

## Supporting Information

### Computational Insights into the Diverse Mechanisms in Cytochrome P450 2D6-Mediated Primaquine Metabolism

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**Table S1.** Binding free energy and its components (kcal·mol<sup>-1</sup>).

Systems	PQ-CYP2D6
$\Delta E_{vdW}$	-37.81
$\Delta E_{ele}$	-6.40
$\Delta G_{GB}$	20.63
$\Delta G_{SA}$	-5.08
$\Delta G_{polar}^a$	14.23
$\Delta G_{nonpolar}^b$	-42.89
$\Delta G_{mmgbsa}^c$	-28.66
$-T\Delta S$	5.93
$\Delta G_{bind}^d$	-8.77

<sup>a</sup>  $\Delta G_{polar} = \Delta E_{ele} + \Delta G_{GB}$ . <sup>b</sup>  $\Delta G_{nonpolar} = \Delta E_{vdW} + \Delta G_{SA}$ .

<sup>c</sup>  $\Delta G_{mmgbsa} = \Delta G_{polar} + \Delta G_{nonpolar}$ . <sup>d</sup>  $\Delta G_{bind} = \Delta G_{mmgbsa} - T\Delta S$ .

**Table S2.** Cartesian coordinates of the first model for analyzing ESP.

N	1.25500000	-2.31100000	0.13400000
C	1.75500000	4.01600000	-0.33300000
O	2.73600000	2.99400000	-0.35800000
N	-0.68200000	-0.45000000	0.08800000
C	2.33400000	1.69400000	-0.24500000
N	-5.65300000	-0.73500000	-1.52000000
C	0.97400000	1.32800000	-0.10400000
C	0.61000000	-0.01200000	0.00100000
C	1.64300000	-1.01800000	-0.00800000
C	3.00600000	-0.61900000	-0.15300000
C	2.18300000	-3.24900000	0.12600000
C	3.56200000	-2.97100000	-0.02500000
C	3.96800000	-1.66400000	-0.16100000
C	3.34100000	0.74600000	-0.27400000
C	-1.82000000	0.38800000	0.43300000
C	-1.75900000	0.86100000	1.89300000
C	-3.09900000	-0.39400000	0.10600000
C	-4.39200000	0.40800000	0.27900000
C	-5.64700000	-0.38400000	-0.09500000
H	1.19900000	4.02400000	0.61300000
H	2.29900000	4.95600000	-0.43600000
H	1.04500000	3.91900000	-1.16400000
H	-0.74300000	-1.44300000	0.28400000
H	-4.98100000	-1.47800000	-1.69600000
H	-6.56000000	-1.11500000	-1.77600000
H	0.20800000	2.08900000	-0.09000000
H	1.84300000	-4.27600000	0.24400000
H	4.27900000	-3.78500000	-0.02700000
H	5.01900000	-1.41400000	-0.27300000
H	-1.79600000	1.26700000	-0.22500000
H	-0.79300000	1.32700000	2.10400000
H	-2.54300000	1.59100000	2.11300000
H	-1.88000000	0.01000000	2.57200000
H	-3.13700000	-1.29100000	0.74300000
H	-3.01400000	-0.73900000	-0.93000000
H	-4.35000000	1.30700000	-0.34800000
H	-4.49100000	0.73800000	1.31900000
H	-5.73400000	-1.25500000	0.58100000
H	-6.52500000	0.24300000	0.09300000
H	4.37200000	1.06200000	-0.38200000

**Table S3.** Cartesian coordinates of the second model for analyzing ESP.

C	0.18500000	0.40000000	7.00400000
C	-0.06300000	-0.25000000	5.65800000
C	-0.61100000	0.51400000	4.60500000
C	0.23700000	-1.63200000	5.48200000
C	-0.84700000	-0.12200000	3.40000000
C	0.07700000	-2.23300000	4.19200000
C	-0.47800000	-1.45000000	3.19300000
H	-0.86300000	1.55900000	4.75800000
H	0.64400000	-2.19700000	6.31500000
H	-1.27900000	0.42500000	2.56900000
H	0.35100000	-3.26900000	4.02000000
H	-0.63400000	-1.87000000	2.20400000
C	6.46900000	4.87800000	-2.38100000
C	4.98900000	4.77000000	-1.88100000
H	7.05200000	4.01200000	-2.05400000
H	4.50800000	3.86900000	-2.27200000
H	4.94800000	4.72600000	-0.78800000
H	4.40000000	5.63200000	-2.20900000
N	-0.86200000	7.66500000	0.58300000
C	0.29000000	7.02900000	-0.17100000
C	-0.17500000	5.75100000	-0.82300000
O	0.09900000	5.46300000	-1.97900000
C	1.55500000	6.81900000	0.60600000
O	1.79000000	7.95000000	1.44200000
H	-0.53100000	8.57600000	0.89700000
H	0.55600000	7.66100000	-1.02900000
H	1.50900000	5.89900000	1.20700000
H	2.39500000	6.72500000	-0.08500000
H	1.21000000	7.85200000	2.20700000
N	-1.12500000	5.01700000	-0.18700000
C	-1.81500000	3.87200000	-0.78000000
C	-2.70500000	4.20100000	-1.95400000
O	-2.50800000	3.64300000	-3.06500000
C	-2.52600000	3.11400000	0.30400000
H	-1.45900000	5.36900000	0.70200000
H	-1.04500000	3.22500000	-1.21200000
H	-2.95800000	2.19100000	-0.09100000
H	-1.81000000	2.83400000	1.07700000
H	-3.33800000	3.70100000	0.75100000
C	-1.60000000	0.53900000	-3.93500000
H	-2.19100000	0.24900000	-4.80700000
H	-1.54700000	1.62500000	-3.86300000

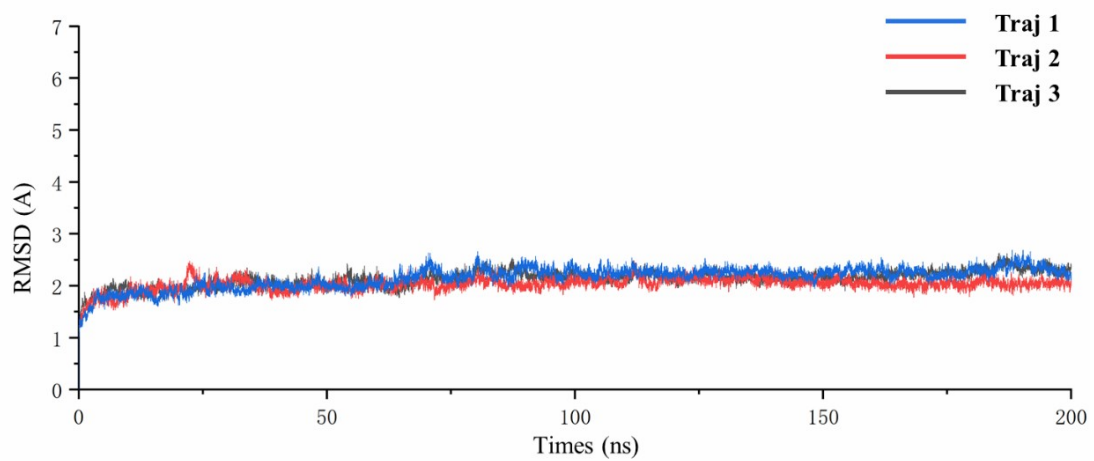
H	-2.07400000	0.14800000	-3.03100000
C	-6.39100000	-4.06500000	-0.72200000
S	-6.58200000	-2.28900000	-0.41600000
C	8.86800000	-2.24200000	-2.68800000
C	8.26800000	-2.94700000	-1.47100000
C	6.87700000	-3.09800000	-1.30700000
C	9.11700000	-3.61800000	-0.62300000
C	6.40400000	-3.82300000	-0.24300000
C	8.65300000	-4.30600000	0.51800000
C	7.28600000	-4.44300000	0.68100000
H	6.18700000	-2.62300000	-1.99900000
H	10.19000000	-3.54000000	-0.78500000
H	5.33100000	-3.92100000	-0.10100000
H	9.35400000	-4.77500000	1.20100000
H	6.87600000	-4.99200000	1.52300000
C	4.05200000	-1.10800000	-4.88900000
C	4.70500000	-0.14300000	-3.88000000
H	4.25300000	0.85200000	-3.93200000
H	4.57400000	-0.51000000	-2.85700000
H	5.77800000	-0.03200000	-4.07000000
N	-3.53800000	-3.12400000	0.05400000
N	-4.47700000	-1.60000000	-2.17700000
N	-4.39800000	-1.08100000	1.83500000
C	-3.54800000	-3.28500000	2.52100000
C	-3.22900000	-3.75200000	-2.31300000
C	-5.66100000	0.47000000	-2.90600000
C	-5.28000000	1.20300000	1.99900000
C	-3.28200000	-3.77400000	1.24500000
C	-3.90100000	-2.65500000	-2.87000000
C	-5.73700000	1.01800000	-1.59700000
C	-4.74800000	0.04700000	2.54500000
C	-2.65100000	-5.04500000	0.98400000
C	-4.12600000	-2.48200000	-4.28300000
C	-6.27500000	2.32300000	-1.30400000
C	-4.56000000	-0.16900000	3.95900000
C	-2.51000000	-5.15100000	-0.36600000
C	-4.83000000	-1.32600000	-4.44700000
C	-6.15800000	2.53100000	0.04100000
C	-4.12000000	-1.44600000	4.10600000
C	-3.08000000	-3.95800000	-0.94300000
C	-5.03800000	-0.75600000	-3.14100000
C	-5.55100000	1.35500000	0.61500000
C	-4.01500000	-2.00400000	2.77900000
N	-5.30600000	0.44000000	-0.40300000

F	-4.28600000	-1.26800000	-0.18000000
H	-3.28700000	-3.91000000	3.36700000
H	-2.82900000	-4.49600000	-2.99200000
H	-6.04000000	1.04800000	-3.73800000
H	-5.53300000	2.02800000	2.65400000
N	2.86700000	-2.14900000	-1.26200000
C	1.18700000	2.98000000	2.12400000
O	0.42900000	2.10700000	1.30900000
N	4.40600000	-0.48800000	0.21600000
C	1.06300000	1.05200000	0.69800000
N	8.98000000	-1.48100000	2.50200000
C	2.46000000	0.85900000	0.78700000
C	3.06700000	-0.21900000	0.14600000
C	2.24600000	-1.12400000	-0.61800000
C	0.83500000	-0.90700000	-0.67300000
C	2.12100000	-2.98900000	-1.96000000
C	0.71300000	-2.88100000	-2.05800000
C	0.07200000	-1.84600000	-1.41900000
C	0.24800000	0.19400000	-0.01300000
C	5.42300000	0.45400000	0.66300000
C	5.55600000	1.64200000	-0.30100000
C	6.73500000	-0.31800000	0.83800000
C	7.87800000	0.47900000	1.46700000
C	9.16300000	-0.34400000	1.59300000
H	1.97900000	3.48300000	1.55500000
H	0.48400000	3.73000000	2.49100000
H	1.63200000	2.45200000	2.97600000
H	4.69600000	-1.25300000	-0.37900000
H	8.43900000	-2.20500000	2.03400000
H	9.88400000	-1.90600000	2.69500000
H	3.06800000	1.54000000	1.36400000
H	2.64400000	-3.79400000	-2.47200000
H	0.15500000	-3.61000000	-2.63700000
H	-1.00500000	-1.72100000	-1.46300000
H	5.11800000	0.83100000	1.65000000
H	4.58300000	2.10100000	-0.48500000
H	6.22300000	2.41200000	0.09800000
H	5.95500000	1.30300000	-1.26300000
H	7.05300000	-0.68900000	-0.14400000
H	6.52300000	-1.20100000	1.44900000
H	7.58400000	0.82600000	2.46500000
H	8.09600000	1.36800000	0.86200000
H	9.49400000	-0.64000000	0.58100000
H	9.95100000	0.29400000	2.00900000

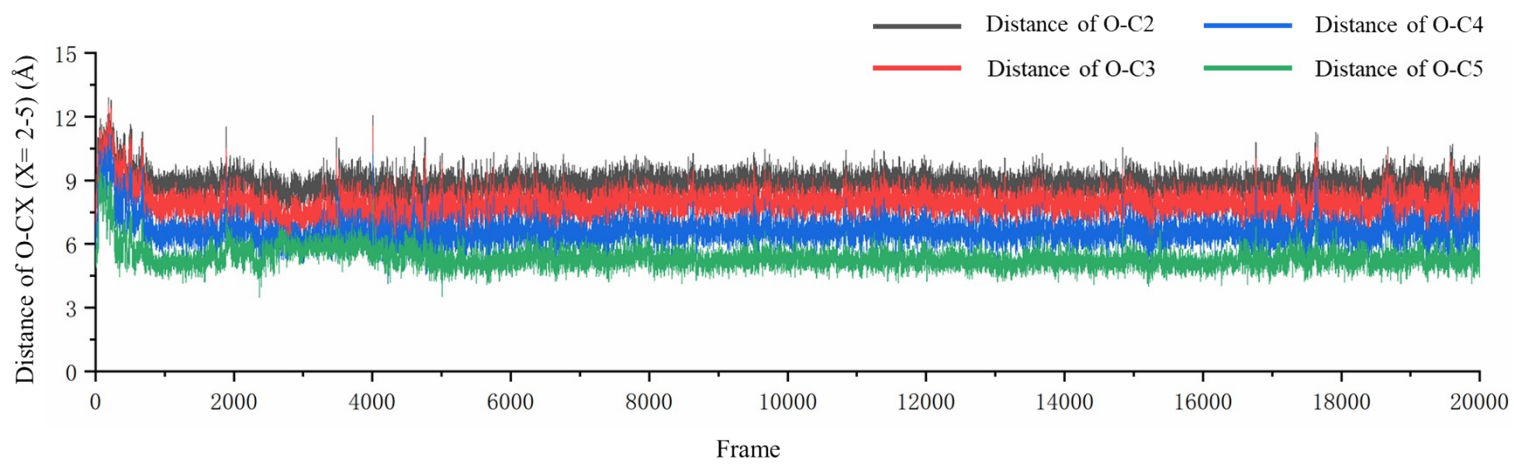
H	-5.81400000	-4.54200000	0.07200000
H	-7.37900000	-4.52000000	-0.81000000
H	-5.85700000	-4.20500000	-1.66800000
H	-4.75200000	0.57100000	4.72400000
H	-6.46100000	3.40100000	0.60700000
H	-6.68800000	2.99300000	-2.04600000
H	-5.16800000	-0.87500000	-5.36900000
H	-3.77900000	-3.16500000	-5.04600000
H	-2.07600000	-5.96200000	-0.93600000
H	-2.34800000	-5.74700000	1.75000000
H	-3.85400000	-1.97100000	5.01200000
H	1.02100000	1.10900000	6.95400000
H	-0.69100000	0.96200000	7.34600000
H	0.43000000	-0.34100000	7.77000000
H	8.88700000	-2.91500000	-3.55300000
H	8.28000000	-1.36400000	-2.97200000
H	9.89300000	-1.91900000	-2.48900000
H	2.98600000	-1.23200000	-4.67200000
H	4.51500000	-2.09900000	-4.84200000
H	6.95000000	5.77900000	-1.99000000
H	4.14800000	-0.74100000	-5.91500000
H	6.50800000	4.92000000	-3.47300000
H	-1.59500000	7.84500000	-0.09800000
O	-2.84300000	-0.54600000	-0.32800000
H	-0.82300000	0.34700000	-0.05900000
H	-0.59500000	0.11700000	-4.01900000
H	-3.52300000	4.93400000	-1.81300000

**Table S4.** The imaginary frequencies of the transition states (TS) in the QM calculation

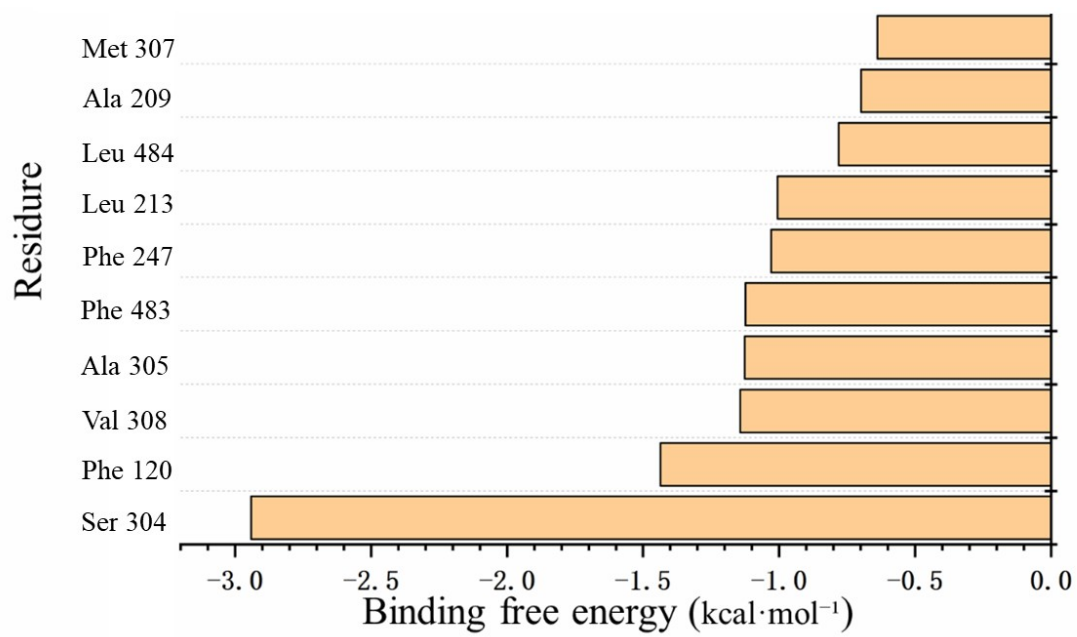
<b>TS</b>	<b>Imaginary Frequency</b>
TS1	-1350.32
TS2	-509.38
TS3	-1884.27
TS4	-264.53
TS5	-893.38



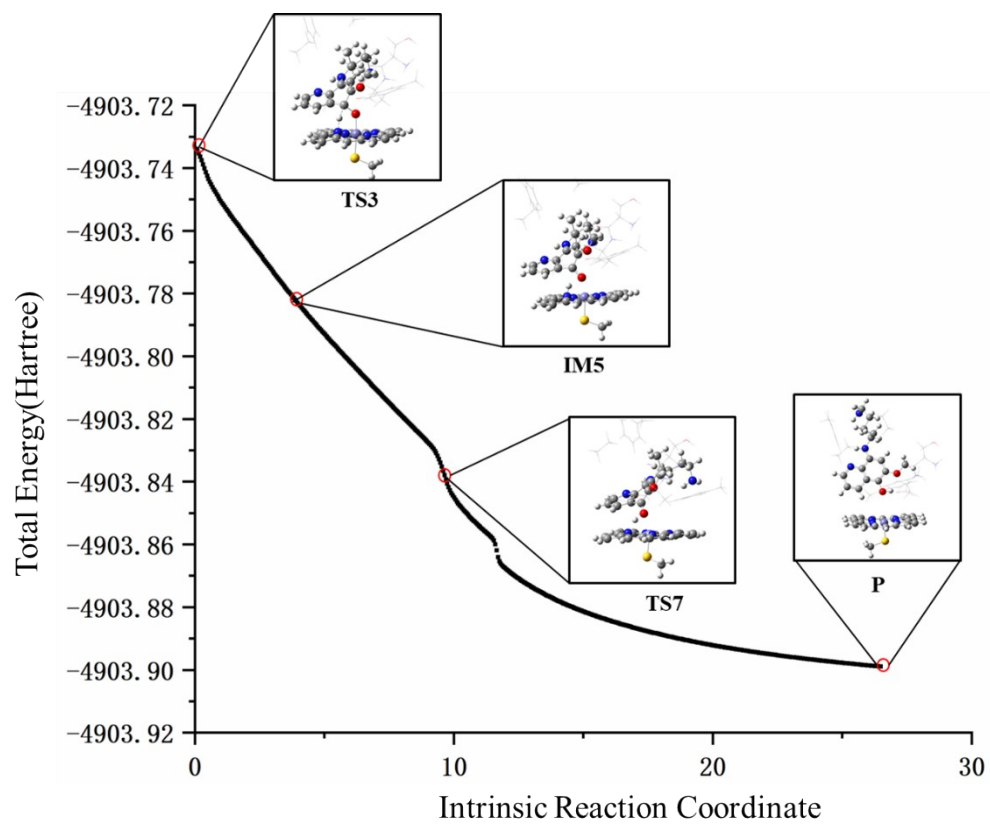
**Figure S1.** RMSDs of the protein backbone atoms in all trajectories.



**Figure S2.** The distances of O-CX ( $X = 2-5$ ).



**Figure S3.** Decomposition of binding free energy on per-residue.



**Figure S4.** The IRC of TS3.

## Cartesian coordinates of all structures in the QM calculation

R			
C	0.18518000	0.40043500	7.00404600
C	-0.06311900	-0.24968300	5.65775200
C	-0.61057400	0.51396500	4.60529000
C	0.23652500	-1.63215000	5.48171500
C	-0.84658800	-0.12162100	3.39951900
C	0.07719500	-2.23303700	4.19243500
C	-0.47769700	-1.45035400	3.19315800
H	-0.86336900	1.55881600	4.75801100
H	0.64374700	-2.19714700	6.31459100
H	-1.27942800	0.42535000	2.56906700
H	0.35061600	-3.26854200	4.02044400
H	-0.63443100	-1.87026000	2.20369000
C	6.46858400	4.87825100	-2.38088200
C	4.98854100	4.76966100	-1.88058200
H	7.05228100	4.01213500	-2.05423400
H	4.50800800	3.86895200	-2.27170200
H	4.94841100	4.72551100	-0.78805600
H	4.40007300	5.63206000	-2.20880900
N	-0.86235900	7.66536200	0.58302700
C	0.28995400	7.02899700	-0.17083400
C	-0.17522500	5.75092900	-0.82310400
O	0.09891000	5.46284100	-1.97850900
C	1.55499200	6.81895200	0.60604700
O	1.79032800	7.95029000	1.44157400
H	-0.53129500	8.57563800	0.89664000
H	0.55582100	7.66109300	-1.02885000
H	1.50895100	5.89882800	1.20733400
H	2.39501500	6.72466900	-0.08465500
H	1.20968500	7.85247100	2.20682900
N	-1.12517500	5.01748100	-0.18706800
C	-1.81481900	3.87240700	-0.77979000
C	-2.70456700	4.20060600	-1.95363300
O	-2.50826700	3.64335200	-3.06542800
C	-2.52649300	3.11400000	0.30350500
H	-1.45932600	5.36946000	0.70200600
H	-1.04474500	3.22532200	-1.21159700
H	-2.95781500	2.19077800	-0.09125000

H	-1.80952600	2.83360600	1.07700400
H	-3.33814000	3.70120000	0.75133800
C	-1.59967900	0.53884300	-3.93507300
H	-2.19126700	0.24901100	-4.80668000
H	-1.54720900	1.62482000	-3.86295100
H	-2.07406300	0.14799300	-3.03100500
C	-6.39077800	-4.06506400	-0.72191000
S	-6.58232300	-2.28870900	-0.41579200
C	8.86803200	-2.24230100	-2.68798300
C	8.26811300	-2.94661200	-1.47099300
C	6.87694700	-3.09827800	-1.30658600
C	9.11704300	-3.61779100	-0.62329100
C	6.40371000	-3.82303200	-0.24250100
C	8.65273400	-4.30605000	0.51807700
C	7.28618100	-4.44340500	0.68053600
H	6.18669000	-2.62339100	-1.99883400
H	10.18965500	-3.54022400	-0.78521700
H	5.33080000	-3.92138500	-0.10121200
H	9.35387200	-4.77481500	1.20108900
H	6.87602800	-4.99168700	1.52300800
C	4.05180000	-1.10794100	-4.88851700
C	4.70483500	-0.14328000	-3.87959500
H	4.25279000	0.85220200	-3.93165700
H	4.57377600	-0.51049600	-2.85714700
H	5.77837800	-0.03231500	-4.07031900
N	-3.53805300	-3.12443500	0.05404700
N	-4.47713400	-1.60029000	-2.17697200
N	-4.39772700	-1.08123600	1.83541100
C	-3.54783100	-3.28523500	2.52089100
C	-3.22878700	-3.75159900	-2.31321500
C	-5.66136600	0.46969200	-2.90637800
C	-5.28014900	1.20310500	1.99919400
C	-3.28159300	-3.77368100	1.24507100
C	-3.90140700	-2.65473500	-2.86959800
C	-5.73653700	1.01809100	-1.59726300
C	-4.74781500	0.04717300	2.54472800
C	-2.65052900	-5.04544800	0.98440900
C	-4.12643000	-2.48152100	-4.28328100
C	-6.27518700	2.32318500	-1.30395600
C	-4.55999400	-0.16850700	3.95942000
C	-2.50970200	-5.15138600	-0.36558000
C	-4.82980500	-1.32638900	-4.44673200
C	-6.15774600	2.53066800	0.04077100
C	-4.12008500	-1.44603000	4.10568500

C	-3.07997700	-3.95819300	-0.94276200
C	-5.03782900	-0.75583500	-3.14148400
C	-5.55064400	1.35536800	0.61548000
C	-4.01508900	-2.00370900	2.77885800
N	-5.30574100	0.44041400	-0.40339200
Fe	-4.28599500	-1.26813200	-0.17983900
H	-3.28656200	-3.91001100	3.36666500
H	-2.82906500	-4.49587300	-2.99150900
H	-6.04011300	1.04826200	-3.73810300
H	-5.53306400	2.02802200	2.65383600
N	2.86650800	-2.14945600	-1.26194600
C	1.18707500	2.97957400	2.12352700
O	0.42947500	2.10694700	1.30894300
N	4.40586800	-0.48839800	0.21643000
C	1.06291400	1.05241800	0.69785300
N	8.98004900	-1.48106100	2.50223800
C	2.45970800	0.85867500	0.78744700
C	3.06672200	-0.21881500	0.14551200
C	2.24583800	-1.12410900	-0.61772000
C	0.83491000	-0.90719500	-0.67323400
C	2.12079200	-2.98879500	-1.95970600
C	0.71292200	-2.88085300	-2.05825900
C	0.07165000	-1.84573500	-1.41876200
C	0.24804700	0.19369300	-0.01256200
C	5.42267800	0.45372500	0.66332900
C	5.55627600	1.64155900	-0.30056400
C	6.73480600	-0.31793200	0.83810300
C	7.87770100	0.47908000	1.46700300
C	9.16293100	-0.34441800	1.59321900
H	1.97907700	3.48328700	1.55468000
H	0.48426100	3.72954100	2.49140500
H	1.63190500	2.45173900	2.97601700
H	4.69617800	-1.25315700	-0.37946100
H	8.43926000	-2.20456600	2.03421500
H	9.88376200	-1.90610600	2.69510200
H	3.06769200	1.54036100	1.36412200
H	2.64447300	-3.79368200	-2.47224900
H	0.15454700	-3.61016300	-2.63682900
H	-1.00548300	-1.72065100	-1.46251300
H	5.11835800	0.83052200	1.65046600
H	4.58290700	2.10056200	-0.48500800
H	6.22330600	2.41170500	0.09776700
H	5.95511900	1.30278700	-1.26286400
H	7.05333500	-0.68852300	-0.14422300

H	6.52259500	-1.20135600	1.44912900
H	7.58386700	0.82584200	2.46540700
H	8.09565300	1.36753800	0.86221800
H	9.49421000	-0.63977100	0.58066400
H	9.95095800	0.29390800	2.00927100
H	-5.81364300	-4.54236300	0.07174300
H	-7.37940400	-4.52022700	-0.80970200
H	-5.85718300	-4.20498900	-1.66792200
H	-4.75240600	0.57143500	4.72392600
H	-6.46107700	3.40119500	0.60698000
H	-6.68783700	2.99279800	-2.04642800
H	-5.16814400	-0.87509700	-5.36928000
H	-3.77852300	-3.16536100	-5.04551300
H	-2.07630600	-5.96165400	-0.93567100
H	-2.34837100	-5.74717000	1.74974100
H	-3.85392500	-1.97065900	5.01243800
H	1.02076800	1.10929200	6.95432800
H	-0.69118900	0.96195700	7.34619800
H	0.42956600	-0.34080600	7.76962500
H	8.88704600	-2.91469400	-3.55311100
H	8.28008600	-1.36354500	-2.97161600
H	9.89272400	-1.91896300	-2.48938500
H	2.98646900	-1.23200200	-4.67161600
H	4.51529000	-2.09919300	-4.84245100
H	6.95037100	5.77942700	-1.98951100
H	4.14806700	-0.74050100	-5.91525800
H	6.50803800	4.91994600	-3.47337800
H	-1.59523200	7.84533600	-0.09829100
O	-2.84293200	-0.54647900	-0.32793000
H	-0.82278200	0.34739700	-0.05921000
H	-0.59509200	0.11705200	-4.01940400
H	-3.52298500	4.93402500	-1.81295700

## TS1

C	0.17719600	0.46030600	7.04050600
C	-0.04638100	-0.19608300	5.69292000
C	-0.59072500	0.55802500	4.63200200
C	0.27304100	-1.57500100	5.52397300
C	-0.80387300	-0.08331100	3.42503900
C	0.13710300	-2.18088700	4.23435200
C	-0.41554400	-1.40770700	3.22646900
H	-0.87331000	1.59533800	4.78489500
H	0.67169100	-2.13435200	6.36475600

H	-1.26591600	0.44341300	2.59872500
H	0.41450300	-3.21679400	4.07129500
H	-0.57789700	-1.83928700	2.24346600
C	6.51646400	4.99640500	-2.27863300
C	5.03194600	4.86998100	-1.79607500
H	7.11010600	4.14158200	-1.93942300
H	4.56828000	3.96063600	-2.18824000
H	4.97792600	4.83348200	-0.70355500
H	4.43545900	5.72153300	-2.13697500
N	-0.88503000	7.69620700	0.58919300
C	0.28440900	7.07291100	-0.14904900
C	-0.15642000	5.78747000	-0.80373200
O	0.13541300	5.50021900	-1.95500500
C	1.54249000	6.88091400	0.64364000
O	1.75315900	8.01712400	1.47914100
H	-0.57405300	8.61494800	0.89839100
H	0.55320700	7.70638900	-1.00509200
H	1.50040900	5.96054200	1.24715400
H	2.39248100	6.79659900	-0.03605400
H	1.15071400	7.92319800	2.22809000
N	-1.10458500	5.04339100	-0.17743800
C	-1.77222300	3.88820900	-0.77562300
C	-2.65181400	4.20217500	-1.96098600
O	-2.43484800	3.64495500	-3.06894100
C	-2.48731900	3.12324700	0.30084500
H	-1.47424700	5.41166900	0.69129200
H	-0.98613300	3.25570800	-1.19877800
H	-2.77156600	2.12855800	-0.05272600
H	-1.84586000	2.98308400	1.16647000
H	-3.40150300	3.63904000	0.62139000
C	-1.47613600	0.55028400	-3.91976900
H	-2.12193800	0.18468900	-4.72092600
H	-1.43882000	1.63927100	-3.93587200
H	-1.88306600	0.22711900	-2.95789100
C	-6.27697200	-3.82465200	-0.89864500
S	-6.29308100	-2.23045000	-0.01481100
C	9.01035800	-2.09348600	-2.53888500
C	8.40473800	-2.80261300	-1.32755800
C	7.01372500	-2.97177600	-1.17954200
C	9.25181700	-3.46085500	-0.46791300
C	6.53691500	-3.69993500	-0.11951000
C	8.78250900	-4.15235600	0.66944500
C	7.41595900	-4.30681900	0.81565900
H	6.32982500	-2.51594600	-1.89110300

H	10.32502200	-3.37168800	-0.61807000
H	5.46464100	-3.82729200	0.00440000
H	9.48078500	-4.61050100	1.36220300
H	7.00254100	-4.86148900	1.65220200
C	4.20715800	-1.02602500	-4.80059700
C	4.83539200	-0.05081600	-3.78605400
H	4.66277600	0.99117700	-4.07313900
H	4.40255800	-0.19942000	-2.79267200
H	5.91882500	-0.19962300	-3.70898600
N	-3.36626400	-3.10506800	0.05330900
N	-4.27882400	-1.58478900	-2.20138700
N	-4.24235100	-1.05864800	1.82232500
C	-3.45356800	-3.28339300	2.52158000
C	-3.06987300	-3.75692200	-2.30713300
C	-5.54879900	0.43147600	-2.94025300
C	-5.23662400	1.18116900	1.96773700
C	-3.16702900	-3.76665400	1.24845000
C	-3.71779200	-2.65034800	-2.87481900
C	-5.63774800	0.98619900	-1.63756500
C	-4.66619500	0.04891400	2.52125000
C	-2.57915800	-5.05970100	0.99634800
C	-3.95937100	-2.50581600	-4.29127100
C	-6.24755500	2.26112600	-1.34479200
C	-4.54394200	-0.18313900	3.94263800
C	-2.42408900	-5.17445800	-0.35179700
C	-4.68067800	-1.36353300	-4.46301600
C	-6.14764600	2.47337900	0.00045300
C	-4.08928200	-1.45389900	4.09594700
C	-2.94182300	-3.96351500	-0.93952100
C	-4.87747700	-0.77642200	-3.15956100
C	-5.47834400	1.33146800	0.57770300
C	-3.90907200	-1.99748700	2.76980400
N	-5.16988700	0.44454700	-0.44126800
Fe	-4.15657000	-1.26928400	-0.20433000
H	-3.23763900	-3.92218700	3.36933800
H	-2.70076300	-4.52334100	-2.97837400
H	-5.96435200	0.97816800	-3.77571200
H	-5.55681800	1.98323700	2.62130600
N	2.73927900	-2.27876200	-1.49793400
C	0.79117600	2.74821200	1.81965200
O	0.05574200	1.77864600	1.08555400
N	4.13495300	-0.54758500	0.04647400
C	0.71186900	0.71622800	0.55816800
N	8.58730900	-1.31645600	2.66440100

C	2.10311500	0.59149600	0.68863200
C	2.79326000	-0.41322900	0.00482100
C	2.04161300	-1.34633000	-0.81409600
C	0.61929700	-1.22798000	-0.85481000
C	2.05766100	-3.11291000	-2.27559500
C	0.65505500	-3.07955800	-2.40292000
C	-0.06498500	-2.14333400	-1.68944900
C	-0.07346000	-0.27262600	-0.06066100
C	5.06269700	0.41900900	0.63524500
C	5.14961000	1.68441900	-0.22897000
C	6.41815000	-0.26284200	0.83378600
C	7.45398800	0.58980000	1.56758400
C	8.77395500	-0.15584500	1.78792900
H	1.58366900	3.19587500	1.20910100
H	0.07415000	3.52322200	2.08845000
H	1.21665400	2.30918900	2.72879800
H	4.49959400	-1.29583000	-0.53286000
H	8.19348200	-2.08804800	2.13194900
H	9.49344100	-1.64766000	2.98518900
H	2.65888700	1.28059600	1.30633200
H	2.64302000	-3.84373700	-2.82878700
H	0.15237700	-3.78747900	-3.05312300
H	-1.14266500	-2.07501800	-1.75679200
H	4.66962200	0.68647600	1.62513300
H	4.15572900	2.08496000	-0.43982300
H	5.72891300	2.46320900	0.27301100
H	5.63151000	1.45853000	-1.18527700
H	6.81539200	-0.55024000	-0.14716500
H	6.25278600	-1.19176600	1.38850100
H	7.05869300	0.89234700	2.54507000
H	7.66208100	1.50369900	0.99866200
H	9.20798700	-0.41149200	0.80443100
H	9.47968700	0.52545500	2.27607500
H	-5.58071400	-4.53317400	-0.44572500
H	-7.28995900	-4.23080500	-0.82623900
H	-6.02770300	-3.69486700	-1.95364700
H	-4.79742200	0.54068000	4.70512700
H	-6.50603900	3.32242400	0.56758900
H	-6.69720100	2.90559400	-2.08832600
H	-5.04725500	-0.93443600	-5.38562600
H	-3.62275400	-3.20602300	-5.04391700
H	-2.02069600	-6.00462900	-0.91568900
H	-2.32161100	-5.77342600	1.76713000
H	-3.87075000	-1.98925100	5.00938800

H	1.03382200	1.14519100	7.01217400
H	-0.69375900	1.04873100	7.34861600
H	0.37606300	-0.27992800	7.82013000
H	9.03237100	-2.76232900	-3.40652000
H	8.42531900	-1.21253000	-2.82227500
H	10.03434100	-1.77210900	-2.33468600
H	3.12514700	-0.87739800	-4.86551400
H	4.37947300	-2.06531700	-4.50273500
H	6.97988500	5.90688600	-1.88726000
H	4.62736600	-0.88785700	-5.80166700
H	6.56880000	5.03195200	-3.37065100
H	-1.61555900	7.85763800	-0.09932500
O	-2.63772300	-0.42918000	-0.34819200
H	-1.53988000	-0.40167200	-0.05091800
H	-0.47202900	0.13569300	-4.04627600
H	-3.48267300	4.92245300	-1.82911200

## IM1

C	0.17530300	0.37909300	7.00280500
C	-0.06366800	-0.26744400	5.65310300
C	-0.60716900	0.49804600	4.59995400
C	0.24062800	-1.64855800	5.47444300
C	-0.83459000	-0.13430400	3.39089500
C	0.09019000	-2.24582200	4.18240300
C	-0.46111100	-1.46144600	3.18246900
H	-0.86606200	1.54095300	4.75460200
H	0.64377400	-2.21565700	6.30767300
H	-1.26222000	0.42192700	2.56390600
H	0.36521400	-3.28042300	4.00869000
H	-0.60698500	-1.88417900	2.19240700
C	6.50000600	4.90272500	-2.33227500
C	5.01742500	4.78866300	-1.84075000
H	7.08689600	4.04205100	-1.99672200
H	4.54448200	3.88290700	-2.22957500
H	4.97051600	4.75080900	-0.74817500
H	4.42611000	5.64562000	-2.17773900
N	-0.85491800	7.66138100	0.59867100
C	0.30331000	7.03039700	-0.15062300
C	-0.15479300	5.75317100	-0.80950800
O	0.12664200	5.46942500	-1.96423500
C	1.56447900	6.82121600	0.63276800
O	1.79210000	7.95053600	1.47315000
H	-0.53367300	8.57736100	0.90568000

H	0.57251400	7.66584300	-1.00507800
H	1.51707500	5.89882700	1.23125900
H	2.40902600	6.73161100	-0.05295200
H	1.19302800	7.85813800	2.22491700
N	-1.10640300	5.01524800	-0.18116800
C	-1.78964000	3.87029200	-0.78134300
C	-2.67362200	4.19977300	-1.95921800
O	-2.46952700	3.64658200	-3.07161800
C	-2.50552200	3.10659600	0.29546400
H	-1.45009200	5.36610400	0.70478100
H	-1.01563200	3.22672100	-1.21103500
H	-2.90143000	2.16745900	-0.09984600
H	-1.80193400	2.85349000	1.08892700
H	-3.34268200	3.67739600	0.71660900
C	-1.54788300	0.54716400	-3.94578400
H	-2.15358900	0.25569800	-4.80690400
H	-1.47143900	1.63298300	-3.89385500
H	-2.02193900	0.18420700	-3.03064800
C	-6.40098300	-3.84552000	-0.84500800
S	-6.42874500	-2.21256300	-0.03401200
C	8.91986800	-2.21054100	-2.64799700
C	8.31490600	-2.92025300	-1.43666600
C	6.92323600	-3.07608300	-1.28048800
C	9.16079000	-3.59184600	-0.58623700
C	6.44591700	-3.80534200	-0.22145200
C	8.69183900	-4.28487400	0.55033900
C	7.32473800	-4.42630200	0.70460700
H	6.23731700	-2.60169600	-1.97749700
H	10.23402100	-3.51139900	-0.74210900
H	5.37280400	-3.91100600	-0.08679100
H	9.39017900	-4.75373300	1.23604500
H	6.91121000	-4.97911900	1.54242100
C	4.11327200	-1.08172400	-4.87241800
C	4.75793400	-0.11863200	-3.85658600
H	4.37892000	0.90088900	-3.97893400
H	4.53359500	-0.43377200	-2.83300600
H	5.84716900	-0.08538300	-3.97387100
N	-3.51867400	-3.14010300	0.01898600
N	-4.39949600	-1.58733100	-2.21557700
N	-4.31776600	-1.07756500	1.79908300
C	-3.52253800	-3.30223700	2.48703600
C	-3.17491500	-3.75261000	-2.34662000
C	-5.61513400	0.46418600	-2.94039300
C	-5.26361400	1.18320500	1.96953000

C	-3.27583500	-3.79390200	1.21019900
C	-3.82137000	-2.63947500	-2.90044000
C	-5.70832400	1.00464100	-1.63412700
C	-4.70831400	0.03990700	2.50945700
C	-2.65360300	-5.06754500	0.94805800
C	-4.03090000	-2.46130000	-4.31616000
C	-6.25860500	2.30314000	-1.33539800
C	-4.54609400	-0.19031600	3.92433000
C	-2.50590800	-5.17154900	-0.40178400
C	-4.74274300	-1.31149200	-4.47966100
C	-6.14707400	2.50561900	0.01078200
C	-4.10130400	-1.46613400	4.06933600
C	-3.06073000	-3.97463400	-0.98161200
C	-4.96640000	-0.75219100	-3.17052500
C	-5.53007100	1.33471100	0.58437900
C	-3.96830500	-2.01733800	2.74371000
N	-5.27416100	0.43283400	-0.43818000
Fe	-4.35486200	-1.32683400	-0.22198300
H	-3.27462400	-3.93386000	3.33126800
H	-2.78035100	-4.49862600	-3.02561000
H	-5.99869900	1.03611600	-3.77423000
H	-5.54319800	1.99697800	2.62670600
N	2.79145900	-2.13082900	-1.33619200
C	1.10746900	2.95184100	2.13476900
O	0.33679900	2.06462400	1.34359900
N	4.31700200	-0.51605500	0.21806700
C	0.96827200	1.01382700	0.73682700
N	8.89120600	-1.45645800	2.53327000
C	2.36661700	0.79984300	0.82677700
C	2.97605300	-0.25490200	0.14897600
C	2.16619000	-1.13797800	-0.65489600
C	0.74344900	-0.93168400	-0.71697600
C	2.06044000	-2.93665300	-2.08731400
C	0.65516500	-2.82421600	-2.20655600
C	-0.00552000	-1.82889700	-1.52561600
C	0.21171300	0.12160800	0.02477800
C	5.32106000	0.43318600	0.68473900
C	5.43734300	1.64199800	-0.25475700
C	6.64486200	-0.31971900	0.84860900
C	7.77244600	0.48948300	1.48986900
C	9.06712400	-0.31746600	1.62597700
H	1.90190100	3.43018600	1.54915300
H	0.41202000	3.71749600	2.48209700
H	1.54574500	2.43949800	2.99943100

H	4.61828100	-1.25483700	-0.40467100
H	8.37340100	-2.19146200	2.05749000
H	9.79957200	-1.86321100	2.74266400
H	2.97214900	1.45777300	1.43411500
H	2.59559100	-3.71403100	-2.62869400
H	0.10858300	-3.52078100	-2.83377300
H	-1.08004500	-1.69735700	-1.58435400
H	5.00952900	0.78428700	1.67885900
H	4.45801000	2.09092500	-0.43340300
H	6.09137700	2.41337500	0.16168700
H	5.84466200	1.32998900	-1.22238400
H	6.97060800	-0.67151100	-0.13812500
H	6.44768300	-1.21463700	1.44767300
H	7.46539000	0.82872800	2.48690200
H	7.98401600	1.38272400	0.88997900
H	9.41136400	-0.60804100	0.61653200
H	9.84246100	0.33157400	2.04899300
H	-5.73015700	-4.53452000	-0.32948300
H	-7.42040800	-4.23647900	-0.80296100
H	-6.09598600	-3.75432300	-1.88912400
H	-4.76269100	0.54087200	4.69085200
H	-6.45664300	3.37204400	0.57995000
H	-6.67115000	2.97379200	-2.07699500
H	-5.07918700	-0.85654500	-5.40112200
H	-3.67372700	-3.14251800	-5.07639000
H	-2.07222800	-5.98192200	-0.97158300
H	-2.35927600	-5.77158500	1.71430200
H	-3.85570300	-1.99830700	4.97751000
H	1.01020000	1.08915200	6.96014800
H	-0.70415400	0.93813000	7.34061800
H	0.41577600	-0.36411700	7.76754700
H	8.94301100	-2.87933800	-3.51576700
H	8.33305600	-1.33069000	-2.93071100
H	9.94348400	-1.88767600	-2.44351800
H	3.02890200	-1.12464300	-4.73237400
H	4.50185500	-2.09853700	-4.75197900
H	6.97406400	5.80894900	-1.94332500
H	4.30910100	-0.76792600	-5.90268300
H	6.54621500	4.93807800	-3.42468300
H	-1.58991300	7.82895800	-0.08353500
O	-2.74436700	-0.51783100	-0.39028400
H	-2.18626000	-0.58475800	0.40052500
H	-0.55331300	0.10241400	-4.03405300
H	-3.49565000	4.92930000	-1.81970100

## TS4

C	0.17726600	0.50753700	7.05844600
C	-0.04517600	-0.15868700	5.71550800
C	-0.58215000	0.58946700	4.64666700
C	0.26781700	-1.54052800	5.55886100
C	-0.79446100	-0.06056800	3.44424800
C	0.13308900	-2.15623200	4.27376200
C	-0.41229600	-1.38851000	3.25779300
H	-0.85642400	1.63039900	4.78967500
H	0.66235500	-2.09454700	6.40506300
H	-1.24311400	0.46412700	2.61126100
H	0.41114100	-3.19306100	4.11842000
H	-0.56602900	-1.82328000	2.27420900
C	6.57056800	4.93531700	-2.27589800
C	5.08387600	4.82021200	-1.79724700
H	7.15590200	4.07622900	-1.93340100
H	4.61529200	3.91344500	-2.18819500
H	5.02659200	4.78543400	-0.70510700
H	4.49513200	5.67609200	-2.14161400
N	-0.82658800	7.69585300	0.54489200
C	0.34210900	7.06064500	-0.18430600
C	-0.10305700	5.77215300	-0.82996300
O	0.19111200	5.47405900	-1.97789700
C	1.59655500	6.86874500	0.61416500
O	1.81021600	8.01065100	1.44110000
H	-0.49883300	8.60114300	0.87603700
H	0.61687400	7.68571100	-1.04459600
H	1.54789200	5.95363200	1.22449100
H	2.44777400	6.77338100	-0.06256400
H	1.23676600	7.90715300	2.21087900
N	-1.05705200	5.03798800	-0.20087800
C	-1.72893900	3.88101900	-0.79171800
C	-2.60182400	4.19102400	-1.98300500
O	-2.38543400	3.62195300	-3.08517600
C	-2.45116100	3.12885500	0.28835000
H	-1.42494600	5.41586800	0.66447700
H	-0.94832500	3.23547000	-1.20656200
H	-2.89757600	2.22698700	-0.13523900
H	-1.77149900	2.83568900	1.07957000
H	-3.27532300	3.71952200	0.70899700
C	-1.43891500	0.51678300	-3.90771700
H	-2.10306600	0.12538300	-4.68163200

H	-1.38385500	1.60295300	-3.97636600
H	-1.83132900	0.24577400	-2.92464500
C	-6.28848200	-3.83936100	-0.86425800
S	-6.34189800	-2.14622000	-0.20296000
C	9.02919600	-2.16902600	-2.46996200
C	8.41594600	-2.86522900	-1.25494200
C	7.02358500	-3.02600700	-1.11025300
C	9.25678900	-3.52076100	-0.38718200
C	6.53955000	-3.74325900	-0.04601800
C	8.78016300	-4.20031300	0.75426200
C	7.41236100	-4.34676000	0.89715600
H	6.34425800	-2.56995000	-1.82556200
H	10.33101500	-3.43700600	-0.53365800
H	5.46615700	-3.85696100	0.07926000
H	9.47388700	-4.65449300	1.45428300
H	6.99323300	-4.89004400	1.73835300
C	4.23911700	-1.09576600	-4.75650100
C	4.86882300	-0.11535300	-3.74783500
H	4.83098000	0.91587300	-4.11308000
H	4.33673500	-0.15331700	-2.79375600
H	5.92014800	-0.36184200	-3.55711000
N	-3.37954700	-3.11215400	0.08715700
N	-4.25454700	-1.59396100	-2.17653400
N	-4.24149100	-1.03402600	1.83746800
C	-3.45743600	-3.25446400	2.55792100
C	-3.06005100	-3.76931000	-2.26544900
C	-5.51550000	0.42627800	-2.94102200
C	-5.21588700	1.21440100	1.96173300
C	-3.17477500	-3.76059300	1.28822700
C	-3.70249900	-2.66717900	-2.84883200
C	-5.58848400	0.99984000	-1.64127100
C	-4.65537500	0.08178000	2.53219500
C	-2.58319400	-5.05792700	1.05027700
C	-3.94289400	-2.53444500	-4.26613600
C	-6.20169000	2.27569200	-1.36150200
C	-4.52353800	-0.13062500	3.95443000
C	-2.42204200	-5.18308400	-0.29552300
C	-4.66024600	-1.39102200	-4.44622600
C	-6.10972700	2.50083900	-0.01785700
C	-4.07050100	-1.40176600	4.11819500
C	-2.94165000	-3.97527300	-0.89319900
C	-4.85259100	-0.78917300	-3.14926600
C	-5.44436300	1.36372300	0.57007900
C	-3.90361100	-1.95937500	2.79666400

N	-5.11225900	0.46504800	-0.43915700
Fe	-4.18114000	-1.30136300	-0.17001300
H	-3.24150200	-3.88347300	3.41342300
H	-2.68142800	-4.53756000	-2.92962600
H	-5.93291600	0.96602900	-3.78015800
H	-5.53552400	2.02244000	2.60886000
N	2.61605300	-2.28460500	-1.53792300
C	0.79167900	2.69605200	1.96111900
O	0.02406500	1.80014100	1.17302600
N	4.07604300	-0.60159700	0.03836200
C	0.65726500	0.76614100	0.54243900
N	8.60346600	-1.25913900	2.57896400
C	2.06210900	0.60814800	0.62711900
C	2.72287000	-0.41433600	-0.04293200
C	1.95084800	-1.32232500	-0.85164000
C	0.52083000	-1.16544700	-0.92121900
C	1.91922100	-3.11237200	-2.29716000
C	0.51302600	-3.04264800	-2.43171600
C	-0.18245400	-2.07296300	-1.75008100
C	-0.06840300	-0.12142500	-0.21165400
C	5.00170500	0.39092400	0.57597900
C	5.08084000	1.64300800	-0.30968100
C	6.36683300	-0.27152100	0.77500400
C	7.40740200	0.60450700	1.47419300
C	8.74456400	-0.11529500	1.67228800
H	1.55430300	3.20607900	1.36121100
H	0.08467000	3.43783200	2.33592900
H	1.25964600	2.18188500	2.80745900
H	4.43296700	-1.30444300	-0.59561300
H	8.15205300	-2.02761900	2.08926400
H	9.52617100	-1.60875000	2.82545300
H	2.63393800	1.30375400	1.22236300
H	2.48439000	-3.86985800	-2.83645500
H	-0.00380100	-3.74587100	-3.07664600
H	-1.25322500	-1.95885900	-1.82177400
H	4.62776700	0.68141800	1.56778800
H	4.08369600	2.02091300	-0.54567400
H	5.63701100	2.44464700	0.18365700
H	5.58305600	1.40880600	-1.25369900
H	6.75490200	-0.57613700	-0.20469900
H	6.21335500	-1.19097300	1.34829400
H	7.03047300	0.91591300	2.45629600
H	7.58831300	1.51376900	0.88868300
H	9.15283000	-0.38552500	0.68121700

H	9.45524800	0.58569200	2.12506500
H	-5.66039600	-4.48551600	-0.24836100
H	-7.31222400	-4.22086800	-0.88130700
H	-5.90074500	-3.84172700	-1.88628500
H	-4.76511500	0.60310800	4.71107700
H	-6.47393500	3.35394100	0.53910400
H	-6.65024000	2.91320100	-2.11168000
H	-5.02251900	-0.96856900	-5.37358400
H	-3.60711100	-3.23947300	-5.01443500
H	-2.00839900	-6.01448400	-0.84971300
H	-2.32145600	-5.76380700	1.82684400
H	-3.84251400	-1.92461600	5.03651000
H	0.35666900	-0.22805800	7.84713200
H	1.04605800	1.17685300	7.03082100
H	-0.68596000	1.11411400	7.35283700
H	9.01577400	-2.83125700	-3.34290900
H	8.47134000	-1.26599600	-2.73874100
H	10.06623700	-1.88445300	-2.27741400
H	3.19044700	-0.84406400	-4.94121600
H	4.26684300	-2.12008400	-4.37209100
H	7.04010900	5.84288300	-1.88470400
H	4.76519700	-1.07806500	-5.71640400
H	6.62638400	4.96846200	-3.36791800
H	-1.53996100	7.88726500	-0.15387900
O	-2.47639100	-0.47137000	-0.29232800
H	-0.44445400	0.07982100	-4.02819800
H	-3.42494200	4.92231400	-1.86256000
H	-2.51615800	0.36586700	0.18853700

## P

C	0.12391000	0.42214600	7.02091400
C	-0.10788900	-0.22575700	5.67061500
C	-0.65254300	0.53675400	4.61590100
C	0.20425300	-1.60524200	5.49291800
C	-0.87321800	-0.09687200	3.40626900
C	0.06057200	-2.20339300	4.20052000
C	-0.49213300	-1.42203900	3.19899600
H	-0.92216600	1.57665800	4.77384200
H	0.60538200	-2.17064700	6.32827400
H	-1.31762700	0.44371000	2.57887200
H	0.33798700	-3.23753400	4.02824700
H	-0.65228700	-1.84779200	2.21265200
C	6.45028900	4.97869000	-2.29704500

C	4.96703000	4.85662600	-1.80951700
H	7.02940800	4.09937100	-1.99882600
H	4.48655100	3.97206000	-2.23618300
H	4.92042300	4.77242900	-0.71946600
H	4.38316500	5.73237200	-2.10950100
N	-0.92728000	7.69837600	0.61330500
C	0.23635600	7.07351000	-0.13272600
C	-0.21311100	5.79381800	-0.79274500
O	0.07299400	5.51150000	-1.94668900
C	1.49644700	6.87109000	0.65417600
O	1.71572900	8.00166800	1.49508800
H	-0.58468800	8.58201800	0.98557600
H	0.50517000	7.71017200	-0.98625000
H	1.45285900	5.94819500	1.25228200
H	2.34230300	6.78431900	-0.03056100
H	1.17921100	7.87108100	2.28677700
N	-1.16250600	5.05087300	-0.16702600
C	-1.83835100	3.90185100	-0.76882400
C	-2.71960000	4.22783400	-1.94957100
O	-2.51105600	3.67410300	-3.06093100
C	-2.55274800	3.13484500	0.30594800
H	-1.53453600	5.42972600	0.69658100
H	-1.05826100	3.26551100	-1.19864400
H	-3.02974700	2.24353400	-0.11194300
H	-1.85092900	2.83107300	1.08226600
H	-3.35440000	3.72297600	0.76820200
C	-1.56963300	0.58042600	-3.93243700
H	-2.33520800	0.20192200	-4.61227900
H	-1.63832600	1.66523500	-3.85850900
H	-1.72313900	0.14394000	-2.94201000
C	-6.53389500	-3.76001400	-1.08828300
S	-6.52283900	-2.27679600	-0.02526800
C	8.90882500	-2.12162500	-2.60537300
C	8.30429700	-2.83455600	-1.39574100
C	6.91298400	-2.99766100	-1.24325700
C	9.15137400	-3.50160300	-0.54290100
C	6.43668900	-3.72952700	-0.18563300
C	8.68295700	-4.19679600	0.59249900
C	7.31621800	-4.34557300	0.74304000
H	6.22492000	-2.53050600	-1.94301900
H	10.22462100	-3.41557300	-0.69589100
H	5.36331300	-3.83983500	-0.05684200
H	9.38199800	-4.66213600	1.27996500
H	6.90341400	-4.90011700	1.58003300

C	4.10250700	-1.01861100	-4.84322400
C	4.73916600	-0.05191200	-3.82577200
H	4.32151400	0.95567600	-3.91781200
H	4.55606400	-0.39234300	-2.80220400
H	5.82297200	0.02275100	-3.97087600
N	-3.53377200	-3.10228200	0.02353300
N	-4.40760900	-1.56640000	-2.19074200
N	-4.38757400	-1.07398300	1.79096400
C	-3.54178600	-3.27914200	2.49524300
C	-3.17836400	-3.72801000	-2.33737400
C	-5.63932500	0.47570500	-2.93829500
C	-5.30524000	1.19694800	1.97252100
C	-3.27933800	-3.76073000	1.21637300
C	-3.83302300	-2.62003300	-2.88941000
C	-5.70689200	1.02401700	-1.63245200
C	-4.76921800	0.04454500	2.51378000
C	-2.62891400	-5.02158100	0.95863800
C	-4.05389000	-2.45337900	-4.30363300
C	-6.26562900	2.31760400	-1.33625000
C	-4.59474800	-0.17722400	3.92813300
C	-2.48077700	-5.12899800	-0.39000400
C	-4.77815400	-1.31163700	-4.46650500
C	-6.15973300	2.52295200	0.01026700
C	-4.14070300	-1.44924100	4.07180200
C	-3.06206400	-3.94507600	-0.97104200
C	-4.99339600	-0.74609400	-3.15866300
C	-5.53853800	1.35728400	0.58398800
C	-4.01817400	-2.00283600	2.74565500
N	-5.24182200	0.45127900	-0.43689900
Fe	-4.54798300	-1.39825000	-0.19906000
H	-3.28200300	-3.90511200	3.34033600
H	-2.78027400	-4.47319800	-3.01573600
H	-6.04080200	1.03669100	-3.77124400
H	-5.59633200	2.00687400	2.63022200
N	2.96393800	-2.39872200	-1.24065200
C	0.91033100	2.78138100	1.85977700
O	0.24342000	1.85232300	1.02085400
N	4.40025600	-0.55466100	0.13746700
C	0.96367800	0.79711200	0.50690400
N	8.92291700	-1.30332900	2.57166600
C	2.36578600	0.69749300	0.60426300
C	3.04593000	-0.37805000	0.04126800
C	2.28209100	-1.37453900	-0.66132500
C	0.85657500	-1.26299800	-0.73585400

C	2.27810000	-3.32448700	-1.88800600
C	0.86816900	-3.31068900	-2.00424600
C	0.15820800	-2.28191200	-1.43101900
C	0.20385600	-0.16467500	-0.13556900
C	5.34119600	0.44972800	0.61064300
C	5.45707500	1.63020200	-0.36541600
C	6.68481400	-0.24398800	0.85758600
C	7.75215900	0.61577500	1.53362800
C	9.07739200	-0.13498400	1.69843300
H	1.70082000	3.31285900	1.31700000
H	0.15292000	3.50177100	2.17143500
H	1.33137000	2.28428700	2.74063600
H	4.75612200	-1.33873400	-0.39133900
H	8.45234500	-2.04822100	2.06288700
H	9.84100600	-1.67480400	2.80289900
H	2.91766400	1.46225100	1.13036800
H	2.85602100	-4.12538600	-2.34501500
H	0.36108100	-4.10338000	-2.54444600
H	-0.92116600	-2.22919900	-1.50379900
H	4.97112500	0.82444900	1.57668500
H	4.47085800	2.02624100	-0.61709500
H	6.05014300	2.44554200	0.05891900
H	5.93368300	1.30459100	-1.29587700
H	7.07026800	-0.60286600	-0.10454600
H	6.49364500	-1.13337400	1.46655200
H	7.40198200	0.93402100	2.52326700
H	7.94000400	1.52150300	0.94442300
H	9.46785600	-0.38423400	0.69444900
H	9.80836300	0.53698400	2.16262700
H	-5.78438700	-4.48505500	-0.76648200
H	-7.52604200	-4.20899100	-0.99266300
H	-6.36099000	-3.50090700	-2.13411900
H	-4.80238800	0.55719700	4.69419700
H	-6.48333300	3.38551600	0.57788300
H	-6.68758000	2.98262100	-2.07802700
H	-5.12568300	-0.86508500	-5.38827800
H	-3.69453600	-3.13370500	-5.06370900
H	-2.02998800	-5.93205800	-0.95696400
H	-2.31907000	-5.71715800	1.72674300
H	-3.87899200	-1.97531900	4.97924400
H	0.31395100	-0.32403900	7.79692300
H	0.98939400	1.09567300	6.99465200
H	-0.73939100	1.02014100	7.33198500
H	8.92692000	-2.78612400	-3.47656800

H	8.32447800	-1.23823100	-2.88239100
H	9.93420000	-1.80357500	-2.40217100
H	3.02341100	-1.09907900	-4.68022900
H	4.52551800	-2.02416400	-4.74836500
H	6.93229800	5.86348300	-1.87037800
H	4.26446400	-0.68191100	-5.87213000
H	6.49603000	5.05991300	-3.38698500
H	-1.63026200	7.93398300	-0.08253000
O	-1.17009200	-0.08634100	-0.20100500
H	-0.58154200	0.29145100	-4.29987500
H	-3.53961700	4.95924000	-1.81474600
H	-1.43359500	0.75639600	0.19306600

## TS2

C	0.89387100	-1.00835400	6.71775800
C	0.69960900	-1.29774500	5.24284000
C	-0.04289800	-0.39906200	4.44809500
C	1.24900400	-2.48872600	4.68455600
C	-0.21981000	-0.71097900	3.11201500
C	1.13570600	-2.72970800	3.27818600
C	0.38523600	-1.82939500	2.53990700
H	-0.49323200	0.48354200	4.89266500
H	1.82491100	-3.16799600	5.30494300
H	-0.83114700	-0.08367300	2.46921900
H	1.56788700	-3.61586500	2.82943000
H	0.19964600	-2.01776300	1.48977400
C	5.65988100	7.04993100	-1.02594000
C	4.25932800	6.51278900	-0.57598900
H	6.46704800	6.48359900	-0.55145300
H	4.13840800	5.45988500	-0.84847900
H	4.14034700	6.59688900	0.50924300
H	3.45013600	7.07560200	-1.05036600
N	-1.89089600	7.38327400	2.60294500
C	-0.68214400	7.22389600	1.70040400
C	-0.92898900	6.10921900	0.71452900
O	-0.67022100	6.21218300	-0.47522700
C	0.64146700	7.06546100	2.38666400
O	0.70168000	7.94553600	3.50706800
H	-1.70781400	8.19872700	3.18439400
H	-0.59063300	8.10814400	1.05537800
H	0.80815700	6.02491600	2.70532000
H	1.44313100	7.33578600	1.69670500
H	0.22331900	7.51359700	4.22589400

N	-1.68285000	5.05397700	1.11819900
C	-2.17178000	4.00330700	0.22700100
C	-3.17256900	4.45543600	-0.80678700
O	-2.93634800	4.28139400	-2.03091500
C	-2.66241300	2.84855300	1.05276800
H	-2.05852000	5.09820500	2.05885600
H	-1.31683500	3.67323000	-0.36718800
H	-2.78015200	1.95008700	0.44437700
H	-1.94664900	2.61088600	1.84009800
H	-3.62831900	3.06939000	1.52403700
C	-1.49790600	1.78218300	-3.73938500
H	-1.86131400	2.07647600	-4.72731900
H	-0.43801800	1.53270600	-3.81187300
H	-1.64484700	2.61672900	-3.05219800
C	-6.75786100	-2.42553500	0.38825800
S	-5.56221400	-3.04574600	-0.83157100
C	9.36208900	0.92131500	-3.32581700
C	8.97860200	-0.19776000	-2.35724000
C	7.65244600	-0.66128600	-2.24073200
C	9.98690400	-0.89189100	-1.73242800
C	7.38988700	-1.73324500	-1.42476500
C	9.72866500	-1.94673400	-0.83091800
C	8.42537400	-2.39475600	-0.71414100
H	6.85102200	-0.15768300	-2.77400200
H	11.01394300	-0.56011900	-1.86657400
H	6.37057800	-2.09925900	-1.32965100
H	10.54359800	-2.43254200	-0.30430200
H	8.17690300	-3.22808900	-0.06354900
C	4.30121800	1.63139400	-5.11880000
C	4.81327800	2.38630000	-3.87796100
H	4.06716800	3.09791000	-3.51045600
H	5.04051700	1.69511200	-3.05890900
H	5.72614900	2.94807300	-4.10239300
N	-2.41271700	-3.13211700	-0.94432700
N	-3.66996100	-1.17579400	-2.65593700
N	-3.51947500	-1.84347100	1.36186600
C	-2.30785600	-3.98365600	1.37786600
C	-2.17839600	-3.02425000	-3.39196600
C	-5.40636400	0.62051800	-2.77211300
C	-4.89711100	0.03263700	2.14140600
C	-2.01931900	-4.03935600	0.01522200
C	-3.04435800	-1.94608900	-3.61509900
C	-5.47039900	0.78765700	-1.36417800
C	-4.10564100	-1.08462100	2.35050900

O	-1.84798900	-0.48496600	-0.39063400
C	-1.23292400	-5.08166500	-0.60455700
C	-3.46713800	-1.52279100	-4.92778900
C	-6.33252600	1.73994100	-0.71145000
C	-3.88169300	-1.69472100	3.64176500
C	-1.15891800	-4.79298300	-1.93346000
C	-4.38754500	-0.53218800	-4.75516700
C	-6.17521200	1.59204500	0.63820100
C	-3.18972800	-2.84385100	3.41928300
C	-1.92146900	-3.58484900	-2.14482400
C	-4.52811300	-0.31348900	-3.33704000
C	-5.21974900	0.53448500	0.85525000
C	-2.97242000	-2.93368300	1.99408900
N	-4.77584100	0.07446900	-0.38011000
Fe	-3.35611500	-1.37103700	-0.64053000
H	-1.93060300	-4.78251500	2.00541700
H	-1.75166700	-3.50911200	-4.26089000
H	-6.02051400	1.24260800	-3.40869000
H	-5.34221800	0.52766000	2.99597200
N	2.25669700	-2.53763100	-1.98384800
C	0.77405500	2.51159600	1.45480700
O	0.00683400	1.83480100	0.46479900
N	3.19337500	-1.78312900	0.40964400
C	0.47478700	0.66090000	-0.02243500
N	4.16799000	-4.66891200	4.57583800
C	1.61521500	0.06000300	0.48770400
C	2.14448900	-1.09652700	-0.09764900
C	1.57602800	-1.55972100	-1.34137700
C	0.43504500	-0.90166000	-1.87999100
C	1.89337700	-2.83865200	-3.22291700
C	0.85806200	-2.17262400	-3.89438300
C	0.11806900	-1.22141000	-3.21054500
C	-0.28899500	0.11559800	-1.11802700
C	3.92370900	-1.43542600	1.62117900
C	4.97423700	-0.34848700	1.35515300
C	4.51654100	-2.71169800	2.23108000
C	4.99958300	-2.51874900	3.67206000
C	5.35745400	-3.82888800	4.37707100
H	3.52203100	-2.53205400	-0.19011200
H	3.87539200	-5.07174600	3.68935400
H	4.40096500	-5.45740200	5.17401000
H	2.09935800	0.47391300	1.35766800
H	2.46042200	-3.62402100	-3.71885200
H	0.63042400	-2.41697900	-4.92639900

H	-0.70229900	-0.71708900	-3.69734900
H	3.18327200	-1.05790100	2.33463000
H	4.51446100	0.52374400	0.88215200
H	5.44327900	-0.02086200	2.28759300
H	5.75866200	-0.71909700	0.68807400
H	5.33993400	-3.07767200	1.60043700
H	3.73015600	-3.47231200	2.20803700
H	4.20793900	-2.02807700	4.24979400
H	5.87670200	-1.86134700	3.68675000
H	6.16830600	-4.33278200	3.82050100
H	5.76004000	-3.59308900	5.36821600
H	-7.09025600	-1.41316000	0.15090100
H	-7.62406400	-3.09588000	0.35136600
H	-6.34546500	-2.45044300	1.39885400
H	-4.23269700	-1.28951900	4.58111400
H	-6.68151500	2.13057600	1.42862000
H	-6.98613600	2.42669400	-1.23278200
H	-4.93574600	0.01135900	-5.51271200
H	-3.11911600	-1.95914500	-5.85448400
H	-0.65633200	-5.34550000	-2.71539400
H	-0.80145600	-5.91978900	-0.07416400
H	-2.83924400	-3.57120600	4.13836600
H	-0.06096100	-0.80387200	7.21499800
H	1.36757500	-1.84916300	7.23090100
H	1.52912800	-0.12723000	6.87003900
H	10.28770100	1.41152000	-3.01392400
H	9.51706100	0.52229200	-4.33481100
H	8.57707300	1.68101200	-3.39211100
H	3.39310200	1.06502200	-4.88858700
H	5.04982900	0.92316600	-5.48897500
H	5.78052500	8.10295900	-0.75450100
H	4.06534800	2.32302300	-5.93354100
H	5.77896600	6.96460900	-2.11013700
H	-2.67524100	7.62818300	2.00405000
H	-0.81066600	0.85777000	-1.70063600
H	1.79036100	2.71029100	1.09532300
H	0.25892800	3.45456100	1.63375900
H	0.82045500	1.93181800	2.38360900
H	-4.10783100	4.94048400	-0.46625700
H	-2.07606500	0.92411000	-3.39705600

IM2

C	0.87733500	-1.01802700	6.71156600
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C	0.68725900	-1.30586200	5.23579300
C	-0.05461500	-0.40732500	4.44029700
C	1.23992500	-2.49529900	4.67742300
C	-0.22765800	-0.71783900	3.10337900
C	1.13055300	-2.73467100	3.27043200
C	0.38054600	-1.83460200	2.53143700
H	-0.51613000	0.46798000	4.88814400
H	1.80541700	-3.18063300	5.30042200
H	-0.86016700	-0.11469700	2.45767000
H	1.55443200	-3.62875100	2.82891900
H	0.16585200	-2.02199900	1.48514200
C	5.65052700	7.05730300	-1.00992500
C	4.24966800	6.51744100	-0.56420100
H	6.45761000	6.48587700	-0.54137700
H	4.12739200	5.46729900	-0.84710800
H	4.13135600	6.59147600	0.52187200
H	3.44085500	7.08556000	-1.03273800
N	-1.90993000	7.37446700	2.60020600
C	-0.69864900	7.21808300	1.70053600
C	-0.94127500	6.10426600	0.71264300
O	-0.67965300	6.20912200	-0.47632200
C	0.62346000	7.06082300	2.38995400
O	0.67947500	7.93958200	3.51160800
H	-1.73562000	8.19553300	3.17632800
H	-0.60654800	8.10319100	1.05685400
H	0.79088900	6.01990600	2.70831200
H	1.42682700	7.33365300	1.70302300
H	0.18179500	7.51499600	4.22185100
N	-1.69451800	5.04735400	1.11308100
C	-2.17957100	3.99705400	0.21930900
C	-3.17843100	4.44895300	-0.81639800
O	-2.93889500	4.27681100	-2.04017200
C	-2.67049200	2.84048900	1.04237200
H	-2.08212800	5.09630000	2.04894000
H	-1.32250800	3.67550400	-0.37660100
H	-2.75745200	1.93097800	0.44506800
H	-1.98056400	2.62576200	1.85901300
H	-3.65449400	3.04615000	1.48075000
C	-1.49216400	1.78197700	-3.74814300
H	-1.82366400	2.03420200	-4.75885300
H	-0.43549300	1.50979400	-3.77853600
H	-1.64022100	2.64797000	-3.10181300
C	-6.50616100	-2.55328400	0.44504800
S	-5.33041000	-2.86025400	-0.91436600

C	9.36800200	0.93728500	-3.30807200
C	8.98378800	-0.18359400	-2.34187300
C	7.65807100	-0.64930600	-2.22930700
C	9.99157200	-0.87695700	-1.71537400
C	7.39507000	-1.72268800	-1.41535600
C	9.73267600	-1.93332300	-0.81583800
C	8.42978400	-2.38350300	-0.70293200
H	6.85809300	-0.14721000	-2.76624400
H	11.01844900	-0.54404200	-1.84713000
H	6.37699900	-2.09475600	-1.32811600
H	10.54692900	-2.41910900	-0.28831600
H	8.18184100	-3.21955900	-0.05558600
C	4.31060300	1.64182400	-5.11299700
C	4.81835100	2.39595600	-3.86991900
H	4.06613600	3.09832300	-3.49708000
H	5.05621200	1.70339800	-3.05470300
H	5.72454800	2.96826700	-4.09425500
N	-2.41266000	-3.13438200	-0.96222300
N	-3.66964500	-1.19281100	-2.66598500
N	-3.53144500	-1.85472600	1.32967900
C	-2.30626000	-3.99155200	1.35987100
C	-2.16618200	-3.02595500	-3.40841500
C	-5.40132000	0.61307300	-2.79219700
C	-4.90366700	0.01976700	2.12185500
C	-2.00899400	-4.03804900	-0.00307300
C	-3.03606500	-1.95059800	-3.63107300
C	-5.46273300	0.77782500	-1.38189600
C	-4.10822100	-1.09479400	2.32476000
O	-1.47993600	-0.55587200	-0.21357400
C	-1.19417600	-5.06491400	-0.61770400
C	-3.44100100	-1.51368900	-4.94611000
C	-6.30763500	1.74962300	-0.73224900
C	-3.86875000	-1.69283700	3.61969400
C	-1.11810200	-4.77503000	-1.94545600
C	-4.36320400	-0.52568200	-4.77313400
C	-6.15727800	1.60168300	0.61756800
C	-3.17778700	-2.84144000	3.39673100
C	-1.90774500	-3.58206700	-2.15893200
C	-4.52189400	-0.32479100	-3.35285000
C	-5.22049300	0.52623800	0.83617100
C	-2.97742900	-2.93959300	1.96796800
N	-4.77593900	0.05516300	-0.39532900
Fe	-3.57269300	-1.53241100	-0.66570100
H	-1.92417500	-4.78598000	1.99036800

H	-1.73713200	-3.51054300	-4.27736800
H	-6.00761300	1.24233800	-3.42929400
H	-5.34608000	0.51418700	2.97850200
N	2.30478500	-2.38160900	-1.98128300
C	0.71404700	2.54059400	1.57609600
O	-0.00236600	1.85843200	0.53626700
N	3.18335900	-1.67521500	0.40157700
C	0.45381400	0.70585400	0.07461900
N	4.10055100	-4.77998600	4.40207200
C	1.61579100	0.14210500	0.55894900
C	2.13392200	-1.00848300	-0.05153200
C	1.55608300	-1.48098300	-1.32237800
C	0.38123500	-0.89154000	-1.81043300
C	1.93765500	-2.69776500	-3.22309900
C	0.84579500	-2.09729100	-3.84938700
C	0.05704800	-1.20233200	-3.13145500
C	-0.47629100	0.04943600	-0.94425100
C	3.92691800	-1.39540800	1.63292500
C	5.00063000	-0.32942900	1.38893000
C	4.48526500	-2.71497900	2.17801100
C	4.97346900	-2.59783100	3.62516500
C	5.30371300	-3.94870000	4.26483400
H	3.48286700	-2.42557200	-0.22030200
H	3.84697900	-5.18302500	3.50396500
H	4.29362800	-5.56816000	5.01408300
H	2.11783700	0.54941400	1.42209600
H	2.55275400	-3.42850000	-3.74200300
H	0.60840100	-2.33860500	-4.87993900
H	-0.80088900	-0.74174900	-3.59427600
H	3.19339500	-1.02994600	2.35776900
H	4.55940600	0.57923800	0.97013900
H	5.49588800	-0.06508500	2.32690700
H	5.76071500	-0.69122800	0.68991400
H	5.29729100	-3.07156800	1.52801200
H	3.67894400	-3.45265400	2.12873500
H	4.19007800	-2.12133000	4.22525200
H	5.86376800	-1.95972900	3.66993800
H	6.11691200	-4.43392000	3.69578200
H	5.69429700	-3.76744400	5.27176600
H	-6.86226100	-1.52109700	0.44137200
H	-7.35678800	-3.22063300	0.28147600
H	-6.06526300	-2.77554000	1.41879400
H	-4.20778600	-1.27904800	4.55991200
H	-6.65452800	2.15152800	1.40627700

H	-6.94568200	2.44896900	-1.25668900
H	-4.89918500	0.02962900	-5.53123300
H	-3.07920000	-1.93767900	-5.87358800
H	-0.60059400	-5.31764000	-2.72521300
H	-0.74857100	-5.89425300	-0.08429000
H	-2.81420100	-3.56214800	4.11646500
H	-0.07390700	-0.77426500	7.19722200
H	1.31219500	-1.87447500	7.23333000
H	1.54534900	-0.16192300	6.86788200
H	10.28563100	1.43622400	-2.98675500
H	9.53809900	0.53743800	-4.31421100
H	8.57710200	1.68977200	-3.38474700
H	3.40799500	1.06606700	-4.88416200
H	5.06516000	0.94286300	-5.48857300
H	5.77213500	8.10748900	-0.72844600
H	4.06607800	2.33519800	-5.92344700
H	5.76864600	6.98242900	-2.09495500
H	-2.69578400	7.60831300	1.99880600
H	-0.83423400	0.85643100	-1.60073100
H	1.73494100	2.76232700	1.25089700
H	0.16813900	3.46700500	1.74233300
H	0.72939700	1.93551900	2.48706800
H	-4.11638100	4.92839600	-0.47665200
H	-2.09473600	0.95213700	-3.37923300

### TS3

C	0.80654800	-0.60220800	6.90586500
C	0.63848700	-0.97607400	5.44680300
C	-0.07371400	-0.11601600	4.58446400
C	1.18123000	-2.20567900	4.97194600
C	-0.22764800	-0.50435700	3.26567400
C	1.09341900	-2.52825300	3.58012100
C	0.37207500	-1.66311400	2.77394400
H	-0.51944900	0.79731800	4.96689200
H	1.73278700	-2.85390800	5.64461100
H	-0.82413700	0.08444200	2.57353000
H	1.52674200	-3.44515200	3.20019700
H	0.20151500	-1.90654700	1.73186200
C	5.85332700	6.91442800	-1.19644200
C	4.43580700	6.42405200	-0.74587700
H	6.64201500	6.36077800	-0.67795400
H	4.30215400	5.36039200	-0.96594800
H	4.29859300	6.56633200	0.33106100

H	3.64512100	6.97429400	-1.26415600
N	-1.76495700	7.56774600	2.24267700
C	-0.54036900	7.33822800	1.37746600
C	-0.78360300	6.17037900	0.45413800
O	-0.49873000	6.19879500	-0.73377800
C	0.76631400	7.20250300	2.10007300
O	0.81660200	8.14665200	3.16765600
H	-1.57868800	8.40994100	2.78355000
H	-0.42236700	8.18098500	0.68303300
H	0.90973500	6.18015500	2.48225800
H	1.58588500	7.42060700	1.41258900
H	0.32437700	7.76152400	3.90348000
N	-1.56154300	5.15159300	0.90318300
C	-2.04781500	4.05668000	0.06535600
C	-3.02002000	4.46041500	-1.01465000
O	-2.76124000	4.21060600	-2.22099400
C	-2.57283600	2.95999500	0.94722300
H	-1.95316900	5.25537500	1.83252900
H	-1.20445500	3.69249300	-0.51947600
H	-2.75285700	2.04672000	0.38092000
H	-1.86415400	2.72435300	1.74265700
H	-3.51781800	3.25271700	1.42222200
C	-1.32569400	1.59445900	-3.74722700
H	-1.31852300	2.45628100	-4.42075800
H	-0.30368400	1.26528300	-3.56549900
H	-1.78393100	1.89468400	-2.80831900
C	-6.56508500	-2.38883000	0.44681100
S	-5.34587600	-2.76217000	-0.86151300
C	9.50903300	0.60891100	-3.04929900
C	9.08887200	-0.44578900	-2.02484200
C	7.75223000	-0.87983800	-1.90963600
C	10.07325500	-1.11510300	-1.33861100
C	7.45793700	-1.90044000	-1.03763400
C	9.78040400	-2.11055500	-0.38180000
C	8.46840400	-2.53293900	-0.26714100
H	6.97047900	-0.39846300	-2.49040900
H	11.10775600	-0.80696200	-1.47107200
H	6.43473700	-2.25668100	-0.95112200
H	10.57670300	-2.57559100	0.19004500
H	8.19408000	-3.32372000	0.42480600
C	4.49685200	1.28237100	-4.99032300
C	4.99733100	2.09843100	-3.78449600
H	4.27455300	2.86951300	-3.49951800
H	5.15742200	1.45743800	-2.91027000

H	5.94564300	2.59853400	-4.00783100
N	-2.43170700	-3.18791600	-0.69535300
N	-3.28318000	-1.04816300	-2.52569700
N	-3.57457600	-1.73424600	1.50467400
C	-2.32872900	-3.84503100	1.68361400
C	-2.08606600	-3.17289500	-3.13073000
C	-5.27054200	0.54682700	-2.79734000
C	-4.87208600	0.24515200	2.15218400
C	-2.04068100	-4.01998500	0.33134300
C	-2.85688000	-2.06798400	-3.44221700
C	-5.36521500	0.79018200	-1.39068600
C	-4.12878600	-0.89169700	2.43910700
O	-1.76575900	-0.74052800	-0.22523500
C	-1.23085300	-5.09422000	-0.20422200
C	-3.36369300	-1.79354800	-4.74243400
C	-6.23869000	1.78611400	-0.81730100
C	-3.89820500	-1.39621200	3.77528700
C	-1.13880000	-4.89216500	-1.54836100
C	-4.23999100	-0.74565400	-4.64327700
C	-6.09620100	1.73494100	0.53940200
C	-3.21083800	-2.56061400	3.63762500
C	-1.89938200	-3.69684700	-1.84314200
C	-4.29286600	-0.31547600	-3.28625700
C	-5.15699300	0.67803600	0.83574500
C	-3.01509300	-2.76119600	2.21873800
N	-4.69104400	0.13407300	-0.35965300
Fe	-3.50077200	-1.50880800	-0.49447000
H	-1.94023300	-4.58337300	2.37628400
H	-1.72918800	-3.77065300	-3.96082500
H	-5.93588100	1.05821900	-3.47908900
H	-5.30945700	0.80588300	2.96976600
N	2.07011000	-2.73590200	-2.13935900
C	0.56746300	2.42826500	0.79462400
O	-0.30413300	1.68429000	-0.07134300
N	2.85571200	-1.85470900	0.26379500
C	0.09803700	0.47549200	-0.47887600
N	4.21680400	-4.27128900	4.60208700
C	1.30623700	-0.01381300	0.03606900
C	1.80340600	-1.26491000	-0.31136800
C	1.24354800	-1.87961000	-1.50877300
C	0.04482100	-1.34491500	-2.03821000
C	1.81651800	-3.02266500	-3.41413100
C	0.81558300	-2.35920300	-4.12172800
C	-0.05589700	-1.52315200	-3.42648200

C	-0.85326500	-0.37640000	-1.24826200
C	3.61556300	-1.32293700	1.39503300
C	4.60559200	-0.23668200	0.95418500
C	4.28773700	-2.49229400	2.12423500
C	4.79609100	-2.11891900	3.51935100
C	5.30168700	-3.32051800	4.32123900
H	3.20045000	-2.66300000	-0.24658800
H	3.99579500	-4.80400300	3.76478100
H	4.52834200	-4.95367300	5.28825200
H	1.83514300	0.53900400	0.79212300
H	2.47948900	-3.73629600	-3.89776000
H	0.71953900	-2.48812500	-5.19474900
H	-0.80029200	-0.97109400	-3.97471300
H	2.87933300	-0.89011700	2.07988700
H	4.10266700	0.53957200	0.37161400
H	5.06501800	0.23834700	1.82544900
H	5.40477200	-0.65819400	0.33895800
H	5.11318400	-2.88360800	1.51144900
H	3.54326400	-3.28935500	2.21339900
H	3.97913100	-1.65213600	4.08073700
H	5.60780900	-1.38646100	3.43838000
H	6.16201400	-3.77305800	3.79568000
H	5.67988300	-2.96056800	5.28408400
H	-6.89195300	-1.34704100	0.40060500
H	-7.43196000	-3.03565800	0.28922300
H	-6.15702900	-2.58674300	1.44058700
H	-4.23089600	-0.91044700	4.68253000
H	-6.60643400	2.33028400	1.28526000
H	-6.87542700	2.44376100	-1.39435800
H	-4.86686800	-0.33853300	-5.42552700
H	-3.14625000	-2.39162900	-5.61732300
H	-0.60886800	-5.48192800	-2.28379600
H	-0.79654800	-5.88996500	0.38608000
H	-2.84648700	-3.22627500	4.40786000
H	-0.15221500	-0.33415400	7.36331200
H	1.23649900	-1.42516400	7.48262700
H	1.46971800	0.26392300	7.02048600
H	10.43572300	1.10330800	-2.74754200
H	9.67780700	0.14890200	-4.02967600
H	8.73737500	1.37454000	-3.17620800
H	3.55300200	0.77745900	-4.76108200
H	5.22297000	0.51510100	-5.27862900
H	5.98676000	7.97804900	-0.97755300
H	4.32826600	1.92485900	-5.86006200

H	5.99052400	6.77099000	-2.27232300
H	-2.53182100	7.79351700	1.61436100
H	-2.19085500	-0.38402400	-2.21627800
H	1.54825700	2.55985100	0.32918900
H	0.11144700	3.40132500	0.94000600
H	0.67369000	1.92574000	1.76089700
H	-3.95482100	4.97834700	-0.72339600
H	-1.90422400	0.79530000	-4.21014400

## TS5

C	0.91133500	-1.17955000	6.55145800
C	0.67166200	-1.45201500	5.07999600
C	-0.06170700	-0.52484500	4.30987400
C	1.16955400	-2.65542700	4.50044600
C	-0.28128400	-0.82136200	2.97661100
C	1.01411900	-2.88244200	3.09568900
C	0.27401600	-1.95391900	2.38240200
H	-0.47017100	0.37105300	4.76811800
H	1.74605800	-3.35360200	5.09767600
H	-0.87796600	-0.16097100	2.35544900
H	1.42236800	-3.77296200	2.63117400
H	0.08660300	-2.11639600	1.32442900
C	5.73455900	6.78258500	-1.25604500
C	4.32940900	6.28587100	-0.77487700
H	6.53639900	6.20869300	-0.78150300
H	4.18152500	5.23047000	-1.02358900
H	4.22839300	6.39537900	0.31002200
H	3.52557100	6.85633900	-1.24898200
N	-1.71002800	7.32452600	2.56205500
C	-0.52953500	7.13414500	1.62866800
C	-0.83558100	6.03496200	0.64198800
O	-0.60311800	6.13841100	-0.55315000
C	0.80505600	6.92955300	2.28057000
O	0.92046300	7.79911100	3.40489700
H	-1.52245100	8.16999200	3.09712200
H	-0.42645300	8.01990300	0.98755300
H	0.94789200	5.88204000	2.58861100
H	1.59830100	7.18108700	1.57418900
H	0.37653900	7.41418900	4.10420500
N	-1.61167800	5.00057800	1.05755400
C	-2.15529800	3.97260700	0.17165900
C	-3.16848800	4.46337800	-0.83369000
O	-2.96366000	4.28860600	-2.06515400

C	-2.66115000	2.82724700	1.00190900
H	-1.95037600	5.03412200	2.01199200
H	-1.32930400	3.61176400	-0.44809600
H	-2.87616400	1.96604100	0.36980800
H	-1.89428600	2.50966700	1.70627800
H	-3.56973300	3.09971000	1.55436400
C	-1.65098800	1.76174700	-3.82303000
H	-2.01297800	1.00973600	-4.52755200
H	-0.61535700	2.01905300	-4.06245100
H	-2.26688000	2.65922700	-3.87875200
C	-6.81484200	-2.49296800	0.50788100
S	-5.71336200	-2.90344700	-0.88745300
C	9.18495300	0.55841200	-3.68740000
C	8.79066200	-0.55523800	-2.71690800
C	7.45391700	-0.97796700	-2.57031000
C	9.79185500	-1.28494600	-2.12192700
C	7.17815500	-2.04720000	-1.75510700
C	9.52306000	-2.33776700	-1.22114700
C	8.20964700	-2.74580000	-1.07479100
H	6.65450900	-0.44440400	-3.07670500
H	10.82520500	-0.98474200	-2.27962400
H	6.14955400	-2.38183400	-1.64384900
H	10.33513800	-2.85281900	-0.71846100
H	7.95203100	-3.57777500	-0.42586100
C	4.10602500	1.43888600	-5.34896800
C	4.67203500	2.16836900	-4.11639300
H	4.04912400	3.02530600	-3.84139300
H	4.71740300	1.50138600	-3.24841000
H	5.68497300	2.54036500	-4.30427100
N	-2.70114200	-3.13948300	-1.03778000
N	-3.97060100	-1.20692500	-2.68670000
N	-3.73124000	-1.87220500	1.26830500
C	-2.51305800	-4.01464900	1.27382700
C	-2.47159600	-3.02509100	-3.49144200
C	-5.56745200	0.71394300	-2.76754700
C	-4.95551800	0.07468100	2.12778400
C	-2.27465400	-4.06270500	-0.09653400
C	-3.31671900	-1.92333000	-3.67716900
C	-5.62168500	0.84769200	-1.35618800
C	-4.21061500	-1.07597400	2.29507800
O	-1.20620300	0.43757500	-0.50220700
C	-1.48922900	-5.09200100	-0.73347800
C	-3.67280200	-1.40650200	-4.97643500
C	-6.34667200	1.89283500	-0.67991500

C	-3.89838400	-1.65575300	3.57796200
C	-1.44315900	-4.79718600	-2.06097400
C	-4.56199600	-0.39535700	-4.77689200
C	-6.16173100	1.73093200	0.66390000
C	-3.25498000	-2.82729400	3.33191500
C	-2.21784200	-3.59593700	-2.25091100
C	-4.75081300	-0.26057400	-3.35341700
C	-5.32305900	0.57517300	0.85430700
C	-3.15434100	-2.95729900	1.89921500
N	-4.98657800	0.04898600	-0.39362300
Fe	-3.96810500	-1.61873200	-0.71775000
H	-2.10559300	-4.80579800	1.89172800
H	-2.04816800	-3.49285900	-4.37246600
H	-6.11485800	1.41004700	-3.38837100
H	-5.30470100	0.61245000	3.00077900
N	2.75147300	-2.04598200	-1.68559200
C	1.05019900	2.72399500	2.18147400
O	0.28556800	1.87577900	1.32867800
N	4.01110600	-1.07300800	0.45581800
C	0.91164500	0.96021800	0.57571700
N	3.98125400	-4.70131400	4.25560900
C	2.23652300	0.53219300	0.84978400
C	2.80814500	-0.52766600	0.16886700
C	2.09912400	-1.09702700	-0.97925100
C	0.79417200	-0.66984900	-1.28458600
C	2.12622800	-2.57859900	-2.73048900
C	0.82660800	-2.21783000	-3.11408000
C	0.14799100	-1.26471800	-2.37273900
C	0.05660500	0.35404400	-0.46790500
C	4.67057000	-1.02816700	1.75939900
C	6.04118300	-0.35605100	1.64256200
C	4.73349800	-2.45450900	2.33739800
C	5.05465900	-2.50366900	3.83420700
C	5.22319100	-3.92673000	4.37223200
H	4.25213900	-1.83677000	-0.16777400
H	3.79180000	-4.90430900	3.27741700
H	4.09574100	-5.60360500	4.71025900
H	2.78689200	1.02207900	1.63929600
H	2.67674500	-3.33237700	-3.28902200
H	0.36104500	-2.69109000	-3.97029800
H	-0.86636000	-0.96159500	-2.59902700
H	4.03020700	-0.43797900	2.42190400
H	5.93650200	0.65820600	1.24784500
H	6.53843600	-0.29679200	2.61495100

H	6.68653800	-0.91651600	0.95850000
H	5.47628500	-3.03621000	1.77069900
H	3.75498400	-2.91527100	2.16849600
H	4.24465700	-2.01223100	4.38595000
H	5.97919300	-1.95143900	4.04018500
H	6.08624100	-4.39723000	3.86677200
H	5.47730600	-3.87200700	5.43662000
H	-7.13248700	-1.44956900	0.46953800
H	-7.69426800	-3.13579500	0.41464400
H	-6.33254500	-2.68797700	1.46721700
H	-4.15016700	-1.20936700	4.53024300
H	-6.56017500	2.33657100	1.46720600
H	-6.92133100	2.65883900	-1.18349000
H	-5.04494800	0.22764800	-5.51743800
H	-3.28794500	-1.78610300	-5.91338300
H	-0.94661900	-5.33841100	-2.85492000
H	-1.03511900	-5.92423100	-0.21257400
H	-2.85005100	-3.53782000	4.03913300
H	-0.03256300	-1.06171300	7.09630200
H	1.47066000	-1.99184900	7.02259500
H	1.48128100	-0.25415200	6.69711500
H	10.13827900	1.00996000	-3.40188600
H	9.29120500	0.16416800	-4.70451600
H	8.42767300	1.34790100	-3.72087800
H	3.09598500	1.06441600	-5.15510200
H	4.73114100	0.58310200	-5.62476300
H	5.88191700	7.83811700	-1.00866200
H	4.05340500	2.10587600	-6.21506700
H	5.83551900	6.67215600	-2.33978800
H	-2.51700100	7.52838200	1.97809900
H	0.76112100	1.40777000	-0.91181100
H	1.86656500	3.20558000	1.63275500
H	0.35079900	3.48387000	2.52908800
H	1.44621400	2.16294400	3.03463000
H	-4.08296900	4.96810600	-0.46437900
H	-1.70302100	1.36766600	-2.80454900

#### IM4

C	1.00805800	-1.42090300	6.46805600
C	0.75562400	-1.63256100	4.98874600
C	0.00393300	-0.68155100	4.26686400
C	1.26039300	-2.80419900	4.35278600
C	-0.22671900	-0.92298800	2.92438700

C	1.09250400	-2.97230500	2.94118900
C	0.33458100	-2.02252000	2.27624400
H	-0.39585900	0.19747600	4.76292100
H	1.84841300	-3.52195800	4.91663000
H	-0.80933600	-0.22086400	2.33717900
H	1.50315600	-3.83564800	2.42959200
H	0.14679400	-2.14046300	1.21272200
C	5.65970900	6.92411900	-1.03786800
C	4.26533000	6.39116900	-0.56419900
H	6.47297600	6.35878100	-0.57285100
H	4.13938800	5.33683800	-0.82922600
H	4.16314700	6.48043200	0.52234100
H	3.44967900	6.95303900	-1.02853800
N	-1.74900100	7.21637700	2.87608800
C	-0.57656700	7.07979000	1.92332200
C	-0.88111900	6.02063500	0.89334100
O	-0.66260200	6.17800800	-0.29853000
C	0.76709800	6.86260400	2.55209500
O	0.88501700	7.68427400	3.71162600
H	-1.53892300	8.01127300	3.47647100
H	-0.48976500	7.99331500	1.31965900
H	0.92557700	5.80654400	2.81466600
H	1.54903500	7.15274400	1.84760600
H	0.40970700	7.23220800	4.42014900
N	-1.64131200	4.96053600	1.27187500
C	-2.18302100	3.96571400	0.34806000
C	-3.21273400	4.48693400	-0.62474500
O	-3.01845800	4.36855300	-1.86458800
C	-2.66740000	2.77976300	1.13329100
H	-1.96130700	4.94456800	2.23305800
H	-1.36047900	3.63916400	-0.29503300
H	-3.01410200	1.99340400	0.46232100
H	-1.84348700	2.36322000	1.71275100
H	-3.49595700	3.04684400	1.80145600
C	-1.69757700	1.93420100	-3.74321300
H	-2.22215100	1.89362900	-4.69991400
H	-0.63573700	1.72705200	-3.90421500
H	-1.82255500	2.91601600	-3.28698400
C	-6.78276100	-2.57006400	0.46223600
S	-5.70104800	-2.91022000	-0.96723700
C	9.15185600	0.85004400	-3.77053200
C	8.78022700	-0.30875600	-2.84499800
C	7.44986400	-0.75263200	-2.70309100
C	9.79568100	-1.05187300	-2.29228800

C	7.19454200	-1.85895100	-1.93187100
C	9.54811900	-2.14546400	-1.43504300
C	8.24091000	-2.57438800	-1.29301100
H	6.63907700	-0.20415300	-3.17446600
H	10.82387500	-0.73216100	-2.44609100
H	6.16834500	-2.19428500	-1.80131200
H	10.37142600	-2.67123600	-0.96237800
H	7.99827400	-3.43263500	-0.67324400
C	4.04605800	1.74311700	-5.34049800
C	4.61721400	2.42533900	-4.08347400
H	3.99126300	3.26635300	-3.76857100
H	4.67604300	1.72402200	-3.24404900
H	5.62569800	2.81202800	-4.26462400
N	-2.67335500	-3.09754100	-1.16164300
N	-3.97764100	-1.11105100	-2.71100100
N	-3.69012300	-1.94274600	1.20499300
C	-2.44144200	-4.06534000	1.10843900
C	-2.46193100	-2.87138800	-3.60990300
C	-5.59064700	0.79748600	-2.69380000
C	-4.91929900	-0.04466500	2.16289100
C	-2.22118100	-4.05359200	-0.26536000
C	-3.31904500	-1.77090600	-3.73910100
C	-5.63442200	0.86765300	-1.27796300
C	-4.16278800	-1.19441100	2.27184000
O	-1.05510700	0.49154800	-0.50370500
C	-1.42520900	-5.04089600	-0.95309400
C	-3.68183900	-1.19161900	-5.00891600
C	-6.35876900	1.87696600	-0.54991700
C	-3.82342900	-1.82112100	3.52495000
C	-1.39688200	-4.68858800	-2.26678200
C	-4.58243700	-0.20228100	-4.75783500
C	-6.15729900	1.65959000	0.78388800
C	-3.16925300	-2.97302100	3.22238200
C	-2.19238100	-3.49351500	-2.39811400
C	-4.77099000	-0.14173300	-3.32992400
C	-5.30898100	0.50364200	0.91612500
C	-3.08956500	-3.04454900	1.78464200
N	-4.98145500	0.03263800	-0.35749000
Fe	-3.96820200	-1.62018300	-0.76518200
H	-2.01254300	-4.87365400	1.68827300
H	-2.03644400	-3.29156200	-4.51346400
H	-6.14854300	1.51650500	-3.27814500
H	-5.26060500	0.45348200	3.06203500
N	2.68979400	-2.13466000	-1.75546500

C	1.10315800	3.07586600	1.71686100
O	0.43139100	1.91407100	1.26944200
N	3.78057100	-1.48543000	0.61079100
C	1.12979600	1.22245900	0.25359200
N	4.02584200	-5.01711000	4.45481100
C	2.29411200	0.42696900	0.78631100
C	2.75044400	-0.69500800	0.18004600
C	2.08210100	-1.16683400	-1.05198200
C	0.82109100	-0.64834900	-1.41091200
C	2.08280700	-2.57619300	-2.86414900
C	0.84407700	-2.11345000	-3.30470500
C	0.18609500	-1.15085600	-2.54401200
C	0.15555100	0.35697200	-0.54008600
C	4.36009400	-1.38982100	1.93959100
C	5.55424500	-0.42578000	1.94693500
C	4.71508300	-2.79609300	2.44002600
C	5.08564400	-2.83980600	3.92530900
C	5.28363300	-4.25726900	4.46653600
H	3.95569900	-2.30109500	0.04126200
H	3.76472000	-5.23754400	3.49717400
H	4.16051300	-5.91173100	4.91911900
H	2.77015500	0.81073100	1.67863100
H	2.61363600	-3.34410500	-3.42254500
H	0.39887900	-2.51143700	-4.20837900
H	-0.79587500	-0.78176700	-2.81231900
H	3.57617900	-1.00211300	2.60503000
H	5.25812200	0.54824600	1.54772000
H	5.94574500	-0.27443500	2.95755800
H	6.35807800	-0.81495900	1.31291400
H	5.53718500	-3.20554300	1.83416800
H	3.83621100	-3.42534800	2.26566800
H	4.29029800	-2.35717900	4.50499400
H	6.00796400	-2.27274800	4.09614300
H	6.10105900	-4.74689300	3.90667500
H	5.61538000	-4.19191800	5.50873900
H	-7.10570700	-1.52771600	0.47643000
H	-7.66060000	-3.21244600	0.35319700
H	-6.28451600	-2.80651100	1.40389500
H	-4.06307400	-1.41520500	4.49811500
H	-6.55005900	2.22826000	1.61638900
H	-6.94442800	2.65943400	-1.01386800
H	-5.07390500	0.45135300	-5.46565000
H	-3.29349700	-1.51797500	-5.96424100
H	-0.89683300	-5.18502000	-3.08715900

H	-0.95069000	-5.88565500	-0.47231300
H	-2.74174400	-3.70415300	3.89425300
H	0.07073300	-1.40612400	7.03692600
H	1.63820900	-2.21172800	6.88306400
H	1.50800100	-0.46284600	6.65186400
H	10.10798500	1.29357100	-3.48160400
H	9.24163600	0.50410600	-4.80675500
H	8.39055600	1.63640900	-3.75410600
H	3.03990700	1.35364900	-5.15502900
H	4.67456300	0.90366800	-5.65559900
H	5.78563500	7.97824400	-0.77324400
H	3.98216600	2.44446900	-6.17827300
H	5.76229700	6.83343600	-2.12332400
H	-2.55418300	7.48361800	2.31578200
H	1.48641800	1.96372100	-0.49475900
H	1.25042200	3.79289700	0.89603300
H	0.46228200	3.53326000	2.47120200
H	2.07851000	2.84858500	2.16815100
H	-4.12943900	4.96485800	-0.22857100
H	-2.11748200	1.18214800	-3.07180700

## TS6

C	0.91980000	-1.23126000	6.59639700
C	0.70090300	-1.47508500	5.11669500
C	-0.04809000	-0.54859500	4.36093100
C	1.23406900	-2.65197100	4.51448500
C	-0.24762200	-0.81919700	3.01902300
C	1.09747500	-2.84992100	3.10343600
C	0.34136400	-1.92348100	2.40434800
H	-0.48071800	0.32575500	4.83935400
H	1.81724500	-3.35027600	5.10713000
H	-0.84045000	-0.16489400	2.38809800
H	1.52361600	-3.72098200	2.61852100
H	0.16472800	-2.03346300	1.34030900
C	5.61642500	7.02799200	-0.97618300
C	4.21961600	6.48526000	-0.52078000
H	6.42753100	6.44941700	-0.52367700
H	4.09182900	5.43874200	-0.81370000
H	4.11398900	6.54676000	0.56738000
H	3.40648700	7.06032900	-0.97318700
N	-1.87497400	7.29637800	2.77870100
C	-0.68140300	7.15712200	1.85305000
C	-0.95051100	6.07394400	0.83819100

O	-0.70952700	6.21107700	-0.35187400
C	0.65180800	6.97037400	2.51317100
O	0.73481700	7.81593100	3.65858300
H	-1.67613600	8.09080800	3.38364200
H	-0.59413400	8.05976200	1.23348900
H	0.81827600	5.92024300	2.79831200
H	1.44415600	7.25662300	1.81889500
H	0.26732900	7.36423700	4.37237100
N	-1.70469600	5.01151900	1.22182000
C	-2.21408300	3.99090200	0.30732500
C	-3.22771600	4.47997900	-0.69662500
O	-3.01172700	4.34107400	-1.92904900
C	-2.69910900	2.81483900	1.10572800
H	-2.06626300	5.03081000	2.16887800
H	-1.36835400	3.67017300	-0.30652300
H	-2.93140300	1.97083000	0.45388100
H	-1.92059900	2.47948500	1.79300400
H	-3.59923700	3.05361300	1.68460600
C	-1.61575200	1.88608400	-3.73378300
H	-2.15667200	2.12445700	-4.65253300
H	-0.56842300	1.69092300	-3.97650700
H	-1.69487700	2.72875300	-3.04613000
C	-6.73346600	-2.58026000	0.43615400
S	-5.60687400	-2.94097400	-0.95293800
C	9.24364400	0.94946900	-3.51605600
C	8.86832800	-0.19681200	-2.57614000
C	7.53952200	-0.65212600	-2.45173900
C	9.88158100	-0.91467200	-1.98796000
C	7.28442700	-1.74969800	-1.66503400
C	9.63059600	-1.99444500	-1.11431600
C	8.32649500	-2.43834700	-0.99092900
H	6.73283800	-0.12607800	-2.95422400
H	10.90843900	-0.58493400	-2.12827600
H	6.26250100	-2.10648300	-1.55895300
H	10.45054400	-2.50027800	-0.61497000
H	8.08276400	-3.28970500	-0.36222500
C	4.15922000	1.74393900	-5.20802600
C	4.69852500	2.45352800	-3.95271800
H	3.96844900	3.16505000	-3.55428100
H	4.92533500	1.73502300	-3.15743800
H	5.61711500	3.00773800	-4.17250400
N	-2.58097700	-3.10680700	-1.07223400
N	-3.87168100	-1.16312000	-2.68739200
N	-3.66993300	-1.92537100	1.25193800

C	-2.38300700	-4.02601900	1.22065600
C	-2.32123500	-2.92449200	-3.51979300
C	-5.51605100	0.71884800	-2.74065500
C	-4.93459800	-0.01930600	2.14448800
C	-2.12317200	-4.02873100	-0.14686700
C	-3.19447000	-1.84289800	-3.68940600
C	-5.58347800	0.82081700	-1.32763500
C	-4.17299100	-1.16186400	2.29188100
O	-0.74770000	-0.13739700	-0.01570800
C	-1.27283500	-4.99966600	-0.79403200
C	-3.54989700	-1.30361800	-4.97838200
C	-6.33734700	1.83313600	-0.63499800
C	-3.85567800	-1.76207700	3.56461500
C	-1.21837200	-4.66889100	-2.11212600
C	-4.46624300	-0.31906800	-4.76464900
C	-6.16037200	1.64518300	0.70716000
C	-3.18124300	-2.91091600	3.29794500
C	-2.05342800	-3.50575200	-2.28738900
C	-4.67318900	-0.22331700	-3.34165000
C	-5.29846200	0.50473400	0.87958400
C	-3.06685900	-3.00649400	1.86302900
N	-4.93531200	0.01565700	-0.37683600
Fe	-3.88674100	-1.63251600	-0.72735600
H	-1.95025000	-4.81416900	1.82490400
H	-1.86214500	-3.35151200	-4.40311300
H	-6.07685500	1.41422700	-3.35034300
H	-5.30305400	0.49009600	3.02659800
N	2.58305400	-2.38277000	-1.85097500
C	0.88450000	2.60603600	1.70937500
O	0.48274600	2.13629600	0.41910100
N	3.43529000	-1.67308100	0.55425700
C	0.83228700	0.89340400	0.05687900
N	4.10493000	-4.83246800	4.62154300
C	1.93889800	0.21833300	0.63711700
C	2.45164900	-0.91234500	0.03970800
C	1.91841100	-1.37528400	-1.26320700
C	0.80528500	-0.73648900	-1.83446000
C	2.16313300	-2.79256000	-3.05130300
C	1.08587500	-2.20905900	-3.71603500
C	0.40058200	-1.16550400	-3.09621900
C	0.06823000	0.32628000	-1.06029300
C	4.11014800	-1.42932400	1.82158400
C	5.22936400	-0.39301600	1.65612200
C	4.59775400	-2.76605600	2.39282600

C	5.03611300	-2.66844500	3.85727700
C	5.32698000	-4.02632600	4.50010300
H	3.73384900	-2.43195500	-0.04890600
H	3.81190400	-5.16062600	3.70498800
H	4.29703500	-5.66846000	5.16743000
H	2.33924800	0.55660600	1.58061000
H	2.71628200	-3.61385300	-3.50082800
H	0.78723100	-2.57042200	-4.69428600
H	-0.45177400	-0.70043500	-3.57636800
H	3.34998900	-1.04477500	2.51169700
H	4.83630300	0.52710400	1.21502800
H	5.68135800	-0.14224600	2.62002900
H	6.01286300	-0.77611800	0.99382500
H	5.42146100	-3.15441600	1.77593100
H	3.76617600	-3.47210600	2.30758200
H	4.24223100	-2.18044000	4.43427100
H	5.93437500	-2.04520400	3.93678100
H	6.13590900	-4.52797100	3.93845700
H	5.70915300	-3.85848200	5.51299500
H	-7.06760000	-1.54147000	0.41691900
H	-7.60104100	-3.23471800	0.31663500
H	-6.26068100	-2.78923700	1.39726000
H	-4.12275300	-1.34176400	4.52452900
H	-6.58234600	2.22167300	1.51994500
H	-6.92701900	2.59573400	-1.12634700
H	-4.95828200	0.30803800	-5.49577800
H	-3.14812100	-1.65224700	-5.92031800
H	-0.67491300	-5.15792100	-2.90885100
H	-0.78156300	-5.81736000	-0.28407500
H	-2.76081500	-3.62483500	3.99250900
H	1.46148400	-0.29363100	6.76964800
H	-0.03163600	-1.15379500	7.13569600
H	1.49846600	-2.03826500	7.05323700
H	10.17908000	1.42222600	-3.20647900
H	9.37637100	0.58156500	-4.53997000
H	8.46403900	1.71711400	-3.54345400
H	3.24587000	1.18415300	-4.98186100
H	4.89195300	1.03611100	-5.60944800
H	5.74366900	8.07471400	-0.68400000
H	3.92238600	2.46266000	-5.99868000
H	5.72219400	6.96536800	-2.06331000
H	-2.66596100	7.56739900	2.20012500
H	-0.39554000	1.06196400	-1.72338400
H	1.96360100	2.79152200	1.73762300

H	0.34698600	3.54173900	1.85671600
H	0.61128400	1.88780800	2.48811900
H	-4.15422300	4.96065800	-0.32698200
H	-2.06960900	1.00220000	-3.28135600

### IM3

C	0.92129800	-1.28373100	6.57480600
C	0.69701700	-1.51657900	5.09414200
C	-0.05405700	-0.58412400	4.34783800
C	1.22730400	-2.68934600	4.48144800
C	-0.25850400	-0.84476900	3.00470000
C	1.08559700	-2.87687400	3.06948000
C	0.32760600	-1.94487900	2.37987500
H	-0.48198900	0.28882700	4.83239700
H	1.81627300	-3.38967900	5.06613700
H	-0.85991700	-0.17999600	2.39360700
H	1.51564500	-3.73888100	2.57284700
H	0.16303300	-2.05770200	1.31457000
C	5.59635200	7.02790500	-0.95367900
C	4.20081800	6.48270200	-0.49731900
H	6.40813500	6.43330600	-0.52369200
H	4.06278000	5.44442300	-0.81326000
H	4.10678300	6.51841200	0.59300600
H	3.38688800	7.07376300	-0.92728200
N	-1.88155300	7.27333600	2.82956600
C	-0.69135000	7.14013800	1.89870100
C	-0.96473100	6.06458600	0.87689800
O	-0.72786900	6.21028400	-0.31297700
C	0.64406800	6.94775000	2.55271300
O	0.73166100	7.78484500	3.70398500
H	-1.66878100	8.04957000	3.45322800
H	-0.60588200	8.04722900	1.28542800
H	0.81144700	5.89596100	2.82926000
H	1.43357200	7.23784800	1.85673900
H	0.29501900	7.31516400	4.42537500
N	-1.71822800	4.99983700	1.25540500
C	-2.23149100	3.98625500	0.33527100
C	-3.24835700	4.48328800	-0.66147700
O	-3.03681600	4.35328200	-1.89564100
C	-2.71443600	2.80467100	1.12675400
H	-2.07357300	5.01170700	2.20483400
H	-1.38570200	3.66775400	-0.28151600
H	-3.00971300	1.98892400	0.46423000

H	-1.91439500	2.43124400	1.76825000
H	-3.57981000	3.05402900	1.75248600
C	-1.64878500	1.91072800	-3.72323200
H	-2.25239500	2.14206500	-4.60348600
H	-0.61055700	1.76615600	-4.03232100
H	-1.72288600	2.73862000	-3.01687300
C	-6.76331600	-2.60759600	0.45230800
S	-5.65919700	-2.95089500	-0.95938200
C	9.21071700	0.96594500	-3.55081400
C	8.83800100	-0.18696100	-2.61799300
C	7.50935500	-0.64236600	-2.49222500
C	9.85287200	-0.90972500	-2.03867500
C	7.25634700	-1.74551600	-1.71267900
C	9.60429300	-1.99571500	-1.17207700
C	8.30035500	-2.43971600	-1.04732800
H	6.70084900	-0.11084600	-2.98591700
H	10.87940900	-0.57912600	-2.17966700
H	6.23407800	-2.09859500	-1.59913400
H	10.42570800	-2.50521400	-0.67882100
H	8.05766500	-3.29415000	-0.42246000
C	4.12084700	1.77587500	-5.21891100
C	4.66503700	2.47592300	-3.96035800
H	3.93884900	3.18829600	-3.55651800
H	4.88909400	1.75216400	-3.16928400
H	5.58586600	3.02705400	-4.17853300
N	-2.61090400	-3.09853800	-1.09407500
N	-3.91430600	-1.15367600	-2.69084000
N	-3.69181900	-1.93797000	1.23867600
C	-2.40226400	-4.03703500	1.19047200
C	-2.35655500	-2.90085700	-3.54197400
C	-5.54628700	0.73862000	-2.72487600
C	-4.94803400	-0.03564700	2.15264200
C	-2.14837800	-4.02966000	-0.17761900
C	-3.23320400	-1.82028100	-3.70038200
C	-5.61230900	0.82799900	-1.31142200
C	-4.18879900	-1.18067100	2.28837300
O	-0.37641000	0.20513000	0.07220800
C	-1.29796100	-4.99284200	-0.83426400
C	-3.58534900	-1.26481800	-4.98303900
C	-6.35567300	1.84032500	-0.60865000
C	-3.86426800	-1.78855300	3.55473000
C	-1.24710400	-4.65137600	-2.14974700
C	-4.50033500	-0.28132300	-4.75946500
C	-6.17429000	1.64184900	0.73145800

C	-3.19229500	-2.93643000	3.27742400
C	-2.08428300	-3.48930500	-2.31464500
C	-4.71040500	-0.20257100	-3.33612700
C	-5.31997000	0.49481100	0.89280400
C	-3.08610600	-3.02384600	1.84214700
N	-4.96584200	0.01017200	-0.36932400
Fe	-3.94077400	-1.64629400	-0.73914000
H	-1.96555300	-4.82844000	1.78744300
H	-1.89554900	-3.31753100	-4.42906700
H	-6.10282600	1.44370500	-3.32732200
H	-5.30891000	0.47028600	3.03979500
N	2.53202900	-2.47706000	-1.79524000
C	0.91648300	2.63765700	1.71180800
O	0.76308800	2.27779200	0.34044500
N	3.47887100	-1.73663900	0.56763000
C	0.89635700	0.92968900	0.06527300
N	4.09160900	-4.83958300	4.68578500
C	2.06505600	0.22528400	0.60885000
C	2.51443900	-0.92942100	0.04218800
C	1.95361600	-1.39519000	-1.24585200
C	0.90471900	-0.69070700	-1.87359700
C	2.10419700	-2.88480600	-2.99280600
C	1.09800100	-2.23620200	-3.70639900
C	0.49184100	-1.12056000	-3.13359700
C	0.28802500	0.46941100	-1.19208600
C	4.16083000	-1.48179200	1.82292300
C	5.30451300	-0.47195100	1.64846000
C	4.62103600	-2.81453900	2.42687100
C	5.05207100	-2.69809700	3.89208900
C	5.32322800	-4.04732000	4.56073900
H	3.76160400	-2.50468700	-0.02625800
H	3.79445000	-5.16240800	3.76854700
H	4.27726200	-5.67916600	5.22870100
H	2.50696000	0.59663600	1.52169100
H	2.59397500	-3.76546500	-3.40271800
H	0.79096300	-2.60303600	-4.67971400
H	-0.30932500	-0.59994600	-3.64523700
H	3.41029700	-1.06464100	2.50699600
H	4.93604800	0.44286000	1.17635600
H	5.75114500	-0.20185500	2.61030700
H	6.08797500	-0.88791500	1.00605200
H	5.44177400	-3.23101100	1.82416600
H	3.77748400	-3.50716400	2.34765200
H	4.26184600	-2.18918000	4.45613700

H	5.95735000	-2.08445900	3.96671500
H	6.13003900	-4.56754800	4.01315800
H	5.69974000	-3.86798800	5.57396300
H	-7.09068900	-1.56651400	0.45564500
H	-7.63696100	-3.25407500	0.33421300
H	-6.27774200	-2.83655200	1.40237500
H	-4.12418500	-1.37327800	4.51871200
H	-6.58714600	2.21694000	1.54978300
H	-6.94094200	2.61127400	-1.09201200
H	-4.98861200	0.35629500	-5.48393600
H	-3.18055000	-1.60125900	-5.92802300
H	-0.70312600	-5.13210300	-2.95093700
H	-0.80231300	-5.81235400	-0.33177300
H	-2.76718000	-3.65382300	3.96540800
H	1.44758700	-0.33856400	6.75315400
H	-0.02777700	-1.22857400	7.12110300
H	1.51712100	-2.08509200	7.01910800
H	10.15138800	1.43103300	-3.24546400
H	9.33204400	0.60709300	-4.57939400
H	8.43491000	1.73785000	-3.56378800
H	3.20630700	1.21740700	-4.99375700
H	4.85013400	1.06777700	-5.62617000
H	5.73364100	8.06646500	-0.63762000
H	3.88449700	2.49984400	-6.00503000
H	5.69106700	6.99098300	-2.04307200
H	-2.66905100	7.57065300	2.25924300
H	-0.22972900	1.19208100	-1.81277300
H	1.97500200	2.72617400	1.98550700
H	0.43319200	3.60808900	1.82771200
H	0.43610300	1.91144200	2.37677900
H	-4.17193300	4.96442600	-0.28521000
H	-2.03864900	0.99886800	-3.26549000