

Supporting information to:

The Energetics of N₂ Reduction by Vanadium Containing Nitrogenase

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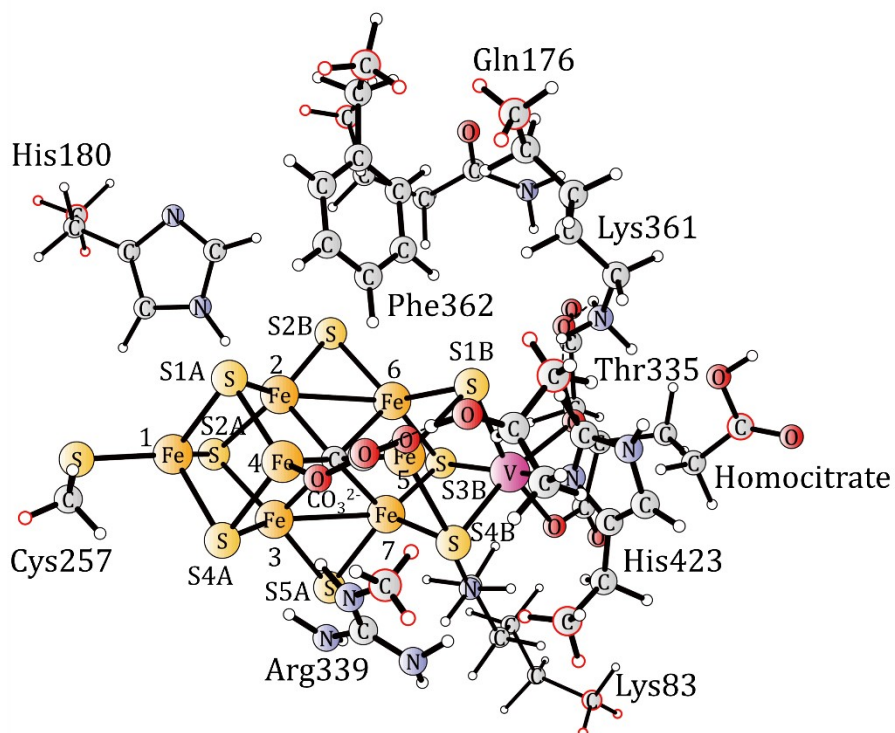


Figure S1. The model used for the present study. Atoms marked with red circles were fixed at their X-ray structure positions during the geometry optimizations.

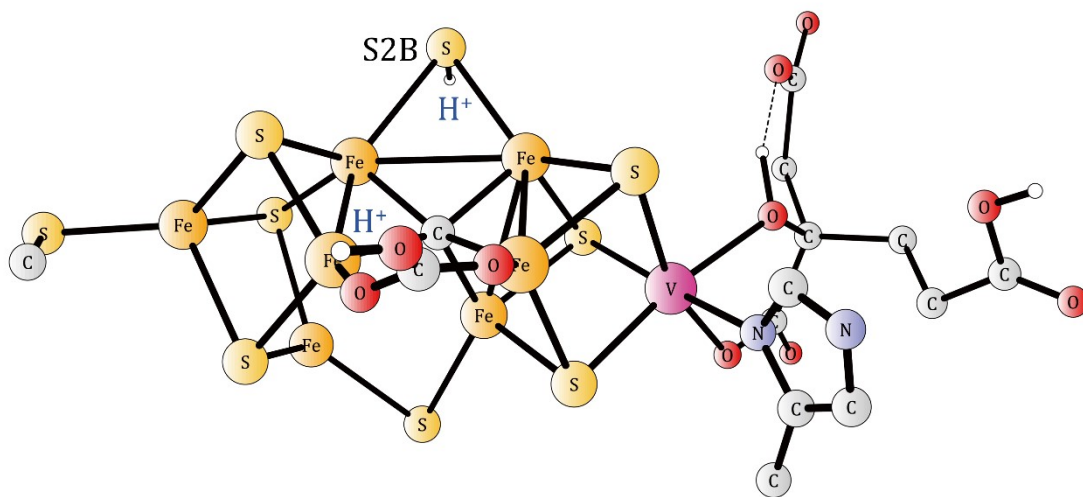


Figure S2. The optimized structure of A_2 . For clarity, only the core of the model is shown. For the full model, see Figure S1.

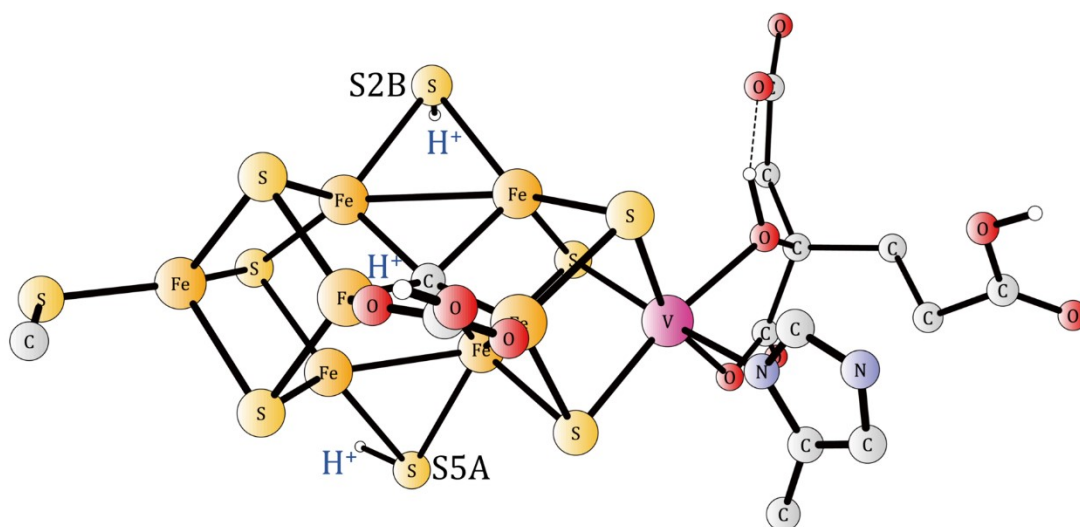


Figure S3. The optimized structure of A_3 . For clarity, only the core of the model is shown. For the full model, see Figure S1.

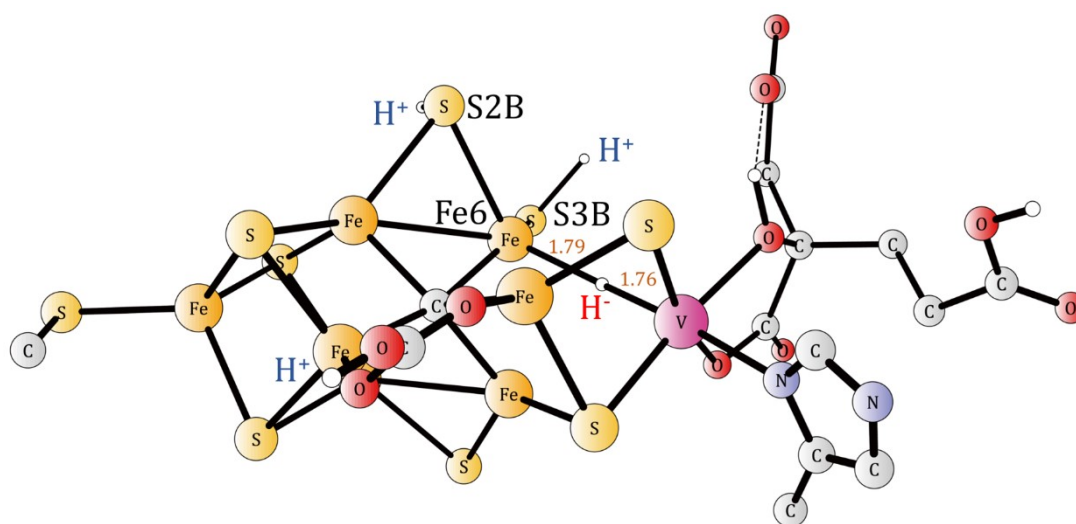


Figure S4. The optimized structure of A_4 . For clarity, only the core of the model is shown. For the full model, see Figure S1.

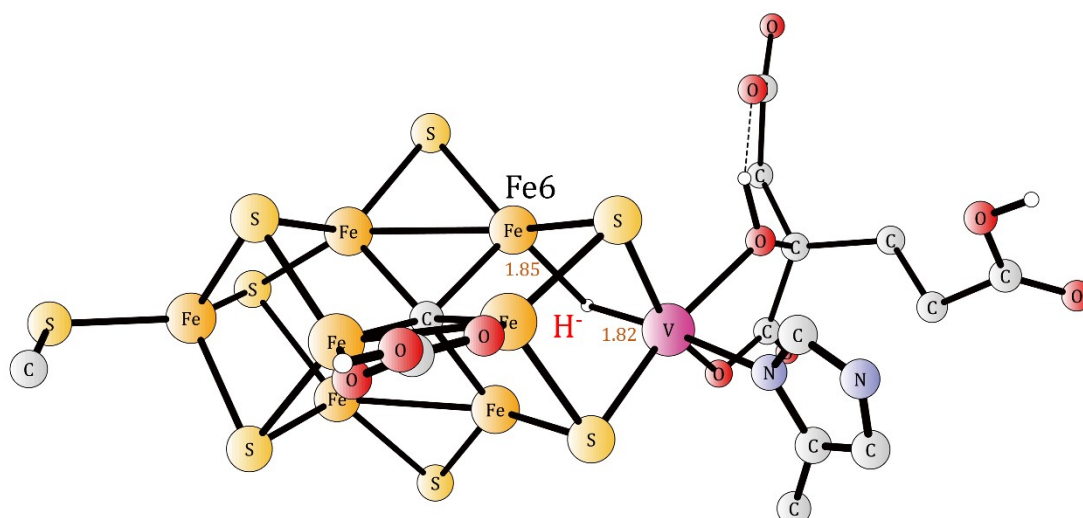


Figure S5. The optimized structure of A_4' . For clarity, only the core of the model is shown. For the full model, see Figure S1.

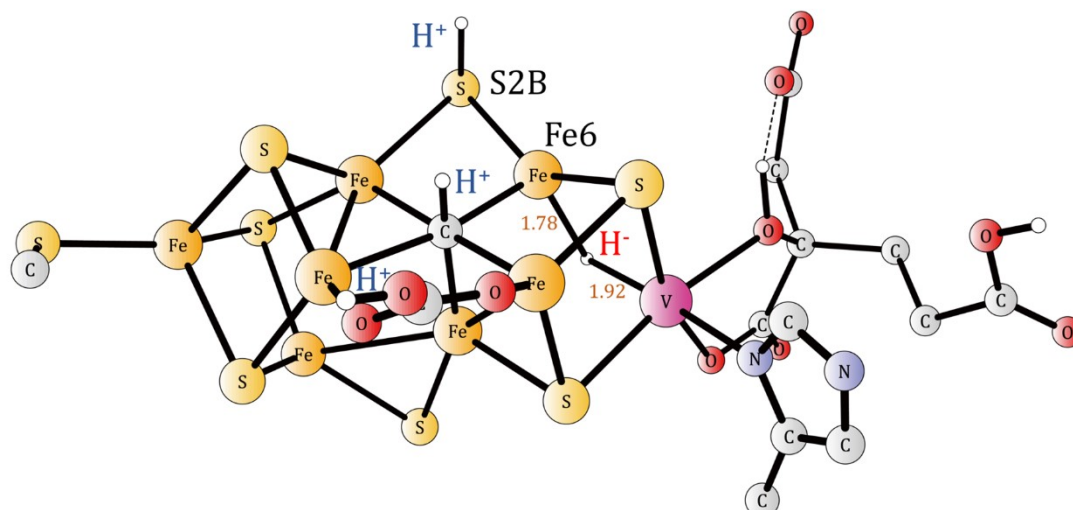


Figure S6. The optimized structure of E_1 . For clarity, only the core of the model is shown. For the full model, see Figure S1.

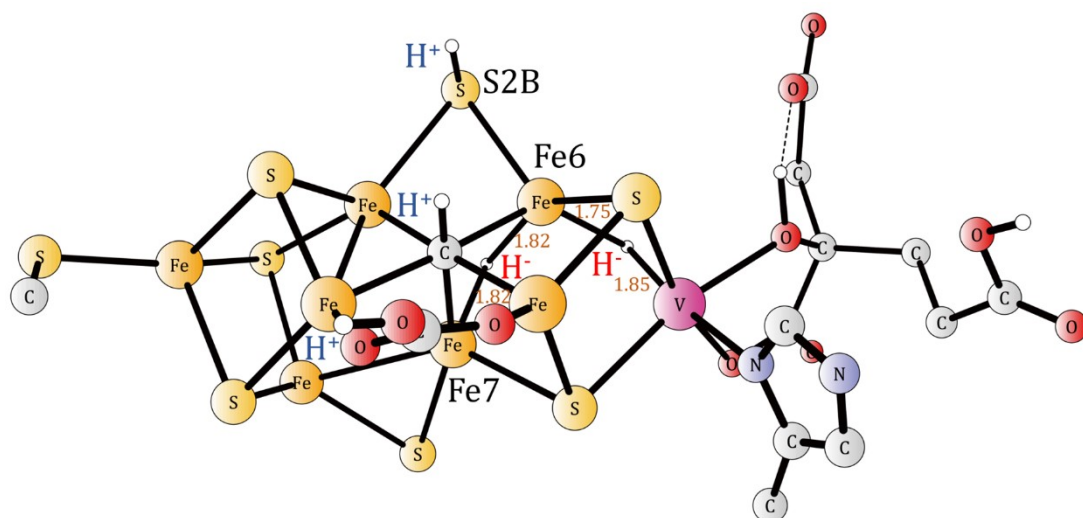


Figure S7. The optimized structure of E_2 . For clarity, only the core of the model is shown. For the full model, see Figure S1.

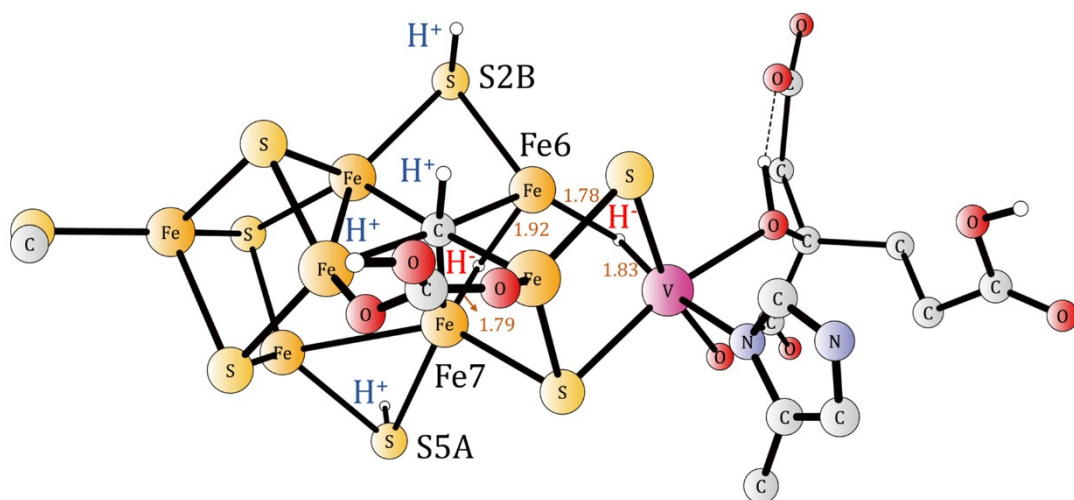


Figure S8. The optimized structure of E_3 . For clarity, only the core of the model is shown. For the full model, see Figure S1.

Coordinates for all structures:

A₀:

E=-7814.105458 solv=-0.118032 disp=-228.01 Z0=885.95

V	99.6843637246	62.5161944316	7.2469784738
Fe	104.7716979715	59.5874295974	1.9747425135
Fe	102.4155051467	61.3384542517	2.4438961529
Fe	104.3475384268	60.9696158300	4.5870534818
Fe	102.6021833964	58.9596262985	3.8044641450
Fe	100.5799896938	60.0622044461	5.4970685284
Fe	100.7929869307	62.5311446660	4.2018107330
Fe	102.4908274864	61.9634632365	6.1407782551
C	102.2507439533	60.9128916179	4.4387774655
S	104.9014964347	58.7319342455	4.2913297811
S	104.7202378199	61.9889181540	6.5687057804
S	104.7819938939	61.8992770445	2.4661546998
S	102.3883904950	59.2277002161	1.5117313872
S	101.0643798443	63.0331098453	2.0473710639
S	98.7856068282	61.7422988038	5.1825346811
S	101.2797840890	60.8128798150	7.7343344612
C	100.4294689608	57.3105381998	5.0169329493
O	101.7191798003	57.5220301937	4.7181113914
O	99.7194163034	58.3768333207	5.3223057459
O	99.9674375725	56.1653203737	5.0671161058
C	97.8137577371	66.4164667985	5.6561458477
C	98.7712531698	66.3845742717	6.8796872805
C	98.4622966192	65.2698286448	7.9249677724
C	97.2214514417	65.6661140428	8.7556259304
C	96.7658166040	64.5738202612	9.7587698752
C	95.2679301067	64.4454875808	9.8432462647
C	99.6735540898	64.9919680345	8.8438803449
O	97.3000848654	65.2560546321	5.3429429783
O	97.6365778120	67.4584738070	5.0292155903
O	94.7368418157	63.9784095482	8.6553513406
O	94.5471819267	64.6918178462	10.7805749757
O	100.1098229024	63.7614385611	8.8092769333
O	100.1690009655	65.8827687457	9.5369040120
O	98.1919974977	64.0346128673	7.2341641793
H	97.8682786931	64.4007391427	6.2816293948
H	99.7743036223	66.2173537457	6.4705627644
H	98.7737470561	67.3635871345	7.3636532155
H	97.4438448175	66.5930380141	9.2921133752

H	96.4180887814	65.8862163350	8.0437493546
H	97.1586456786	63.6047522510	9.4343758436
H	97.1400813123	64.7780885351	10.7638008358
C	106.5349855467	56.8890771769	1.3248933370
H	105.7701827211	56.2216189946	0.9175920699
H	106.4732910530	56.8859159758	2.4156322988
S	106.3303165392	58.5952726162	0.6540346138
C	93.8072701759	61.0298119949	1.8673687043
C	93.6557869026	61.1382765269	3.3853066040
C	94.6639710597	62.1747318228	3.8993155331
C	94.5650035689	62.4517910893	5.3916100589
N	95.7766925269	63.1865119771	5.8665521860
C	93.0790262916	59.8959601518	1.1410743922
H	94.8748944474	60.9393406456	1.6384148114
H	93.4954295726	61.9860931742	1.4234404799
H	93.8557507145	60.1673890696	3.8618077941
H	92.6271125657	61.4195465272	3.6577746977
H	95.6730827276	61.8104444999	3.6709644175
H	94.5472878114	63.1162030172	3.3460288242
H	94.5155606616	61.5215887971	5.9674098115
H	93.6902801807	63.0565980624	5.6499944016
H	95.7464244607	63.3734463187	6.8777606700
H	96.6450144672	62.6440743309	5.6685211890
H	95.9644871112	64.1106615280	5.4084157089
H	91.9880005441	59.9542820977	1.2423894473
H	93.4048998749	58.9145809255	1.4526838954
C	100.0989993722	60.0520006882	10.8889971414
C	99.2117314332	61.2986675822	10.6693747094
C	98.0906582282	61.0405488249	9.7216324868
N	98.1727702199	61.2794652068	8.3589847391
C	96.9122514338	60.3888503429	9.9906564471
C	97.0901998952	60.7406901506	7.8186614387
N	96.2889777676	60.2122002405	8.7727466799
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H	98.7874567378	61.5848988848	11.6409715471
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H	95.4581482357	59.6650593474	8.5992411672
H	96.8997972982	60.6620367882	6.7602093606
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C	103.3724300048	57.9106413205	8.0707709051

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C	103.8574728621	63.8372868785	-2.5184989178
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C	102.1638211956	63.6659556588	-1.2112850891
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H	101.1665241570	63.6006607933	-0.8033209941
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C	97.0341376038	56.9677409711	6.8377511031
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H	98.1474811478	56.1070217753	8.4886026099
H	96.4381494221	55.6485696922	8.4585201869
H	96.9166477780	57.2752021713	9.0129474959
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H	98.2376751619	56.0156890039	5.6062251226
H	97.7535234201	57.7829667720	6.6843300531
C	98.4859997435	66.3580013373	-1.7130007656
C	98.8231691461	65.6319119545	-0.3927634838
C	98.2800052167	66.2636863121	0.8955831947
C	96.7992237537	66.0104075432	1.1774602728
O	96.0698370835	65.3316032808	0.4527050994
N	96.3200765437	66.6193611209	2.3065309105
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H	97.4191306883	66.2612454477	-1.9445774250

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H	99.9150479735	65.5904509591	-0.2973516693
H	98.8430414742	65.8703516368	1.7540681389
H	98.4519281692	67.3498581918	0.9033236531
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C	103.9162979280	67.9349574781	9.6453653034
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H	102.6370768811	68.0813031541	11.9830053842
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H	105.5175884582	68.4014599993	11.0250341365
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H	104.0723630996	65.8570247924	7.6935292299
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H	102.0846384310	64.2556810781	9.2187219496
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H	95.6198512737	57.7972836219	5.4686068333
H	93.3471302870	60.0483404823	0.1060382914
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S	101.3439196198	63.9953434230	5.9552851172
H	94.8291922960	59.8672858579	-1.0815087559
C	95.2420434820	60.2379266224	-2.0081033962
H	95.8060990000	59.4731290000	-2.5212650000
C	96.2118299809	61.3953728499	-1.6916354617
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C	97.8056214663	59.7985108629	-0.5186743225
C	97.1330589761	61.8117585634	0.6233135961
C	98.4892744552	59.3707483160	0.6198302124
C	97.8183729061	61.3856873655	1.7621570368
C	98.4794090096	60.1561073292	1.7744681136
H	94.4259996474	60.5555671281	-2.6694208907
H	96.8071389957	61.6300399477	-2.5850926042

H	95.6629244716	62.3092943706	-1.4379917365
H	96.6250904571	62.7744650631	0.6201203677
H	97.8129184471	59.1725069945	-1.4081268021
H	97.8622845692	62.0264830769	2.6350309585
H	99.0022542037	59.8253282704	2.6660638054
H	99.0332380607	58.4304655675	0.6074036260

A₁:

E=-7814.687452 solv=-0.120258 disp=-228.57 Z0=890.63

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Fe	105.1675048128	59.8531056827	1.9663211455
Fe	102.7169006919	61.6100097650	2.5189775029
Fe	104.4794823278	61.0095175029	4.6699637631
Fe	102.6068753526	59.0614739052	3.6427319192
Fe	100.5916843743	60.1648964227	5.4142725516
Fe	100.8010575501	62.6905300544	4.1942279804
Fe	102.5058704146	62.0828919884	6.0796449461
C	102.2701522020	61.1422666541	4.3854615354
S	104.9680820945	58.8205375893	4.2682482237
S	104.6939497286	62.0036947605	6.6936685306
S	105.0170400060	62.1543162118	2.6611009677
S	102.7025171885	59.6440961440	1.3510731203
S	101.3070315766	63.5086983639	1.9891233181
S	98.8026235069	61.8998094316	5.1140084477
S	101.2734176482	60.9035570990	7.6668949552
C	100.3085179042	57.5874434823	5.0522756797
O	101.5945524633	57.9823416415	4.9060099454
O	99.4788909894	58.5811491862	5.2472098528
O	99.9951773352	56.3924211584	5.0766391138
C	97.8391721853	66.5361914769	5.6957559151
C	98.7731786065	66.4816833883	6.9380269211
C	98.4584406031	65.3435038156	7.9562305054
C	97.2118428156	65.7147774390	8.7897903437
C	96.7642635694	64.6002865177	9.7731402577
C	95.2679301346	64.4454876009	9.8432462381
C	99.6645855733	65.0461210008	8.8773171374
O	97.3181157565	65.3872915186	5.3574943864
O	97.6903261985	67.5890220218	5.0778607857
O	94.7554668172	63.9845561453	8.6447903334
O	94.5347596418	64.6688852830	10.7768697965
O	100.1024012519	63.8161599732	8.8187365112
O	100.1508540314	65.9204644267	9.5961900332
O	98.1944033052	64.1245844773	7.2355514850

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H	99.7845246317	66.3306810507	6.5433350624
H	98.7611847870	67.4505776469	7.4420148572
H	97.4239489622	66.6339164376	9.3435368627
H	96.4087214523	65.9397691312	8.0790476500
H	97.1758536517	63.6425245536	9.4386230224
H	97.1267668204	64.7965818537	10.7840156664
C	106.5542248090	57.0243425559	1.1450188063
H	105.8226934892	56.5448349994	0.4881866551
H	106.2321771919	56.9140079486	2.1835958722
S	106.7496382698	58.8093083043	0.7022798932
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C	93.7105180018	61.1636139268	3.3666400146
C	94.7237526516	62.2109891995	3.8514597950
C	94.6209679012	62.5197385929	5.3382026104
N	95.8187992638	63.2809901230	5.8054635442
C	93.0790262515	59.8959601555	1.1410743695
H	94.8984563481	60.9220560433	1.6024748225
H	93.5291054660	61.9833841272	1.3965098657
H	93.9170758892	60.2011526879	3.8569610092
H	92.6858768249	61.4497421275	3.6489091591
H	95.7337998447	61.8425276568	3.6317217277
H	94.6051507600	63.1397180534	3.2773600260
H	94.5844489636	61.6004680146	5.9320743739
H	93.7349829336	63.1142429869	5.5817306320
H	95.7997763981	63.4488726256	6.8205256924
H	96.7005363971	62.7640903487	5.5873906485
H	95.9790654508	64.2167368366	5.3641265743
H	91.9907791925	59.9674121358	1.2533118326
H	93.4048998871	58.9145809321	1.4526839044
C	100.0989993737	60.0520008091	10.8889970621
C	99.2218578746	61.3036411321	10.6486060546
C	98.1173961851	61.0570718720	9.6755630528
N	98.1993177311	61.3472416300	8.3214439634
C	96.9461582011	60.3813707651	9.9151554055
C	97.1254285873	60.8144428546	7.7586431186
N	96.3283321331	60.2424205242	8.6902973304
H	100.7720112040	59.8784109586	10.1700238655
H	99.4654981416	59.1641474642	11.0128040977
H	100.5712426720	60.2159537713	11.7550862226
H	98.7791898929	61.5950215819	11.6105720515
H	99.8337800040	62.1422974544	10.3111141991
H	96.5235974434	59.9802716862	10.8232767823
H	95.5044369649	59.6927772283	8.4945747103

H	96.9418208581	60.7667873059	6.6972398397
C	101.6500025575	56.1420056576	7.7050016543
N	102.7827136829	56.9821976316	7.3112721742
C	103.3481210398	57.9355402867	8.0464511044
N	102.9733823280	58.1115837718	9.3453081522
N	104.3713306129	58.6491501625	7.5590714098
H	101.6888187391	55.2540728314	7.0689355878
H	100.7886342881	56.5995586888	7.4843450607
H	101.6262277359	55.8261439710	8.6535096511
H	102.7862159741	57.1589551215	6.3001619149
H	103.3987852883	58.9007859989	9.8145405384
H	101.9843574466	58.0178448474	9.5401859393
H	104.6495291830	58.4887513763	6.5835484025
H	104.4472461162	59.6390296120	7.8021303195
C	104.8710010363	65.5940001655	-4.0429948518
C	104.6529988246	64.0691737359	-3.8759416615
C	103.7946250939	63.5737106783	-2.7549644246
N	102.4747886734	63.9619792850	-2.6096181415
C	104.0988589330	62.5878809055	-1.8439581636
C	101.9982704651	63.2183316397	-1.6306048410
N	102.9389334375	62.3659163284	-1.1349504925
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H	103.9196899197	66.1260601834	-4.1326664650
H	105.3923871666	65.6470936021	-4.8946699846
H	105.6372911942	63.5879545402	-3.7922878745
H	104.2224873810	63.6997544861	-4.8195079773
H	105.0001916022	62.0248670664	-1.6519150632
H	102.8120373519	61.6811355417	-0.3977557896
H	100.9935118238	63.2579267704	-1.2343135546
C	95.6299756841	57.4820324106	6.4910615233
C	97.0393626401	56.9932220544	6.8504625187
O	97.3629030741	55.9407468328	5.9577979286
C	97.1295773345	56.4886668897	8.2963639933
H	95.2861945555	58.3082415146	7.1282408425
H	98.1454703150	56.1352996777	8.5072609748
H	96.4461928025	55.6437986438	8.4470230309
H	96.8838195446	57.2728760761	9.0259529176
H	94.9092300127	56.6615598245	6.5980950753
H	98.2632838389	56.1051308133	5.5934617997
H	97.7419845000	57.8247228174	6.7134207609
C	98.4859995980	66.3580013543	-1.7130008099
C	98.8230722763	65.6394242525	-0.3882927684
C	98.3176522698	66.3088005490	0.8979003862
C	96.8352193013	66.1050165631	1.2131134520

O	96.0747916543	65.4258873862	0.5204301372
N	96.3919237064	66.7578100225	2.3315720198
H	98.7144620192	67.3289719310	-1.6420951217
H	97.4186823055	66.2631909395	-1.9432882401
H	99.0290071663	65.9401255045	-2.4413701656
H	98.4515925559	64.6097894415	-0.4196040455
H	99.9151682258	65.5677544115	-0.3086317360
H	98.8836936111	65.9163014657	1.7549523527
H	98.5209794115	67.3893836161	0.8821578872
H	97.0072519262	67.0755079879	3.0816333691
H	95.4509428162	66.5226377831	2.6184554380
C	103.6859930662	68.3259923543	12.1929977138
C	104.4547232038	68.6420299532	10.8896056588
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C	103.8043934379	66.3840661576	9.8287633739
C	103.3325001865	65.7636603249	8.5240922967
N	102.8968090933	64.3419890999	8.6613632095
H	104.1085749484	67.5601822981	12.6777192244
H	102.6369259954	68.0818047038	11.9833487523
H	103.6948492606	69.1366815072	12.7784182631
H	104.4056208039	69.7188049211	10.6834424109
H	105.5202626536	68.4127237900	11.0322342392
H	102.9335419272	68.2956039403	9.4039457617
H	104.5755411202	68.1228602759	8.7941011923
H	104.7651316278	65.9470975051	10.1381590569
H	103.0700807452	66.1642592003	10.6132604375
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H	95.6198512602	57.7972836104	5.4686068299
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H	102.2697704975	64.3571820857	2.4189355736
S	101.3770733743	64.1393571677	5.9654152289
H	94.8291929030	59.8672864771	-1.0815082439
C	95.2420431008	60.2379264318	-2.0081037070
H	95.8060990000	59.4731290000	-2.5212650000
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C	97.1412469332	61.1975184370	-0.6318272541
C	97.9919540650	60.0802017576	-0.6599692663
C	97.1940578927	62.0514569502	0.4774832008

C	98.8535343054	59.8064101437	0.4026728543
C	98.0502484303	61.7752121250	1.5471533297
C	98.8717126557	60.6465445060	1.5194569098
H	94.4072386866	60.5126178836	-2.6668653034
H	96.6695170940	61.7226630265	-2.6748485536
H	95.5386243806	62.3291927179	-1.4788417607
H	96.5773649238	62.9476394297	0.4964059723
H	97.9810441319	59.4148369811	-1.5205240217
H	98.0833902808	62.4462520686	2.3993134694
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E=-7815.264388 solv=-0.126663 disp=-231.42 Z0=897.71

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Fe	102.8516149854	61.4286270020	2.9008481452
Fe	105.1188021487	60.9671165345	5.2523612598
Fe	102.7727913879	59.0836238056	3.8617598251
Fe	100.2227940051	59.7964582722	5.4377836717
Fe	100.5091634355	62.1658440127	4.1960229169
Fe	102.5196210146	61.4721732280	6.1447170259
C	101.6870656874	60.6917886821	4.3919551668
S	104.9143158395	58.6742969527	4.7104040220
S	104.5862615377	61.7121371226	7.3634648466
S	105.0397669512	62.1346374876	3.2353279183
S	103.0585944066	59.4812923005	1.5616106977
S	101.2425640386	63.1858343306	2.1264562257
S	98.4303345891	61.4169879516	5.1760204422
S	100.9485376220	60.3824247800	7.6395077637
C	100.4564750769	57.1394761363	4.3944790194
O	101.6921651407	57.3505897314	4.2372623785
O	99.6252857011	57.8681949907	5.0133250860
O	99.9468657597	55.9976908819	3.8856994636
C	97.7796024401	66.2396515717	5.4884274032
C	98.7654373565	66.1680020749	6.6878058534
C	98.4247295597	65.0903841355	7.7573846322
C	97.2168078279	65.5499394997	8.6072523164
C	96.7616955211	64.5021233145	9.6579971999
C	95.2679300914	64.4454875706	9.8432462851
C	99.6376952097	64.7737079642	8.6647006063
O	97.2520277728	65.0968775739	5.1445143307
O	97.6020823788	67.3083153649	4.9008504219

O	94.6366158692	64.0074903941	8.6928385082
O	94.6223080669	64.7200829886	10.8263192415
O	99.9907289126	63.5219897629	8.6819666490
O	100.1944882806	65.6665821720	9.3107905649
O	98.0927031867	63.8555764436	7.0936655046
H	97.8410040165	64.1812016899	6.1379031454
H	99.7456494866	65.9277117785	6.2580974524
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H	97.4803417321	66.4857630517	9.1088213693
H	96.3989282003	65.7732156578	7.9126208823
H	97.0850604511	63.5090960566	9.3301390898
H	97.2106478313	64.7013778285	10.6329945402
C	106.6738013019	57.1224459320	1.3749833031
H	105.8269491635	56.9591094719	0.7020279869
H	106.4018945179	56.7883419632	2.3806315136
S	107.1701604119	58.9061337317	1.3890089754
C	93.8180202663	61.0235562929	1.8648198922
C	93.5923497498	61.1764222575	3.3672504566
C	94.5996723090	62.1934396867	3.9121059924
C	94.4034436810	62.5263350286	5.3832327315
N	95.6256249780	63.1878079420	5.9212792745
C	93.0790262863	59.8959601421	1.1410744358
H	94.8924167049	60.8908149446	1.6868882662
H	93.5608082455	61.9773673829	1.3827665980
H	93.7328040772	60.2125564462	3.8787712807
H	92.5589226072	61.4951679206	3.5724030160
H	95.6098313924	61.7873115532	3.7747025097
H	94.5585057522	63.1180564756	3.3215283938
H	94.2436096117	61.6195518774	5.9775265823
H	93.5543683651	63.1954551478	5.5541882557
H	95.5459032349	63.4014540509	6.9235616341
H	96.4583030790	62.5748940979	5.7845085962
H	95.9174493470	64.0822642802	5.4417678627
H	91.9891384794	59.9623152836	1.2453375140
H	93.4048998648	58.9145809186	1.4526838852
C	100.0989992940	60.0520006029	10.8889972253
C	99.1796044617	61.2758051660	10.6859260422
C	97.9854425827	61.0025626495	9.8325389076
N	97.9672160977	61.1902420432	8.4592106713
C	96.7868028217	60.4549947360	10.2204951707
C	96.8019465293	60.7360864695	8.0300218711
N	96.0458271377	60.2953806588	9.0648570949
H	100.7720111947	59.8784111352	10.1700238744
H	99.4901629529	59.1461554626	11.0201940503

H	100.5712427323	60.2159537800	11.7550861881
H	98.8180424268	61.5858196287	11.6757161905
H	99.7435633250	62.1139487826	10.2741653062
H	96.4113914181	60.1662571892	11.1900057148
H	95.1474031694	59.8420685886	8.9860741863
H	96.5119194661	60.6597632737	6.9942354294
C	101.6500025842	56.1420052209	7.7050017582
N	102.8237805470	56.9751886229	7.4259915730
C	103.3533571696	57.8788415309	8.2553183812
N	102.7493755458	58.1114770938	9.4550495940
N	104.5120748676	58.4787086827	7.9699194495
H	101.7302163629	55.2565067878	7.0665688665
H	100.7886343771	56.5995588297	7.4843450065
H	101.6262276944	55.8261440559	8.6535096783
H	103.1290826167	57.0368486030	6.4565459532
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H	101.7434678826	58.2348063431	9.3905551199
H	104.8976121382	58.2871001421	7.0382536599
H	104.5815493832	59.4946393778	8.1644690177
C	104.8710010927	65.5940002891	-4.0429953461
C	104.5777251973	64.0952722891	-3.8272608841
C	104.0256757391	63.7005941467	-2.4918182311
N	103.1514063623	62.6350399315	-2.3909302644
C	104.3167722653	64.1907886552	-1.2383673182
C	102.9216017223	62.4860675655	-1.1021050690
N	103.6043855164	63.4005306377	-0.3606724108
H	105.4142233245	65.9758307739	-3.2952586306
H	103.9447048749	66.1732701442	-4.1331363813
H	105.3923871639	65.6470938498	-4.8946699709
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H	103.8783966478	63.7402153565	-4.5932688562
H	104.9540745914	64.9907418475	-0.8927862574
H	103.5687841073	63.4756417136	0.6473948945
H	102.2827097892	61.7424464636	-0.6482486849
C	95.6299757077	57.4820326637	6.4910615995
C	97.0376376219	57.2386518083	7.0509456125
O	97.7189109732	56.2549259262	6.2857001861
C	96.9844420247	56.7353459305	8.4942213268
H	95.0957422539	58.2416074395	7.0824958404
H	97.9983366582	56.6099513605	8.8880519613
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C	98.2240416321	66.2331884764	0.8855321908
C	96.7355070188	65.9729961742	1.1221328197
O	96.0332380410	65.2882656282	0.3757619128
N	96.2217820086	66.5840561771	2.2344106801
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H	99.8959616363	65.5826769402	-0.2750117008
H	98.7596276946	65.8269586527	1.7554945151
H	98.3939839108	67.3191561090	0.9161446776
H	96.8043518009	66.8777153152	3.0226654056
H	95.2826033848	66.2958387204	2.4764849699
C	103.6859927444	68.3259922934	12.1929977105
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C	103.2738336511	65.7936543412	8.3660566895
N	102.8929359019	64.3491514215	8.4082328213
H	104.1085750625	67.5601823537	12.6777192128
H	102.6323744217	68.0756750836	12.0088043237
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H	104.3918711941	69.6788929163	10.6436148819
H	105.4797684265	68.3444713060	10.9625164459
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H	104.4295026750	68.1657521457	8.7468944765
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H	102.3728194187	66.3201945567	8.0452269659
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H	103.6837270918	63.6795745801	8.4844735341
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H	95.6198511489	57.7972834644	5.4686067860
H	93.3471300446	60.0483401280	0.1060380297
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S	101.2210106011	63.5662824751	5.8697020550
H	101.8653282313	64.1574349898	2.8329616920
H	94.8291929628	59.8672868416	-1.0815080649

C	95.2420430633	60.2379261298	-2.0081038609
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C	97.2287056535	61.8128537435	0.5143708877
C	98.9991879624	59.6861570980	0.1456942722
C	98.1041958231	61.4442498719	1.5373497380
C	98.9854674738	60.3745648974	1.3621474071
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H	95.5963726346	62.3116871508	-1.4234819538
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Fe	102.4812795881	59.1791544481	3.6088010510
Fe	100.6108759330	60.0951676241	5.5337021856
Fe	100.6123949293	62.5251278187	4.2058623182
Fe	102.5095204564	62.0558191904	6.0962464004
C	102.0441453060	61.0135941443	4.4285565953
S	104.6405712899	58.5823439718	4.5005438484
S	104.6841901952	61.8264500582	7.2739922180
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S	101.3738804907	63.5996282346	2.2083212827
S	98.6043203299	61.5584070120	5.1693786041
S	101.2434950144	60.7728191457	7.7505983294
C	100.2463929773	57.4300997232	4.2455905363
O	101.2860471017	57.5504699233	3.5438001656
O	99.8739113947	58.1416825349	5.2267066910
O	99.4252860257	56.3968477900	3.9440127847
C	97.7648719369	66.4195620810	5.5330393451
C	98.7014325414	66.3802929855	6.7728437356
C	98.3897035960	65.2593404031	7.8066048107

C	97.1611473781	65.6583558331	8.6540881768
C	96.7562594603	64.5824611562	9.6948786019
C	95.2679302282	64.4454875938	9.8432462049
C	99.5792511489	64.9473086248	8.7436038081
O	97.3115031883	65.2575030847	5.1521067783
O	97.5579395263	67.4871375805	4.9523707451
O	94.6903223319	63.9891159398	8.6736623707
O	94.5854951709	64.6783505174	10.8133430876
O	99.8972422569	63.6911309870	8.8163570569
O	100.1442527875	65.8431896712	9.3841865598
O	98.1090124575	64.0260561536	7.1155613284
H	97.8733466674	64.3633058399	6.1559553602
H	99.7113393805	66.2194008982	6.3792565167
H	98.6909028380	67.3563395856	7.2626512754
H	97.3789946478	66.6015328283	9.1641784666
H	96.3364879882	65.8485957975	7.9579510216
H	97.1454707996	63.6108491332	9.3745030402
H	97.1718012638	64.8078810242	10.6788844902
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H	105.8161193090	56.7826269414	0.5835737397
H	106.3031697058	56.7752268192	2.2978634990
S	106.9623418543	58.8729964280	1.1903399247
C	93.8346914405	61.0242647955	1.8497480224
C	93.6723784350	61.1727370887	3.3612313651
C	94.6933869269	62.2001545969	3.8620123727
C	94.5691954878	62.5234934376	5.3437087690
N	95.7958417152	63.2207973511	5.8186803065
C	93.0790263164	59.8959601376	1.1410744381
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H	93.5546307865	61.9785926948	1.3815988029
H	93.8449805538	60.2099190474	3.8647546084
H	92.6462794314	61.4814790298	3.6127645746
H	95.7006740002	61.8086517539	3.6706065476
H	94.6090644867	63.1270192747	3.2792554783
H	94.4699845243	61.6094457734	5.9395889146
H	93.7086714484	63.1631598000	5.5638016097
H	95.7775648076	63.4090991630	6.8281403827
H	96.6536117677	62.6429270306	5.6239865315
H	96.0165481507	64.1392969842	5.3552931233
H	91.9904406274	59.9680188352	1.2521708337
H	93.4048998571	58.9145809149	1.4526838815
C	100.0989992235	60.0520007218	10.8889969882
C	99.2094728579	61.2968200295	10.6779106132
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C	96.8113882251	60.5516404633	10.1312550914
C	96.8933686953	60.8718515777	7.9479623924
N	96.0953916420	60.4385833815	8.9543656799
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H	99.4737085929	59.1575674802	11.0195430268
H	100.5712426964	60.2159537988	11.7550862039
H	98.8251694310	61.5978489492	11.6622920368
H	99.8024358725	62.1301303782	10.2984909648
H	96.4023061964	60.2582999738	11.0857600075
H	95.1896664020	60.0077164220	8.8431313847
H	96.6332116890	60.8222789164	6.9029744022
C	101.6500025775	56.1420055728	7.7050019661
N	102.8278494646	56.9528972732	7.3855814533
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N	102.8229884701	58.1368075573	9.3880522441
N	104.5296554591	58.4603179306	7.8115007078
H	101.7105259011	55.2501046304	7.0731080727
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H	104.7057590369	59.4118174758	8.1321248164
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C	103.4916606248	63.8177702168	-2.7940537222
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C	101.8489192219	62.7923683573	-1.8637508325
N	102.2664594311	63.7358086451	-0.9781756737
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H	103.9610251073	66.1974518821	-4.1527215090
H	105.3923871567	65.6470937044	-4.8946699842
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H	103.8547875370	65.1869689300	-1.0436026942
H	101.9428092170	63.8377361781	-0.0208469639
H	101.0307166058	62.1203632614	-1.6433844668
C	95.6299761223	57.4820326466	6.4910614639
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C	96.8880111070	56.9270844322	8.6054607740

H	94.9646166839	58.1603226618	7.0490444941
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H	96.1940520948	57.5391509019	9.1931346711
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C	98.7937548066	65.6317534298	-0.3862667682
C	98.2323993757	66.2788071004	0.8883678551
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H	98.7144620015	67.3289719358	-1.6420951275
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H	99.8835713915	65.5728793587	-0.2721322461
H	98.7665243541	65.8789624897	1.7622020868
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H	96.8336769935	66.9956092419	3.0270528312
H	95.3007593406	66.4338316532	2.4960737216
C	103.6859926779	68.3259919759	12.1929974984
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H	107.5224144432	56.5249259744	1.0242612873
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C	96.1379754736	61.4701032305	-1.7679880033
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C	97.2599245976	61.9073363084	0.4588406234
C	99.1883814540	59.9459636058	-0.0219921323
C	98.2217192062	61.6159181716	1.4307422758
C	99.1816048253	60.6292128389	1.1976779327
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H	98.2248181825	59.6846775214	-1.9275663891
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Fe	102.6970606576	58.7991202820	4.0415688330
Fe	100.1285888855	60.0171458001	5.0578537803
Fe	101.4901405376	62.6053687169	4.7435232689
Fe	102.2225725757	60.8744190082	6.6943395629
C	102.1534737631	60.6511386791	4.6656091814
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S	102.9180761361	59.1825069377	1.6442245274
S	101.1621438114	62.9373561828	2.2866429420
S	97.8633519100	60.9175306306	5.3350907881
S	100.3981422696	59.7878481011	7.5523922889

C	100.4978304138	57.0513045846	4.2806172564
O	101.7712791870	57.0432350209	4.4084580744
O	99.7173942529	58.0152117839	4.4634952213
O	99.9249489561	55.8840224545	3.9182868982
C	97.7018646040	65.8853881292	5.3751873416
C	98.7500639024	65.7611014840	6.5146187660
C	98.3791296826	64.7600933818	7.6442380880
C	97.2710080411	65.3578040441	8.5381288960
C	96.7572309665	64.3793923579	9.6279450025
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C	99.6414390937	64.3718392724	8.4422576309
O	97.0136751262	64.8072815078	5.1421070051
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O	94.5692010434	63.9750385674	8.7497540019
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O	100.0180352319	63.1469586388	8.3151412807
O	100.2498685509	65.2274346515	9.1117495716
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H	97.5837866964	63.8680891496	6.1073309658
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H	97.6514528277	66.2693810513	9.0075391511
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C	94.1443212054	62.3134292375	5.5325659933
N	95.3837159112	62.9104034183	6.0947658315
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H	93.5123433567	61.9808088281	1.4322480806
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H	95.3753397167	61.8414451056	3.8598074817
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H	93.2964906105	62.9561231328	5.7912450842
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H	96.1882645142	62.2456791574	5.9297449054
H	95.6810094431	63.7913107227	5.6111884279
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C	99.1717333608	61.2741150102	10.6954234375
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C	96.4314211144	60.5934302763	8.4523237725
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H	104.7180183469	59.3531869577	8.0323289094
C	104.8710010702	65.5940003073	-4.0429953322
C	104.5576392532	64.1020972031	-3.8292418987
C	103.8487722185	63.7575167060	-2.5575446417
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H	103.9489980498	66.1799796083	-4.1398242890
H	105.3923871825	65.6470938017	-4.8946699624
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N	96.1088110298	66.3453698533	2.1804150015
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C	95.2420430907	60.2379261408	-2.0081037633
H	95.8060990000	59.4731290000	-2.5212650000
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Fe4	104.5528220000	61.0625100000	5.2839870000
Fe5	102.9547520000	58.9897820000	4.1278410000
Fe6	100.0402030000	60.0627550000	5.0697470000
Fe7	101.2764810000	62.5185830000	4.6579190000
Fe8	102.1736010000	60.9577860000	6.6392570000

C9	102.1721500000	60.7609830000	4.6896820000
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S12	105.2188320000	61.9420820000	3.1813150000
S13	103.2004180000	59.2796750000	1.7361540000
S14	101.5502080000	63.2415120000	2.4693240000
S15	98.0144650000	61.2867460000	5.2155740000
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O20	100.0425750000	56.0915800000	3.6893540000
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C23	98.3903900000	64.9871660000	7.6869920000
C24	97.2587140000	65.5206510000	8.5967750000
C25	96.7630280000	64.4787020000	9.6377070000
C26	95.2679300000	64.4454880000	9.8432460000
C27	99.6450580000	64.5873790000	8.4902320000
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O29	97.6641950000	67.2562350000	4.8422570000
O30	94.5945480000	64.0982650000	8.6874360000
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O32	99.9718930000	63.3426380000	8.4249320000
O33	100.3042800000	65.4496350000	9.0950410000
O34	97.9377410000	63.7901080000	7.0332060000
H35	97.6577910000	64.1439110000	6.0855220000
H36	99.7237120000	65.7413630000	6.1529820000
H37	98.9294870000	67.0148360000	7.0722210000
H38	97.6143220000	66.4188080000	9.1103620000
H39	96.4360100000	65.8247140000	7.9397300000
H40	97.0535920000	63.4801460000	9.2967120000
H41	97.2176890000	64.6499150000	10.6154910000
C42	106.6262690000	57.0987870000	1.2951770000
H43	105.8610350000	56.9559520000	0.5272980000
H44	106.2484580000	56.7316900000	2.2533350000
S45	107.0780060000	58.8872340000	1.4169830000
C46	93.7940120000	61.0324700000	1.8687710000
C47	93.4715990000	61.2256900000	3.3469650000
C48	94.4010740000	62.3016220000	3.9080750000
C49	94.1779680000	62.6108750000	5.3810130000
N50	95.4132820000	63.2288430000	5.9378180000
C51	93.0790260000	59.8959600000	1.1410740000
H52	94.8764970000	60.8853630000	1.7604550000

H53	93.5731190000	61.9739310000	1.3463030000
H54	93.6234950000	60.2862650000	3.8988180000
H55	92.4148110000	61.5045770000	3.4769350000
H56	95.4347920000	61.9558140000	3.7821810000
H57	94.3109410000	63.2251080000	3.3213210000
H58	93.9935720000	61.6955430000	5.9543370000
H59	93.3411380000	63.2951250000	5.5530700000
H60	95.3303810000	63.4602730000	6.9358710000
H61	96.2179570000	62.5685350000	5.8108000000
H62	95.7348620000	64.0983870000	5.4462500000
H63	91.9873480000	59.9556520000	1.2361420000
H64	93.4049000000	58.9145810000	1.4526840000
C65	100.0989990000	60.0520010000	10.8889970000
C66	99.1630960000	61.2648440000	10.6683840000
C67	97.8816520000	60.9542800000	9.9565480000
N68	97.6763660000	61.2015330000	8.6061870000
C69	96.7511430000	60.3626380000	10.4665310000
C70	96.4711920000	60.7479340000	8.3084590000
N71	95.8672720000	60.2409090000	9.4104450000
H72	100.7720110000	59.8784110000	10.1700240000
H73	99.5054420000	59.1366280000	11.0146540000
H74	100.5712430000	60.2159540000	11.7550860000
H75	98.9023220000	61.6654890000	11.6574390000
H76	99.6910510000	62.0570410000	10.1356030000
H77	96.5062990000	60.0234100000	11.4614100000
H78	94.9702230000	59.7788700000	9.4309630000
H79	96.0535280000	60.7132750000	7.3141770000
C80	101.6500030000	56.1420050000	7.7050020000
N81	102.8567420000	56.9180390000	7.4164410000
C82	103.3688520000	57.8634230000	8.2061540000
N83	102.6561960000	58.2662080000	9.2890780000
N84	104.5971570000	58.3593350000	7.9991810000
H85	101.7049010000	55.2485170000	7.0741240000
H86	100.7886340000	56.5995590000	7.4843450000
H87	101.6262280000	55.8261440000	8.6535100000
H88	103.2134780000	56.8773060000	6.4662260000
H89	103.0836530000	59.0320280000	9.7987870000
H90	101.6757360000	58.4574920000	9.0717520000
H91	105.0644580000	58.0721030000	7.1378360000
H92	104.6824180000	59.3811070000	8.1311840000
C93	104.8710010000	65.5940000000	-4.0429950000
C94	104.5166960000	64.1044870000	-3.8462440000
C95	103.6387600000	63.7538100000	-2.6804370000
N96	102.6857850000	62.7594270000	-2.8101460000

C97	103.631360000	64.2426950000	-1.3925210000
C98	102.121840000	62.6519340000	-1.6214680000
N99	102.6541220000	63.5299370000	-0.7289730000
H100	105.4142230000	65.9758310000	-3.2952590000
H101	103.9587720000	66.1944240000	-4.1488210000
H102	105.3923870000	65.6470940000	-4.8946700000
H103	105.4552720000	63.5296360000	-3.7935370000
H104	104.0033680000	63.7421270000	-4.7449960000
H105	104.2137520000	65.0034310000	-0.8943080000
H106	102.4027600000	63.6019960000	0.2549290000
H107	101.3250690000	61.9713640000	-1.3525480000
C108	95.6299760000	57.4820330000	6.4910620000
C109	97.0669810000	57.4538610000	7.0422130000
O110	97.9212350000	56.6777340000	6.2049630000
C111	97.1246520000	56.8253290000	8.4337450000
H112	94.9900490000	58.1597820000	7.0750530000
H113	98.1422540000	56.8804070000	8.8331420000
H114	96.8296380000	55.7701110000	8.3814120000
H115	96.4521880000	57.3375060000	9.1326110000
H116	95.1871620000	56.4789830000	6.5358360000
H117	98.2540110000	57.2441840000	5.4837360000
H118	97.4533380000	58.4802750000	7.0983920000
C119	98.4860000000	66.3580010000	-1.7130010000
C120	98.8066060000	65.6178820000	-0.3974720000
C121	98.2337630000	66.2355930000	0.8837360000
C122	96.7336370000	66.0254420000	1.0920920000
O123	96.0261690000	65.3670020000	0.3299320000
N124	96.2183410000	66.6515260000	2.1967560000
H125	98.7144620000	67.3289720000	-1.6420950000
H126	97.4204500000	66.2646420000	-1.9518310000
H127	99.0290070000	65.9401250000	-2.4413700000
H128	98.4638460000	64.5806120000	-0.4717360000
H129	99.8972100000	65.5721160000	-0.2814650000
H130	98.7428360000	65.7991440000	1.7553100000
H131	98.4426370000	67.3142350000	0.9291320000
H132	96.8018610000	66.9118280000	2.9951260000
H133	95.2705940000	66.3812580000	2.4255040000
C134	103.6859930000	68.3259930000	12.1929980000
C135	104.4790890000	68.6292310000	10.8951270000
C136	103.9462240000	67.9937880000	9.6025850000
C137	103.7835810000	66.4619960000	9.5874820000
C138	103.4941640000	66.0223360000	8.1502320000
N139	102.8521630000	64.6762430000	8.0222700000
H140	104.1085750000	67.5601820000	12.6777190000

H141	102.6397070000	68.0785540000	11.9740900000
H142	103.6948490000	69.1366810000	12.7784180000
H143	104.5017950000	69.7142820000	10.7293020000
H144	105.5271040000	68.3307400000	11.0391900000
H145	102.9676670000	68.4354870000	9.3662630000
H146	104.6158880000	68.2855660000	8.7806080000
H147	104.6882760000	65.9657780000	9.9640650000
H148	102.9514020000	66.1699170000	10.2395630000
H149	102.7892100000	66.7133230000	7.6814710000
H150	104.3960080000	66.0101590000	7.5341380000
H151	103.4652260000	63.8590940000	8.2056990000
H152	101.9951910000	64.6380160000	8.6086300000
H153	102.5610380000	64.5690220000	7.0257460000
H154	93.6474240000	64.1310060000	8.9212680000
H155	95.6198510000	57.7972830000	5.4686070000
H156	93.3471300000	60.0483400000	0.1060380000
H157	107.5224150000	56.5249250000	1.0242610000
H158	100.7991130000	55.5008430000	3.5332510000
H159	100.4531470000	62.7081860000	6.1625420000
H160	102.2744860000	64.3426570000	3.5173450000
S161	102.6430710000	65.3005000000	4.7909570000
H162	101.5156690000	66.0264620000	4.6238440000
H163	94.8291930000	59.8672870000	-1.0815080000
C164	95.2420430000	60.2379260000	-2.0081040000
H165	95.8060990000	59.4731290000	-2.5212650000
C166	96.1471680000	61.4626620000	-1.7717010000
C167	97.3099210000	61.1426660000	-0.8564590000
C168	98.2761630000	60.1968600000	-1.2296790000
C169	97.4272280000	61.7605420000	0.3955600000
C170	99.3214000000	59.8622280000	-0.3679070000
C171	98.4693640000	61.4272360000	1.2641980000
C172	99.4147960000	60.4718050000	0.8864930000
H173	94.3980900000	60.5072310000	-2.6590340000
H174	96.5198730000	61.8148840000	-2.7438810000
H175	95.5669520000	62.2903560000	-1.3476330000
H176	96.7156770000	62.5350620000	0.6743300000
H177	98.2150600000	59.7226970000	-2.2076740000
H178	98.5512100000	61.9174690000	2.2287200000
H179	100.2376740000	60.2225700000	1.5484370000
H180	100.0696900000	59.1348950000	-0.6729360000

A₄':

E=-7417.084609 solv=-0.124097 disp=-220.89 Z0=896.67

V	99.5606825865	62.0838318900	7.2918774629
Fe	105.2472743824	59.7013318345	2.6414727615
Fe	103.0191065916	61.5646709938	3.1299188102
Fe	104.6344521150	60.8080909792	5.2880183830
Fe	102.8239993131	58.9893981267	3.9844463606
Fe	100.5011759426	59.8487534948	5.3053533458
Fe	101.0267382312	62.4355612286	4.6685639207
Fe	102.4924717655	61.0750070779	6.7947769338
C	102.2952361023	60.7538505137	4.8233942976
S	105.0969726575	58.5258546046	4.7219941357
S	104.5982385383	61.6017642864	7.5169170289
S	105.3884674208	61.9221277957	3.2866531223
S	103.0858418278	59.6560228150	1.6888736501
S	101.8327278614	63.4501589092	2.8450120701
S	98.7481537018	61.5665963875	5.1465481756
S	100.6868968616	60.0239382276	7.7368659435
C	100.5987013371	57.1065592434	4.3019322692
O	101.8592746525	57.1808001283	4.1894246174
O	99.8205576248	57.9571228246	4.8248144858
O	100.0024476260	55.9866357733	3.8436271960
C	97.9616480135	66.2044769061	5.5982838428
C	98.9361460855	66.0806893888	6.8059732429
C	98.5292224018	65.0110299777	7.8641065405
C	97.2967278242	65.4969797808	8.6648018802
C	96.7746693568	64.4781329189	9.7157305044
C	95.2679300213	64.4454875340	9.8432462286
C	99.7288140867	64.6926437448	8.7816281930
O	97.4187547986	65.0780546592	5.2366829790
O	97.8069281177	67.2897321969	5.0381223625
O	94.6870758344	63.9856540979	8.6783252128
O	94.5890615562	64.7516301023	10.7940878567
O	100.1783190602	63.4728652013	8.6988437678
O	100.2314377924	65.5768655333	9.4826949384
O	98.2102327167	63.7896501678	7.1777203553
H	97.9627239365	64.1357903094	6.2265762451
H	99.9080427656	65.7958270426	6.3795301737
H	99.0609682756	67.0552035424	7.2816068492
H	97.5567802025	66.4357844421	9.1623413321
H	96.5113950041	65.7226373511	7.9347410922
H	97.0902291723	63.4719732097	9.4219301494
H	97.1875575906	64.6892228975	10.7042486044
C	106.6276909282	57.0481112358	1.3876730221
H	105.7834352549	56.8020963705	0.7371767090
H	106.4096050208	56.7121249436	2.4049317566

S	106.9521474526	58.8666736247	1.3646164735
C	93.8276362891	61.0260765579	1.8500003071
C	93.6849290382	61.1386377291	3.3647869832
C	94.7054280912	62.1588026521	3.8761339782
C	94.5975811625	62.4304193314	5.3679382698
N	95.8421013260	63.0859584928	5.8544631641
C	93.0790262245	59.8959601620	1.1410744081
H	94.8939134604	60.9247209219	1.6105326827
H	93.5215264925	61.9828165407	1.4037382762
H	93.8719666208	60.1650050097	3.8418682700
H	92.6601910802	61.4330576908	3.6386349773
H	95.7125145908	61.7828886419	3.6538166512
H	94.6050432417	63.1024576738	3.3240015579
H	94.4833801719	61.4984768829	5.9323652004
H	93.7537938257	63.0806773427	5.6188281242
H	95.8275601898	63.2636771925	6.8654955276
H	96.6846336508	62.4954316512	5.6461158561
H	96.0819433622	64.0035001705	5.4008010387
H	91.9901723846	59.9648728150	1.2516627203
H	93.4048998872	58.9145809298	1.4526838969
C	100.0989993674	60.0520007254	10.8889969645
C	99.1498875528	61.2556137914	10.7055041287
C	97.9462476316	60.9695827757	9.8677083995
N	97.9191647355	61.1782699848	8.4991541741
C	96.7520634132	60.4088366566	10.2513459120
C	96.7577544925	60.7255621538	8.0650160358
N	96.0077410269	60.2627408920	9.0956964679
H	100.7720113283	59.8784109931	10.1700240420
H	99.5067948735	59.1345854909	11.0184647281
H	100.5712426423	60.2159537996	11.7550862333
H	98.7999263398	61.5538354787	11.7029084664
H	99.6940666097	62.1069378860	10.2927123877
H	96.3794243895	60.1048244358	11.2172229329
H	95.1101315132	59.8081311315	9.0142426425
H	96.4641253749	60.6586993888	7.0297857888
C	101.6500025681	56.1420052469	7.7050017406
N	102.8454214072	56.9303265284	7.4085157872
C	103.4375815251	57.7820537593	8.2443828243
N	102.8358550608	58.0678257273	9.4317848815
N	104.6488717964	58.2877300558	7.9775826241
H	101.7064749190	55.2470483483	7.0750225683
H	100.7886343612	56.5995587959	7.4843449978
H	101.6262277141	55.8261440640	8.6535096816
H	103.1531888188	56.9612833959	6.4389539647

H	103.3264412773	58.7646370596	9.9812282182
H	101.8460606681	58.2888592474	9.3355608571
H	105.0353634880	58.0810598734	7.0505870206
H	104.7824500609	59.2870702983	8.1984357870
C	104.8710008956	65.5940004129	-4.0429950314
C	104.5873449119	64.1009983931	-3.7513504312
C	104.0270665084	63.8346605531	-2.3881674920
N	102.7131284983	64.1249239123	-2.0706898247
C	104.6742276612	63.3143629204	-1.2901069570
C	102.5759174775	63.7810499827	-0.8039448433
N	103.7345871364	63.2926382655	-0.2827996367
H	105.4142233796	65.9758308916	-3.2952587306
H	103.9371905315	66.1591932325	-4.1296920740
H	105.3923872364	65.6470935380	-4.8946699459
H	105.5263819124	63.5406936631	-3.8597022794
H	103.9000931682	63.7065004604	-4.5115611195
H	105.6825934619	62.9596006467	-1.1367850884
H	103.8592135365	62.9396975783	0.6582581770
H	101.6730974523	63.8485625982	-0.2138887526
C	95.6299757305	57.4820327412	6.4910616085
C	97.0644097387	57.3401261871	7.0290302580
O	97.8170388120	56.4500297659	6.2142575848
C	97.0824393885	56.7812044379	8.4522604335
H	95.0473357598	58.2030486707	7.0840937530
H	98.1076061236	56.7560636492	8.8349999379
H	96.6894465626	55.7572209630	8.4556585885
H	96.4760533593	57.3881138414	9.1353542760
H	95.1151199698	56.5148022412	6.5440320596
H	98.3310755851	56.9800105324	5.5754667860
H	97.5487520033	58.3264352890	7.0333691754
C	98.4859996148	66.3580013517	-1.7130007866
C	98.8421928358	65.6382211797	-0.3936847960
C	98.3160481228	66.2776456517	0.8983081251
C	96.8323303163	66.0550679790	1.1906065240
O	96.0755942139	65.4172082587	0.4560281180
N	96.3823905828	66.6483227332	2.3402307934
H	98.7144620224	67.3289719301	-1.6420951188
H	97.4178284322	66.2568234294	-1.9345556720
H	99.0290071473	65.9401254950	-2.4413701743
H	98.5071449741	64.5969426697	-0.4380595682
H	99.9360617281	65.6041727525	-0.3148392127
H	98.8787810400	65.8790543680	1.7546232044
H	98.5062209948	67.3609445113	0.9029486659
H	97.0009704555	66.9090296825	3.1104152507

H	95.4418922079	66.3907278741	2.6093804335
C	103.6859931304	68.3259924761	12.1929978666
C	104.3649228326	68.5537093709	10.8197513579
C	103.7093265964	67.8527097464	9.6085501196
C	103.6561496399	66.3072755355	9.6000833345
C	103.1920723743	65.8341971641	8.2157562755
N	102.8717519507	64.3656792747	8.1275205168
H	104.1085749227	67.5601822624	12.6777191902
H	102.6267142927	68.0707386069	12.0435995015
H	103.6948492247	69.1366815086	12.7784182617
H	104.3669465955	69.6271567175	10.5904835378
H	105.4229974428	68.2625144555	10.8792124826
H	102.6802869201	68.2241589423	9.5041679561
H	104.2454989005	68.1844342456	8.7073971769
H	104.6424135842	65.8826025622	9.8323804922
H	102.9466949191	65.9507286900	10.3561366090
H	102.2704063270	66.3502115369	7.9396505108
H	103.9490022748	66.0318665635	7.4515679460
H	103.6803481573	63.7108865726	8.2208558688
H	102.1206133557	64.0850954918	8.7849170293
H	102.4808189273	64.1187606580	7.2029775656
H	93.7244272010	64.0292730733	8.8333289556
H	95.6198510793	57.7972834192	5.4686067728
H	93.3471300164	60.0483400105	0.1060379870
H	107.5224146709	56.5249255497	1.0242611578
H	100.7038007146	55.4494211951	3.4356858936
H	101.0069218830	62.8313903852	6.4728399361
H	94.8291929469	59.8672869102	-1.0815080541
C	95.2420431227	60.2379261136	-2.0081037557
H	95.8060990000	59.4731290000	-2.5212650000
C	96.1576931540	61.4362650496	-1.6966949697
C	97.1595953282	61.1338336163	-0.5972187232
C	97.9469235780	59.9720064951	-0.6232700693
C	97.3186921856	62.0245701736	0.4750515131
C	98.8732611495	59.7094417849	0.3883481507
C	98.2463861688	61.7646518280	1.4878830704
C	99.0259462982	60.6063872669	1.4478776334
H	94.4155264063	60.5330592643	-2.6673483918
H	96.6838120710	61.7396943497	-2.6134519443
H	95.5558643629	62.3018618347	-1.3958846335
H	96.7370558775	62.9442710775	0.4965148175
H	97.8523722216	59.2721918132	-1.4507358702
H	98.3869336243	62.4731514256	2.2976979538
H	99.7676563352	60.4273022154	2.2183567046

H 99.4947760731 58.8190743687 0.3385776104

A₅ (E₀):

E=-7417.665898 solv=-0.127710 disp=-223.50 Z0=901.48

V	99.4601583819	62.0649471480	7.2956573210
Fe	105.2672272263	59.8573373023	2.3982032311
Fe	102.8538099811	61.5679386831	3.0504675980
Fe	104.4709064766	60.9074912363	5.1530055672
Fe	102.7146627834	58.9879455356	3.8797065022
Fe	100.3974321688	59.8082561607	5.2744092429
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H	102.0003547356	64.2650374526	8.6615591760
H	102.4048398391	64.3223590746	7.0901497614
H	93.6546171184	63.9927497999	8.9579531441
H	95.6198511854	57.7972834899	5.4686067936
H	93.3471300271	60.0483400537	0.1060380186
H	107.5224147565	56.5249253651	1.0242612115
H	100.6363359922	55.7027560301	2.7590519583
H	101.0354976198	62.8686660655	6.2768339300
H	98.1750115149	61.4961121760	3.5503298968
H	94.8291928824	59.8672868565	-1.0815081026
C	95.2420431499	60.2379261097	-2.0081038374
H	95.8060990000	59.4731290000	-2.5212650000
C	96.0946478441	61.4937555854	-1.7569694235
C	97.2433244767	61.3035912223	-0.7825396959
C	98.1983603537	60.2868401148	-0.9488751845

C	97.4040845275	62.1986757562	0.2838158145
C	99.2936842757	60.1803921797	-0.0897704015
C	98.5096409176	62.1026537465	1.1361455568
C	99.4608220668	61.0928440809	0.9570488249
H	94.3972057821	60.4907160193	-2.6626023007
H	96.4942209755	61.8505549502	-2.7175355394
H	95.4542019010	62.3021999182	-1.3852964215
H	96.6905883445	63.0089140573	0.4137662074
H	98.1032004175	59.5860285962	-1.7753924792
H	98.6418095840	62.8522555948	1.9152247293
H	100.3342654231	61.0219544493	1.5992164754
H	100.0408360614	59.4079073482	-0.2493798967
H	101.1606182273	63.9800457408	2.0628536144

E1 TS_{C-H}

E=-7418.213186 solv=-0.124185 disp=-228.15 Z0=904.12

V	99.533109	62.175424	7.269395
Fe	105.295744	59.884531	2.589235
Fe	102.941567	61.809346	3.132733
Fe	105.046104	61.075948	5.379602
Fe	102.636966	59.125038	3.904279
Fe	100.405338	59.756986	5.241598
Fe	100.595038	62.569078	4.604093
Fe	102.388252	61.404461	6.402367
C	101.902252	60.926739	4.622377
S	104.814868	58.791002	4.819351
S	104.442596	61.829618	7.486277
S	105.315691	62.185040	3.364341
S	102.964378	59.920762	1.705512
S	101.618602	63.924803	2.904558
S	98.577354	61.424710	5.024210
S	100.846579	60.032815	7.514350
C	100.707674	56.940265	4.518480
O	101.905352	57.174468	4.195848
O	99.902473	57.716937	5.111554
O	100.219213	55.708769	4.239047
C	97.982771	66.289228	5.585401
C	98.920449	66.174995	6.821654
C	98.522548	65.082677	7.858348
C	97.270958	65.532458	8.650823
C	96.771613	64.486097	9.684698
C	95.267930	64.445488	9.843246
C	99.716021	64.777765	8.794238

O	97.443999	65.166315	5.206351
O	97.855086	67.370961	5.012220
O	94.661863	64.002297	8.685052
O	94.610947	64.733766	10.814022
O	100.171805	63.563607	8.768638
O	100.206289	65.700637	9.458331
O	98.223380	63.871737	7.143474
H	97.960610	64.230699	6.201484
H	99.912489	65.929583	6.417238
H	99.004902	67.147784	7.309189
H	97.500931	66.472383	9.160998
H	96.484995	65.743414	7.916379
H	97.084611	63.489309	9.357457
H	97.204586	64.674141	10.669433
C	106.673226	57.058612	1.477058
H	105.758405	56.756620	0.957965
H	106.597511	56.767981	2.528985
S	106.943965	58.883202	1.315513
C	93.828958	61.030208	1.846627
C	93.674583	61.170926	3.359417
C	94.678199	62.217095	3.856716
C	94.581302	62.502862	5.348488
N	95.837228	63.151389	5.821675
C	93.079026	59.895960	1.141074
H	94.897394	60.918252	1.619228
H	93.532181	61.981622	1.382883
H	93.872956	60.209902	3.856432
H	92.644025	61.456792	3.618868
H	95.690389	61.855297	3.634349
H	94.555964	63.153058	3.295722
H	94.469721	61.576298	5.921558
H	93.744025	63.160424	5.601259
H	95.837869	63.317714	6.834467
H	96.669470	62.549261	5.595956
H	96.074693	64.068352	5.373554
H	91.990445	59.966805	1.252018
H	93.404900	58.914581	1.452684
C	100.098999	60.052001	10.888997
C	99.150177	61.252777	10.674865
C	97.969520	60.947159	9.809901
N	97.960959	61.169849	8.442057
C	96.784414	60.348749	10.166529
C	96.818144	60.689065	7.983181
N	96.064770	60.195995	8.997550

H	100.772011	59.878411	10.170024
H	99.505714	59.135562	11.021385
H	100.571243	60.215954	11.755086
H	98.776425	61.559040	11.661088
H	99.699994	62.101717	10.262659
H	96.404278	60.022386	11.122469
H	95.185409	59.711477	8.894706
H	96.548553	60.622520	6.941172
C	101.650003	56.142005	7.705002
N	102.816419	56.990813	7.451930
C	103.327906	57.858648	8.323927
N	102.738776	57.996999	9.546543
N	104.470896	58.505694	8.065803
H	101.740121	55.262519	7.059933
H	100.788634	56.599559	7.484345
H	101.626228	55.826144	8.653510
H	103.092130	57.123879	6.479702
H	103.173214	58.697766	10.135525
H	101.729895	58.102587	9.506809
H	104.850442	58.377532	7.120198
H	104.509932	59.502709	8.322014
C	104.871001	65.594000	-4.042995
C	104.585588	64.083977	-3.849710
C	103.933213	63.629285	-2.578499
N	102.652503	64.004797	-2.214963
C	104.427651	62.712761	-1.675732
C	102.387030	63.319801	-1.118975
N	103.429882	62.525609	-0.745646
H	105.414223	65.975831	-3.295259
H	103.938781	66.161542	-4.132112
H	105.392387	65.647094	-4.894670
H	105.535709	63.540906	-3.948879
H	103.964896	63.756494	-4.697105
H	105.365072	62.179111	-1.617585
H	103.441802	61.850684	0.014965
H	101.461369	63.350952	-0.559452
C	95.629976	57.482033	6.491062
C	97.055622	57.248240	7.012431
O	97.717035	56.300777	6.187476
C	97.046796	56.706781	8.445638
H	95.091287	58.229080	7.092679
H	98.072539	56.585133	8.809299
H	96.559871	55.724248	8.468528
H	96.515972	57.374126	9.135731

H	95.060883	56.545237	6.549815
H	98.399440	56.777873	5.675604
H	97.607382	58.198962	6.995136
C	98.486000	66.358001	-1.713001
C	98.852434	65.660914	-0.382910
C	98.345943	66.344812	0.895152
C	96.857999	66.160049	1.194062
O	96.092180	65.527022	0.466136
N	96.421578	66.779009	2.333965
H	98.714462	67.328972	-1.642095
H	97.417318	66.253610	-1.926013
H	99.029007	65.940125	-2.441370
H	98.503994	64.623157	-0.398533
H	99.948466	65.622765	-0.315992
H	98.900845	65.962294	1.764033
H	98.559547	67.423222	0.868181
H	97.044025	67.029875	3.105046
H	95.473883	66.549366	2.602925
C	103.685993	68.325992	12.192998
C	104.406911	68.593704	10.847573
C	103.764257	67.956091	9.601429
C	103.646949	66.419325	9.585447
C	103.136045	65.969204	8.214663
N	102.796988	64.510353	8.146548
H	104.108575	67.560182	12.677719
H	102.631143	68.072965	12.017835
H	103.694849	69.136681	12.778418
H	104.444498	69.675450	10.664956
H	105.454218	68.268977	10.921617
H	102.756008	68.374379	9.472170
H	104.342800	68.273493	8.721715
H	104.619537	65.954178	9.797446
H	102.937597	66.088593	10.353326
H	102.214381	66.501145	7.970924
H	103.874832	66.157033	7.429939
H	103.604014	63.849625	8.230881
H	102.051068	64.239549	8.815809
H	102.398225	64.255432	7.229456
H	93.703212	64.035237	8.864971
H	95.619851	57.797283	5.468607
H	93.347130	60.048340	0.106038
H	107.522415	56.524925	1.024261
H	100.922124	55.244733	3.751724
H	101.128762	62.937023	6.324915

H	100.758951	59.481288	3.669308
H	94.856552	59.832907	-1.094580
C	95.234825	60.257974	-2.027867
H	95.806099	59.473129	-2.521265
C	96.108281	61.490074	-1.772911
C	97.240821	61.280543	-0.788494
C	98.199629	60.272688	-0.971354
C	97.348111	62.110995	0.334890
C	99.233260	60.093280	-0.051250
C	98.376951	61.927283	1.262252
C	99.320485	60.915506	1.075997
H	94.381167	60.504187	-2.670958
H	96.517784	61.827955	-2.736708
H	95.482451	62.316371	-1.414516
H	96.641379	62.927376	0.467511
H	98.144290	59.627452	-1.846015
H	98.433272	62.567094	2.138421
H	100.119753	60.762533	1.793284
H	99.979227	59.318574	-0.207312
H	100.753838	63.497510	1.954953

E1 CH product

E=-7418.256586 solv=-0.130979 disp=-224.33 Z0=905.73

V	99.6097125199	62.2978105616	7.2170678766
Fe	105.7224767352	60.0156397393	2.5110107668
Fe	103.2168253437	61.7774487349	3.1103085775
Fe	105.3957413257	61.1650490258	5.2740290225
Fe	103.1185650189	59.1374834107	3.8483302553
Fe	100.3061991844	59.8879862570	5.4848438371
Fe	100.8769617156	62.6334304194	4.5739265171
Fe	102.7037803942	61.2853286343	6.0534636599
C	101.7909620300	60.7495791348	4.2691499980
S	105.3021229022	58.8647747362	4.8031464711
S	104.5705936796	61.8930270640	7.3218683881
S	105.5466259588	62.3613891965	3.3131716858
S	103.4350491355	59.8335884367	1.6588834056
S	101.8756708177	63.9785599521	2.8531967520
S	98.6448613370	61.6659515163	5.1155982536
S	101.0619695667	60.5314995516	7.6780525772
C	100.7708791521	57.1711112936	4.6232304629
O	102.0090382597	57.3822355762	4.5820463092
O	99.8662747271	57.9357800577	5.0980165596
O	100.3051109055	55.9936285899	4.1474419283

C	97.8305018805	66.3104598150	5.5336859028
C	98.8084524576	66.2389771537	6.7431796861
C	98.4559646708	65.1592782612	7.8101133977
C	97.2229551505	65.5974877427	8.6351507456
C	96.7661536799	64.5463831940	9.6842699733
C	95.2679299194	64.4454875681	9.8432463491
C	99.6739942294	64.8791377827	8.7184414906
O	97.3194087548	65.1627976222	5.1879127423
O	97.6458674140	67.3782925169	4.9494635250
O	94.6739847913	64.0044484362	8.6748385556
O	94.5996696872	64.6854493906	10.8191076264
O	100.1367101187	63.6622640216	8.6557982238
O	100.1631680121	65.7812088744	9.4034498778
O	98.1663378476	63.9250315638	7.1352409563
H	97.8902995471	64.2535328407	6.1866004867
H	99.7928207961	65.9993341009	6.3182940920
H	98.8890230244	67.2224706656	7.2098866576
H	97.4579447653	66.5403185415	9.1376071648
H	96.4144994497	65.8005982207	7.9236437821
H	97.1197091768	63.5578410580	9.3730331503
H	97.1889159778	64.7634740607	10.6669803868
C	106.7642708487	57.2041396359	1.4289663810
H	105.8637712332	57.1322097507	0.8134192405
H	106.5248080085	56.8911307659	2.4487964069
S	107.4295068828	58.9300448805	1.4175351090
C	93.8478217807	61.0156473176	1.8516900600
C	93.6659880490	61.1656369013	3.3605325597
C	94.6921430873	62.1750937430	3.8862785750
C	94.5210561198	62.5040917608	5.3617715568
N	95.7371549690	63.1925862929	5.8786774620
C	93.0790262292	59.8959601458	1.1410743610
H	94.9166897522	60.8693723932	1.6451007634
H	93.5897792997	61.9738800333	1.3792921168
H	93.8115082079	60.1986079250	3.8645780097
H	92.6407292290	61.4912167435	3.5930399665
H	95.6987167620	61.7654073748	3.7305790323
H	94.6446029999	63.1011967324	3.2981926468
H	94.3925211487	61.5935219660	5.9576790208
H	93.6604314778	63.1535287940	5.5499986914
H	95.6772789107	63.3855231786	6.8862863739
H	96.5931102127	62.6131636533	5.7086476635
H	95.9850636114	64.1036564797	5.4136608414
H	91.9921256725	59.9759723688	1.2570643763
H	93.4048998939	58.9145809357	1.4526839086

C	100.0989993337	60.0520006461	10.8889970057
C	99.2029535458	61.2909315026	10.6642728721
C	98.0300205236	61.0301056762	9.7774786027
N	98.0450223386	61.2468579875	8.4084147497
C	96.8274148935	60.4626362417	10.1229904521
C	96.8958465218	60.7911872492	7.9406810177
N	96.1182299622	60.3206498468	8.9457450685
H	100.7720113387	59.8784111180	10.1700240486
H	99.4756814771	59.1564506762	11.0189820371
H	100.5712426463	60.2159538082	11.7550862295
H	98.8221932310	61.6124485461	11.6429380847
H	99.7932203260	62.1176353788	10.2631813523
H	96.4310346885	60.1472923218	11.0757173935
H	95.2290226496	59.8562487156	8.8337810978
H	96.6337573765	60.7358580029	6.8963867539
C	101.6500025475	56.1420051136	7.7050016696
N	102.8157544308	56.9876923334	7.4239743217
C	103.3499790245	57.8891054448	8.2527439264
N	102.7989778229	58.0625923496	9.4913610884
N	104.4674520301	58.5413413239	7.9281360328
H	101.7340864803	55.2586761980	7.0647685155
H	100.7886343882	56.5995588696	7.4843450448
H	101.6262277127	55.8261440922	8.6535096909
H	103.0400331178	57.1027967254	6.4359407313
H	103.2266832187	58.8066207353	10.0302362896
H	101.7866410728	58.1281591386	9.4956165163
H	104.8479577724	58.4051994845	6.9770508383
H	104.5450208578	59.5315389834	8.1961065793
C	104.8710009858	65.5940002216	-4.0429951298
C	104.5673984408	64.1088612663	-3.7380764715
C	103.8505021222	63.8826935007	-2.4389351171
N	102.5479746370	63.4249886161	-2.4241771422
C	104.2883717783	64.0897519272	-1.1475254036
C	102.2106545774	63.3555196141	-1.1515794596
N	103.2289271572	63.7472273552	-0.3371436934
H	105.4142233594	65.9758308144	-3.2952586767
H	103.9437515495	66.1700531397	-4.1397599703
H	105.3923871987	65.6470937869	-4.8946699534
H	105.5183338974	63.5565108087	-3.7478511894
H	103.9456173397	63.6783227769	-4.5304709024
H	105.2327412139	64.4118997847	-0.7354883655
H	103.1871716428	63.7985915411	0.6769764795
H	101.2603651514	63.0111372050	-0.7671430977
C	95.6299755263	57.4820326835	6.4910616552

C	97.0597354498	57.2939271630	7.0227873059
O	97.7707822881	56.3706530170	6.2110123269
C	97.0622345289	56.7548695350	8.4551262718
H	95.0707585880	58.2184461902	7.0879828471
H	98.0884870896	56.6777945493	8.8291454509
H	96.6161509504	55.7531845227	8.4771051129
H	96.4965904254	57.4020162551	9.1363658274
H	95.0872372457	56.5304460366	6.5479808486
H	98.3747685851	56.8760384818	5.6330951564
H	97.5753883078	58.2650829344	7.0112547869
C	98.4859996122	66.3580013639	-1.7130007970
C	98.8178697828	65.6327758897	-0.3909473593
C	98.2484992849	66.2685114570	0.8849976813
C	96.7773865126	65.9596866986	1.1697483953
O	96.0837977660	65.2255796763	0.4657797175
N	96.2698540397	66.5886565143	2.2762589593
H	98.7144620317	67.3289719296	-1.6420951404
H	97.4195947818	66.2607588795	-1.9470367881
H	99.0290071534	65.9401254937	-2.4413701690
H	98.4799561650	64.5929858202	-0.4482703768
H	99.9103855126	65.5983877150	-0.2870123518
H	98.8215640231	65.9228591349	1.7575684919
H	98.3764027385	67.3601758972	0.8698784172
H	96.8606910545	66.9221909214	3.0405398430
H	95.3480703449	66.2766816868	2.5519390544
C	103.6859932711	68.3259925467	12.1929978970
C	104.3866962628	68.5788110952	10.8340752701
C	103.7348981196	67.9222869861	9.5993584425
C	103.6525604645	66.3811593319	9.5685977311
C	103.1641275906	65.9322912514	8.1865267058
N	102.8226354124	64.4723374697	8.1001225995
H	104.1085749052	67.5601822397	12.6777191698
H	102.6291577779	68.0720425390	12.0293297133
H	103.6948491352	69.1366814925	12.7784182853
H	104.4116188171	69.6583427600	10.6368791316
H	105.4381666227	68.2658793379	10.8987824991
H	102.7148316498	68.3166191845	9.4892606996
H	104.2896475908	68.2579488834	8.7110708456
H	104.6322730312	65.9343113895	9.7857734515
H	102.9447746936	66.0284071216	10.3286058936
H	102.2481250216	66.4675662829	7.9279349182
H	103.9152077093	66.1227370798	7.4146008988
H	103.6349306503	63.8070848725	8.1241838464
H	102.1114949782	64.1933258911	8.7976890068

H	102.3701713426	64.2437038905	7.1998458161
H	93.7152519631	64.0010221995	8.8573383830
H	95.6198512441	57.7972834509	5.4686067811
H	93.3471300418	60.0483400679	0.1060380265
H	107.5224148629	56.5249253222	1.0242611859
H	101.0717056569	55.5325604477	3.7640409126
H	100.9576254122	63.2018107463	6.2669554373
H	101.0860036943	60.5187854407	3.4410285726
H	94.8291928993	59.8672868365	-1.0815081044
C	95.2420431294	60.2379261443	-2.0081038253
H	95.8060990000	59.4731290000	-2.5212650000
C	96.1160951492	61.4926058378	-1.7922009477
C	97.3754556379	61.2371466326	-0.9868229273
C	98.3955954418	60.4198740901	-1.5016453130
C	97.5623432139	61.8204653201	0.2744256568
C	99.5681399162	60.1933641607	-0.7834361962
C	98.7328755652	61.5866088120	1.0050519499
C	99.7413121841	60.7731629300	0.4778407961
H	94.3898877250	60.4911745939	-2.6548052832
H	96.3973388753	61.8876808953	-2.7785791838
H	95.5284327300	62.2808930269	-1.3067592511
H	96.8071049736	62.4990667252	0.6649549203
H	98.2794073653	59.9764436488	-2.4889752494
H	98.8521678724	62.0379331457	1.9869899719
H	100.6663288926	60.5965621030	1.0203997652
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Fe	103.4224000963	62.0335351218	3.5272170203
Fe	105.5976048547	60.9093989407	5.5444201237
Fe	103.2506114401	59.3234014101	4.1234350504
Fe	100.3795857526	60.2961737034	5.7684858001
Fe	101.0908591160	62.9500543762	4.8781491313
Fe	103.0181483046	61.4389869216	6.1058228425
C	101.8758712621	60.9604801219	4.5108013873
S	105.4314925281	58.6889034673	4.8340359849
S	104.8439651344	61.5972932227	7.6008945082
S	105.8663811673	62.3057201999	3.7495717403

S	103.5226277365	60.2367378418	1.9672469610
S	101.9850090882	63.9563420678	2.8594716450
S	98.7122990449	61.8940330569	5.1883321212
S	101.2805462398	60.9583475468	7.7885124254
C	100.7817790688	57.5575141971	4.7060384619
O	102.0313859136	57.6835316796	4.5833071031
O	99.9689273471	58.3283963299	5.3022866786
O	100.2141147061	56.4494584126	4.1776157780
C	97.9581546264	66.5825003949	5.7855614642
C	98.8708277018	66.4810309281	7.0424141133
C	98.4718194625	65.3860407196	8.0779451192
C	97.2333560422	65.8069737639	8.8938641044
C	96.7531972805	64.6916006343	9.8641505599
C	95.2679300971	64.4454876509	9.8432462679
C	99.6700767642	65.0738750741	9.0054131926
O	97.3787159747	65.4626055155	5.4528967148
O	97.8747080426	67.6384442946	5.1601917700
O	94.8229741540	64.0662166323	8.5904863737
O	94.4873234803	64.5304514946	10.7621369520
O	100.1594638409	63.8692645148	8.8848567939
O	100.1088223186	65.9454469321	9.7572386327
O	98.1477277715	64.1737612151	7.3719653452
H	97.8477394134	64.5672310443	6.4355335535
H	99.8730730452	66.2476203397	6.6602229123
H	98.9317523300	67.4557354212	7.5311419511
H	97.4742709345	66.7111449840	9.4596895221
H	96.4422008365	66.0621497892	8.1801766498
H	97.2288360856	63.7469898181	9.5794228771
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C	106.7763044154	57.2013712746	1.4633240737
H	105.8377790242	57.0870254819	0.9119247914
H	106.6147313372	56.9134456723	2.5061325235
S	107.3853983620	58.9476475481	1.3576852144
C	93.8671215364	61.0261942640	1.8233716550
C	93.7354195442	61.2261989274	3.3325675231
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C	94.6464566174	62.6406967865	5.2550301477
N	95.8565869291	63.3723442401	5.7273485261
C	93.0790261780	59.8959601795	1.1410742998
H	94.9294808287	60.8722043351	1.5913117661
H	93.6011737621	61.9739503351	1.3343357720
H	93.8933328200	60.2764839811	3.8649398013
H	92.7203288539	61.5662656152	3.5884232261
H	95.7840755559	61.8203263248	3.6326694612

H	94.7373106965	63.1477901779	3.1612975165
H	94.5462194844	61.7539589589	5.8905815599
H	93.7767391037	63.2811200226	5.4333588077
H	95.8284002545	63.5635682183	6.7390817394
H	96.7331074971	62.8193661212	5.5361661154
H	96.0471875962	64.2949303989	5.2754644882
H	91.9937778567	59.9834901896	1.2638299228
H	93.4048999179	58.9145809522	1.4526839356
C	100.0989992450	60.0520007078	10.8889967560
C	99.2239767218	61.3111264868	10.6929162053
C	98.0518798242	61.1063221854	9.7932518716
N	98.0781328733	61.4024114061	8.4422006733
C	96.8384964344	60.5398842659	10.1022203082
C	96.9206390003	61.0022696562	7.9439890417
N	96.1299464442	60.4857069401	8.9161771679
H	100.7720114131	59.8784110368	10.1700242001
H	99.4651562742	59.1641487088	11.0163444291
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H	98.8455990951	61.6085621794	11.6801227057
H	99.8317805425	62.1401847973	10.3225651551
H	96.4324537949	60.1766827439	11.0336068506
H	95.2299444990	60.0510778321	8.7752997466
H	96.6621095256	61.0227899202	6.8974678654
C	101.6500025455	56.1420050292	7.7050015864
N	102.8354393865	56.9571599596	7.4216989549
C	103.4101233635	57.8411100168	8.2458718160
N	102.8123414570	58.1252453954	9.4382511715
N	104.5951080641	58.3769815327	7.9593591451
H	101.7193673660	55.2524286155	7.0704981589
H	100.7886343837	56.5995588818	7.4843450882
H	101.6262277353	55.8261441325	8.6535097049
H	103.1220868250	57.0133581083	6.4474540715
H	103.2711842181	58.8634372616	9.9609097628
H	101.8099985189	58.2694450483	9.3857391918
H	105.0032664027	58.1665799796	7.0386333334
H	104.7392390281	59.3774534249	8.1874575175
C	104.8710008554	65.5940001583	-4.0429944264
C	104.6244562768	64.0823573303	-3.8171442637
C	103.9750349654	63.6864017914	-2.5284283604
N	102.6639213870	64.0112724888	-2.2317867401
C	104.5156732334	62.9298017601	-1.5137793036
C	102.4263767111	63.4567471258	-1.0598336297
N	103.5110150425	62.7855982524	-0.5826670986
H	105.4142233118	65.9758310722	-3.2952587737

H	103.9268678214	66.1411249148	-4.1283642820
H	105.3923871822	65.6470934926	-4.8946699817
H	105.5896298938	63.5616469843	-3.8839272630
H	104.0194782516	63.7050536205	-4.6545846494
H	105.4894450718	62.4839504254	-1.3739298320
H	103.5683825960	62.2489631676	0.2781701577
H	101.4870794810	63.4987476157	-0.5252123307
C	95.6299756888	57.4820327262	6.4910616038
C	97.0422645431	57.4467887638	7.0926798352
O	97.9000677110	56.6139016599	6.3203127417
C	97.0273301530	56.8973504788	8.5208580308
H	94.9721711643	58.1521844017	7.0649155555
H	98.0308331380	56.9442857547	8.9559489752
H	96.7083284918	55.8481208292	8.5126767459
H	96.3450586164	57.4608341364	9.1683165346
H	95.1892838752	56.4780496359	6.5278193869
H	98.4573614745	57.1912962813	5.7664377176
H	97.4477037711	58.4679919904	7.1105967374
C	98.4859995290	66.3580013806	-1.7130008685
C	98.8537494319	65.6385618356	-0.3935939993
C	98.3884533251	66.3034665301	0.9116399559
C	96.9668148026	65.9755250037	1.3747186206
O	96.2339901078	65.1490259979	0.8277867452
N	96.5508466406	66.6907164109	2.4660513189
H	98.7144620540	67.3289719229	-1.6420951224
H	97.4168384904	66.2589429766	-1.9355242739
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H	98.4851204049	64.6080341774	-0.4172278724
H	99.9484905248	65.5755714933	-0.3506426234
H	99.0551000001	65.9928148749	1.7298201131
H	98.4920121199	67.3961019837	0.8544906043
H	97.2040526063	67.1100146517	3.1282742462
H	95.6919352470	66.3622833185	2.8874525493
C	103.6859932140	68.3259924958	12.1929978020
C	104.3554255382	68.5446016759	10.8166868315
C	103.6999314064	67.8099917724	9.6276981247
C	103.6078067475	66.2689706003	9.6948532243
C	103.2200970364	65.7325186013	8.3124116762
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H	102.6258987129	68.0707974187	12.0482184347
H	103.6948491526	69.1366814739	12.7784183111
H	104.3425827286	69.6136327867	10.5676013288
H	105.4171794823	68.2665967091	10.8755693363

H	102.6807122899	68.1976055074	9.4928404395
H	104.2571973098	68.0889659026	8.7213267230
H	104.5682653441	65.8341761967	10.0052486361
H	102.8455470908	65.9713255325	10.4242181337
H	102.3307574524	66.2490377365	7.9437212169
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H	103.6535293233	63.6406608793	8.5619878189
H	102.0017744959	64.0481866659	8.8001750281
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H	95.6198511104	57.7972834376	5.4686067782
H	93.3471300347	60.0483399607	0.1060380078
H	107.5224149944	56.5249251915	1.0242612430
H	100.9204039442	55.9759148702	3.7041363669
H	100.6697761746	63.7872871404	6.3588001605
H	101.2246584719	63.2883324118	1.9610610836
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H	94.8291929373	59.8672868858	-1.0815080789
C	95.2420430888	60.2379261311	-2.0081038582
H	95.8060990000	59.4731290000	-2.5212650000
C	96.1556929414	61.4474049694	-1.7282142231
C	97.3063721106	61.1214473089	-0.7934702606
C	98.2002203207	60.0785972508	-1.0867422752
C	97.5095094025	61.8650899901	0.3783423713
C	99.2698490259	59.7890092457	-0.2397477107
C	98.5775808172	61.5724083440	1.2347656461
C	99.4611485002	60.5340459847	0.9273729919
H	94.4082433972	60.5272004053	-2.6610806087
H	96.5524964853	61.8211947629	-2.6830500584
H	95.5696562956	62.2696657653	-1.3011114758
H	96.8561306169	62.7059679758	0.6015942064
H	98.0724707316	59.4983499853	-1.9983449466
H	98.7192911038	62.1524728786	2.1426631386
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Fe	105.6654975785	60.9984313400	5.2659166508

Fe	103.2244906621	59.3033461780	4.0045629516
Fe	100.4951428504	60.3136802770	5.7659659322
Fe	101.1835366797	63.0256146737	4.8948009804
Fe	103.0216761039	61.5077060832	6.0475464760
C	101.9553191453	60.9709708389	4.4852300240
S	105.4576192007	58.7886861103	4.7856998245
S	105.1800778201	61.8041707624	7.4959882677
S	105.8759175699	62.3398869486	3.4577110002
S	103.5176054861	60.0595140970	1.8024647242
S	102.0741581528	64.0236869543	2.8447766478
S	98.8240076151	61.8901657956	5.1568989542
S	101.4197109209	60.9687617590	7.8141555642
C	100.8068798637	57.5706797138	4.7096939833
O	102.0715296623	57.6317279130	4.6784350085
O	100.0103522610	58.3284088389	5.3409383575
O	100.2114939875	56.5648918129	4.0312270907
C	97.9126729582	66.5047255245	5.6709540790
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C	98.4486671152	65.3609258993	7.9835759951
C	97.1992378604	65.7759045041	8.7893507256
C	96.7531519141	64.6935028740	9.8120828804
C	95.2679300856	64.4454876708	9.8432463624
C	99.6460010298	65.1016677880	8.9267973438
O	97.4190813691	65.3539947323	5.3141309187
O	97.7627757293	67.5646962334	5.0612059721
O	94.7989511601	64.0065428494	8.6203547421
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O	100.1299387574	63.8893660408	8.8888728526
O	100.0886468599	66.0185250007	9.6220514486
O	98.1622195686	64.1237802560	7.3026614127
H	97.9221248447	64.4675229338	6.3434131878
H	99.8311298338	66.2257199250	6.5525254527
H	98.8622210962	67.4299506690	7.4023610738
H	97.4147671903	66.7110287762	9.3136873260
H	96.3974247753	65.9780698073	8.0704957710
H	97.2244327268	63.7401069430	9.5489219200
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C	106.7345165673	57.2659993341	1.2010286303
H	106.0219730354	57.2268163157	0.3718936712
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C	93.7565360967	61.1881196255	3.3429433346
C	94.8145485447	62.1971178139	3.8114084740

C	94.6942549847	62.5585641855	5.2850470238
N	95.9109592202	63.2785438568	5.7534942234
C	93.0790261900	59.8959601248	1.1410742400
H	94.9313549339	60.8709675555	1.5814728362
H	93.5975906609	61.9740601834	1.3590217149
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H	95.8101334948	61.7710065631	3.6325077573
H	94.7597284316	63.1097371363	3.2026685129
H	94.5998912513	61.6586087326	5.9028290873
H	93.8272303276	63.1956012645	5.4877233121
H	95.8936836230	63.4629493175	6.7653360057
H	96.7890149985	62.7275717052	5.5513435683
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H	93.4048999104	58.9145809491	1.4526839338
C	100.0989992852	60.0520005754	10.8889968915
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C	96.8479662422	60.5126023476	10.0508131870
C	96.9936325954	60.9229507305	7.8856303118
N	96.1767156628	60.4241134858	8.8458862412
H	100.7720113621	59.8784110869	10.1700241272
H	99.4663245228	59.1627733661	11.0196909281
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H	99.8190819333	62.1401676857	10.3249034355
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H	95.2858038853	59.9766997842	8.6876179394
H	96.7699646447	60.9134121437	6.8308480489
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N	102.8032693079	56.9982457131	7.4195040267
C	103.3952790678	57.8173693921	8.2835634765
N	102.9011438937	57.9305426726	9.5521800245
N	104.5302491890	58.4406756890	7.9564222653
H	101.7374639585	55.2589386273	7.0643033779
H	100.7886343814	56.5995588643	7.4843450608
H	101.6262277402	55.8261441297	8.6535097041
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H	103.3637279297	58.6207543648	10.1311214715
H	101.8917217839	58.0043200119	9.6119473048
H	104.8895905007	58.3909263402	6.9862402538
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C	104.5731725693	64.1027189260	-3.7678951030
C	103.9091735444	63.8350104411	-2.4514315814
N	102.5939689221	63.4188796035	-2.3832480695
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C	102.3336485687	63.2871081480	-1.0968000933
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H	103.9424086746	66.1687229542	-4.1364171476
H	105.3923872063	65.6470935916	-4.8946699610
H	105.5196551917	63.5459304838	-3.8293926214
H	103.9246769506	63.7012918509	-4.5545084711
H	105.4103497966	64.2257212717	-0.8146116045
H	103.4370833757	63.6039531037	0.6852950933
H	101.3965976048	62.9543173952	-0.6717695477
C	95.6299754893	57.4820327236	6.4910616521
C	97.0572907210	57.4342714679	7.0617253500
O	97.8909388810	56.6089256284	6.2573622336
C	97.0729266795	56.8705448090	8.4838398440
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N	96.4176257856	66.6236603251	2.3944440359
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C	99.4021994696	59.9592540367	-0.4191806713
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C	98.7188168939	66.4480739824	6.7885885045
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Fe6	100.3841390000	60.0915690000	5.8481970000
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O30	94.7303040000	63.9850450000	8.6584510000
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H43	107.2891310000	57.0897530000	-0.6457400000
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H61	96.7081610000	62.6171700000	5.6187560000
H62	96.0345330000	64.1072790000	5.3537130000
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H74	100.5712430000	60.2159540000	11.7550860000
H75	98.8909770000	61.6375230000	11.6986580000
H76	99.8280050000	62.1354160000	10.2922930000
H77	96.4371730000	60.2009250000	11.1486010000
H78	95.2135500000	59.9675490000	8.9107900000
H79	96.6212720000	60.8549370000	6.9764100000
C80	101.6500030000	56.1420050000	7.7050010000
N81	102.7793340000	57.0229090000	7.4027620000
C82	103.3772590000	57.8386720000	8.2564840000
N83	102.9433450000	57.9067460000	9.5515500000
N84	104.4805280000	58.5156240000	7.9017850000
H85	101.7423460000	55.2628090000	7.0593890000
H86	100.7886340000	56.5995590000	7.4843450000
H87	101.6262280000	55.8261440000	8.6535100000
H88	102.8607320000	57.2425580000	6.3977570000
H89	103.4287110000	58.5806970000	10.1301660000
H90	101.9369150000	57.9681770000	9.6576700000
H91	104.8248620000	58.4650250000	6.9300080000
H92	104.6344800000	59.4181310000	8.3355620000
C93	104.8710010000	65.5940000000	-4.0429950000
C94	104.5661300000	64.1051970000	-3.7544400000
C95	103.8796580000	63.8578870000	-2.4440670000
N96	102.5126670000	63.6677540000	-2.3771210000
C97	104.4215260000	63.8163750000	-1.1779440000
C98	102.2377450000	63.5119110000	-1.0971380000
N99	103.3591570000	63.6013450000	-0.3259370000
H100	105.4142230000	65.9758310000	-3.2952590000
H101	103.9435550000	66.1703340000	-4.1375080000
H102	105.3923870000	65.6470940000	-4.8946700000
H103	105.5120130000	63.5463800000	-3.7870480000
H104	103.9312690000	63.6985170000	-4.5497210000
H105	105.4332050000	63.9003610000	-0.8098690000
H106	103.4058080000	63.5185160000	0.6834690000
H107	101.2539510000	63.3273040000	-0.6852670000
C108	95.6299750000	57.4820330000	6.4910620000
C109	97.0817040000	57.3835950000	6.9926400000
O110	97.8404580000	56.5604210000	6.1149290000
C111	97.1627590000	56.7904820000	8.4018770000
H112	95.0387390000	58.1871490000	7.0932080000
H113	98.1994730000	56.7888040000	8.7553180000
H114	96.8054090000	55.7538020000	8.3911230000
H115	96.5578120000	57.3584230000	9.1197930000
H116	95.1431100000	56.5009880000	6.5463970000
H117	98.5021990000	57.1150330000	5.6567860000

H118	97.5140270000	58.3932280000	7.0074410000
C119	98.4860000000	66.3580010000	-1.7130010000
C120	98.8184220000	65.6355080000	-0.3885080000
C121	98.2718480000	66.2761820000	0.8956560000
C122	96.7891400000	66.0254470000	1.1772650000
O123	96.0726830000	65.3079980000	0.4759790000
N124	96.2956730000	66.6828010000	2.2718890000
H125	98.7144620000	67.3289720000	-1.6420950000
H126	97.4195030000	66.2611860000	-1.9453770000
H127	99.0290070000	65.9401260000	-2.4413700000
H128	98.4697710000	64.5985750000	-0.4406920000
H129	99.9112830000	65.5916380000	-0.2939290000
H130	98.8314190000	65.8922750000	1.7612780000
H131	98.4457180000	67.3616640000	0.8963610000
H132	96.8893350000	67.0062680000	3.0397940000
H133	95.3633370000	66.4000900000	2.5453530000
C134	103.6859930000	68.3259930000	12.1929980000
C135	104.3579000000	68.5573990000	10.8196080000
C136	103.6849870000	67.8503040000	9.6245140000
C137	103.5322660000	66.3175980000	9.7160980000
C138	103.1340160000	65.7556400000	8.3486290000
N139	102.7516090000	64.3019250000	8.3910390000
H140	104.1085750000	67.5601820000	12.6777190000
H141	102.6256620000	68.0727720000	12.0480040000
H142	103.6948490000	69.1366820000	12.7784180000
H143	104.3658710000	69.6305410000	10.5900040000
H144	105.4138880000	68.2568310000	10.8714840000
H145	102.6836030000	68.2762940000	9.4757430000
H146	104.2610170000	68.0955380000	8.7203260000
H147	104.4739820000	65.8543940000	10.0462820000
H148	102.7540410000	66.0634410000	10.4447010000
H149	102.2602440000	66.2810620000	7.9593830000
H150	103.9525080000	65.8514450000	7.6288410000
H151	103.4593340000	63.7151260000	8.8443860000
H152	101.7907950000	64.1413470000	8.8214810000
H153	102.6606580000	63.9092890000	7.4417230000
H154	93.7738650000	63.8949970000	8.8304010000
H155	95.6198510000	57.7972830000	5.4686070000
H156	93.3471300000	60.0483400000	0.1060380000
H157	107.5224150000	56.5249260000	1.0242610000
H158	101.3974430000	57.1056240000	2.6966240000
H159	100.8244170000	63.5276780000	6.0653380000
H160	101.2128600000	60.3891070000	3.4920930000
H161	100.9182030000	63.4034170000	1.7900770000

H162	101.9395330000	63.1485280000	5.6074640000
H163	105.3078910000	63.4552050000	6.3162300000
H164	103.0036920000	59.5876550000	0.9334710000
H165	94.8291930000	59.8672870000	-1.0815080000
C166	95.2420430000	60.2379260000	-2.0081040000
H167	95.8060990000	59.4731290000	-2.5212650000
C168	96.1501350000	61.4613500000	-1.7653720000
C169	97.3436400000	61.1561100000	-0.8788730000
C170	98.2414610000	60.1272070000	-1.2071970000
C171	97.5765790000	61.8972800000	0.2883200000
C172	99.3346720000	59.8378720000	-0.3898130000
C173	98.6673520000	61.6057360000	1.1157280000
C174	99.5466780000	60.5728310000	0.7803020000
H175	94.4008580000	60.5125690000	-2.6590090000
H176	96.5061180000	61.8301860000	-2.7379560000
H177	95.5714460000	62.2816930000	-1.3249020000
H178	96.9193770000	62.7290170000	0.5327430000
H179	98.0916040000	59.5514320000	-2.1181930000
H180	98.8229680000	62.1708850000	2.0301300000
H181	100.3888230000	60.3372660000	1.4239300000
H182	100.0224940000	59.0420220000	-0.6633500000

E₄-H₂:

E=-7418.805768 solv=-0.126742 disp=-219.97 Z0=912.05

V	99.3419603927	62.2438675322	7.3458828526
Fe	105.6261958434	59.8508360717	2.1116324734
Fe	102.7668731355	61.9293141547	3.1009935752
Fe	104.9793475420	61.4030814789	4.5095804908
Fe	103.2443100027	59.2469558036	3.9407103313
Fe	100.2181516671	59.9938485534	5.6813385822
Fe	100.1559932228	62.0351618813	4.1278268490
Fe	102.5213265372	61.4948342741	5.6767344969
C	101.6811559693	60.5712037227	4.0894311939
S	105.5172592438	59.2003753504	4.6558577483
S	104.4616243728	62.9726768174	6.3720092376
S	105.0058427197	62.2026856107	2.3257569781
S	103.5112206030	58.4213316064	1.5968154725
S	101.1811024829	63.8267503874	2.7802757602
S	98.2383977018	61.3142696016	5.2936038469
S	101.4032189463	60.8175762126	7.6680587275
C	101.0573287061	57.5158271210	4.4719540394
O	102.3096954152	57.4317889123	4.6964822063
O	100.1831061207	57.8877845276	5.3148326825

O	100.6219161155	57.2110063366	3.2384797168
C	97.5984106359	66.1957450675	5.4457124279
C	98.6375049754	66.1804389720	6.6052766465
C	98.3252111341	65.1816155255	7.7564814777
C	97.1191568337	65.6683764978	8.5899815214
C	96.7493430118	64.7091228125	9.7557876676
C	95.2679299516	64.4454876816	9.8432466558
C	99.5719965813	64.9964063508	8.6479279654
O	96.9484008511	65.0833209995	5.2740643824
O	97.4963681812	67.2055083346	4.7464174630
O	94.7034418897	64.8453938376	10.9979020230
O	94.6045553375	63.9118974126	8.9614800354
O	100.1077443926	63.8041593958	8.6229769253
O	100.0111451246	65.9501825121	9.2959985235
O	98.0079967397	63.9062453750	7.1745797547
H	97.6154025888	64.1808448148	6.2567512393
H	99.5969781438	65.9021399943	6.1473159518
H	98.7567230607	67.1911704147	7.0008031963
H	97.3452304812	66.6607491821	8.9895447205
H	96.2748685166	65.7702544873	7.9000847560
H	97.2076553376	63.7309343228	9.5740398338
H	97.1210787594	65.0871919590	10.7099679519
C	106.9286360880	57.2473498887	0.4506855249
H	107.1283190807	57.0898319511	-0.6138883521
H	105.8677037851	57.0666728927	0.6368876867
S	107.3864001375	58.9887055477	0.8772804326
C	93.8113007402	61.0033810146	1.9075432331
C	93.5428302485	61.1007905289	3.4104820778
C	94.5184365152	62.1011609580	4.0405472472
C	94.2722298061	62.3512531630	5.5233083328
N	95.4430931044	63.0637580296	6.1171743272
C	93.0790262864	59.8959600207	1.1410742500
H	94.8890657302	60.8603356095	1.7575720151
H	93.5763380045	61.9742179468	1.4494225520
H	93.6732628400	60.1166831841	3.8844506503
H	92.4998782783	61.4022298755	3.5924098027
H	95.5407233627	61.7212357528	3.9174486539
H	94.4764081819	63.0571880070	3.5017432449
H	94.1590170971	61.4089531031	6.0706403260
H	93.3802290704	62.9573197447	5.7084022043
H	95.3223747302	63.2703140009	7.1226493834
H	96.3109717627	62.4899852419	5.9809280574
H	95.6829103452	63.9675010348	5.6423573432
H	91.9887634423	59.9610170834	1.2423579599

H	93.4048998960	58.9145809269	1.4526838786
C	100.0989994288	60.0520002989	10.8889973403
C	99.2145043759	61.3110502595	10.7215298722
C	97.9568018465	61.0496275517	9.9701087687
N	97.8839304998	61.2105507394	8.5993561722
C	96.7759365619	60.5146948588	10.4236103026
C	96.6991607359	60.7508888615	8.2265128710
N	95.9901394322	60.3307444985	9.3012259150
H	100.7720111624	59.8784112627	10.1700239397
H	99.4678413101	59.1630144605	11.0181665004
H	100.5712426781	60.2159539797	11.7550861797
H	98.9481213966	61.6699752453	11.7247281140
H	99.7768187194	62.1117455537	10.2342716932
H	96.4437117009	60.2369851729	11.4118457639
H	95.0746253015	59.9067706381	9.2710903066
H	96.3695486502	60.6567413626	7.2046335264
C	101.6500024717	56.1420048671	7.7050012277
N	102.7830381972	57.0058999736	7.3686960653
C	103.3019803952	57.9316914950	8.1586750642
N	102.8596614069	58.0582778786	9.4460214086
N	104.3498651821	58.6748126972	7.7595934112
H	101.7269804881	55.2573815113	7.0653877395
H	100.7886343488	56.5995589210	7.4843453045
H	101.6262277914	55.8261442367	8.6535097409
H	102.8436314932	57.1831697884	6.3495783693
H	103.2486784757	58.8464093024	9.9480065494
H	101.8530771345	58.0074120783	9.5513040414
H	104.6900512801	58.5955762229	6.7898359575
H	104.3558122494	59.6364491974	8.0815736530
C	104.8710008268	65.5940002333	-4.0429947813
C	104.4922311003	64.1312175938	-3.7330940206
C	103.7691196786	63.9710919740	-2.4272944123
N	102.4405815004	63.5953273921	-2.3843891584
C	104.2453011745	64.1572690705	-1.1475008904
C	102.1228505406	63.5681030739	-1.1043944785
N	103.1781336283	63.9103847189	-0.3135420179
H	105.4142234317	65.9758308992	-3.2952587725
H	103.9636427456	66.2024738087	-4.1450530408
H	105.3923871904	65.6470936342	-4.8946699680
H	105.4006131970	63.5118336418	-3.7416370612
H	103.8406475873	63.7366476333	-4.5205546992
H	105.2204176096	64.4032175209	-0.7553770636
H	103.2123423576	63.8682941300	0.6987518693
H	101.1465607415	63.3322796629	-0.7039243950

C	95.6299752577	57.4820327132	6.4910617008
C	97.0829669290	57.3963422416	6.9837063784
O	97.8278131955	56.5485149229	6.1166028779
C	97.1770940579	56.8481347306	8.4110130547
H	95.0373733223	58.1853537856	7.0942538283
H	98.2180758817	56.8520011120	8.7525550371
H	96.8149532238	55.8133179897	8.4391736158
H	96.5837479324	57.4429362507	9.1176787764
H	95.1491260747	56.4977132602	6.5484076616
H	98.5454357318	57.0765183612	5.7127107771
H	97.5147157417	58.4063312328	6.9621324773
C	98.4859998146	66.3580012676	-1.7130009238
C	98.8079234926	65.6210425660	-0.3965608585
C	98.1485869790	66.1792762962	0.8701410681
C	96.6880041241	65.7698853675	1.0719199900
O	96.0754599819	65.0230164619	0.3078608888
N	96.0972258907	66.3195756891	2.1780874688
H	98.7144619427	67.3289719409	-1.6420950074
H	97.4207289136	66.2594700235	-1.9526588819
H	99.0290070848	65.9401255304	-2.4413702410
H	98.5289989407	64.5658410254	-0.4972325124
H	99.8952268455	65.6449129124	-0.2478168568
H	98.7032140298	65.8355277865	1.7548474754
H	98.2096017094	67.2766951834	0.8963638823
H	96.6425899707	66.6746114482	2.9683712955
H	95.1948203997	65.9277607829	2.4142118378
C	103.6859934727	68.3259927689	12.1929980688
C	104.3596423233	68.5568709564	10.8248494119
C	103.7255680217	67.7561563549	9.6725764962
C	103.5491779679	66.2502865948	9.9373224458
C	103.1628928839	65.5264530174	8.6508835028
N	102.7746234820	64.0888885001	8.8793263503
H	104.1085748123	67.5601821431	12.6777190980
H	102.6249637217	68.0773648283	12.0468689903
H	103.6948490738	69.1366814775	12.7784183072
H	104.3130143366	69.6198221985	10.5568902352
H	105.4285947063	68.3120259378	10.8967522919
H	102.7353300588	68.1738831015	9.4460770153
H	104.3347084445	67.8962930861	8.7684894084
H	104.4804802036	65.8191088156	10.3358052113
H	102.7623431667	66.0965096028	10.6854176780
H	102.2989335186	66.0050991212	8.1877743201
H	103.9930985738	65.5182591168	7.9399313795
H	103.2192862038	63.7025468204	9.7150267629

H	101.7185431746	63.9590506898	8.9461702324
H	103.1004429411	63.5104421858	8.0718993973
H	93.7528595854	64.6299205460	10.9305088294
H	95.6198514253	57.7972834390	5.4686067755
H	93.3471299997	60.0483402012	0.1060380514
H	107.5224149812	56.5249253785	1.0242611400
H	101.4167397938	57.1158772706	2.6672288573
H	101.1227524502	60.0468656321	3.2854511630
H	102.9325455831	59.3887901720	0.8529523930
H	104.2816430860	63.9978197085	5.5099584164
H	100.5729528161	63.3856035443	1.6520200164
H	94.8291928814	59.8672868581	-1.0815080931
C	95.2420430298	60.2379260013	-2.0081039438
H	95.8060990000	59.4731290000	-2.5212650000
C	96.1460027879	61.4706609703	-1.7805617951
C	97.4026786559	61.1148953315	-1.0152713356
C	98.4613177250	60.4489973873	-1.6528111762
C	97.5134052500	61.3821206873	0.3551648682
C	99.5895984281	60.0419845476	-0.9402051108
C	98.6285644238	60.9529737550	1.0794143629
C	99.6688349927	60.2788697729	0.4351189374
H	94.3933261611	60.5070673744	-2.6525484673
H	96.4178418294	61.8893291641	-2.7586841677
H	95.5992941166	62.2581138289	-1.2489075927
H	96.7274369955	61.9439492806	0.8531108674
H	98.4036242423	60.2556006082	-2.7223819356
H	98.6726643124	61.1313413266	2.1515042663
H	100.5335726401	59.9377514228	0.9964252360
H	100.4039554855	59.5377408624	-1.4532408938

E₄-H₂+N₂:

E=-7528.325102 solv=-0.125513 disp=-228.50 Z0=917.57

V	99.3444026141	62.4239355603	7.2481404312
Fe	105.5311852272	59.6764729239	2.0859204592
Fe	102.8647174939	61.7783159566	3.0925525940
Fe	105.0500102295	61.1738354139	4.5683644104
Fe	103.1557125596	59.1539238149	3.9630005341
Fe	100.1949254882	60.0298051855	5.8239499759
Fe	100.4332756875	62.4185517389	4.4112468642
Fe	102.6569588216	61.4026706909	5.7521709598
C	101.6885270847	60.5876227023	4.2208642389
S	105.4414793246	58.9272125061	4.6403566192
S	104.6714838449	62.6468019955	6.5734213444

S	105.0993007560	62.0578422598	2.4129876049
S	103.3515359383	58.3453748178	1.6082681644
S	101.1415260787	63.4249059107	2.3115658723
S	98.3479793893	61.4104342378	5.2089472361
S	101.3231409418	60.8603075200	7.7001000145
C	100.9016748232	57.5295531553	4.4833322124
O	102.1470968061	57.4042154232	4.7127634953
O	100.0424837262	57.9479702996	5.3181113921
O	100.4551507082	57.2213135704	3.2550490947
C	97.4565828293	66.3495576206	5.4381517596
C	98.4808691275	66.3854159056	6.6059723859
C	98.2625268142	65.3222771907	7.7212832678
C	97.0694145908	65.7372687580	8.6093938151
C	96.7442252117	64.7229335989	9.7377038127
C	95.2679299571	64.4454876642	9.8432466085
C	99.5390519878	65.1476456696	8.5736745377
O	96.9180485354	65.1864403332	5.2050283358
O	97.2671254759	67.3670585439	4.7725496568
O	94.7326823060	64.7164253335	11.0467903381
O	94.5844968032	63.9987124249	8.9289882067
O	100.0689260224	63.9527086566	8.5539504301
O	99.9906575075	66.1036649972	9.2062647573
O	97.9723570723	64.0549283134	7.1062924228
H	97.5943307814	64.3398906333	6.1761068272
H	99.4666475994	66.2308044951	6.1532071917
H	98.4932118108	67.3869188552	7.0412460727
H	97.2880667332	66.7149487427	9.0479058097
H	96.2031230045	65.8549824030	7.9493844794
H	97.2027703258	63.7580103868	9.4933694392
H	97.1391915567	65.0544846287	10.6998987034
C	106.8849835817	57.1600745179	0.3994080483
H	107.1058218752	56.9467025370	-0.6512859523
H	105.8360928784	56.9199207438	0.5922123802
S	107.2283519082	58.9476726669	0.7187917744
C	93.8203414014	61.0088926624	1.8977834228
C	93.5539716612	61.1430302225	3.3998774661
C	94.5312427808	62.1587587981	4.0113618095
C	94.2402895014	62.4762351159	5.4738869473
N	95.3861095459	63.2163896529	6.0900060754
C	93.0790262759	59.8959600311	1.1410742722
H	94.8967043664	60.8546126144	1.7495932939
H	93.5929879269	61.9730049317	1.4219499720
H	93.6797871901	60.1704991415	3.8982675604
H	92.5120246821	61.4530711110	3.5731706824

H	95.5519913028	61.7625700960	3.9324929550
H	94.5154153078	63.0906547665	3.4308846659
H	94.1031768372	61.5610330744	6.0602225669
H	93.3444418757	63.0920366099	5.5978453244
H	95.2196485326	63.4487253763	7.0856131080
H	96.2546311015	62.6499993421	6.0159729410
H	95.6526411616	64.1106518671	5.6006997809
H	91.9892883205	59.9641364406	1.2454227932
H	93.4048998940	58.9145809260	1.4526838781
C	100.0989994092	60.0520002798	10.8889973433
C	99.2157874025	61.3072069251	10.6808374196
C	97.9918934216	61.0389996687	9.8729802145
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C	96.8318168313	60.4129105836	10.2624972676
C	96.7763858136	60.8065370683	8.0883991320
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H	100.7720111624	59.8784112777	10.1700239361
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C	103.3324926511	57.9006367645	8.1862163897
N	102.9007264791	58.0072090655	9.4792837119
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H	101.7330546193	55.2595851257	7.0633716163
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N	102.4198549568	63.6054847412	-2.4750817490
C	104.2454998341	64.0052974173	-1.2055682642
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H	101.1137993091	63.3159616103	-0.7976748874
C	95.6299752713	57.4820327184	6.4910617019
C	97.0650476620	57.3346675451	7.0183074282
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H	96.4896015647	57.3258348943	9.1354267014
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H	98.4816038799	57.0356324182	5.7013343197
H	97.5308419641	58.3302346516	7.0474641485
C	98.4859998204	66.3580012255	-1.7130009438
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C	98.1378245527	66.1948842750	0.8692464238
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N	96.0394191880	66.4823957653	2.0875541928
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H	97.4216623054	66.2645576014	-1.9594431287
H	99.0290070816	65.9401255562	-2.4413702582
H	98.4983916331	64.5709344368	-0.4892847559
H	99.8794950644	65.6268966376	-0.2359008338
H	98.6513358071	65.7938760556	1.7549281606
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H	96.5581345450	66.8335420447	2.8958878422
H	95.1084815496	66.1412659131	2.2890944304
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C	104.3748127764	68.5684123959	10.8330310894
C	103.7520293948	67.7939677176	9.6571187397
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H	102.7725727333	68.2279090362	9.4156522835
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H	104.4571730922	65.8397883558	10.3259151438
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H	100.9811638330	60.1669980841	3.4820963884
H	102.7784670888	59.3252521439	0.8760995363
H	104.5972300871	63.7161433554	5.7487910478
H	100.5811962989	62.5466725569	1.4445993832
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C	98.3407597715	60.0916554073	-1.4364722872
C	97.4733427025	61.3013620109	0.4545541691
C	99.3487136939	59.5545554130	-0.6377663574
C	98.4703613777	60.7533916394	1.2658830434
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H	95.6882572529	62.2452223678	-1.2399368618
H	96.7668690968	62.0155397488	0.8714833933
H	98.2989140130	59.8337125468	-2.4930735465
H	98.5100738747	61.0138867797	2.3198411518
H	100.1672950001	59.4215062324	1.3520152056
H	100.0879720492	58.8860766476	-1.0720306597
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TS_{N2H}

1. E=7528.292320 solv=-0.125251 disp=-227.74 Z0=915.41

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Fe	100.1679460000	60.0369630000	5.7652030000
Fe	100.4502900000	62.3330930000	4.2731460000
Fe	102.6407370000	61.3439400000	5.7531920000
C	101.6833840000	60.5703630000	4.1574400000
S	105.3921500000	58.7137840000	4.6722270000
S	104.6720340000	62.5026360000	6.6325420000
S	105.2336870000	61.9269350000	2.5723130000
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S	98.3855380000	61.5383300000	5.1777930000
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C	100.7862840000	57.5134350000	4.4406620000
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C	98.6627950000	66.5053540000	6.9234610000
C	98.3503090000	65.4109280000	7.9892020000
C	97.1559790000	65.8537020000	8.8626730000
C	96.7288940000	64.8073130000	9.9283550000
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H	95.4948430000	63.5060760000	6.9416970000
H	96.4550350000	62.7659670000	5.7628760000
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C	96.8440340000	60.4550580000	10.1878610000
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H	99.8231720000	62.1082490000	10.2084360000
H	96.4912720000	60.0712880000	11.1330630000
H	95.2033390000	59.9079800000	8.9248530000
H	96.5300090000	60.9003450000	6.9897540000
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C	104.4936590000	64.1338870000	-3.7134990000
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C	102.7935190000	64.3864470000	-0.5694190000
N	103.7834180000	63.5427480000	-0.1716260000
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H	103.9624850000	66.1984650000	-4.1349740000
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C	95.6299760000	57.4820330000	6.4910620000
C	97.0498010000	57.3524590000	7.0629720000
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H	103.2259820000	63.7320600000	9.6879140000
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H	103.0787700000	63.5031950000	8.0657320000
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H	102.8442700000	59.3482420000	0.8855730000
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Fe	105.1772240165	61.4284204514	4.6340541673
Fe	103.1736033920	59.4460915524	4.0017104019
Fe	100.2289652199	60.0921699625	5.8611411165
Fe	100.3048607691	62.5467472868	4.2757527598
Fe	102.4845635041	61.7115367236	5.7412954302
C	101.6812123861	60.7750130574	4.1695509395
S	105.4687493133	59.2075644537	4.6643588727
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C	96.3044530000	61.3086090000	-1.6329710000
C	97.4129410000	60.5977230000	-0.8797490000
C	98.3260810000	59.7873130000	-1.5762640000
C	97.4731950000	60.6007950000	0.5207260000
C	99.2403200000	58.9787830000	-0.8992830000
C	98.3693160000	59.7725850000	1.2072990000
C	99.2520810000	58.9530380000	0.4985710000
H	94.4411220000	60.6309900000	-2.6435160000
H	96.7095710000	61.7732260000	-2.5409110000
H	95.8711690000	62.1131780000	-1.0285220000
H	96.8121300000	61.2541800000	1.0827200000
H	98.3177810000	59.7931480000	-2.6648440000
H	98.3738560000	59.7883030000	2.2928640000
H	99.9639670000	58.3221630000	1.0226950000
H	99.9476480000	58.3724200000	-1.4586490000
N	100.5570080000	63.1687570000	5.7608800000
N	101.4331560000	64.0585020000	5.8507200000
O	100.5236960000	62.1095120000	-0.2107060000
H	101.7064370000	61.2904710000	-0.3699360000
H	99.7047920000	61.5993250000	-0.0846140000
O	102.6630550000	60.8310070000	-0.5295330000
H	102.8819020000	59.9935530000	0.1674710000
H	103.3335480000	61.5321250000	-0.3730650000

E'_{N2H}

$E=-7528.306758$ solv=-0.125370 disp=234.64 Z0=918.78

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Fe	105.4745063142	60.0058602941	2.1156299928
Fe	102.6803135931	61.4736939212	2.7701519415
Fe	105.2179105166	61.1689452225	4.7530109016
Fe	103.0425993544	58.9536144643	3.7710034593
Fe	100.1913289681	59.8400073249	5.8905838135
Fe	100.3222490055	62.1053912924	4.3882298811
Fe	102.6498475678	61.0984148540	5.6337428791
C	101.5501331351	60.3773434469	4.2029944953

S	105.3193537001	58.9371609574	4.6297142801
S	104.7333193488	62.3540524762	6.7802532187
S	105.0407827976	62.3373683191	2.8263136274
S	103.1856253411	59.4784598273	1.4811928418
S	101.1124572371	63.3630115118	2.4343674445
S	98.2968351805	61.1854347063	5.3003235262
S	101.4051846351	60.6753682018	7.6746346500
C	100.8467998831	57.1759366083	4.5799794030
O	102.1191794439	57.2217402803	4.6091087388
O	100.0574673987	57.7691772934	5.3667100203
O	100.2731092166	56.3955404686	3.6407636232
C	97.6597542720	66.1940523116	5.4676678465
C	98.6539376361	66.2138104738	6.6626014858
C	98.3345365944	65.2082864592	7.8082165701
C	97.1186856999	65.6956835710	8.6256284824
C	96.7406463741	64.7532377366	9.8003824264
C	95.2679302591	64.4454877275	9.8432464474
C	99.5586107802	65.0228114831	8.7343604386
O	97.0875096792	65.0449053704	5.2459125736
O	97.5160278792	67.2057639078	4.7780722504
O	94.6701606059	64.7630964885	11.0079568995
O	94.6349333097	63.9395561900	8.9235001050
O	100.0544697524	63.8161433482	8.7781263540
O	99.9957294564	65.9867531327	9.3699762560
O	98.0205804164	63.9275116473	7.2295897260
H	97.6699515390	64.2036486750	6.2897115335
H	99.6404796682	65.9681041886	6.2519868491
H	98.7175274504	67.2283844070	7.0612168125
H	97.3406636829	66.6931340895	9.0146662869
H	96.2781689122	65.7894257567	7.9294976009
H	97.2367941073	63.7857527637	9.6601242034
H	97.0673129047	65.1612063219	10.7586823720
C	106.7058250850	57.1873633482	1.3300716616
H	105.8230716822	56.9608434104	0.7244037662
H	106.4738203381	57.0035232734	2.3826376646
S	107.2323079774	58.9466718576	1.0847659557
C	93.8214366816	61.0006872844	1.9037368006
C	93.5807142640	61.0991310576	3.4122421519
C	94.5853309353	62.0829499087	4.0264295535
C	94.3564200971	62.3546341245	5.5085014183
N	95.5367024743	63.0650203710	6.0876055569
C	93.0790263092	59.8959599939	1.1410742737
H	94.8955174975	60.8539014393	1.7371776904
H	93.5835649875	61.9730497227	1.4504782020

H	93.7028362654	60.1123677393	3.8828173461
H	92.5467131825	61.4181777971	3.6141498776
H	95.5979123962	61.6793332859	3.8981671784
H	94.5600448957	63.0343447632	3.4784336269
H	94.2366862281	61.4214753542	6.0697241951
H	93.4729455398	62.9734028430	5.6920087969
H	95.4160785206	63.2957347626	7.0881027870
H	96.3956896732	62.4806638619	5.9743215961
H	95.7900296991	63.9580146511	5.5967831162
H	91.9892861606	59.9641275550	1.2457224917
H	93.4048998805	58.9145809172	1.4526838642
C	100.0989993937	60.0520005043	10.8889969228
C	99.2299798820	61.3250555786	10.7398003419
C	97.9850250017	61.0984683112	9.9609963299
N	97.9571011232	61.2167223052	8.5856559469
C	96.7770315379	60.6169653817	10.4051161908
C	96.7700816977	60.7790965113	8.2012802017
N	96.0155543007	60.4165110905	9.2686882566
H	100.7720112776	59.8784110622	10.1700240961
H	99.4601244231	59.1681102027	11.0158442008
H	100.5712425857	60.2159540459	11.7550862176
H	98.9478313171	61.6529365861	11.7494990221
H	99.8061381106	62.1365839360	10.2889304532
H	96.4126985111	60.3832451785	11.3936885239
H	95.0846660316	60.0286923982	9.2280061489
H	96.4631005625	60.6582846652	7.1747171201
C	101.6500023662	56.1420046415	7.7050009646
N	102.7829140244	57.0137261724	7.3815775159
C	103.3461842868	57.8841714885	8.2069972031
N	102.8965557052	57.9842516281	9.4940805706
N	104.4362120085	58.5752005076	7.8373930333
H	101.7346880728	55.2579155922	7.0651029314
H	100.7886343400	56.5995589497	7.4843453987
H	101.6262278707	55.8261444120	8.6535098012
H	102.8901130588	57.1854064364	6.3746340188
H	103.3432371643	58.7083497823	10.0426117887
H	101.8867256606	58.0183234899	9.5819045368
H	104.7545089480	58.5292885231	6.8552591632
H	104.5530912312	59.4970134198	8.2422466415
C	104.8710003563	65.5940000768	-4.0429939310
C	104.5904390262	64.1007511720	-3.7644383544
C	104.0356484381	63.8610180939	-2.3997093933
N	102.7453433411	64.2315926355	-2.0740303771
C	104.6777614404	63.3530398364	-1.2950577192

C	102.6167368766	63.9463661195	-0.7942252826
N	103.7589612720	63.4179961280	-0.2722165733
H	105.4142236009	65.9758309969	-3.2952589453
H	103.9358771175	66.1566868796	-4.1285100717
H	105.3923872632	65.6470933406	-4.8946699416
H	105.5270093226	63.5370275410	-3.8730618132
H	103.8989229942	63.7106083015	-4.5229575999
H	105.6705769946	62.9556288876	-1.1452086662
H	103.9117004034	63.1124309811	0.6823222744
H	101.7278333732	64.0935475537	-0.2002564580
C	95.6299754317	57.4820327609	6.4910616685
C	97.0670888310	57.3342252994	7.0046141676
O	97.7551719877	56.3755738986	6.2079997411
C	97.1133828822	56.8787374458	8.4648995556
H	95.0638305697	58.2112683588	7.0892397628
H	98.1510045334	56.8213127910	8.8121514351
H	96.6680123470	55.8811366275	8.5618454019
H	96.5700030063	57.5683517710	9.1227276455
H	95.1083214299	56.5189502850	6.5543289854
H	98.4542775657	56.8451877007	5.7143646184
H	97.5675645615	58.3092626455	6.9222395194
C	98.4859997138	66.3580011999	-1.7130009289
C	98.8192614068	65.6308648310	-0.3941325512
C	98.1549813446	66.1870876388	0.8719823595
C	96.6970155257	65.7702472018	1.0810509892
O	96.0780622270	65.0336566484	0.3126881641
N	96.1153957856	66.3064176252	2.1992566627
H	98.7144619950	67.3289719260	-1.6420949715
H	97.4197982233	66.2559178659	-1.9472682953
H	99.0290071076	65.9401255986	-2.4413702628
H	98.5616843012	64.5701146707	-0.4884683114
H	99.9062146214	65.6798489037	-0.2487509118
H	98.7129970943	65.8496956864	1.7570559651
H	98.2075231306	67.2851387401	0.8953133708
H	96.6668379971	66.6556371382	2.9879507182
H	95.2149373827	65.9120323119	2.4383465995
C	103.6859932634	68.3259926243	12.1929979453
C	104.3516434663	68.5438451267	10.8183057698
C	103.7077389856	67.7462414185	9.6658589623
C	103.4897900913	66.2430916926	9.9276614831
C	103.1734875615	65.5164877382	8.6215138435
N	102.7171663244	64.1001869847	8.8410763864
H	104.1085748799	67.5601821905	12.6777191146
H	102.6241505961	68.0763060563	12.0533477481

H	103.6948491636	69.1366814795	12.7784183029
H	104.3141791921	69.6061947119	10.5460618305
H	105.4189374461	68.2900447154	10.8861335959
H	102.7305495303	68.1852488160	9.4246424099
H	104.3303155436	67.8711517353	8.7683825275
H	104.3857705399	65.7990815526	10.3888295912
H	102.6527839169	66.1077652428	10.6222912134
H	102.3663882754	65.9997935994	8.0729056732
H	104.0559925688	65.4727820566	7.9767738364
H	103.2073965043	63.6603418285	9.6234036129
H	101.6605225251	64.0265674324	8.9845364329
H	102.9149236872	63.5195155534	8.0093846888
H	93.7296728267	64.5172416400	10.9103604083
H	95.6198513773	57.7972834039	5.4686067653
H	93.3471301324	60.0483404375	0.1060381924
H	107.5224147836	56.5249257589	1.0242611368
H	100.9962070651	56.0439576141	3.0895825170
H	100.8572495113	59.8877005037	3.4932590368
H	100.3192328490	62.7082515597	1.5569609879
H	104.7980349975	63.5069501214	6.0746084647
H	101.9887134358	64.4943438409	5.1399239929
H	94.8291928409	59.8672864785	-1.0815082568
C	95.2420430022	60.2379261311	-2.0081039642
H	95.8060990000	59.4731290000	-2.5212650000
C	96.1878473518	61.4291942443	-1.7406846085
C	97.3948703936	60.9770728006	-0.9501397887
C	98.4031649604	60.2202726838	-1.5670453658
C	97.5036813374	61.2404388875	0.4210160457
C	99.4814217474	59.7287241098	-0.8339300646
C	98.5674513806	60.7262045199	1.1680141603
C	99.5597981782	59.9674337087	0.5408673050
H	94.4063331776	60.5384262846	-2.6536641146
H	96.5096690156	61.8522615420	-2.7017834755
H	95.6702935672	62.2328629710	-1.2042417611
H	96.7607291422	61.8722973456	0.9005645299
H	98.3478463939	60.0271622638	-2.6372180283
H	98.6138980510	60.9210231198	2.2372080690
H	100.4085842099	59.5821435477	1.0962531638
H	100.2680033775	59.1646173581	-1.3277749867
N	100.7419206851	63.3135925381	5.9159626573
N	101.4985035521	64.3060251166	6.0454493937

TS_{N2H2}

E=-7528.281644 solv=-0.135461 disp=-230.20 Z0=918.22

V	99.4909310000	62.3243550000	7.1456530000
Fe	105.3990860000	59.8281670000	2.4438320000
Fe	102.6219620000	61.2518510000	2.6343440000
Fe	104.9135740000	61.4426650000	4.8435320000
Fe	102.7751790000	58.6810750000	3.6653220000
Fe	99.9030710000	59.7393120000	5.6379680000
Fe	100.3822610000	62.0661140000	4.2720780000
Fe	102.5011360000	60.6140630000	5.6741710000
C	101.4016460000	60.2966020000	4.0719700000
S	104.7524140000	59.1354500000	5.0414050000
S	104.0835940000	62.4564200000	6.7942340000
S	104.9604480000	62.1949370000	2.7331010000
S	103.2478160000	59.2043080000	1.4699510000
S	100.9316130000	62.9678990000	2.0852510000
S	98.2288660000	61.3791380000	5.1191300000
S	101.0594290000	60.2431600000	7.5539050000
C	100.5233050000	56.9274020000	4.4889170000
O	101.7882190000	57.0307540000	4.4724620000
O	99.6786940000	57.7376690000	4.9550850000
O	99.9961910000	55.7914370000	3.9669760000
C	97.7911870000	66.4119690000	5.6459610000
C	98.7697680000	66.3184670000	6.8544160000
C	98.4306300000	65.2030760000	7.8885350000
C	97.2087560000	65.6462440000	8.7279220000
C	96.7654070000	64.6153930000	9.7987610000
C	95.2679300000	64.4454880000	9.8432460000
C	99.6385680000	64.9139990000	8.8040560000
O	97.2403560000	65.2832550000	5.2962970000
O	97.6430780000	67.4860390000	5.0652480000
O	94.7080340000	64.7126750000	11.0388110000
O	94.5942590000	64.0825990000	8.8878080000
O	100.1432410000	63.7143820000	8.7222010000
O	100.0716720000	65.8046620000	9.5424400000
O	98.1182620000	63.9914880000	7.1838830000
H	97.7724510000	64.3556480000	6.2685970000
H	99.7641730000	66.1271830000	6.4315830000
H	98.8201500000	67.2894570000	7.3512980000
H	97.4512340000	66.5955530000	9.2133930000
H	96.3888750000	65.8333220000	8.0256550000
H	97.1613610000	63.6303460000	9.5267330000
H	97.1506840000	64.8768360000	10.7863660000
C	106.8117920000	57.0539850000	1.6657590000
H	105.8147190000	56.9794180000	1.2221260000

H	106.8027790000	56.5759560000	2.6503420000
S	107.3500120000	58.8176120000	1.8000610000
C	93.8219230000	61.0296390000	1.8672210000
C	93.5933130000	61.2087340000	3.3701600000
C	94.5703220000	62.2654790000	3.9085710000
C	94.3637120000	62.5989570000	5.3827140000
N	95.5721240000	63.2839730000	5.9382200000
C	93.0790260000	59.8959600000	1.1410740000
H	94.8985770000	60.8884410000	1.7010240000
H	93.5734430000	61.9779060000	1.3707330000
H	93.7572290000	60.2579610000	3.8985500000
H	92.5506760000	61.5029670000	3.5639070000
H	95.5941240000	61.8934810000	3.7756030000
H	94.4935660000	63.1851150000	3.3136280000
H	94.2234610000	61.6894850000	5.9768010000
H	93.5004510000	63.2486690000	5.5539000000
H	95.4726120000	63.4914550000	6.9441280000
H	96.4172960000	62.6766860000	5.7973910000
H	95.8379730000	64.1814590000	5.4691590000
H	91.9899560000	59.9657090000	1.2472760000
H	93.4049000000	58.9145810000	1.4526840000
C	100.0989990000	60.0520010000	10.8889970000
C	99.2117240000	61.2968020000	10.6542370000
C	97.9776210000	61.0282910000	9.8585870000
N	97.9258380000	61.2413520000	8.4930570000
C	96.7806900000	60.4974880000	10.2799260000
C	96.7378570000	60.8233680000	8.0939390000
N	96.0034940000	60.3742190000	9.1438280000
H	100.7720110000	59.8784110000	10.1700240000
H	99.4760280000	59.1564610000	11.0177790000
H	100.5712430000	60.2159540000	11.7550860000
H	98.9158760000	61.6980840000	11.6328740000
H	99.7885330000	62.0709440000	10.1432940000
H	96.4268440000	60.1983280000	11.2550200000
H	95.0793140000	59.9726420000	9.0882430000
H	96.4151170000	60.7784190000	7.0655030000
C	101.6500030000	56.1420050000	7.7050010000
N	102.7834780000	57.0457330000	7.4864200000
C	103.2520320000	57.8777970000	8.4073010000
N	102.6862370000	57.8800990000	9.6512290000
N	104.3512330000	58.6171600000	8.1837270000
H	101.7756340000	55.2798710000	7.0456250000
H	100.7886340000	56.5995590000	7.4843450000
H	101.6262280000	55.8261440000	8.6535100000

H	103.0101650000	57.2583500000	6.5150370000
H	103.0923310000	58.5447260000	10.2975350000
H	101.6727280000	57.9264900000	9.6460870000
H	104.6939100000	58.6600990000	7.2078090000
H	104.3548380000	59.5363420000	8.6137100000
C	104.8710000000	65.5940000000	-4.0429940000
C	104.5065920000	64.1303100000	-3.7274610000
C	103.9720350000	63.9918970000	-2.3372880000
N	102.8283270000	64.6579350000	-1.9366960000
C	104.5342180000	63.3317690000	-1.2695980000
C	102.7082100000	64.3960190000	-0.6492040000
N	103.7148740000	63.6001060000	-0.1967840000
H	105.4142240000	65.9758310000	-3.2952590000
H	103.9584170000	66.1930780000	-4.1342430000
H	105.3923870000	65.6470930000	-4.8946700000
H	105.3963320000	63.4953620000	-3.8341220000
H	103.7732780000	63.7685830000	-4.4620090000
H	105.4173870000	62.7178520000	-1.1723900000
H	103.8472540000	63.2583650000	0.7491930000
H	101.9173880000	64.7372460000	0.0016170000
C	95.6299760000	57.4820330000	6.4910620000
C	97.0301460000	57.2813030000	7.0851030000
O	97.7579730000	56.2974670000	6.3653810000
C	96.9488960000	56.8077770000	8.5380960000
H	95.0659670000	58.2280600000	7.0714240000
H	97.9552650000	56.7010560000	8.9567320000
H	96.4549630000	55.8295070000	8.5853530000
H	96.3885850000	57.5121490000	9.1636800000
H	95.0734370000	56.5374230000	6.5474920000
H	98.2628900000	56.7574030000	5.6662470000
H	97.5697690000	58.2408530000	7.0582690000
C	98.4860000000	66.3580010000	-1.7130010000
C	98.7727640000	65.6287410000	-0.3848770000
C	98.2769440000	66.3236430000	0.8906630000
C	96.7633880000	66.3003330000	1.1030330000
O	95.9719480000	65.8143820000	0.2966940000
N	96.3355880000	66.8997590000	2.2584710000
H	98.7144620000	67.3289720000	-1.6420950000
H	97.4210440000	66.2796250000	-1.9588950000
H	99.0290070000	65.9401260000	-2.4413700000
H	98.3555450000	64.6161810000	-0.4263490000
H	99.8574800000	65.5067410000	-0.2840770000
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H	107.5224150000	56.5249260000	1.0242610000
H	100.7443240000	55.2855530000	3.6054270000
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