528748712	2.757955032	0.384612819
H	-3.396332208	2.144268251	0.658412250
H	-2.551606825	3.687303499	0.968127136
H	-2.603520399	3.002505154	-0.682133620
P	-1.217098687	-1.636671406	0.786814919
C	-2.943745598	-2.241462580	0.656330107
H	-3.114236347	-3.109534941	1.305516384
H	-3.638518707	-1.439562204	0.937343695
H	-3.151443202	-2.524523814	-0.383198657
C	-0.953330711	-1.709241075	2.599084100
H	0.074606482	-1.419424973	2.844607484
H	-1.644001198	-1.024129907	3.104904142
H	-1.135550912	-2.728207767	2.966025061
C	-0.201945698	-3.048754626	0.151554097
H	-0.721982959	-4.008619480	0.275711020
H	0.713737266	-3.073338905	0.760157440
C	0.144346739	-2.741522930	-1.297127491
H	-0.703191155	-3.008331501	-1.952412092
H	1.009700227	-3.334896757	-1.632794357
C	0.718554430	2.575072243	-1.287498386
H	1.713034805	2.962315406	-1.561323275
H	-0.001793804	3.009398878	-2.002250534
C	0.348186603	2.973265386	0.132376966
H	1.203757272	2.818985505	0.805497585
H	0.032765705	4.022551299	0.212594509
C	1.346232679	-0.872970452	-2.296353369
H	1.927999256	-1.560947173	-2.911937965
C	1.495074348	0.501020218	-2.288601076

H	2.205757583	1.057138623	-2.901227296
C	3.563947520	-0.149144853	1.220535969
H	4.133084414	-0.128021851	2.161619428
C	4.095094859	0.927254851	0.295534274
H	5.150854091	0.749987495	0.055015549
H	3.528775114	0.932765777	-0.648138152
H	4.011583428	1.919054864	0.756580980
C	3.666915289	-1.531985757	0.607947759
H	3.301195923	-2.296746616	1.304042917
H	3.070221315	-1.585155487	-0.316242275
H	4.707048558	-1.771251023	0.352799368
O	2.218145850	0.134158610	1.613784177
H	1.644271296	0.130737469	0.819011036

K
 G°_{solv} -2563.036466

Fe	-0.000540074	0.352026003	0.139216789
P	1.744035019	-0.970052728	-0.226830428
O	-0.027799593	-0.072593896	3.000817269
N	-1.238262867	1.724627618	-0.243242992
N	1.209914984	1.735357628	-0.281749665
C	-0.015791377	0.080331352	1.831753323
C	1.827714622	-2.301444525	-1.483936945
H	2.867429258	-2.622761855	-1.632150290
H	1.239025247	-3.165036479	-1.151782662
H	1.422950293	-1.945275068	-2.438011891
C	2.519728643	-1.798373251	1.214549296
H	1.811565137	-2.512830605	1.653507926
H	3.433805975	-2.332611456	0.925793756
H	2.767865009	-1.049767369	1.976959402
P	-1.723065227	-0.988806018	-0.257373341
C	-2.452325908	-1.905301648	1.153280821
H	-3.353914455	-2.454229707	0.852979183
H	-1.716874896	-2.615450377	1.553039900
H	-2.712222042	-1.198823763	1.951365702
C	-1.799619019	-2.256212078	-1.579469874
H	-1.429360260	-1.836684742	-2.521809606
H	-1.177855971	-3.118487752	-1.310382979
H	-2.833427921	-2.599063340	-1.720543745
C	-3.049009616	0.210502620	-0.741335045
H	-4.044283693	-0.144345649	-0.440101684
H	-3.025219854	0.279251873	-1.838439653
C	-2.681866065	1.553293767	-0.130273390
H	-2.980133709	1.578452309	0.932324216
H	-3.210660073	2.377865239	-0.632635809
C	2.659588036	1.588443265	-0.209466832
H	3.158945411	2.406339939	-0.751467863

H	2.990944197	1.650555598	0.841685239
C	3.030622759	0.234730526	-0.792433077
H	2.968481687	0.268477811	-1.889742202
H	4.042207366	-0.092172622	-0.515225992
C	-0.713545592	2.962223922	-0.404836014
H	-1.347250488	3.839753368	-0.540013370
C	0.667843464	2.969273971	-0.426700190
H	1.288271059	3.853096673	-0.580309477