

Supporting Information

Origin of metabolic sites selectivity of 7, 12-dimethylbenz[a]anthracene catalysed by cytochrome P450 1B1: An in silico protocol

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Table S1. Classification and binding energy of the 50 docking results

Rank_SubRank	docked energy	Rank_SubRank	docked energy
1_1	-11.44	2_3	-11.32
1_2	-11.44	2_4	-11.32
1_3	-11.44	2_5	-11.32
1_4	-11.44	2_6	-11.31
1_5	-11.44	2_7	-11.31
1_6	-11.44	2_8	-11.31
1_7	-11.44	2_9	-11.31
1_8	-11.44	3_1	-8.52
1_9	-11.44	3_2	-8.52
1_10	-11.43	4_1	-7.98
1_11	-11.43	4_2	-7.97
1_12	-11.40	4_3	-7.97
1_13	-11.40	4_4	-7.97
1_14	-11.40	4_5	-7.97
1_15	-11.40	4_6	-7.97
1_16	-11.40	4_7	-7.97
1_17	-11.40	4_8	-7.97
1_18	-11.39	4_9	-7.97
1_19	-11.39	4_10	-7.97
1_20	-11.39	4_11	-7.97
1_21	-11.38	4_12	-7.97
1_22	-11.36	4_13	-7.96
1_23	-11.36	4_14	-7.96
2_1	-11.32	4_15	-7.96
2_2	-11.32	5_1	-7.80

Table S2. Binding free energy of mode I and mode II (ΔG_{bind}) (Unit: kcal·mol⁻¹)

	ΔE_{ele}	ΔE_{vdW}	ΔG_{GB}	ΔG_{SA}	$^a\Delta G_{polar}$	$^b\Delta G_{nonpolar}$	$^c\Delta G_{MM-GBSA}$	TAS	$^d\Delta G_{bind}$
Mode I	-3.96	-45.18	15.43	-4.85	11.47	-50.03	-38.56	-18.53	-20.03
Mode II	-3.60	-45.93	15.23	-4.86	11.63	-50.79	-39.16	-17.20	-21.96

$^a\Delta G_{polar} = \Delta E_{ele} + \Delta G_{GB}$
 $^b\Delta G_{nonpolar} = \Delta E_{vdW} + \Delta G_{SA}$
 $^c\Delta G_{MM-GBSA} = \Delta E_{ele} + \Delta E_{vdW} + \Delta G_{GB} + \Delta G_{SA}$
 $^d\Delta G_{bind} = \Delta G_{MM-GBSA} - TAS$

Table S3. Decomposition of binding free energy (kcal·mol⁻¹) on per residue basis for mode I and mode II

Residues	Mode I					Mode II				
	^a vdW	^b Ele	^c Polar	^d Nonpolar	Total I	^a vdW	^b Ele	^c Polar	^d Nonpolar	Total
Gly329	-1.96	-0.52	0.15	-0.15	-2.48	-1.83	-1.00	0.22	-0.15	-2.76
Phe231	-3.34	0.54	1.02	-0.29	-2.06	-3.37	0.61	0.91	-0.27	-2.11
Ala330	-1.94	-0.11	0.24	-0.20	-2.00	-1.78	-0.05	0.13	-0.18	-1.88
Gln332	-0.60	-0.56	-0.17	-0.03	-1.36	-0.69	-0.76	-0.01	-0.05	-1.51
Val126	-0.67	-0.02	-0.30	-0.05	-1.04	-0.93	-0.14	-0.39	-0.05	-1.51
Phe268	-1.59	0.33	0.36	-0.10	-1.00	-1.82	0.40	0.48	-0.14	-1.08

^avdW is the van der Waals energy
^bEle is the electrostatic interaction energy
^cPolar is the polar solvation energy
^dNonpolar is the nonpolar solvation energy

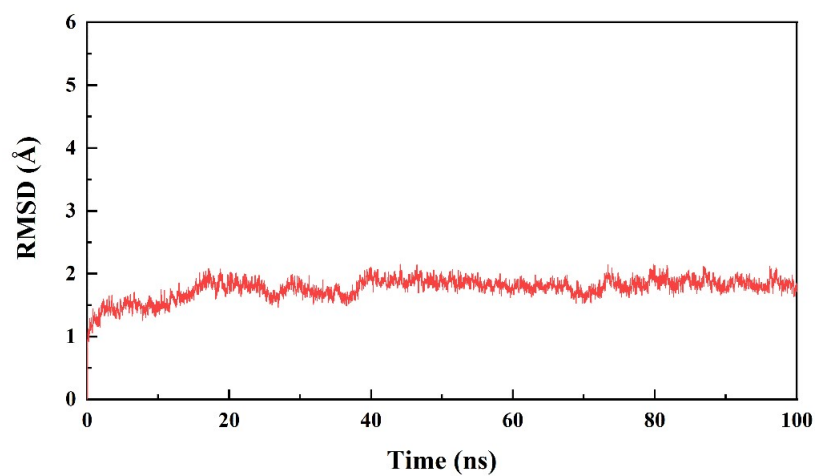


Figure S1. RMSD of completed CYP1B1 structure optimization.

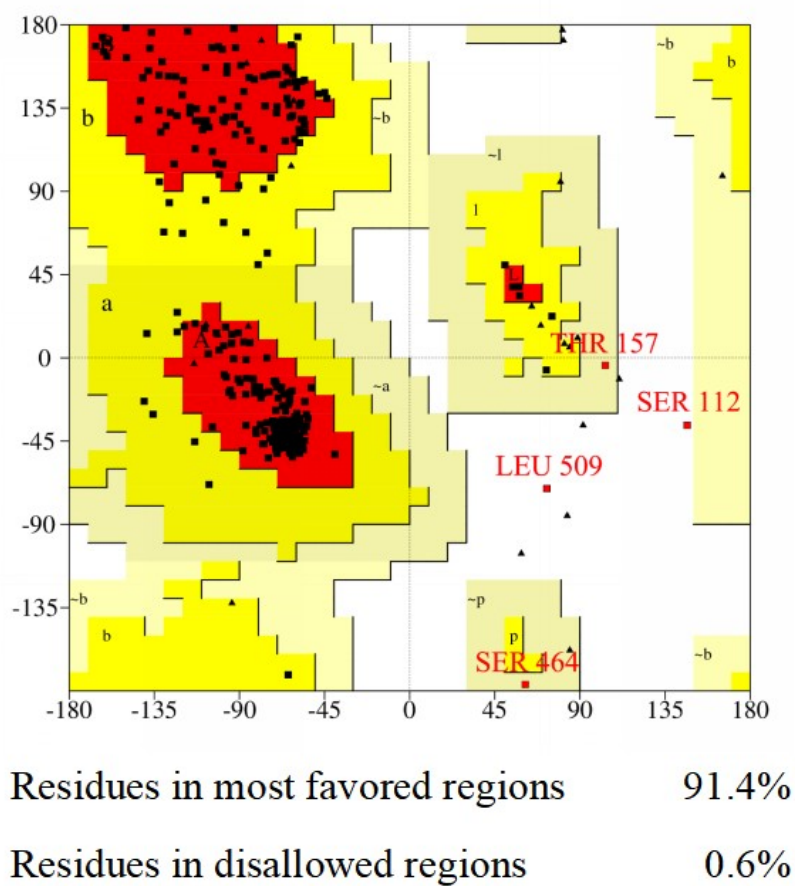


Figure S2. The Ramachandran plot and its detailed information calculated by SAVES.

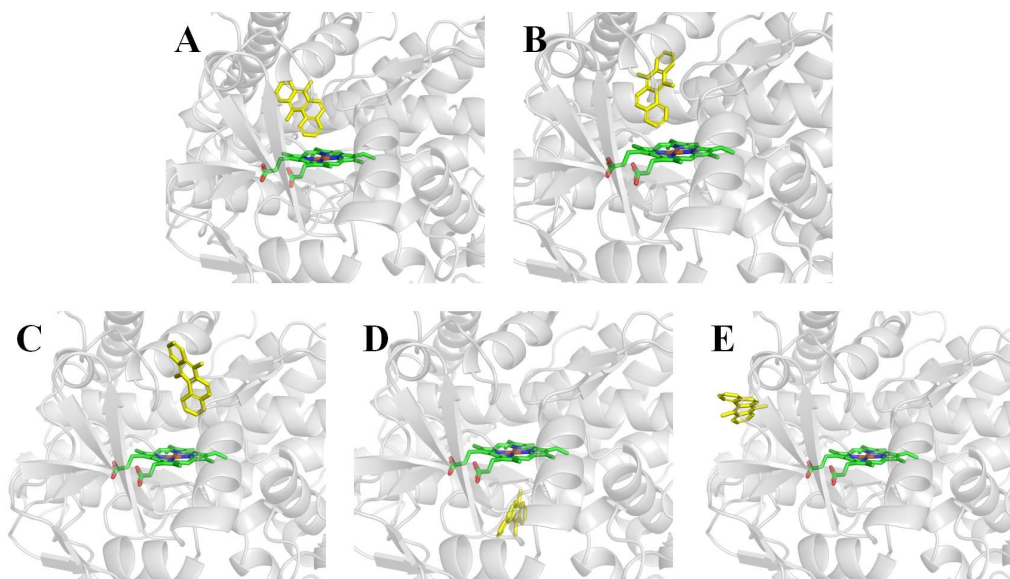


Figure S3. Representative conformations of the five DMBA-CYP1B1 docking poses

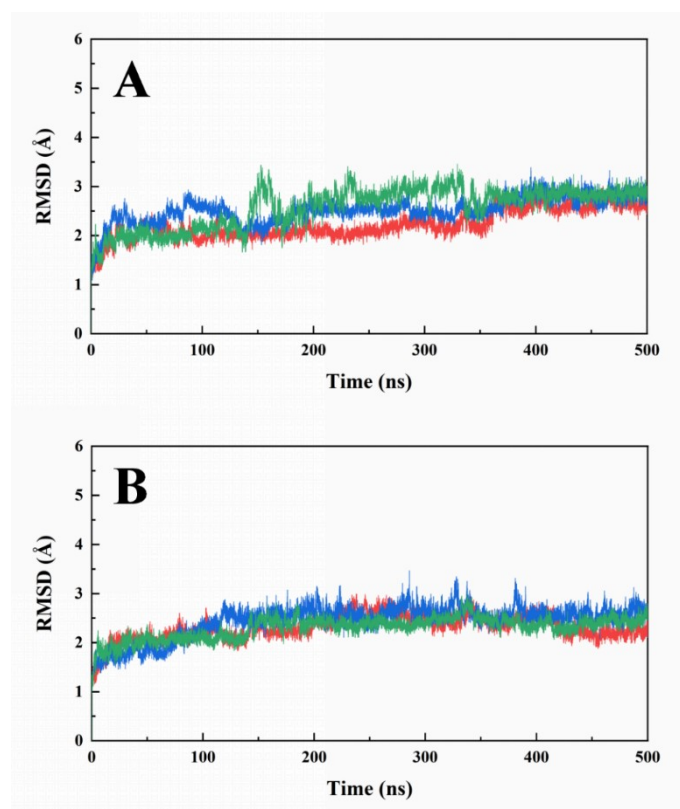


Figure S4. RMSDs of binding mode I (A) and mode II (B).

Cartesian coordinates of all structures in the QM calculation.

The first model for analyzing ESP and ALIE.

C	1.89174600	2.97621700	-0.20817600
C	1.37454800	1.56073200	-0.09055000
C	0.00874500	1.27614100	0.04154900
C	-0.95610700	2.33286700	0.24797600
C	-2.28000900	2.08891700	0.38450800
C	-2.81331200	0.77115200	0.18062500
C	-4.20545700	0.56580100	0.12287200
C	-4.73175700	-0.66608400	-0.22367900
C	-3.85961200	-1.71005000	-0.55881100
C	-2.48612900	-1.53070800	-0.47996700
C	-1.91805100	-0.31136500	-0.05029400
C	-0.46848400	-0.09345800	0.06851200
C	0.45848300	-1.13440600	0.22866500
C	0.06020900	-2.53137400	0.65684600
C	1.84906900	-0.85526000	0.09436000
C	2.82219800	-1.89784000	0.12653300
C	4.16214100	-1.64152200	-0.03060900
C	4.61215000	-0.31419900	-0.21818600
C	3.70753200	0.71767000	-0.25388400
C	2.30705300	0.49117200	-0.10605100
H	2.59007600	3.06169500	-1.04590400
H	1.10111300	3.70060900	-0.39217600
H	2.43115300	3.28875800	0.69396900
H	-0.60133900	3.34953800	0.35264100
H	-2.97216900	2.90163100	0.58559600
H	-4.86235300	1.40688800	0.32693900
H	-5.80646000	-0.81085300	-0.27212100
H	-4.25514300	-2.66257600	-0.89769900
H	-1.84465500	-2.33747900	-0.80315400
H	0.05277200	-3.25669100	-0.16640100
H	0.76899100	-2.90209600	1.40155200
H	-0.92634300	-2.54020700	1.11769300
H	2.49709500	-2.92320300	0.24925600
H	4.87635100	-2.45904200	-0.01612200
H	5.67241400	-0.11242900	-0.33563100
H	4.06875400	1.72904700	-0.39187700

The second model for analyzing ESP and ALIE.

C	0	-8.64521100	1.99605200	-0.58202600
S	0	-8.01291100	0.57363900	-1.50585100
H	0	-8.75282500	1.76462300	0.47922400
H	0	-9.59751900	2.31890500	-1.00980100
N	0	-6.20872700	1.11726700	1.32974400
N	0	-6.55115600	-1.68315900	0.75208200
N	0	-5.18432500	1.51541800	-1.36090100
C	0	-5.51484600	3.25367300	0.36945900
C	0	-7.07422600	-0.57594500	2.88207900
C	0	-6.31025500	-3.43432800	-0.97770000
C	0	-4.57773600	0.37525200	-3.44134400
C	0	-6.01326600	2.47528000	1.42016600
C	0	-7.00627400	-1.68468800	2.05015600
C	0	-5.76190500	-2.68543100	-2.01647500
C	0	-4.68307300	1.52245900	-2.65349400
O	0	-4.19385000	-0.44135800	0.29894100
C	-1	-6.42095300	2.95051000	2.75180200
C	-1	-7.43728900	-3.01012400	2.43967000
C	-1	-5.37894100	-3.18464700	-3.35045400
C	-1	-4.31089400	2.90023100	-3.03500400
C	0	-6.84446500	1.85069300	3.43044600
C	0	-7.22543800	-3.80480900	1.34522200
C	0	-4.88630300	-2.08526300	-4.00290200
C	0	-4.59340000	3.66968100	-1.94345700
C	0	-6.71094500	0.71740400	2.54405500
C	0	-6.66689000	-2.97253400	0.29561600
C	0	-4.96726600	-0.93471900	-3.10879600
C	0	-5.12716400	2.81005100	-0.89993100
N	0	-5.50447800	-1.33247000	-1.91440500
Fe	0	-5.69073900	-0.14355900	-0.22997700
H	0	-5.39949700	4.31601000	0.56093400
H	0	-7.46012500	-0.73452600	3.88365600
H	0	-6.47410400	-4.49060700	-1.16733300
H	0	-4.16807300	0.50960900	-4.43783700
C	0	4.51609200	-1.40986400	2.19638800
C	0	3.85642000	-0.33361100	1.36922900
C	0	2.49794700	-0.01257300	1.48466000

C	0	1.63085700	-0.78842800	2.34269000
C	0	0.29225900	-0.58740800	2.38237400
C	0	-0.31643800	0.52012400	1.69917500
C	0	-1.69293300	0.77890500	1.83928700
C	0	-2.26238300	1.92348900	1.31022400
C	0	-1.43853600	2.86501300	0.68072900
C	0	-0.08387500	2.61092300	0.50905500
C	0	0.50426000	1.39842000	0.93463100
C	0	1.90198500	1.02990200	0.66520400
C	0	2.65232500	1.58864600	-0.38144900
C	0	2.04147200	2.38197700	-1.51793200
C	0	4.04533400	1.30681500	-0.46830300
C	0	4.87852000	1.96688000	-1.42065200
C	0	6.22518500	1.70508100	-1.50562600
C	0	6.81320300	0.74616200	-0.64979100
C	0	6.04355000	0.08983400	0.27701200
C	0	4.65169800	0.35440100	0.41676300
H	0	3.87068100	-1.84793800	2.95314300
H	0	4.86505400	-2.22418200	1.55021600
H	0	5.39101500	-1.00406500	2.71504800
H	0	2.05169600	-1.58582900	2.93963300
H	0	-0.34210200	-1.22531100	2.99206500
H	0	-2.31066200	0.06163300	2.37054500
H	0	-3.32629600	2.09508900	1.40832600
H	0	-1.85812900	3.80084800	0.32260100
H	0	0.53210700	3.37953200	0.06483700
H	0	2.17228100	3.46749100	-1.41852100
H	0	2.51268800	2.08914500	-2.45998900
H	0	0.97635000	2.18417800	-1.61658800
H	0	4.45080600	2.71925000	-2.07137100
H	0	6.83758600	2.23933200	-2.22663400
H	0	7.87384400	0.53192000	-0.72001500
H	0	6.51637600	-0.62320900	0.93827000
C	-1	5.96247500	7.06438100	-0.72865100
C	-1	5.47439100	5.67130300	-1.14320100
H	0	5.19465400	7.82478600	-0.90521600
H	0	5.21862900	5.63741500	-2.20787800
H	0	6.23569300	4.90520500	-0.96490100
H	0	4.58107700	5.37610000	-0.58210700
C	-1	8.34539200	0.18485400	4.46362900
C	-1	7.56072100	1.15752400	3.53352600

C	-1	8.24050000	1.74113300	2.44709400
C	-1	6.21909300	1.47831500	3.80923000
C	-1	7.57229400	2.71999300	1.66425200
C	-1	5.60275500	2.43887100	2.96303500
C	-1	6.23715800	3.09333600	1.91006600
H	0	9.10660500	-0.36422700	3.90252800
H	0	7.67361700	-0.53723800	4.93629700
H	0	9.26889700	1.47146900	2.23156100
H	0	5.67579400	1.01764300	4.62571300
H	0	8.10795900	3.17362200	0.83395700
H	0	4.55665900	2.67121500	3.15568300
H	0	5.71969700	3.81236600	1.28835900
C	-1	8.60215200	-0.70477200	-4.77360800
C	-1	8.28254400	-1.80391600	-3.79694900
C	-1	8.90208300	-3.07924300	-3.81508000
C	-1	7.30804300	-1.54360400	-2.88768000
C	-1	8.59578300	-4.03468300	-2.81693500
C	-1	6.92768600	-2.51852400	-1.92843600
C	-1	7.53984300	-3.79162200	-1.94640800
H	0	8.94037700	0.19612200	-4.24941300
H	0	7.71795400	-0.42522100	-5.35707300
H	0	9.68371200	-3.28311400	-4.54191600
H	0	6.81614100	-0.57736900	-2.87197000
H	0	9.10818700	-4.99230300	-2.81462400
H	0	6.13299600	-2.30033300	-1.22311800
H	0	7.24392800	-4.53984400	-1.21667100
C	-1	3.45734300	-1.48729100	-2.91338000
C	-1	2.34436800	-1.57010100	-1.85942900
O	-1	2.54574600	-2.26487600	-0.87279800
H	0	3.69232600	-2.50623300	-3.22824700
H	0	4.35357400	-1.06655700	-2.45406400
N	-1	1.17331900	-1.01726200	-2.19499300
C	-1	-0.00887500	-1.32232100	-1.39128300
C	-1	-0.99674300	-0.28565400	-1.72554300
H	0	1.06024200	-0.56860700	-3.08923900
H	0	0.28652500	-1.30150300	-0.34184600
H	0	-1.93780200	-0.41629300	-1.18053400
H	0	-0.62538700	0.70968900	-1.47491700
H	0	-1.24784900	-0.29851000	-2.79540100
C	-1	2.02253200	-4.45050000	2.25427200
C	-1	2.50761800	-4.61327000	3.67843200

O	-1	2.79705000	-3.63323100	4.32413200
O	-1	2.57273900	-5.78912500	4.13397200
H	0	2.75310800	-3.87614500	1.68090200
H	0	1.10554300	-3.85634100	2.26816700
H	0	-6.37224300	3.97935300	3.08034800
H	0	-7.22218900	1.79253400	4.44246800
H	0	-7.84134000	-3.27560700	3.40621000
H	0	-7.42486200	-4.86304300	1.23858100
H	0	-5.48148700	-4.20299600	-3.69529400
H	0	-4.50159800	-2.03392300	-5.01352700
H	0	-3.90071500	3.19208300	-3.99101900
H	0	-4.45625300	4.73765300	-1.83310800
H	0	-7.92583400	2.81741500	-0.68068800
H	0	1.82931900	-5.40150300	1.75402200
H	0	8.85113300	0.74423700	5.25857000
H	0	9.38842900	-0.99034300	-5.47941500
H	0	6.85452100	7.35741300	-1.29199500
H	0	6.21902100	7.09326900	0.33533600
H	0	-0.36885000	-2.33684500	-1.61208600
H	0	3.20261200	-0.88698600	-3.79358900
H	0	2.89003800	-5.73211400	5.05281100

The third model for analyzing ESP and ALIE.

C	0	9.14797800	0.30948900	0.66931700
S	0	8.14480200	-1.17218000	0.94627600
H	0	9.16951000	0.50927000	-0.40805400
H	0	10.17257100	0.12843400	1.00364500
C	-1	-6.38135500	5.69365700	3.84064800
C	-1	-5.73878800	4.38137200	3.35188800
H	0	-5.84367700	6.56502900	3.45344000
H	0	-4.69694200	4.29975100	3.67841300
H	0	-6.27779500	3.50724500	3.73194400
H	0	-5.74692200	4.31482000	2.25908600
C	-1	-7.30745300	4.38939500	-3.96575000
C	-1	-5.95241700	4.50227100	-3.24290500
C	-1	-5.87598600	4.28948400	-1.85996300

C	-1	-4.79526000	4.81574700	-3.96809600
C	-1	-4.64305100	4.39207500	-1.20138900
C	-1	-3.56112500	4.91743600	-3.31118800
C	-1	-3.48649800	4.70663000	-1.92748300
H	0	-7.87209000	5.32579200	-3.88731700
H	0	-7.92028600	3.59636700	-3.52761600
H	0	-6.77008200	4.02545300	-1.30270600
H	0	-4.85847400	4.97108900	-5.04132200
H	0	-4.57859200	4.20356700	-0.13405500
H	0	-2.66320400	5.15617200	-3.87380400
H	0	-2.53019500	4.77492900	-1.41747900
N	-1	-1.12809300	-2.66018800	0.50436700
C	-1	-0.21824700	-1.73380400	-0.18464500
C	-1	1.07989400	-1.58751200	0.63104000
H	0	-1.31373800	-2.41513200	1.47283000
H	0	-0.69003400	-0.75906100	-0.33382000
H	0	1.55590600	-2.56351300	0.76248300
H	0	1.78973200	-0.92941700	0.12470200
H	0	0.87753700	-1.16225700	1.61904800
C	-1	-3.69805300	-3.09403800	0.44195400
C	-1	-2.36715800	-2.80004500	-0.27464300
O	-1	-2.33967700	-2.67865400	-1.52666900
H	0	-4.33106000	-3.67963400	-0.22495400
H	0	-4.19001200	-2.13311800	0.63266000
C	-1	-4.47365000	-3.71540900	-3.87399400
N	-1	-3.99673900	-2.47502100	-3.72317000
O	-1	-5.19304700	-3.99638900	-4.86750000
H	0	-4.17272600	-1.83122500	-4.47891700
H	0	-3.33625800	-2.26928100	-2.98199800
C	-1	-11.21611300	-2.89423300	1.38898900
C	-1	-9.88815600	-3.59519200	1.04704900
C	-1	-8.66965800	-2.95611200	1.31376800
C	-1	-9.89821200	-4.87173100	0.46897000
C	-1	-7.46132000	-3.59415700	1.00270400
C	-1	-8.68977200	-5.50949600	0.15771300
C	-1	-7.47131100	-4.87070500	0.42464100
H	0	-11.90738400	-2.92767500	0.54101400
H	0	-11.04988000	-1.84687900	1.65383800
H	0	-8.66338700	-1.96514900	1.75695100
H	0	-10.84503000	-5.36093200	0.25781100
H	0	-6.52132500	-3.08918000	1.20266100

H	0	-8.69734600	-6.49583400	-0.29648700
H	0	-6.53543600	-5.36342200	0.17776100
C	0	-3.52862800	1.05733200	3.96726700
C	0	-3.30801100	1.10317700	2.47192900
C	0	-2.03830100	1.30775000	1.91365600
C	0	-0.85162300	1.27742600	2.74134300
C	0	0.39310300	1.42159500	2.22816100
C	0	0.58877000	1.76574900	0.84760800
C	0	1.88218700	2.03427600	0.36009200
C	0	2.07337500	2.48884900	-0.93289600
C	0	0.95401000	2.73665800	-1.73927900
C	0	-0.32551000	2.44259800	-1.28482000
C	0	-0.54424500	1.87858000	-0.00847400
C	0	-1.86726100	1.45273500	0.47871700
C	0	-2.93621100	1.12052900	-0.37159200
C	0	-2.77024200	0.88054100	-1.85686200
C	0	-4.22742400	0.88743700	0.18942900
C	0	-5.36366200	0.63721300	-0.63829500
C	0	-6.61303400	0.42291400	-0.10808100
C	0	-6.80149700	0.45020500	1.29373000
C	0	-5.73567800	0.69222500	2.12571200
C	0	-4.42273900	0.91799200	1.61295300
H	0	-2.67114500	1.42200000	4.52961900
H	0	-4.37398400	1.69184800	4.24828400
H	0	-3.75565300	0.04338600	4.31959500
H	0	-0.95861600	1.06485700	3.79718100
H	0	1.27031500	1.32035000	2.86143600
H	0	2.73248700	1.87811500	1.01511000
H	0	3.07780700	2.66542300	-1.30264600
H	0	1.08117000	3.16068500	-2.73091500
H	0	-1.16736800	2.68492000	-1.91720300
H	0	-3.37182600	0.02009400	-2.15603500
H	0	-3.09041200	1.73738700	-2.46172600
H	0	-1.73765400	0.64753100	-2.11146300
H	0	-5.24790900	0.63864500	-1.71377000
H	0	-7.45640200	0.23541300	-0.76498800
H	0	-7.79087600	0.28845900	1.71061800
H	0	-5.89539900	0.70420600	3.19666400
N	0	6.23223100	1.47171500	0.02900100
N	0	6.64046700	-0.81371000	-1.60406300
N	0	4.85633100	-0.15741900	1.93409800

C	-1	5.39505100	2.23592200	2.21513000
C	-1	7.33587100	1.48606000	-2.17489300
C	-1	6.25928100	-3.24728300	-1.79246400
C	-1	4.00816700	-2.43081600	2.40128300
C	0	6.02253300	2.43478100	0.99230600
C	0	7.23694600	0.12076300	-2.42880500
C	0	5.53709300	-3.42583700	-0.62396900
C	0	4.17886300	-1.07835700	2.70001300
O	0	4.16549500	-0.13314700	-0.69214100
C	0	6.54580600	3.70179600	0.54100000
C	0	7.76665700	-0.53435800	-3.60026100
C	0	5.00293000	-4.69454700	-0.18661000
C	0	3.70080200	-0.44843500	3.90721800
C	0	7.05986300	3.49793900	-0.70450700
C	0	7.47746300	-1.86058000	-3.48411500
C	0	4.35985000	-4.46388900	0.98976300
C	0	4.11080900	0.85217900	3.86879100
C	0	6.86807000	2.10195500	-1.01587200
C	0	6.76170400	-2.03368900	-2.24432300
C	0	4.50692300	-3.05590500	1.27417500
C	0	4.83036500	1.03004200	2.63007000
N	0	5.22757200	-2.44109700	0.27856600
H	0	5.30107800	3.08836000	2.87859900
H	0	7.82954200	2.10488000	-2.91554700
H	0	6.43445400	-4.11880700	-2.41351000
H	0	3.45097700	-3.03203200	3.11090700
Fe	0	5.55619400	-0.44002000	0.06845200
H	0	-11.71103500	-3.38218000	2.23635200
H	0	-6.37383700	5.75665400	4.93370400
H	0	-7.42205600	5.77157600	3.51003700
H	0	-7.16939700	4.17091200	-5.02790900
H	0	-0.00745000	-2.15559500	-1.16698100
H	0	-3.55683600	-3.61364200	1.39320700
H	0	-4.19907400	-4.42456600	-3.07566400
H	0	7.71521500	-2.66176600	-4.17068600
H	0	8.28955500	-0.02918600	-4.40117200
H	0	5.11679100	-5.62635100	-0.72352400
H	0	3.83598500	-5.16689600	1.62295800
H	0	7.53976700	4.21271200	-1.35931700
H	0	6.51220400	4.61896900	1.11333900
H	0	3.14009400	-0.95319000	4.68233300

H	0	3.95104900	1.62956400	4.60382100
H	0	8.72235300	1.18015700	1.17113100

R1

C	0	-8.64521100	1.99605200	-0.58202600
S	0	-8.01291100	0.57363900	-1.50585100
H	0	-8.75282500	1.76462300	0.47922400
H	0	-9.59751900	2.31890500	-1.00980100
N	0	-6.20872700	1.11726700	1.32974400
N	0	-6.55115600	-1.68315900	0.75208200
N	0	-5.18432500	1.51541800	-1.36090100
C	0	-5.51484600	3.25367300	0.36945900
C	0	-7.07422600	-0.57594500	2.88207900
C	0	-6.31025500	-3.43432800	-0.97770000
C	0	-4.57773600	0.37525200	-3.44134400
C	0	-6.01326600	2.47528000	1.42016600
C	0	-7.00627400	-1.68468800	2.05015600
C	0	-5.76190500	-2.68543100	-2.01647500
C	0	-4.68307300	1.52245900	-2.65349400
O	0	-4.19385000	-0.44135800	0.29894100
C	-1	-6.42095300	2.95051000	2.75180200
C	-1	-7.43728900	-3.01012400	2.43967000
C	-1	-5.37894100	-3.18464700	-3.35045400
C	-1	-4.31089400	2.90023100	-3.03500400
C	0	-6.84446500	1.85069300	3.43044600
C	0	-7.22543800	-3.80480900	1.34522200
C	0	-4.88630300	-2.08526300	-4.00290200
C	0	-4.59340000	3.66968100	-1.94345700
C	0	-6.71094500	0.71740400	2.54405500
C	0	-6.66689000	-2.97253400	0.29561600
C	0	-4.96726600	-0.93471900	-3.10879600
C	0	-5.12716400	2.81005100	-0.89993100
N	0	-5.50447800	-1.33247000	-1.91440500
Fe	0	-5.69073900	-0.14355900	-0.22997700
H	0	-5.39949700	4.31601000	0.56093400
H	0	-7.46012500	-0.73452600	3.88365600

H	0	-6.47410400	-4.49060700	-1.16733300
H	0	-4.16807300	0.50960900	-4.43783700
C	0	4.51609200	-1.40986400	2.19638800
C	0	3.85642000	-0.33361100	1.36922900
C	0	2.49794700	-0.01257300	1.48466000
C	0	1.63085700	-0.78842800	2.34269000
C	0	0.29225900	-0.58740800	2.38237400
C	0	-0.31643800	0.52012400	1.69917500
C	0	-1.69293300	0.77890500	1.83928700
C	0	-2.26238300	1.92348900	1.31022400
C	0	-1.43853600	2.86501300	0.68072900
C	0	-0.08387500	2.61092300	0.50905500
C	0	0.50426000	1.39842000	0.93463100
C	0	1.90198500	1.02990200	0.66520400
C	0	2.65232500	1.58864600	-0.38144900
C	0	2.04147200	2.38197700	-1.51793200
C	0	4.04533400	1.30681500	-0.46830300
C	0	4.87852000	1.96688000	-1.42065200
C	0	6.22518500	1.70508100	-1.50562600
C	0	6.81320300	0.74616200	-0.64979100
C	0	6.04355000	0.08983400	0.27701200
C	0	4.65169800	0.35440100	0.41676300
H	0	3.87068100	-1.84793800	2.95314300
H	0	4.86505400	-2.22418200	1.55021600
H	0	5.39101500	-1.00406500	2.71504800
H	0	2.05169600	-1.58582900	2.93963300
H	0	-0.34210200	-1.22531100	2.99206500
H	0	-2.31066200	0.06163300	2.37054500
H	0	-3.32629600	2.09508900	1.40832600
H	0	-1.85812900	3.80084800	0.32260100
H	0	0.53210700	3.37953200	0.06483700
H	0	2.17228100	3.46749100	-1.41852100
H	0	2.51268800	2.08914500	-2.45998900
H	0	0.97635000	2.18417800	-1.61658800
H	0	4.45080600	2.71925000	-2.07137100
H	0	6.83758600	2.23933200	-2.22663400
H	0	7.87384400	0.53192000	-0.72001500
H	0	6.51637600	-0.62320900	0.93827000
C	-1	5.96247500	7.06438100	-0.72865100
C	-1	5.47439100	5.67130300	-1.14320100
H	0	5.19465400	7.82478600	-0.90521600

H	0	5.21862900	5.63741500	-2.20787800
H	0	6.23569300	4.90520500	-0.96490100
H	0	4.58107700	5.37610000	-0.58210700
C	-1	8.34539200	0.18485400	4.46362900
C	-1	7.56072100	1.15752400	3.53352600
C	-1	8.24050000	1.74113300	2.44709400
C	-1	6.21909300	1.47831500	3.80923000
C	-1	7.57229400	2.71999300	1.66425200
C	-1	5.60275500	2.43887100	2.96303500
C	-1	6.23715800	3.09333600	1.91006600
H	0	9.10660500	-0.36422700	3.90252800
H	0	7.67361700	-0.53723800	4.93629700
H	0	9.26889700	1.47146900	2.23156100
H	0	5.67579400	1.01764300	4.62571300
H	0	8.10795900	3.17362200	0.83395700
H	0	4.55665900	2.67121500	3.15568300
H	0	5.71969700	3.81236600	1.28835900
C	-1	8.60215200	-0.70477200	-4.77360800
C	-1	8.28254400	-1.80391600	-3.79694900
C	-1	8.90208300	-3.07924300	-3.81508000
C	-1	7.30804300	-1.54360400	-2.88768000
C	-1	8.59578300	-4.03468300	-2.81693500
C	-1	6.92768600	-2.51852400	-1.92843600
C	-1	7.53984300	-3.79162200	-1.94640800
H	0	8.94037700	0.19612200	-4.24941300
H	0	7.71795400	-0.42522100	-5.35707300
H	0	9.68371200	-3.28311400	-4.54191600
H	0	6.81614100	-0.57736900	-2.87197000
H	0	9.10818700	-4.99230300	-2.81462400
H	0	6.13299600	-2.30033300	-1.22311800
H	0	7.24392800	-4.53984400	-1.21667100
C	-1	3.45734300	-1.48729100	-2.91338000
C	-1	2.34436800	-1.57010100	-1.85942900
O	-1	2.54574600	-2.26487600	-0.87279800
H	0	3.69232600	-2.50623300	-3.22824700
H	0	4.35357400	-1.06655700	-2.45406400
N	-1	1.17331900	-1.01726200	-2.19499300
C	-1	-0.00887500	-1.32232100	-1.39128300
C	-1	-0.99674300	-0.28565400	-1.72554300
H	0	1.06024200	-0.56860700	-3.08923900
H	0	0.28652500	-1.30150300	-0.34184600

H	0	-1.93780200	-0.41629300	-1.18053400
H	0	-0.62538700	0.70968900	-1.47491700
H	0	-1.24784900	-0.29851000	-2.79540100
C	-1	2.02253200	-4.45050000	2.25427200
C	-1	2.50761800	-4.61327000	3.67843200
O	-1	2.79705000	-3.63323100	4.32413200
O	-1	2.57273900	-5.78912500	4.13397200
H	0	2.75310800	-3.87614500	1.68090200
H	0	1.10554300	-3.85634100	2.26816700
H	0	-6.37224300	3.97935300	3.08034800
H	0	-7.22218900	1.79253400	4.44246800
H	0	-7.84134000	-3.27560700	3.40621000
H	0	-7.42486200	-4.86304300	1.23858100
H	0	-5.48148700	-4.20299600	-3.69529400
H	0	-4.50159800	-2.03392300	-5.01352700
H	0	-3.90071500	3.19208300	-3.99101900
H	0	-4.45625300	4.73765300	-1.83310800
H	0	-7.92583400	2.81741500	-0.68068800
H	0	1.82931900	-5.40150300	1.75402200
H	0	8.85113300	0.74423700	5.25857000
H	0	9.38842900	-0.99034300	-5.47941500
H	0	6.85452100	7.35741300	-1.29199500
H	0	6.21902100	7.09326900	0.33533600
H	0	-0.36885000	-2.33684500	-1.61208600
H	0	3.20261200	-0.88698600	-3.79358900
H	0	2.89003800	-5.73211400	5.05281100

TS1-1

C	0	-8.35071900	1.87693700	-0.59879600
S	0	-7.60262200	0.43728700	-1.41683700
H	0	-8.48554500	1.69654200	0.46969500
H	0	-9.31399800	2.08141200	-1.07302200
N	0	-5.98565800	1.11210300	1.32554100
N	0	-6.26473600	-1.64659100	0.58570700
N	0	-4.97522900	1.70791800	-1.32085700
C	0	-5.38607900	3.33049300	0.49493100

C	0	-6.85083700	-0.68838800	2.76239900
C	0	-6.08602000	-3.25277500	-1.29012600
C	0	-4.31391800	0.69989000	-3.45743200
C	0	-5.83835300	2.46989200	1.50185200
C	0	-6.77647100	-1.73858100	1.85693400
C	0	-5.51668000	-2.44211900	-2.26936900
C	0	-4.44541700	1.79284700	-2.59690700
O	0	-3.82934100	-0.27289200	0.09457900
C	-1	-6.23325900	2.84309900	2.86844100
C	-1	-7.27669700	-3.07423200	2.12258500
C	-1	-5.18884400	-2.84177100	-3.65492300
C	-1	-4.09316700	3.19892900	-2.89651600
C	0	-6.63212200	1.69321700	3.47483800
C	0	-7.05481500	-3.78098500	0.97250100
C	0	-4.67227900	-1.70574600	-4.22022000
C	0	-4.43543800	3.90507400	-1.77925300
C	0	-6.48994000	0.62559000	2.51254300
C	0	-6.42784800	-2.88454400	0.01689200
C	0	-4.69946600	-0.63312500	-3.22465700
C	0	-4.97400400	2.97583000	-0.79704900
N	0	-5.20644400	-1.11686900	-2.05255200
Fe	0	-5.50011700	0.00358500	-0.31682900
H	0	-5.31917000	4.38464700	0.74700300
H	0	-7.26021800	-0.90833100	3.74310600
H	0	-6.30042700	-4.28052900	-1.56765200
H	0	-3.90637500	0.91125900	-4.44181800
C	0	4.37028100	-1.33836800	1.96431000
C	0	3.47719900	-0.27120300	1.37897400
C	0	2.10631500	-0.20294500	1.64179000
C	0	1.48788500	-1.24766900	2.42542300
C	0	0.14810500	-1.40117900	2.47882000
C	0	-0.73596900	-0.41700200	1.91746200
C	0	-2.11350700	-0.58345500	2.02072500
C	0	-3.03505700	0.42294600	1.61345200
C	0	-2.44949800	1.69623400	1.28307400
C	0	-1.09118000	1.86057400	1.17367600
C	0	-0.17240800	0.78539300	1.36253100
C	0	1.26074900	0.83006500	1.04891000
C	0	1.84346200	1.74104400	0.13774300
C	0	1.06567900	2.77437400	-0.64962900
C	0	3.23863200	1.64866800	-0.15764800

C	0	3.87229100	2.53457600	-1.08340700
C	0	5.19132700	2.39098100	-1.44324500
C	0	5.97317900	1.36104300	-0.87510200
C	0	5.41508300	0.51694900	0.05334900
C	0	4.05113200	0.63288800	0.44712800
H	0	3.91872500	-1.89811400	2.77924600
H	0	4.64289300	-2.05571500	1.18062600
H	0	5.29233800	-0.89442700	2.35041300
H	0	2.10896300	-1.97102200	2.93218500
H	0	-0.29161200	-2.24341200	3.00622300
H	0	-2.50040900	-1.50987100	2.43452100
H	0	-3.99385200	0.44472200	2.11569700
H	0	-3.10279500	2.54574300	1.13791700
H	0	-0.71657800	2.85654800	0.99175400
H	0	1.14986800	3.77739000	-0.21044800
H	0	1.44441300	2.83582600	-1.67112800
H	0	0.01009600	2.54170900	-0.72761800
H	0	3.31071000	3.35053700	-1.51771800
H	0	5.63298300	3.07931300	-2.15666200
H	0	7.01875300	1.25356000	-1.14413800
H	0	6.03555500	-0.24409000	0.50594500
C	-1	6.18796800	7.13271400	-0.24588000
C	-1	5.69532000	5.77567700	-0.76207100
H	0	5.41856000	7.90430600	-0.35357100
H	0	5.42915400	5.82289100	-1.82371000
H	0	6.46255400	5.00335600	-0.64960100
H	0	4.81028400	5.43226600	-0.21715600
C	-1	8.51037500	-0.11531300	4.44866300
C	-1	7.73529700	0.92589900	3.58725800
C	-1	8.42357600	1.58273900	2.54905700
C	-1	6.39380200	1.23294400	3.87880000
C	-1	7.76421900	2.61890700	1.83554200
C	-1	5.78655200	2.25517500	3.10105000
C	-1	6.42963200	2.98048800	2.10107800
H	0	9.24876200	-0.65028300	3.84512800
H	0	7.82873300	-0.84598900	4.89266500
H	0	9.45266700	1.32602300	2.32165200
H	0	5.84517300	0.71882900	4.65902400
H	0	8.30926700	3.13227900	1.04626400
H	0	4.74191000	2.48191100	3.30759200
H	0	5.91833200	3.74585200	1.53143600

C	-1	8.81131100	-0.33840900	-4.82731100
C	-1	8.48129000	-1.50339000	-3.93398200
C	-1	9.09473600	-2.77730300	-4.04097700
C	-1	7.50336000	-1.30419300	-3.01304000
C	-1	8.77862700	-3.80055100	-3.11577000
C	-1	7.11314200	-2.34374400	-2.12855900
C	-1	7.71932800	-3.61537800	-2.23513800
H	0	9.57408100	-0.58827500	-5.57121000
H	0	9.18781300	0.50813200	-4.24205100
H	0	9.87709900	-2.93276600	-4.77863300
H	0	7.01477300	-0.33737900	-2.92928300
H	0	9.28550300	-4.75880600	-3.18035300
H	0	6.30800200	-2.17765900	-1.41944400
H	0	7.41505300	-4.41294200	-1.56363200
C	-1	3.65311600	-1.22622500	-3.05346400
C	-1	2.53421600	-1.37896100	-2.01369900
O	-1	2.72707100	-2.14404700	-1.07872300
H	0	3.93026200	-2.22683300	-3.39050100
H	0	4.52780100	-0.78347100	-2.57191200
N	-1	1.36763600	-0.79732100	-2.31424900
C	-1	0.17975700	-1.15337900	-1.54045400
C	-1	-0.80128500	-0.09016200	-1.80387100
H	0	1.25846600	-0.29600800	-3.18079900
H	0	0.47362600	-1.21706400	-0.49405600
H	0	-1.72939000	-0.21923800	-1.23696000
H	0	-0.39308000	0.88595900	-1.55476200
H	0	-1.08690500	-0.06857900	-2.86503500
C	-1	2.17687400	-4.54655000	1.88009700
C	-1	2.65377200	-4.81407300	3.29117100
O	-1	2.94447000	-3.88458100	4.00721100
O	-1	2.71079300	-6.01997800	3.66107400
H	0	2.86344500	-3.86175000	1.38090100
H	0	1.21035800	-4.04006400	1.92669600
H	0	-6.20668300	3.84884700	3.26474700
H	0	-7.00171600	1.56127300	4.48299700
H	0	-7.72701000	-3.40052600	3.04934300
H	0	-7.29392800	-4.81627800	0.76663400
H	0	-5.33637400	-3.82233300	-4.08286600
H	0	-4.31339600	-1.57614300	-5.23362800
H	0	-3.66460200	3.54972900	-3.82441500
H	0	-4.33328300	4.96967900	-1.61134400

H	0	-7.70943100	2.75518900	-0.72261100
H	0	2.07086500	-5.45796800	1.28796300
H	0	9.04260200	0.38798900	5.26348800
H	0	7.92334800	0.00991800	-5.36588500
H	0	7.07358200	7.46950400	-0.79458700
H	0	6.45643100	7.07843900	0.81418200
H	0	-0.18659000	-2.14590600	-1.83648800
H	0	3.38442700	-0.61194300	-3.91926600
H	0	3.01932400	-6.03251400	4.58460600

IM1

C	0	8.27788600	1.95177400	0.64422300
S	0	7.66110200	0.32431700	1.19610300
H	0	8.34279300	2.00986900	-0.44451600
H	0	9.27735100	2.08439700	1.06774400
N	0	5.92672100	1.13234600	-1.33880000
N	0	6.24019600	-1.65142000	-0.59223300
N	0	4.94306900	1.72636200	1.29786700
C	0	5.34558600	3.35650200	-0.51207800
C	0	6.82109000	-0.67033700	-2.76173600
C	0	6.06505700	-3.26452300	1.26740100
C	0	4.35345300	0.71086700	3.45168600
C	0	5.79916700	2.49457800	-1.51450700
C	0	6.75694000	-1.72444200	-1.85991900
C	0	5.51841800	-2.44025200	2.25288800
C	0	4.44955900	1.80514700	2.58392700
O	0	3.74481800	-0.32544200	-0.14169100
C	-1	6.22206700	2.86242100	-2.87331900
C	-1	7.26779000	-3.05624300	-2.14136700
C	-1	5.19622500	-2.83455700	3.64242400
C	-1	4.09822400	3.20749700	2.89829700
C	0	6.61476200	1.70848100	-3.47571100
C	0	7.04162300	-3.77878100	-1.00271900
C	0	4.70566400	-1.69140300	4.21451100
C	0	4.42299600	3.92251700	1.77985800
C	0	6.44876300	0.64113600	-2.51624300

C	0	6.40584900	-2.89462000	-0.03672300
C	0	4.73907800	-0.62053700	3.21689800
C	0	4.94917800	2.99761700	0.78669700
N	0	5.22874000	-1.11304500	2.04083200
Fe	0	5.57012900	0.03391300	0.35269900
H	0	5.29318700	4.41296100	-0.75805300
H	0	7.24313100	-0.88345900	-3.73882500
H	0	6.26986200	-4.29426800	1.54534900
H	0	3.96961800	0.92302500	4.44588700
C	0	-4.30534700	-1.37717000	-2.09443800
C	0	-3.43398700	-0.31029600	-1.47905700
C	0	-2.06376600	-0.20857800	-1.72558500
C	0	-1.41577900	-1.21955600	-2.53211800
C	0	-0.07416600	-1.35580000	-2.55306100
C	0	0.77450600	-0.38748500	-1.91015200
C	0	2.13404400	-0.59681900	-1.79923700
C	0	3.07650600	0.34509200	-1.16894400
C	0	2.43207100	1.65849400	-0.87790300
C	0	1.09949100	1.87541900	-1.04881800
C	0	0.18363600	0.80701100	-1.34901300
C	0	-1.24973800	0.83438400	-1.09681800
C	0	-1.87103800	1.73440200	-0.18790000
C	0	-1.12951600	2.78115900	0.61404000
C	0	-3.26619600	1.60598400	0.08004300
C	0	-3.94301300	2.47609900	0.99308600
C	0	-5.26079100	2.29084900	1.33157900
C	0	-5.99747100	1.22964100	0.75848000
C	0	-5.40099500	0.40359200	-0.16075300
C	0	-4.03820000	0.56703700	-0.53970200
H	0	-3.82775200	-1.94710500	-2.88583200
H	0	-4.61333900	-2.08762600	-1.31814200
H	0	-5.21072300	-0.92854400	-2.51424000
H	0	-2.01872400	-1.93800100	-3.06838400
H	0	0.39730900	-2.17917300	-3.08124600
H	0	2.55915000	-1.54492800	-2.11703200
H	0	3.81262000	0.62433000	-1.97500800
H	0	3.07535000	2.47338400	-0.57649000
H	0	0.71774200	2.87632400	-0.91771300
H	0	-1.15276300	3.76347600	0.12413400
H	0	-1.58019400	2.89673500	1.59873700
H	0	-0.09034700	2.52704300	0.78494900

H	0	-3.41788100	3.31374500	1.43034800
H	0	-5.73720000	2.96853500	2.03231200
H	0	-7.04025000	1.08337800	1.01830200
H	0	-5.98893500	-0.37956400	-0.61758900
C	-1	-6.19046700	7.14580400	0.28394400
C	-1	-5.69632300	5.78783200	0.79623000
H	0	-5.42253200	7.91791100	0.39642500
H	0	-5.43217000	5.83153800	1.85855300
H	0	-6.46282800	5.01522300	0.67837200
H	0	-4.80959100	5.44979500	0.24995500
C	-1	-8.52587000	-0.09360300	-4.41744700
C	-1	-7.74840000	0.94604100	-3.55630500
C	-1	-8.43377000	1.60093200	-2.51495300
C	-1	-6.40774200	1.25367500	-3.85105800
C	-1	-7.77243600	2.63580200	-1.80138100
C	-1	-5.79833400	2.27448600	-3.07313200
C	-1	-6.43861500	2.99792200	-2.07000900
H	0	-9.25483500	-0.63752400	-3.81057500
H	0	-7.84460500	-0.81644200	-4.87450200
H	0	-9.46261400	1.34483100	-2.28610000
H	0	-5.86303400	0.74428800	-4.63714600
H	0	-8.31680600	3.15025300	-1.01231100
H	0	-4.75571100	2.50526600	-3.28598700
H	0	-5.92783800	3.76647700	-1.50434600
C	-1	-8.80064800	-0.33388600	4.85890900
C	-1	-8.47311000	-1.49719900	3.96249700
C	-1	-9.08621200	-2.77133100	4.06886100
C	-1	-7.49778600	-1.29626100	3.03917200
C	-1	-8.77268000	-3.79285200	3.14087400
C	-1	-7.11003000	-2.33415700	2.15167100
C	-1	-7.71587300	-3.60600900	2.25760400
H	0	-9.56374300	-0.58422700	5.60211400
H	0	-9.17579400	0.51490700	4.27606500
H	0	-9.86605300	-2.92825100	4.80870200
H	0	-7.00899300	-0.32907500	2.95908800
H	0	-9.27926800	-4.75117600	3.20502900
H	0	-6.30642400	-2.16820400	1.44066000
H	0	-7.41320400	-4.40255000	1.58423800
C	-1	-3.64744600	-1.21822600	3.06888700
C	-1	-2.53147700	-1.36899500	2.02569100
O	-1	-2.72694300	-2.13235500	1.08984600

H	0	-3.89825000	-2.21692000	3.43176300
H	0	-4.53602300	-0.81002400	2.58300000
N	-1	-1.36407300	-0.78787000	2.32402800
C	-1	-0.17836800	-1.14245000	1.54622800
C	-1	0.80337900	-0.07968700	1.80884800
H	0	-1.24708200	-0.30775900	3.20190700
H	0	-0.47907900	-1.20858600	0.50135800
H	0	1.74091500	-0.22077000	1.25917500
H	0	0.40123900	0.89739300	1.55312300
H	0	1.08023200	-0.05226400	2.87138600
C	-1	-2.18501300	-4.52935500	-1.87495700
C	-1	-2.66587900	-4.79428200	-3.28517400
O	-1	-2.95862300	-3.86347700	-3.99866900
O	-1	-2.72390400	-5.99950300	-3.65714700
H	0	-2.86928200	-3.84465200	-1.37251800
H	0	-1.21752800	-4.02423200	-1.92564600
H	0	6.21543400	3.86889100	-3.26947800
H	0	7.00131600	1.57429900	-4.47741000
H	0	7.72582900	-3.36776600	-3.06957700
H	0	7.28561000	-4.81539400	-0.80808000
H	0	5.33108000	-3.81812900	4.06825900
H	0	4.35877300	-1.55676200	5.23167300
H	0	3.69200700	3.55412900	3.83810900
H	0	4.32349400	4.98921800	1.62240700
H	0	7.63533200	2.75907100	1.00409200
H	0	-2.07672700	-5.44102500	-1.28413300
H	0	-9.06947400	0.41315400	-5.22238300
H	0	-7.91209500	0.01092600	5.39879800
H	0	-7.07751100	7.47840200	0.83253300
H	0	-6.45672100	7.09478300	-0.77672100
H	0	0.19089400	-2.13422000	1.83950300
H	0	-3.38849700	-0.57800900	3.91857300
H	0	-3.03335800	-6.01354900	-4.58035500

TS1-2

C	0	8.24318500	1.85821000	1.04802300
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S	0	7.69838800	0.12520600	1.20633100
H	0	8.28704600	2.16913300	0.00276000
H	0	9.24667600	1.91166500	1.47995700
N	0	6.03289300	1.21665700	-1.20799500
N	0	6.24866700	-1.63610400	-0.72410800
N	0	4.96805900	1.57559300	1.43749100
C	0	5.41598200	3.36063900	-0.21243200
C	0	6.85140600	-0.47606200	-2.79930600
C	0	6.06752900	-3.40166700	0.99309800
C	0	4.34966100	0.38497400	3.49180000
C	0	5.87362000	2.58610900	-1.28105700
C	0	6.77701600	-1.60103600	-1.99350900
C	0	5.51616200	-2.66196100	2.03890900
C	0	4.45800100	1.54926200	2.72156200
O	0	3.52186900	-0.16917100	-0.43047000
C	-1	6.22892100	3.05180800	-2.63011400
C	-1	7.28025900	-2.90590900	-2.38482500
C	-1	5.21779800	-3.15839700	3.40095600
C	-1	4.11406900	2.92324700	3.15367400
C	0	6.61519300	1.94863800	-3.32460300
C	0	7.04611700	-3.72247200	-1.31274300
C	0	4.72108500	-2.06466800	4.05876200
C	0	4.47061600	3.72907700	2.10745400
C	0	6.50214700	0.81573200	-2.43557100
C	0	6.40944800	-2.92409800	-0.27646900
C	0	4.73097100	-0.92205300	3.14499600
C	0	5.00225300	2.89121100	1.04312600
N	0	5.20565800	-1.32227900	1.92519400
Fe	0	5.63326300	-0.02697600	0.36198700
H	0	5.35381900	4.43287400	-0.37182400
H	0	7.25438600	-0.61062100	-3.79806300
H	0	6.27968300	-4.44866700	1.18764000
H	0	3.96453800	0.51300100	4.49953500
C	0	-4.23972700	-1.34102100	-2.09611500
C	0	-3.42089200	-0.26411600	-1.43275700
C	0	-2.04788200	-0.09017000	-1.66579300
C	0	-1.33329600	-1.03096800	-2.48504100
C	0	0.02054500	-1.02156900	-2.56210300
C	0	0.79054100	-0.02830100	-1.87598500
C	0	2.19674500	-0.05211200	-1.96918900
C	0	3.07886600	0.88684900	-1.27061800

C	0	2.32794500	1.94748900	-0.53648100
C	0	0.98420400	1.97898200	-0.48119800
C	0	0.13376200	1.02028200	-1.17063400
C	0	-1.31206500	1.02109500	-1.06403200
C	0	-2.05063800	2.00503200	-0.35025900
C	0	-1.57249100	3.42064000	-0.09335200
C	0	-3.36919900	1.69489800	0.06498600
C	0	-4.04652300	2.49328900	1.04014500
C	0	-5.30893400	2.17865000	1.47361300
C	0	-5.99702200	1.07201900	0.91635000
C	0	-5.38633600	0.28757300	-0.02752600
C	0	-4.05673100	0.55313800	-0.47034800
H	0	-3.75289400	-1.80740200	-2.94855300
H	0	-4.46988300	-2.12836500	-1.36818000
H	0	-5.18784200	-0.92511900	-2.45068500
H	0	-1.88533800	-1.78569700	-3.02625900
H	0	0.54655400	-1.76815500	-3.15014700
H	0	2.68233900	-0.81623600	-2.56475700
H	0	3.87212200	1.31090400	-1.89408300
H	0	2.90181200	2.68276000	0.00770300
H	0	0.53468500	2.71712400	0.15703700
H	0	-0.83968000	3.73578000	-0.83476000
H	0	-2.42103700	4.10384500	-0.17521100
H	0	-1.13736200	3.57182900	0.90251900
H	0	-3.53250100	3.33494500	1.48712800
H	0	-5.78335900	2.78087500	2.24136300
H	0	-7.01164000	0.84929800	1.22748900
H	0	-5.92590600	-0.55133900	-0.44503900
C	-1	-6.18175200	7.05257000	0.88496700
C	-1	-5.68576800	5.65778300	1.28405700
H	0	-5.40693800	7.81074600	1.03820700
H	0	-5.39699100	5.61927800	2.34008200
H	0	-6.45790800	4.89946200	1.12312000
H	0	-4.81438700	5.36051600	0.69207700
C	-1	-8.51924800	0.21857400	-4.38749200
C	-1	-7.74118000	1.18522100	-3.44563700
C	-1	-8.42537100	1.75241600	-2.35330000
C	-1	-6.40122700	1.51704300	-3.71638200
C	-1	-7.76367300	2.72623500	-1.55873600
C	-1	-5.79134000	2.47155800	-2.85874400
C	-1	-6.43055600	3.11022600	-1.79899000

H	0	-9.06056500	0.78794200	-5.15113100
H	0	-9.25017200	-0.37031100	-3.82655800
H	0	-9.45334500	1.47673200	-2.14389800
H	0	-5.85622900	1.07123700	-4.54004000
H	0	-8.30630900	3.17251400	-0.72809300
H	0	-4.74856700	2.71868300	-3.05203800
H	0	-5.91885200	3.82850700	-1.17199500
C	-1	-8.77898300	-0.77755000	4.83879200
C	-1	-8.45200700	-1.86360600	3.85000500
C	-1	-9.06398100	-3.14270700	3.85306100
C	-1	-7.47831500	-1.58719200	2.94464200
C	-1	-8.75117000	-4.08488200	2.84438600
C	-1	-7.09120300	-2.54892400	1.97487000
C	-1	-7.69592000	-3.82571000	1.97767200
H	0	-9.48549300	-1.11185400	5.60469000
H	0	-9.22688600	0.08746600	4.33601400
H	0	-9.84123100	-3.36077800	4.58007700
H	0	-6.98501400	-0.61972100	2.94937800
H	0	-9.25585400	-5.04629400	2.83197300
H	0	-6.28463800	-2.32775200	1.28294800
H	0	-7.39236400	-4.56502100	1.24231000
C	-1	-3.62799200	-1.50845600	2.97470800
C	-1	-2.51358400	-1.57267800	1.92098000
O	-1	-2.70997500	-2.25735900	0.92630700
H	0	-3.87062700	-2.53370300	3.26157600
H	0	-4.52074400	-1.07020900	2.52460400
N	-1	-1.34613900	-1.01679000	2.26391700
C	-1	-0.16141600	-1.30572400	1.45797400
C	-1	0.81995200	-0.26705100	1.80487100
H	0	-1.23103100	-0.59605400	3.17183600
H	0	-0.46166700	-1.27991500	0.41032800
H	0	1.73142500	-0.32458800	1.20180500
H	0	0.39246400	0.72864600	1.66971800
H	0	1.13287900	-0.35206400	2.85477800
C	-1	-2.17099600	-4.40414800	-2.22490700
C	-1	-2.65392200	-4.55362600	-3.65129000
O	-1	-2.94850700	-3.56799800	-4.28606000
O	-1	-2.71163800	-5.72455300	-4.12021100
H	0	-2.84523000	-3.75287500	-1.66946800
H	0	-1.19436600	-3.91374900	-2.23626500
H	0	6.18639400	4.08196200	-2.95681500

H	0	6.95556800	1.88858700	-4.34991500
H	0	7.73953100	-3.13993800	-3.33483100
H	0	7.28340500	-4.77342200	-1.20785300
H	0	5.36732900	-4.16879300	3.75214000
H	0	4.38463700	-2.00827000	5.08667600
H	0	3.69367000	3.19026700	4.11276000
H	0	4.38498800	4.80656300	2.04259500
H	0	7.58472400	2.53390700	1.59684900
H	0	-2.07466300	-5.36086000	-1.70743800
H	0	-7.83824700	-0.46734700	-4.89866700
H	0	-7.87675800	-0.42450100	5.34915600
H	0	-7.05541000	7.34827200	1.47476600
H	0	-6.46993000	7.08133900	-0.17078000
H	0	0.20656000	-2.31978700	1.66405100
H	0	-3.37005300	-0.93352500	3.87028300
H	0	-3.02228000	-5.66233300	-5.04099300

P1

C	0	-8.32703400	1.95802900	-1.13621800
S	0	-7.91271500	0.18542800	-1.24034500
H	0	-8.32821700	2.30476900	-0.10178500
H	0	-9.33291300	2.06591200	-1.55237600
N	0	-6.12792000	1.20554900	1.15706100
N	0	-6.41513000	-1.62228700	0.71977300
N	0	-5.05768600	1.48532000	-1.48550700
C	0	-5.40210800	3.30860500	0.15431600
C	0	-7.01571500	-0.42427600	2.77561300
C	0	-6.16855700	-3.45550200	-0.91973200
C	0	-4.51673900	0.27585100	-3.54538100
C	0	-5.91909300	2.57275300	1.22016900
C	0	-6.92139100	-1.56875600	2.00469400
C	0	-5.64067300	-2.73755700	-1.99027300
C	0	-4.58486800	1.44912300	-2.78836200
O	0	-2.79393200	-0.11351700	1.13014000
C	-1	-6.30426600	3.08339900	2.54801400
C	-1	-7.34655100	-2.88026200	2.45819600

C	-1	-5.28832700	-3.27956500	-3.32081700
C	-1	-4.19384400	2.80814000	-3.23225900
C	0	-6.74667800	2.00404500	3.24679200
C	0	-7.09533500	-3.72406700	1.41031300
C	0	-4.82546400	-2.19452300	-4.01629000
C	0	-4.46588700	3.61937000	-2.16629800
C	0	-6.64275200	0.85102900	2.38311700
C	0	-6.52366300	-2.93930500	0.32957600
C	0	-4.89526500	-1.01696300	-3.15632000
C	0	-5.00415700	2.80462400	-1.08936200
N	0	-5.38747200	-1.37684900	-1.92443000
Fe	0	-5.88544600	-0.05109300	-0.43630000
H	0	-5.28780700	4.37829500	0.30095000
H	0	-7.41925100	-0.53311200	3.77695400
H	0	-6.33168700	-4.51845300	-1.06831400
H	0	-4.13637000	0.37527700	-4.55774200
C	0	4.44942900	-1.35012500	2.03928800
C	0	3.65605400	-0.26568100	1.35326400
C	0	2.29586900	-0.02059200	1.63351300
C	0	1.61056400	-0.82508500	2.59706500
C	0	0.27225500	-0.68477700	2.82041600
C	0	-0.49319200	0.24131600	2.07369800
C	0	-1.96323000	0.22738300	2.26041800
C	0	-2.78862600	1.26241100	1.59263900
C	0	-2.07546400	2.20060600	0.71776000
C	0	-0.75330700	2.07133000	0.48500500
C	0	0.11898700	1.12843900	1.18603600
C	0	1.56528000	1.05966700	0.97613500
C	0	2.29918100	1.95923800	0.16430000
C	0	1.82315700	3.35091100	-0.20849900
C	0	3.61217200	1.61012900	-0.24019500
C	0	4.29778000	2.34812000	-1.25724100
C	0	5.57480600	2.03182800	-1.64316200
C	0	6.26726600	0.96956300	-1.00920800
C	0	5.63860900	0.22123800	-0.04969600
C	0	4.29647400	0.49520800	0.35564700
H	0	3.93999600	-1.80767500	2.88308300
H	0	4.67860700	-2.14652000	1.32090900
H	0	5.39806500	-0.94976600	2.41067500
H	0	2.14888500	-1.57911300	3.15355300
H	0	-0.22967800	-1.32249000	3.54332000

H	0	-2.31378000	-0.21334100	3.19355600
H	0	-3.72815300	1.56852900	2.03874800
H	0	-2.64682400	2.96796700	0.20936500
H	0	-0.32869600	2.71438200	-0.26497600
H	0	1.13638100	3.74759000	0.53843600
H	0	2.67787100	4.03020000	-0.23743700
H	0	1.33339000	3.41512700	-1.18910300
H	0	3.78418700	3.15464100	-1.76490900
H	0	6.05800300	2.60003500	-2.43213200
H	0	7.29519000	0.75248200	-1.27658200
H	0	6.17975800	-0.58582100	0.42497700
C	-1	6.09736300	7.01066000	-1.08001500
C	-1	5.60322800	5.60522100	-1.44238100
H	0	5.34087700	7.77010700	-1.30332900
H	0	5.36474700	5.52380700	-2.50845200
H	0	6.35353900	4.84351200	-1.21211900
H	0	4.69947900	5.34579500	-0.88184900
C	-1	8.44966700	0.31928600	4.36593500
C	-1	7.66934900	1.25999000	3.39998100
C	-1	8.35178800	1.79971200	2.29272900
C	-1	6.32909800	1.59667000	3.66315200
C	-1	7.68794600	2.75158200	1.47373300
C	-1	5.71704800	2.52768800	2.78156000
C	-1	6.35442900	3.13963500	1.70506500
H	0	8.97816400	0.90771000	5.12424400
H	0	9.19178700	-0.27172000	3.82210700
H	0	9.37948700	1.51884800	2.08863500
H	0	5.78382500	1.16859100	4.49594400
H	0	8.22714600	3.17349700	0.62848700
H	0	4.67221100	2.77320800	2.96516300
H	0	5.83980200	3.83635700	1.05668800
C	-1	8.70359200	-0.91538100	-4.83162600
C	-1	8.37909100	-1.97592800	-3.81473200
C	-1	8.99304500	-3.25373900	-3.78513100
C	-1	7.40569200	-1.67761900	-2.91602100
C	-1	8.68250100	-4.16991700	-2.75210000
C	-1	7.02083900	-2.61446100	-1.92133100
C	-1	7.62753700	-3.88997000	-1.89151700
H	0	9.41084100	-1.26779100	-5.58885100
H	0	9.14927700	-0.03644900	-4.35147000
H	0	9.77082300	-3.48935900	-4.50627300

H	0	6.90934000	-0.71335000	-2.94475600
H	0	9.18878700	-5.12997300	-2.71533600
H	0	6.21555700	-2.37415900	-1.23506800
H	0	7.32595100	-4.61041700	-1.13674000
C	-1	3.55523800	-1.60558100	-2.94490000
C	-1	2.44176300	-1.64416500	-1.88893300
O	-1	2.64001100	-2.30250500	-0.87699800
H	0	3.82460000	-2.63735800	-3.17883400
H	0	4.43627700	-1.12174000	-2.51710600
N	-1	1.27317200	-1.09916200	-2.24521100
C	-1	0.08953700	-1.36888500	-1.43099400
C	-1	-0.89369000	-0.34103900	-1.80392100
H	0	1.15967400	-0.69573000	-3.16096600
H	0	0.38621000	-1.30177500	-0.38322700
H	0	-1.78730500	-0.37482700	-1.17482700
H	0	-0.46538900	0.65795300	-1.69463500
H	0	-1.22215200	-0.45427900	-2.84631900
C	-1	2.10683300	-4.36770300	2.32925800
C	-1	2.59117600	-4.47938700	3.75867800
O	-1	2.88474000	-3.47711500	4.36736500
O	-1	2.65108500	-5.63765600	4.25772800
H	0	2.84820700	-3.83468300	1.73102700
H	0	1.20263900	-3.75453700	2.31800000
H	0	-6.22908000	4.11672400	2.85695000
H	0	-7.11552600	1.97032400	4.26338600
H	0	-7.76711000	-3.09996500	3.42900200
H	0	-7.27395300	-4.79007100	1.35295300
H	0	-5.38381500	-4.31071100	-3.62717500
H	0	-4.46267500	-2.16930000	-5.03626400
H	0	-3.78713900	3.05639200	-4.20185200
H	0	-4.31993600	4.68979800	-2.09466000
H	0	-7.63231200	2.56200900	-1.72188100
H	0	1.89468900	-5.33568700	1.87131300
H	0	7.77165300	-0.36496500	4.88354400
H	0	7.80041800	-0.57727600	-5.35038800
H	0	7.00256000	7.27110500	-1.63831000
H	0	6.33456900	7.08245700	-0.01362000
H	0	-0.27458000	-2.39042600	-1.60554100
H	0	3.28458200	-1.08248700	-3.86817600
H	0	2.96878300	-5.55009300	5.17406900

R2

C	0	9.14797800	0.30948900	0.66931700
S	0	8.14480200	-1.17218000	0.94627600
H	0	9.16951000	0.50927000	-0.40805400
H	0	10.17257100	0.12843400	1.00364500
C	-1	-6.38135500	5.69365700	3.84064800
C	-1	-5.73878800	4.38137200	3.35188800
H	0	-5.84367700	6.56502900	3.45344000
H	0	-4.69694200	4.29975100	3.67841300
H	0	-6.27779500	3.50724500	3.73194400
H	0	-5.74692200	4.31482000	2.25908600
C	-1	-7.30745300	4.38939500	-3.96575000
C	-1	-5.95241700	4.50227100	-3.24290500
C	-1	-5.87598600	4.28948400	-1.85996300
C	-1	-4.79526000	4.81574700	-3.96809600
C	-1	-4.64305100	4.39207500	-1.20138900
C	-1	-3.56112500	4.91743600	-3.31118800
C	-1	-3.48649800	4.70663000	-1.92748300
H	0	-7.87209000	5.32579200	-3.88731700
H	0	-7.92028600	3.59636700	-3.52761600
H	0	-6.77008200	4.02545300	-1.30270600
H	0	-4.85847400	4.97108900	-5.04132200
H	0	-4.57859200	4.20356700	-0.13405500
H	0	-2.66320400	5.15617200	-3.87380400
H	0	-2.53019500	4.77492900	-1.41747900
N	-1	-1.12809300	-2.66018800	0.50436700
C	-1	-0.21824700	-1.73380400	-0.18464500
C	-1	1.07989400	-1.58751200	0.63104000
H	0	-1.31373800	-2.41513200	1.47283000
H	0	-0.69003400	-0.75906100	-0.33382000
H	0	1.55590600	-2.56351300	0.76248300
H	0	1.78973200	-0.92941700	0.12470200
H	0	0.87753700	-1.16225700	1.61904800
C	-1	-3.69805300	-3.09403800	0.44195400
C	-1	-2.36715800	-2.80004500	-0.27464300
O	-1	-2.33967700	-2.67865400	-1.52666900
H	0	-4.33106000	-3.67963400	-0.22495400

H	0	-4.19001200	-2.13311800	0.63266000
C	-1	-4.47365000	-3.71540900	-3.87399400
N	-1	-3.99673900	-2.47502100	-3.72317000
O	-1	-5.19304700	-3.99638900	-4.86750000
H	0	-4.17272600	-1.83122500	-4.47891700
H	0	-3.33625800	-2.26928100	-2.98199800
C	-1	-11.21611300	-2.89423300	1.38898900
C	-1	-9.88815600	-3.59519200	1.04704900
C	-1	-8.66965800	-2.95611200	1.31376800
C	-1	-9.89821200	-4.87173100	0.46897000
C	-1	-7.46132000	-3.59415700	1.00270400
C	-1	-8.68977200	-5.50949600	0.15771300
C	-1	-7.47131100	-4.87070500	0.42464100
H	0	-11.90738400	-2.92767500	0.54101400
H	0	-11.04988000	-1.84687900	1.65383800
H	0	-8.66338700	-1.96514900	1.75695100
H	0	-10.84503000	-5.36093200	0.25781100
H	0	-6.52132500	-3.08918000	1.20266100
H	0	-8.69734600	-6.49583400	-0.29648700
H	0	-6.53543600	-5.36342200	0.17776100
C	0	-3.52862800	1.05733200	3.96726700
C	0	-3.30801100	1.10317700	2.47192900
C	0	-2.03830100	1.30775000	1.91365600
C	0	-0.85162300	1.27742600	2.74134300
C	0	0.39310300	1.42159500	2.22816100
C	0	0.58877000	1.76574900	0.84760800
C	0	1.88218700	2.03427600	0.36009200
C	0	2.07337500	2.48884900	-0.93289600
C	0	0.95401000	2.73665800	-1.73927900
C	0	-0.32551000	2.44259800	-1.28482000
C	0	-0.54424500	1.87858000	-0.00847400
C	0	-1.86726100	1.45273500	0.47871700
C	0	-2.93621100	1.12052900	-0.37159200
C	0	-2.77024200	0.88054100	-1.85686200
C	0	-4.22742400	0.88743700	0.18942900
C	0	-5.36366200	0.63721300	-0.63829500
C	0	-6.61303400	0.42291400	-0.10808100
C	0	-6.80149700	0.45020500	1.29373000
C	0	-5.73567800	0.69222500	2.12571200
C	0	-4.42273900	0.91799200	1.61295300
H	0	-2.67114500	1.42200000	4.52961900

H	0	-4.37398400	1.69184800	4.24828400
H	0	-3.75565300	0.04338600	4.31959500
H	0	-0.95861600	1.06485700	3.79718100
H	0	1.27031500	1.32035000	2.86143600
H	0	2.73248700	1.87811500	1.01511000
H	0	3.07780700	2.66542300	-1.30264600
H	0	1.08117000	3.16068500	-2.73091500
H	0	-1.16736800	2.68492000	-1.91720300
H	0	-3.37182600	0.02009400	-2.15603500
H	0	-3.09041200	1.73738700	-2.46172600
H	0	-1.73765400	0.64753100	-2.11146300
H	0	-5.24790900	0.63864500	-1.71377000
H	0	-7.45640200	0.23541300	-0.76498800
H	0	-7.79087600	0.28845900	1.71061800
H	0	-5.89539900	0.70420600	3.19666400
N	0	6.23223100	1.47171500	0.02900100
N	0	6.64046700	-0.81371000	-1.60406300
N	0	4.85633100	-0.15741900	1.93409800
C	-1	5.39505100	2.23592200	2.21513000
C	-1	7.33587100	1.48606000	-2.17489300
C	-1	6.25928100	-3.24728300	-1.79246400
C	-1	4.00816700	-2.43081600	2.40128300
C	0	6.02253300	2.43478100	0.99230600
C	0	7.23694600	0.12076300	-2.42880500
C	0	5.53709300	-3.42583700	-0.62396900
C	0	4.17886300	-1.07835700	2.70001300
O	0	4.16549500	-0.13314700	-0.69214100
C	0	6.54580600	3.70179600	0.54100000
C	0	7.76665700	-0.53435800	-3.60026100
C	0	5.00293000	-4.69454700	-0.18661000
C	0	3.70080200	-0.44843500	3.90721800
C	0	7.05986300	3.49793900	-0.70450700
C	0	7.47746300	-1.86058000	-3.48411500
C	0	4.35985000	-4.46388900	0.98976300
C	0	4.11080900	0.85217900	3.86879100
C	0	6.86807000	2.10195500	-1.01587200
C	0	6.76170400	-2.03368900	-2.24432300
C	0	4.50692300	-3.05590500	1.27417500
C	0	4.83036500	1.03004200	2.63007000
N	0	5.22757200	-2.44109700	0.27856600
H	0	5.30107800	3.08836000	2.87859900

H	0	7.82954200	2.10488000	-2.91554700
H	0	6.43445400	-4.11880700	-2.41351000
H	0	3.45097700	-3.03203200	3.11090700
Fe	0	5.55619400	-0.44002000	0.06845200
H	0	-11.71103500	-3.38218000	2.23635200
H	0	-6.37383700	5.75665400	4.93370400
H	0	-7.42205600	5.77157600	3.51003700
H	0	-7.16939700	4.17091200	-5.02790900
H	0	-0.00745000	-2.15559500	-1.16698100
H	0	-3.55683600	-3.61364200	1.39320700
H	0	-4.19907400	-4.42456600	-3.07566400
H	0	7.71521500	-2.66176600	-4.17068600
H	0	8.28955500	-0.02918600	-4.40117200
H	0	5.11679100	-5.62635100	-0.72352400
H	0	3.83598500	-5.16689600	1.62295800
H	0	7.53976700	4.21271200	-1.35931700
H	0	6.51220400	4.61896900	1.11333900
H	0	3.14009400	-0.95319000	4.68233300
H	0	3.95104900	1.62956400	4.60382100
H	0	8.72235300	1.18015700	1.17113100

TS2-1

C	0	8.77821000	0.00229500	0.83570000
S	0	7.71519300	-1.44164200	1.10371800
H	0	8.77744400	0.24258400	-0.23283000
H	0	9.80316600	-0.24267200	1.12728700
C	-1	-6.61298700	5.38504300	4.79869400
C	-1	-5.99377100	4.10846300	4.19815200
H	0	-6.09536300	6.28072800	4.44131200
H	0	-4.93773500	4.01463300	4.47374300
H	0	-6.51033900	3.21040500	4.55287000
H	0	-6.05250500	4.11514800	3.10429300
C	-1	-7.73112600	4.67637900	-3.05915600
C	-1	-6.35876900	4.72487600	-2.36227100
C	-1	-6.25229400	4.40848900	-1.00131900
C	-1	-5.21591300	5.08340700	-3.08926000

C	-1	-5.00358900	4.45242600	-0.36638300
C	-1	-3.96604000	5.12658200	-2.45607300
C	-1	-3.86133900	4.81211300	-1.09415900
H	0	-8.34352000	5.54205600	-2.78154100
H	0	-8.28459700	3.77656100	-2.77324000
H	0	-7.13769600	4.11542300	-0.44406600
H	0	-5.30327300	5.32058900	-4.14572000
H	0	-4.91743600	4.18815600	0.68180300
H	0	-3.07847300	5.39653400	-3.02091400
H	0	-2.89154900	4.82316200	-0.60578700
N	-1	-1.51399900	-2.73319200	0.72342200
C	-1	-0.61199100	-1.76445800	0.08418700
C	-1	0.70594700	-1.68918900	0.87747600
H	0	-1.66544900	-2.58308100	1.71604200
H	0	-1.08312500	-0.78510900	0.01845800
H	0	1.13097200	-2.68929500	1.00049300
H	0	1.44625700	-1.07371500	0.36162000
H	0	0.54833500	-1.25464000	1.87144800
C	-1	-4.08853300	-3.14242900	0.68976300
C	-1	-2.77190100	-2.80535100	-0.03424500
O	-1	-2.77238100	-2.59066900	-1.27409700
H	0	-4.69265400	-3.77750800	0.04047600
H	0	-4.62492200	-2.19870900	0.84042200
C	-1	-4.96948600	-3.43288300	-3.64077000
N	-1	-4.47775300	-2.21079900	-3.40915900
O	-1	-5.71392000	-3.63341700	-4.63536500
H	0	-4.75044000	-1.48216600	-4.04980000
H	0	-3.90482600	-2.03753000	-2.59079900
C	-1	-11.58055500	-2.95949200	1.82730200
C	-1	-10.26725200	-3.64249700	1.40248400
C	-1	-9.03718300	-3.03409900	1.68723600
C	-1	-10.30221100	-4.87200500	0.73097900
C	-1	-7.84217600	-3.65582100	1.30073800
C	-1	-9.10710600	-5.49342500	0.34431000
C	-1	-7.87707500	-4.88533000	0.62924900
H	0	-12.05917100	-2.46624400	0.97341000
H	0	-11.39905900	-2.20138600	2.59360300
H	0	-9.01569200	-2.08355300	2.21266600
H	0	-11.25766700	-5.34214100	0.51612400
H	0	-6.88976400	-3.18544000	1.52558300
H	0	-9.13362100	-6.44603400	-0.17620100

H	0	-6.95156600	-5.36902000	0.33087600
C	0	-2.25842700	2.31455400	2.87775100
C	0	-2.11211800	1.91262400	1.42690300
C	0	-0.84988400	1.87660500	0.80800800
C	0	0.34422500	2.01017400	1.59981700
C	0	1.58737500	1.83563500	1.07190200
C	0	1.76795800	1.65139900	-0.32361800
C	0	3.11279500	1.54993900	-0.84957600
C	0	3.29114200	1.62726600	-2.26620300
C	0	2.19248500	1.73459200	-3.09223500
C	0	0.88997100	1.75263500	-2.56819000
C	0	0.63800500	1.62757300	-1.18383100
C	0	-0.71260800	1.56990700	-0.60417200
C	0	-1.84102100	1.12859200	-1.31871700
C	0	-1.74239400	0.45742700	-2.67202100
C	0	-3.11927300	1.13984100	-0.68763700
C	0	-4.29624500	0.74673400	-1.39184500
C	0	-5.52326200	0.68071300	-0.78026000
C	0	-5.64778200	1.01032900	0.59084000
C	0	-4.54857900	1.43079100	1.29733100
C	0	-3.25765800	1.52498100	0.69047900
H	0	-1.45270000	2.97361000	3.20087000
H	0	-3.18904500	2.86215000	3.04003000
H	0	-2.26963400	1.44798000	3.55145800
H	0	0.25154800	2.17649500	2.66507700
H	0	2.46468900	1.86088200	1.70852300
H	0	3.88633100	1.98702700	-0.23503200
H	0	4.29823400	1.60628600	-2.66500200
H	0	2.32591500	1.83102300	-4.16565800
H	0	0.07090900	1.92409500	-3.25057000
H	0	-2.41516800	-0.39811800	-2.71237300
H	0	-1.99484800	1.12385400	-3.50612000
H	0	-0.74252300	0.06454500	-2.84708200
H	0	-4.22683900	0.51105500	-2.44482100
H	0	-6.39612100	0.37635200	-1.34873000
H	0	-6.61545700	0.94300800	1.07907900
H	0	-4.66305700	1.68356200	2.34426000
N	0	5.88367100	1.37563800	0.38756700
N	0	6.19976600	-0.78293100	-1.43891200
N	0	4.51542300	-0.38250000	2.19086700
C	-1	5.09093000	1.97323300	2.64008700

C	-1	6.92284900	1.54044200	-1.83851800
C	-1	5.81269100	-3.20028900	-1.78562000
C	-1	3.66664600	-2.68412300	2.50969900
C	0	5.72835400	2.25767100	1.43756200
C	0	6.78816800	0.20268500	-2.20348800
C	0	5.08838200	-3.46153900	-0.63080800
C	0	3.85952100	-1.35877800	2.90499500
O	0	3.64636500	-0.16041000	-0.44289800
C	0	6.28885500	3.54041100	1.08487300
C	0	7.28057700	-0.36531300	-3.43592300
C	0	4.58605000	-4.76746600	-0.25868200
C	0	3.42376600	-0.82170300	4.17274400
C	0	6.77526300	3.42709600	-0.18440000
C	0	6.98948100	-1.69647500	-3.40597000
C	0	3.96952700	-4.62075200	0.94463100
C	0	3.83310800	0.47821800	4.21874200
C	0	6.52796200	2.07082300	-0.61135400
C	0	6.30234000	-1.95500200	-2.16376500
C	0	4.10248300	-3.22701600	1.31178300
C	0	4.51804800	0.74633100	2.97593300
N	0	4.76852600	-2.53930400	0.32970500
H	0	5.02543500	2.77081900	3.37237100
H	0	7.41410700	2.20590500	-2.54002900
H	0	5.99257100	-4.02837000	-2.46264600
H	0	3.14578500	-3.33738900	3.20116400
Fe	0	5.16893600	-0.52327600	0.29040500
H	0	-12.29114500	-3.68919100	2.22679400
H	0	-6.55223200	5.37779500	5.89161200
H	0	-7.66836300	5.47900500	4.52404200
H	0	-7.62001100	4.67916000	-4.14646500
H	0	-0.42702500	-2.11395700	-0.93132000
H	0	-3.93128300	-3.62637600	1.65680900
H	0	-4.66581900	-4.20545100	-2.91536600
H	0	7.20836600	-2.44741800	-4.15310500
H	0	7.78739600	0.19356900	-4.21124400
H	0	4.70687800	-5.66488100	-0.85018100
H	0	3.48064500	-5.37313600	1.54865500
H	0	7.27094600	4.18015000	-0.78222700
H	0	6.30168700	4.40619100	1.73325900
H	0	2.88698800	-1.38316800	4.92568300
H	0	3.69748400	1.19782200	5.01507100

H	0	8.41886400	0.87327500	1.38677700
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IM2

C	0	8.76434800	0.01049600	0.86284400
S	0	7.68731400	-1.39121700	1.28437400
H	0	8.75695900	0.15866100	-0.22174800
H	0	9.78910300	-0.21888300	1.16851800
C	-1	-6.64519600	5.38680900	4.83376100
C	-1	-6.02398200	4.11181500	4.23189800
H	0	-6.16902400	6.28619100	4.43092800
H	0	-4.95337400	4.05015600	4.45634400
H	0	-6.49926000	3.21009600	4.63201600
H	0	-6.13669200	4.09144600	3.14233000
C	-1	-7.77361300	4.67795900	-3.02259800
C	-1	-6.40031700	4.72938000	-2.32777500
C	-1	-6.29106100	4.41282700	-0.96708100
C	-1	-5.25938400	5.09073800	-3.05638300
C	-1	-5.04150000	4.45942500	-0.33401600
C	-1	-4.00865600	5.13657700	-2.42507500
C	-1	-3.90117600	4.82193700	-1.06341700
H	0	-8.36631400	5.56952300	-2.78711800
H	0	-8.34674100	3.80539200	-2.69481300
H	0	-7.17541100	4.11898600	-0.40856000
H	0	-5.34878300	5.32787700	-4.11267500
H	0	-4.95416600	4.19943600	0.71491400
H	0	-3.12273000	5.40923200	-2.99118300
H	0	-2.93085400	4.83669400	-0.57617500
N	-1	-1.53386800	-2.71853600	0.74830800
C	-1	-0.63504200	-1.74755200	0.10800300
C	-1	0.68392000	-1.66951400	0.89932000
H	0	-1.68151100	-2.57384600	1.74220300
H	0	-1.10989400	-0.76905600	0.04116000
H	0	1.09742900	-2.67218900	1.03977700
H	0	1.43389600	-1.07442000	0.37543700
H	0	0.53093100	-1.21836400	1.88664500
C	-1	-4.10750800	-3.13364100	0.71842000

C	-1	-2.79274600	-2.79333900	-0.00747700
O	-1	-2.79559400	-2.57828600	-1.24726100
H	0	-4.71184600	-3.76894900	0.06958200
H	0	-4.64524900	-2.19111800	0.87147600
C	-1	-4.99435000	-3.42480000	-3.61086500
N	-1	-4.50505900	-2.20166600	-3.37962400
O	-1	-5.73983000	-3.62673300	-4.60439200
H	0	-4.78128400	-1.47384900	-4.01972300
H	0	-3.93068800	-2.02770900	-2.56229500
C	-1	-11.59819800	-2.96815500	1.86735000
C	-1	-10.28398200	-3.64803200	1.44033700
C	-1	-9.05487700	-3.03691200	1.72341300
C	-1	-10.31715100	-4.87741300	0.76851000
C	-1	-7.85904000	-3.65578600	1.33491800
C	-1	-9.12121800	-5.49598600	0.37984400
C	-1	-7.89214800	-4.88517000	0.66310600
H	0	-12.08310500	-2.48229900	1.01279600
H	0	-11.41640500	-2.20472600	2.62825700
H	0	-9.03493900	-2.08665000	2.24942800
H	0	-11.27183000	-5.34970700	0.55500200
H	0	-6.90722600	-3.18389000	1.55928800
H	0	-9.14631800	-6.44857000	-0.14075100
H	0	-6.96603100	-5.36697300	0.36354700
C	0	-2.09364100	2.44976800	2.77488100
C	0	-1.99374600	2.00012600	1.33466100
C	0	-0.74712700	1.92401100	0.68367600
C	0	0.46449100	2.04560800	1.43969400
C	0	1.69191200	1.76103100	0.89952500
C	0	1.82626600	1.48737300	-0.47222800
C	0	3.20567700	1.15166700	-0.98715900
C	0	3.30239400	1.09247600	-2.47214800
C	0	2.22586700	1.36196700	-3.26074100
C	0	0.94105900	1.60036200	-2.70331500
C	0	0.69188300	1.53234200	-1.31697900
C	0	-0.65201000	1.56795100	-0.72058000
C	0	-1.80629700	1.14161900	-1.39889300
C	0	-1.75500100	0.45571100	-2.74664400
C	0	-3.06697400	1.18304100	-0.73131700
C	0	-4.26749400	0.78542500	-1.39019200
C	0	-5.47328300	0.72861700	-0.73573300
C	0	-5.55128200	1.07515400	0.63422700

C	0	-4.42970900	1.50929000	1.29555600
C	0	-3.16057600	1.59537100	0.64320900
H	0	-1.28152800	3.12429600	3.04664400
H	0	-3.02231800	2.99622900	2.95104700
H	0	-2.07350400	1.60595900	3.47646000
H	0	0.40630500	2.27867200	2.49494500
H	0	2.57885900	1.75814800	1.52199200
H	0	3.90242200	1.92452300	-0.62932200
H	0	4.26869300	0.83784600	-2.89128100
H	0	2.32460200	1.36969800	-4.34253300
H	0	0.13809800	1.86183400	-3.37774600
H	0	-2.45489500	-0.37808300	-2.77133500
H	0	-1.99797100	1.12445200	-3.58156800
H	0	-0.77094800	0.02912400	-2.93595200
H	0	-4.23506400	0.53434500	-2.44129000
H	0	-6.36488300	0.41751800	-1.27038000
H	0	-6.50123000	1.01294800	1.15652500
H	0	-4.50845700	1.77838300	2.34169600
N	0	5.85249800	1.41963400	0.39798200
N	0	6.16752300	-0.74679800	-1.43830000
N	0	4.49643800	-0.35913900	2.22317700
C	-1	5.06319400	2.00238000	2.65641100
C	-1	6.88931500	1.57512400	-1.82509200
C	-1	5.79006300	-3.16814500	-1.77196100
C	-1	3.64935000	-2.65817600	2.52675700
C	0	5.68381000	2.29749000	1.44536000
C	0	6.76224100	0.23724000	-2.19480500
C	0	5.07869500	-3.44177500	-0.61125800
C	0	3.84190000	-1.33551800	2.93242700
O	0	3.55305400	-0.10741300	-0.39747800
C	0	6.23051300	3.58645700	1.08777100
C	0	7.25475100	-0.32979100	-3.42781200
C	0	4.57316700	-4.74782900	-0.24051800
C	0	3.40596900	-0.79843600	4.20166600
C	0	6.72272800	3.47484500	-0.17975600
C	0	6.96045000	-1.66134400	-3.39864100
C	0	3.95611000	-4.60171800	0.96331300
C	0	3.81833800	0.50082300	4.24850900
C	0	6.49301800	2.11323700	-0.60266100
C	0	6.27266400	-1.92017600	-2.15607200
C	0	4.09316600	-3.20856300	1.33405700

C	0	4.50198700	0.77088600	3.00327200
N	0	4.76347300	-2.52591900	0.35439000
H	0	4.99654900	2.80067300	3.38805000
H	0	7.38078000	2.24048900	-2.52695700
H	0	5.97046500	-3.99386000	-2.45213700
H	0	3.12381700	-3.31201000	3.21472400
Fe	0	5.19631700	-0.51039600	0.32194200
H	0	-12.30363400	-3.69854100	2.27465700
H	0	-6.53027900	5.40686100	5.92210100
H	0	-7.71491300	5.44821300	4.61025100
H	0	-7.66282100	4.62735800	-4.10881600
H	0	-0.45108800	-2.09705400	-0.90775900
H	0	-3.94781000	-3.61846100	1.68459400
H	0	-4.68764100	-4.19697200	-2.88640300
H	0	7.18120800	-2.41223100	-4.14536000
H	0	7.76632600	0.22752400	-4.20110500
H	0	4.68903200	-5.64482500	-0.83375600
H	0	3.46410700	-5.35462200	1.56420100
H	0	7.21165700	4.23209500	-0.77786100
H	0	6.23292800	4.45486200	1.73289500
H	0	2.86911300	-1.35893800	4.95534900
H	0	3.68368900	1.21916200	5.04629400
H	0	8.42659200	0.93257300	1.34052900

TS2-2

C	0	8.61737300	-0.20027000	0.68261500
S	0	7.25618700	-1.22483600	1.33943700
H	0	8.68278100	-0.28553600	-0.40430100
H	0	9.54663100	-0.57282800	1.12221000
C	-1	-6.60727200	5.45251800	4.74164400
C	-1	-5.98794300	4.16700000	4.15809500
H	0	-6.05878500	6.34008700	4.41129100
H	0	-4.94596000	4.05176300	4.47585100
H	0	-6.53537800	3.27707700	4.48587400
H	0	-6.00381900	4.18246100	3.06253000
C	-1	-7.75091900	4.63400000	-3.10088100

C	-1	-6.37642100	4.69589700	-2.40941700
C	-1	-6.26423500	4.39857200	-1.04479900
C	-1	-5.23701300	5.04779900	-3.14514300
C	-1	-5.01371100	4.45451400	-0.41408000
C	-1	-3.98516400	5.10333200	-2.51681200
C	-1	-3.87506400	4.80775300	-1.15128100
H	0	-8.36874000	3.83794400	-2.67546900
H	0	-7.64347700	4.45025700	-4.17316700
H	0	-7.14750300	4.11225200	-0.48088400
H	0	-5.32823200	5.26973600	-4.20458900
H	0	-4.92514700	4.21383800	0.63934300
H	0	-3.10074600	5.36969100	-3.08820800
H	0	-2.90400200	4.83301100	-0.66572400
N	-1	-1.49887800	-2.70602800	0.75934500
C	-1	-0.60205100	-1.74296100	0.10418400
C	-1	0.71835000	-1.65327400	0.89196900
H	0	-1.63988200	-2.55630100	1.75326700
H	0	-1.08121300	-0.76878100	0.02581500
H	0	1.12259500	-2.65493900	1.06133900
H	0	1.47903700	-1.08455200	0.35242900
H	0	0.57105400	-1.17425800	1.86681700
C	-1	-4.07233200	-3.12296600	0.74025700
C	-1	-2.75942400	-2.79203800	0.00706500
O	-1	-2.76452600	-2.59312100	-1.23529600
H	0	-4.67885500	-3.76560700	0.10074800
H	0	-4.61025000	-2.17926900	0.88492800
C	-1	-4.96675300	-3.47431400	-3.58324700
N	-1	-4.47859500	-2.24768200	-3.36937700
O	-1	-5.71446800	-3.69017200	-4.57223800
H	0	-4.76590800	-1.52793700	-4.01370100
H	0	-3.90948100	-2.06099100	-2.55122800
C	-1	-11.56100200	-2.94672100	1.90087800
C	-1	-10.24711800	-3.63151500	1.48072400
C	-1	-9.01790600	-3.01569000	1.75302400
C	-1	-10.28070500	-4.87004100	0.82595000
C	-1	-7.82237300	-3.63912900	1.37084600
C	-1	-9.08507400	-5.49309600	0.44353000
C	-1	-7.85592400	-4.87761400	0.71606600
H	0	-11.37211600	-2.13356400	2.60640800
H	0	-12.24173300	-3.66082600	2.37423500
H	0	-8.99791900	-2.05823000	2.26582300

H	0	-11.23543900	-5.34566400	0.62019000
H	0	-6.87034700	-3.16388200	1.58732100
H	0	-9.11048200	-6.45266000	-0.06401000
H	0	-6.93011600	-5.36309100	0.42150700
C	0	-2.35304400	2.46126200	2.75016100
C	0	-2.16102400	1.99452600	1.32470400
C	0	-0.87478900	1.92379000	0.74892600
C	0	0.28010100	2.08441400	1.57655800
C	0	1.55072100	1.84465200	1.12374200
C	0	1.77142400	1.53370100	-0.22949700
C	0	3.19056100	1.26533100	-0.65931300
C	0	3.39295700	1.18097400	-2.11327200
C	0	2.32744500	1.25807000	-2.99382300
C	0	1.03599300	1.46877900	-2.51718700
C	0	0.69453100	1.48625200	-1.13141700
C	0	-0.68465400	1.53624300	-0.63770200
C	0	-1.79707200	1.09899500	-1.38214800
C	0	-1.66184500	0.37450800	-2.70482300
C	0	-3.09446000	1.15724000	-0.79821600
C	0	-4.25459600	0.76365100	-1.53175200
C	0	-5.49607100	0.70506500	-0.95243500
C	0	-5.65938800	1.04431400	0.41361200
C	0	-4.58387800	1.48167100	1.14196200
C	0	-3.27656300	1.57479400	0.56723100
H	0	-1.57383700	3.15754000	3.06009500
H	0	-3.30097900	2.98923000	2.86482900
H	0	-2.35589400	1.62634500	3.46212400
H	0	0.14571800	2.33000700	2.62210500
H	0	2.39898800	1.89560800	1.79736800
H	0	3.85992200	1.97758700	-0.16769100
H	0	4.40568200	1.00796300	-2.44881500
H	0	2.49220100	1.18500000	-4.06383200
H	0	0.26124500	1.65860100	-3.24593300
H	0	-2.39255400	-0.42898400	-2.77258200
H	0	-1.79821900	1.02696000	-3.57603400
H	0	-0.68902400	-0.10858100	-2.79291000
H	0	-4.15805500	0.51965200	-2.58044000
H	0	-6.35334700	0.39576800	-1.54131900
H	0	-6.63930000	0.97496100	0.87561600
H	0	-4.72695900	1.75060200	2.18111100
N	0	5.92052300	1.39926300	0.35574900

N	0	6.17142800	-0.75416600	-1.47246400
N	0	4.50037300	-0.31439500	2.15905700
C	-1	5.09839400	2.04533000	2.59002500
C	-1	6.91637400	1.55775500	-1.88865600
C	-1	5.82052500	-3.18512000	-1.76819800
C	-1	3.68752300	-2.61752100	2.52706100
C	0	5.75718800	2.29743300	1.39159900
C	0	6.76971200	0.21693400	-2.24332600
C	0	5.11603600	-3.42670000	-0.59955500
C	0	3.85084500	-1.28107200	2.89110200
O	0	3.55177600	-0.08873300	-0.40749700
C	0	6.29979500	3.58207500	1.01603800
C	0	7.25750400	-0.36334800	-3.47379500
C	0	4.61786500	-4.72976200	-0.21057300
C	0	3.40255300	-0.72166800	4.14712100
C	0	6.77864600	3.45705600	-0.25419000
C	0	6.97027300	-1.69442300	-3.42278500
C	0	4.00546900	-4.56911900	0.99203600
C	0	3.80887700	0.57851200	4.17197200
C	0	6.54538300	2.09080700	-0.65831400
C	0	6.28899600	-1.93499200	-2.17072400
C	0	4.13584500	-3.16937100	1.33783100
C	0	4.50900200	0.82489100	2.92897300
N	0	4.79541300	-2.49014400	0.34902300
H	0	5.03205100	2.85357800	3.31012300
H	0	7.40537400	2.21632400	-2.59824400
H	0	6.00394200	-4.02335000	-2.43149500
H	0	3.17753400	-3.26823600	3.22902600
Fe	0	5.36004100	-0.53623300	0.34907900
H	0	-12.07830500	-2.52544100	1.03134300
H	0	-6.59058400	5.43712500	5.83585700
H	0	-7.64861800	5.56757500	4.42515600
H	0	-8.29496900	5.57762300	-2.97695800
H	0	-0.41975600	-2.10775000	-0.90654600
H	0	-3.90997900	-3.59697800	1.71129500
H	0	-4.65572300	-4.23702000	-2.85078800
H	0	7.18987000	-2.45710200	-4.15809800
H	0	7.76480000	0.18634000	-4.25553700
H	0	4.73500900	-5.63245300	-0.79504300
H	0	3.51551100	-5.31224900	1.60682700
H	0	7.25742500	4.20748600	-0.86917200

H	0	6.30128700	4.45791900	1.65125800
H	0	2.86317200	-1.27174800	4.90693400
H	0	3.67064900	1.31161800	4.95590500
H	0	8.49215700	0.85087200	0.95085200

P2

C	0	8.71234500	-0.28079600	0.51094700
S	0	7.34749600	-1.19373200	1.30545700
H	0	8.74840400	-0.48144000	-0.56113800
H	0	9.63801200	-0.63676400	0.97180500
C	-1	-6.50908800	5.41639300	4.81846700
C	-1	-5.89188500	4.13478700	4.22403000
H	0	-5.92908500	6.30072500	4.53662900
H	0	-4.86647900	3.98882700	4.57864900
H	0	-6.47060700	3.24789000	4.50276300
H	0	-5.86144000	4.18319100	3.12985300
C	-1	-7.70854900	4.63498000	-3.01948800
C	-1	-6.32915200	4.69575800	-2.33775200
C	-1	-6.20651900	4.39183400	-0.97549300
C	-1	-5.19572100	5.05324200	-3.07999400
C	-1	-4.95152400	4.44675600	-0.35363100
C	-1	-3.93941300	5.10777000	-2.46052900
C	-1	-3.81887400	4.80558200	-1.09732300
H	0	-8.05637300	3.59915100	-3.10564500
H	0	-7.66929800	5.06168800	-4.02474900
H	0	-7.08601600	4.10799800	-0.40454700
H	0	-5.29676100	5.28926700	-4.13541600
H	0	-4.85398400	4.20415500	0.69908100
H	0	-3.06003100	5.38246500	-3.03568900
H	0	-2.84481300	4.83165200	-0.61809500
N	-1	-1.41640100	-2.71359800	0.75841700
C	-1	-0.52597000	-1.74576700	0.10155800
C	-1	0.79999300	-1.65777600	0.88013800
H	0	-1.55636300	-2.55860000	1.75193200
H	0	-1.00411800	-0.77159300	0.03089400
H	0	1.21298100	-2.65779100	1.03845800

H	0	1.53765200	-1.07594100	0.32649700
H	0	0.66077700	-1.18057300	1.85652100
C	-1	-3.98923400	-3.13477700	0.75599600
C	-1	-2.68226100	-2.79802800	0.01491400
O	-1	-2.69674300	-2.59285800	-1.22634600
H	0	-4.59619000	-3.78023400	0.11969200
H	0	-4.53084100	-2.19345400	0.90264400
C	-1	-4.91456500	-3.46611700	-3.56258200
N	-1	-4.42691100	-2.23972300	-3.34613800
O	-1	-5.66912200	-3.67831000	-4.54716400
H	0	-4.75949700	-1.50944000	-3.95540500
H	0	-3.87895600	-2.04291800	-2.51627500
C	-1	-11.46952100	-2.97696600	1.97199900
C	-1	-10.15760700	-3.65744100	1.53887400
C	-1	-8.92746000	-3.04090400	1.80528400
C	-1	-10.19391900	-4.89274700	0.87818900
C	-1	-7.73371600	-3.66041400	1.41129800
C	-1	-9.00008100	-5.51187000	0.48396600
C	-1	-7.76999700	-4.89567800	0.75061100
H	0	-11.27857200	-2.18044300	2.69574900
H	0	-12.15407000	-3.69865500	2.42793000
H	0	-8.90499900	-2.08569000	2.32210100
H	0	-11.14937800	-5.36895500	0.67709100
H	0	-6.78115000	-3.18375000	1.62181700
H	0	-9.02764800	-6.46884500	-0.02838700
H	0	-6.84551800	-5.37762200	0.44626200
C	0	-2.92592400	2.16875100	2.68160400
C	0	-2.59012200	1.81501600	1.24991800
C	0	-1.24347600	1.84345300	0.82592400
C	0	-0.21167200	2.09120600	1.78650800
C	0	1.10825000	1.95039300	1.47158400
C	0	1.49846200	1.64355800	0.14636200
C	0	2.93615100	1.48823100	-0.12899900
C	0	3.39621500	1.34875400	-1.53547800
C	0	2.36076900	1.48187200	-2.56524800
C	0	1.05075900	1.55415600	-2.24425000
C	0	0.55084500	1.52693400	-0.87268300
C	0	-0.86826700	1.51004500	-0.53851800
C	0	-1.87759700	1.07430700	-1.43070900
C	0	-1.57254800	0.37915000	-2.74309800
C	0	-3.23286600	1.10571700	-1.01793600

C	0	-4.28721600	0.78842100	-1.93231300
C	0	-5.59258000	0.69368500	-1.53276000
C	0	-5.93165100	0.90239300	-0.17069400
C	0	-4.96589500	1.26845900	0.72742400
C	0	-3.59372200	1.42267700	0.34172100
H	0	-2.41466500	3.08475800	2.99061000
H	0	-3.98901000	2.34781000	2.82540000
H	0	-2.62670300	1.37900900	3.38185600
H	0	-0.48474600	2.33370400	2.80484200
H	0	1.87611500	2.06303500	2.23102600
H	0	3.61137300	1.89225800	0.60993300
H	0	4.40579400	1.64151200	-1.79255500
H	0	2.67923100	1.63096100	-3.59218100
H	0	0.34575000	1.75106600	-3.03810500
H	0	-2.27600200	-0.43633200	-2.90649800
H	0	-1.62552100	1.04486300	-3.61360500
H	0	-0.58513100	-0.07808300	-2.72970000
H	0	-4.04473100	0.64423100	-2.97696400
H	0	-6.36759600	0.45307700	-2.25317400
H	0	-6.96210900	0.79104100	0.15254200
H	0	-5.25221700	1.44421100	1.75652800
N	0	5.99558400	1.40173600	0.32308200
N	0	6.20043700	-0.73209600	-1.52127500
N	0	4.57228600	-0.31465600	2.10557500
C	-1	5.18616400	2.03973100	2.56467900
C	-1	6.97223000	1.57752200	-1.92950100
C	-1	5.88515200	-3.16773800	-1.82473100
C	-1	3.78260800	-2.62514100	2.48873700
C	0	5.85925000	2.28980900	1.37268500
C	0	6.77962900	0.24981300	-2.30111500
C	0	5.19924000	-3.41442000	-0.64851200
C	0	3.93319700	-1.28596600	2.84647600
O	0	3.36892300	0.19391200	-0.64270200
C	0	6.43510500	3.56371200	1.01616300
C	0	7.24088000	-0.31818200	-3.54519700
C	0	4.72300900	-4.72076300	-0.25254900
C	0	3.48623000	-0.73030200	4.10165600
C	0	6.90978300	3.44575800	-0.25645800
C	0	6.96912300	-1.65229300	-3.49645900
C	0	4.11661900	-4.56692400	0.95421300
C	0	3.88590900	0.57221300	4.12685900

C	0	6.63699400	2.09540100	-0.68283800
C	0	6.32122100	-1.90860100	-2.23176300
C	0	4.22875600	-3.16796100	1.29800700
C	0	4.58359800	0.82390000	2.88689100
N	0	4.87059600	-2.47490900	0.30011500
H	0	5.12602800	2.84177300	3.29168400
H	0	7.46124800	2.23592000	-2.63874300
H	0	6.07156900	-4.00275200	-2.49070500
H	0	3.28440500	-3.28044600	3.19433800
Fe	0	5.48270800	-0.54682300	0.33205300
H	0	-11.98337700	-2.53384400	1.11125200
H	0	-6.53835000	5.37043900	5.91170800
H	0	-7.53382600	5.56335400	4.46312600
H	0	-8.45745400	5.18606600	-2.44187000
H	0	-0.34977600	-2.10578400	-0.91192100
H	0	-3.81964500	-3.60786400	1.72633600
H	0	-4.58950300	-4.23440500	-2.84189500
H	0	7.17722300	-2.40769900	-4.24237600
H	0	7.72312800	0.24203600	-4.33507300
H	0	4.84637800	-5.62207000	-0.83766400
H	0	3.63886700	-5.31509200	1.57219500
H	0	7.40273300	4.19415000	-0.86240100
H	0	6.45633100	4.43040900	1.66327100
H	0	2.94874800	-1.28304300	4.86056500
H	0	3.74509200	1.30375200	4.91151600
H	0	8.62141700	0.79414700	0.67576400