

## *Supporting Information*

# **A Mechanistic Study of Chiral Manganese Porphyrin-Catalyzed Enantioselective C–H Hydroxylation Reaction**

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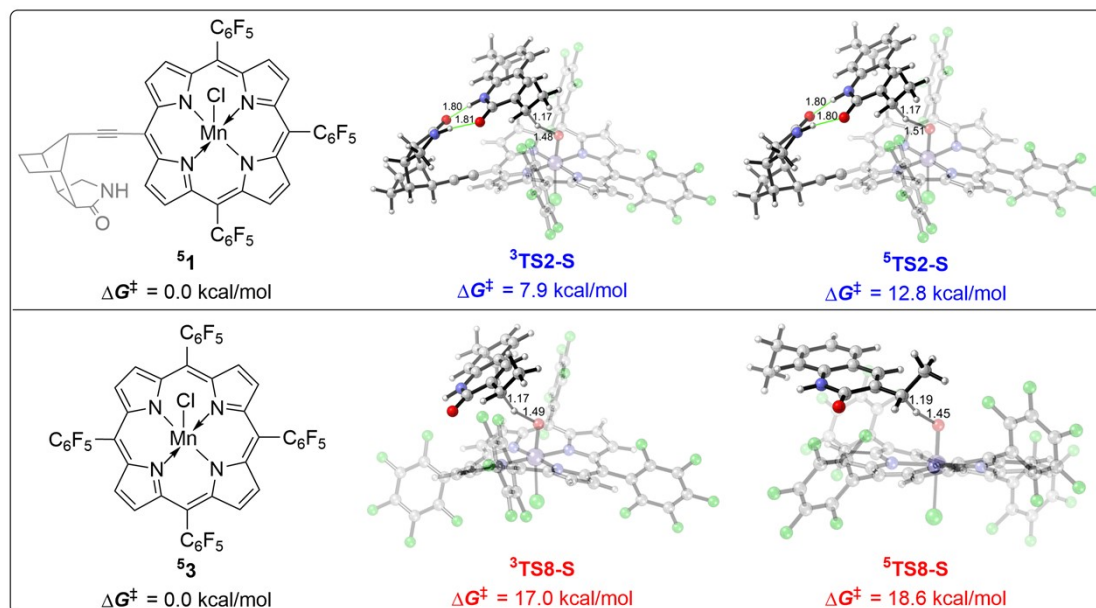
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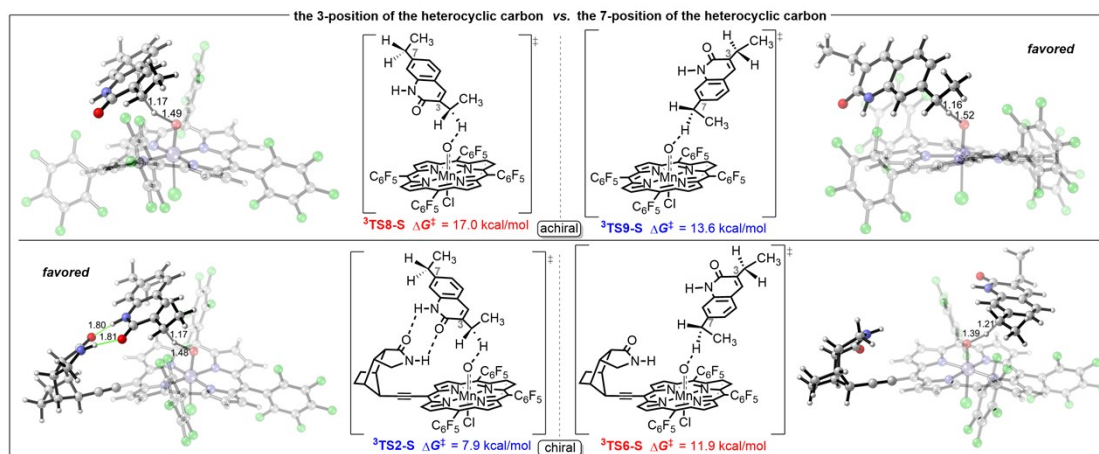
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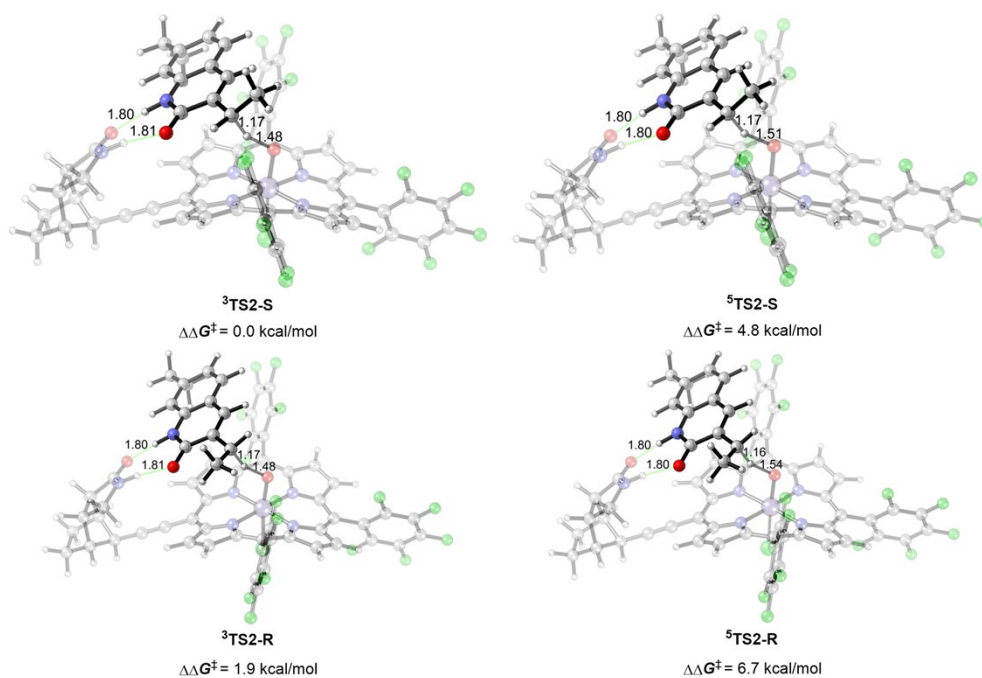
**Fig. S1** The barrier for hydroxylation reaction of the methylene *pro*-(*S*) C–H bond at the heterocyclic C-3 position of the heterocyclic carbon skeleton in chiral and achiral catalyst systems. Gibbs free energies are shown in kcal/mol. The distances are in Å.

The barrier for the hydroxylation reaction of the methylene *pro*-(*S*) C–H bond at the heterocyclic C-3 position of the heterocyclic carbon skeleton in the chiral catalyst **51** system is much lower than that in the achiral catalyst **53** system. The chiral system has a 9.1 kcal/mol barrier advantage over the achiral system. The two-point hydrogen bonding interaction between chiral catalyst **51** and substrate can contribute to the stability of high valent metal intermediates, effectively stabilizing the transition state structure, reducing the energy of the system, and reducing the energy barrier for hydrogen atom abstraction transition state. Therefore, catalysts with chiral lactam units had a rate accelerating effect than **Mn**[TPFPP]Cl catalysts.

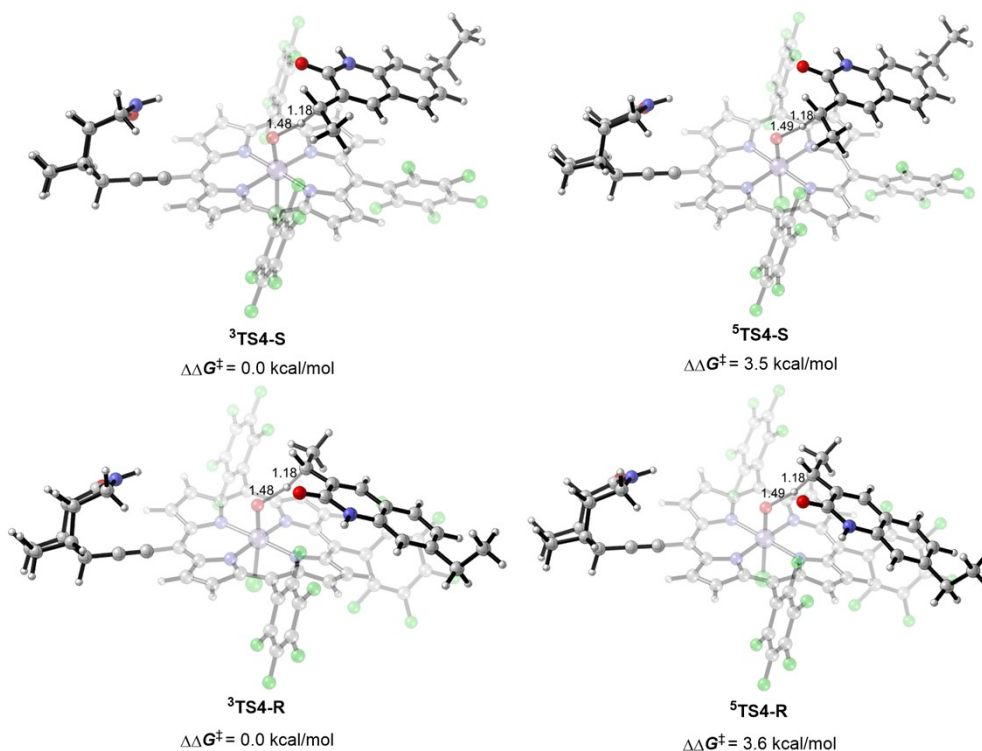


**Fig. S2** The key transition state structures that determine enantioselectivity and site-selectivity. Gibbs free energies are shown in kcal/mol. The distances are in Å.

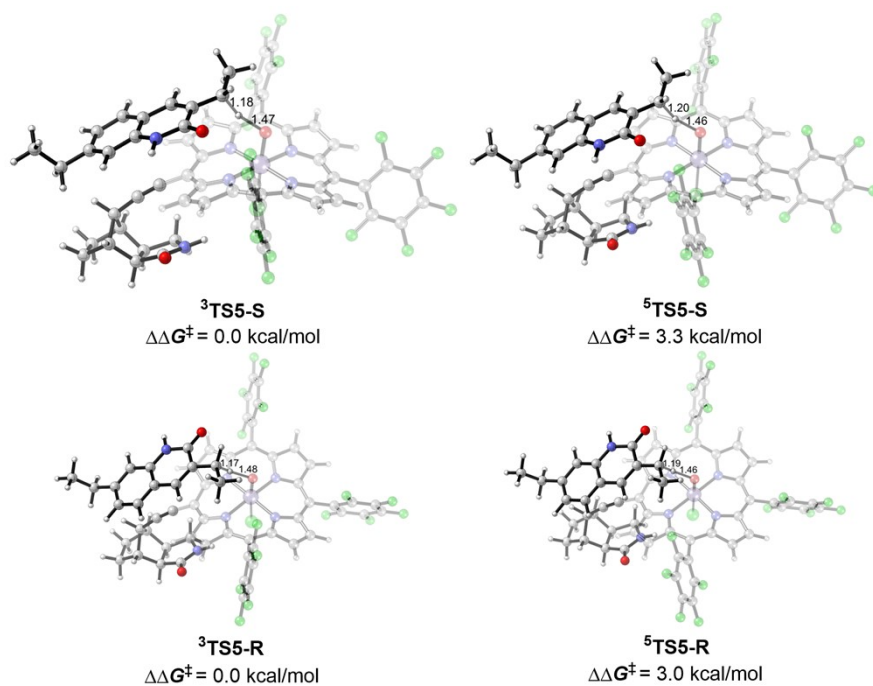
In the achiral **Mn**[**TPFPP**]**Cl** system, the transition state energy barrier for hydrogen atom abstraction of the methylene *pro*-(*S*) C–H bond at the heterocyclic C-3 position is 3.4 kcal/mol higher than the methylene *pro*-(*S*) C–H bond at the heterocyclic C-7 position. In the chiral catalyst system, the presence of two-point hydrogen bonding interactions orients the methylene *pro*-(*S*) C–H bond at the heterocyclic C-3 position of the substrate close to the Mn-oxo center. The presence of directing groups can shorten the distance between substrate reaction sites and catalyst active centers, and the barrier of abstraction of the methylene *pro*-(*S*) C–H bond at the heterocyclic C-3 position decreased to 7.9 kcal/mol leading to the reversal of site-selectivity.



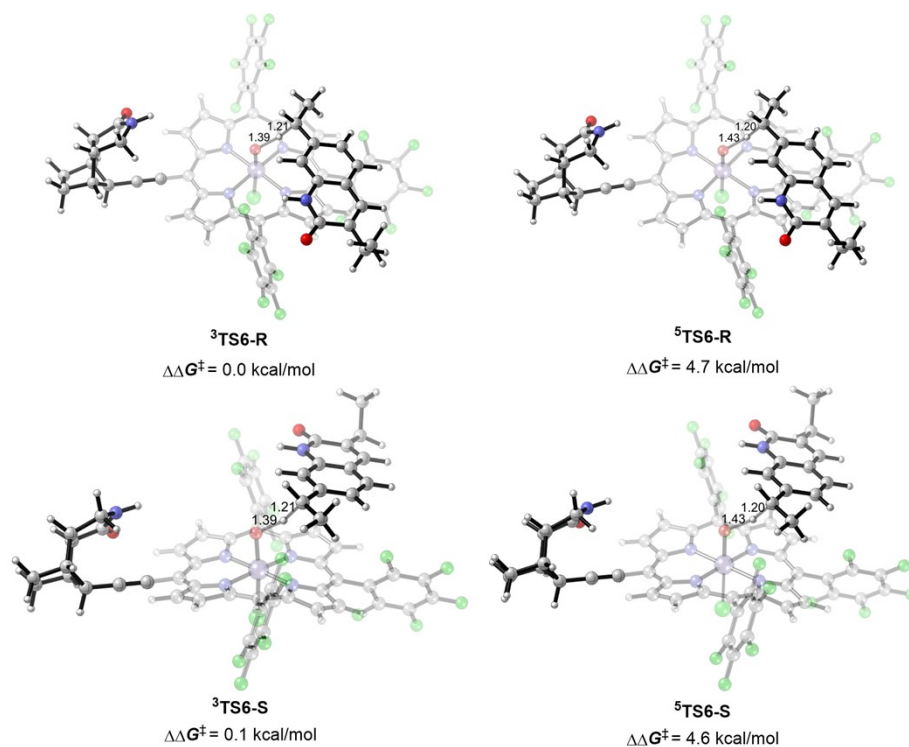
**Fig. S3** Optimized geometries and Gibbs free energy for C-3 position methylene H-abstraction transition state **TS2** with the chiral directing group forming H-bonding interaction. The distances are in Å.



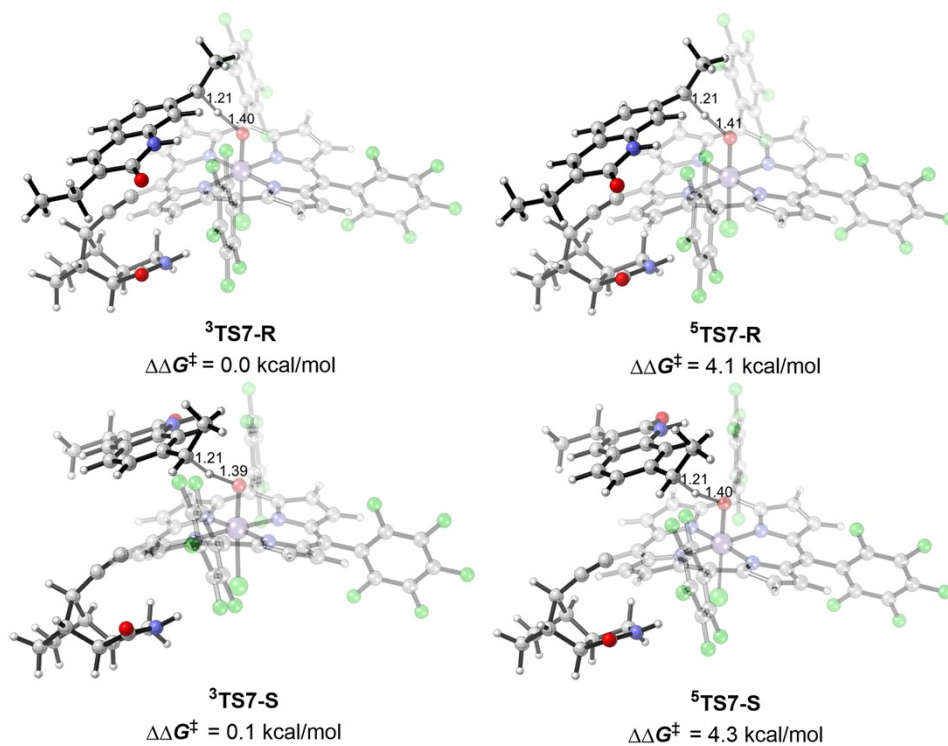
**Fig. S4** Optimized geometries and Gibbs free energy for C-3 position methylene H-abstraction transition state **TS4** with the chiral directing group not forming H-bonding interaction. The distances are in Å.



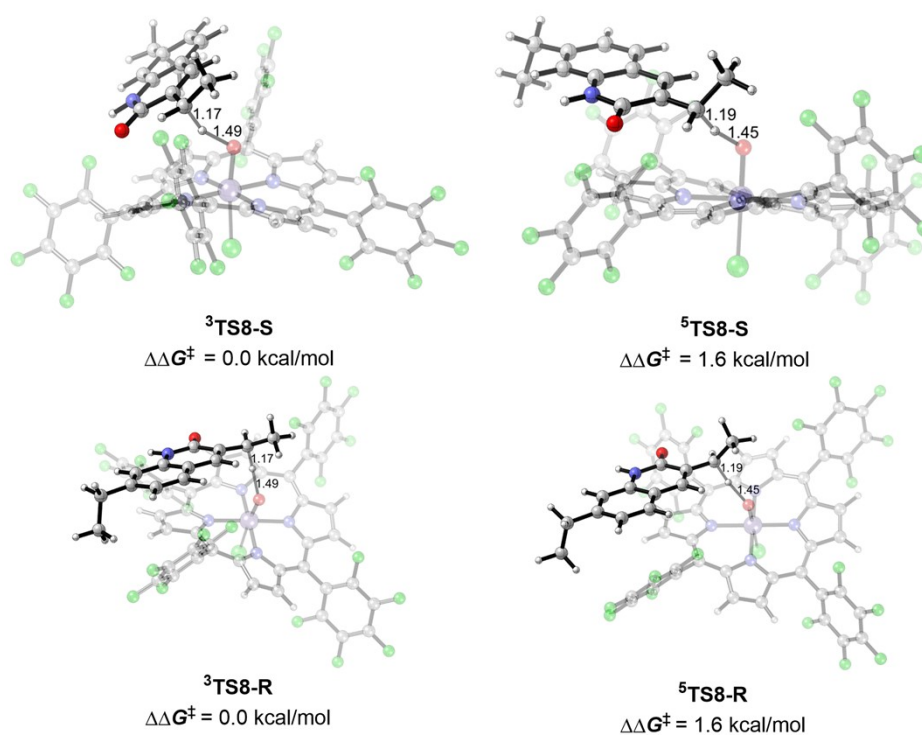
**Fig. S5** Optimized geometries and Gibbs free energy for C-3 position methylene H-abstraction transition state **TS5** with the chiral directing group on the Mn–Cl side. The distances are in Å.



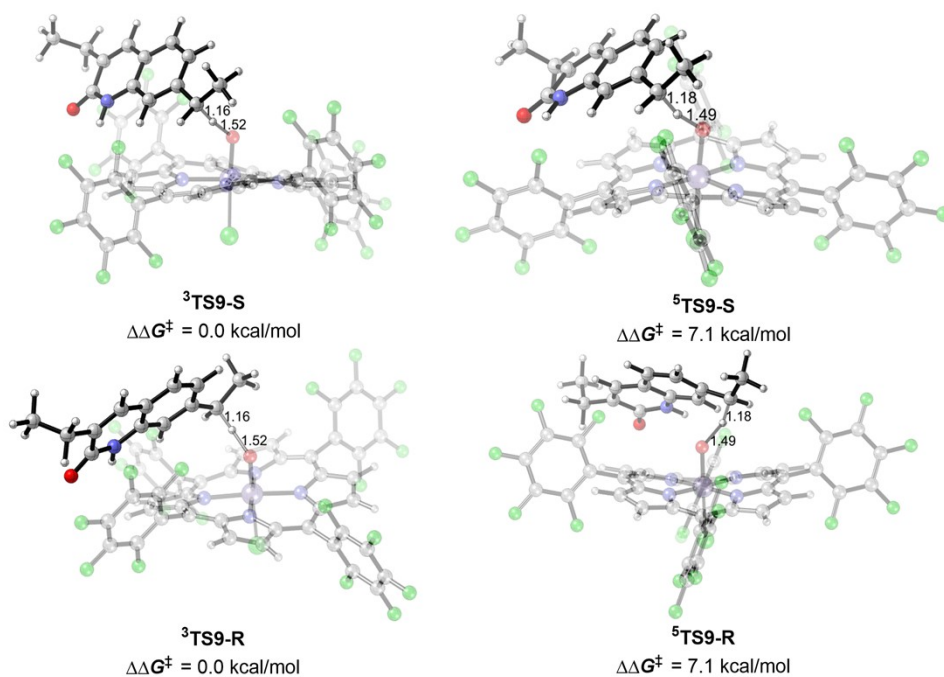
**Fig. S6** Optimized geometries and Gibbs free energy for C-7 position methylene H-abstraction transition state **TS6** with the chiral directing group not forming H-bonding interaction. The distances are in Å.



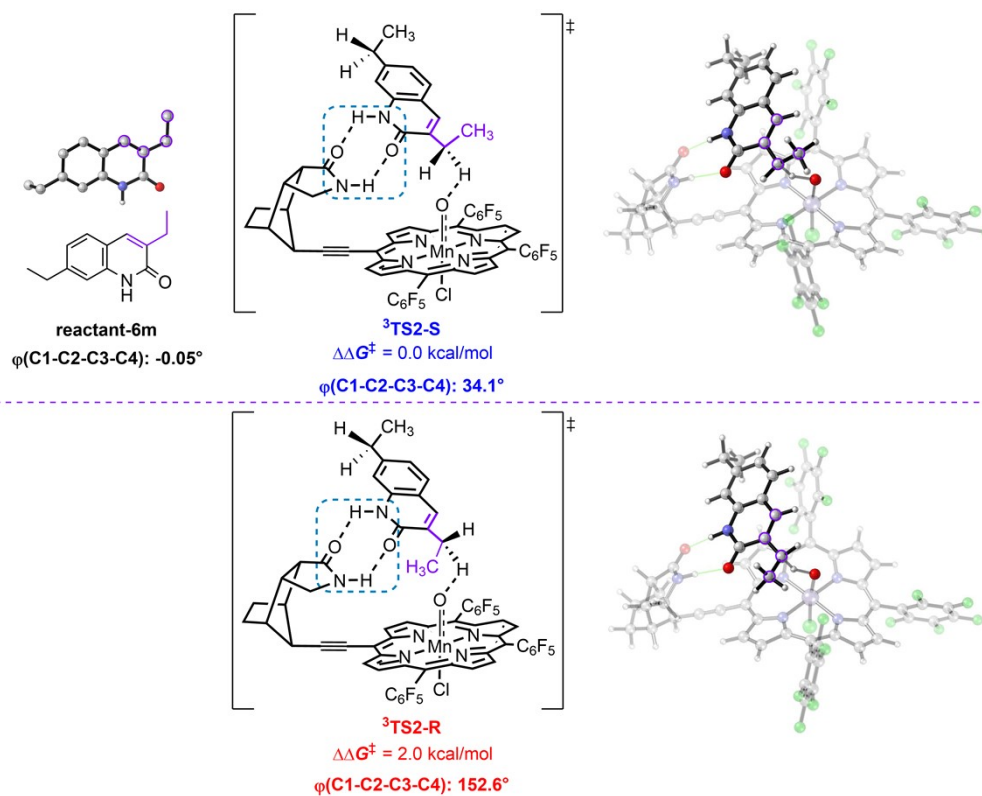
**Fig. S7** Optimized geometries and Gibbs free energy for C-7 position methylene H-abstraction transition state **TS7** with the chiral directing group on the Mn–Cl side. The distances are in Å.



**Fig. S8** Optimized geometries and Gibbs free energy for C-3 position methylene H-abstraction transition state **TS8** without the chiral directing group. The distances are in Å.



**Fig. S9** Optimized geometries and Gibbs free energy for C-7 position methylene H-abstraction transition state **TS9** without the chiral directing group. The distances are in Å.



**Fig. S10** The dihedral angle analysis of substrate distortion in  ${}^3\text{TS2-R}$  vs.  ${}^3\text{TS2-S}$ .



**Table S1. Electronic Energies and Free Energies (in Hartree) of the Structures Calculated at the (U)B3LYP-D3/def2-TZVP (SMD: Dichloromethane)//(U)B3LYP-D3/6-31G(d)-LANL2DZ Level**

Structures	ZPVE	TCE	TCH	TCG	E	G(E+TCG)	Imaginary Frequenc y	$\Delta G^\ddagger$
PhIO	0.091911	0.099402	0.100346	0.057877	-604.708416	-604.650539	—	—
PhI	0.090333	0.096218	0.097163	0.058573	-529.550400	-529.491827	—	—
Sub	0.254723	0.268373	0.269317	0.213853	-634.724002	-634.510149	—	—
<sup>1</sup> I	0.600103	0.658619	0.659564	0.500838	-5338.707056	-5338.206218	—	29.3
<sup>3</sup> I	0.600121	0.658599	0.659543	0.499999	-5338.722332	-5338.222333	—	19.2
<sup>3</sup> INT1	0.694940	0.761454	0.762398	0.588553	-5943.479022	-5942.890469	—	8.1
<sup>3</sup> TS1	0.693098	0.759819	0.760763	0.584133	-5943.466083	-5942.881950	706.09i	13.5
<sup>3</sup> INT2	0.600573	0.660591	0.661535	0.498439	-5413.900742	-5413.402303	—	5.8
<sup>3</sup> INT3-S	0.858157	0.932389	0.933333	0.745129	-6048.657494	-6047.912365	—	5.9
<sup>3</sup> TS2-S	0.856393	0.929576	0.930521	0.745552	-6048.654675	-6047.909123	367.91i	7.9
<sup>3</sup> INT4-S	0.857578	0.931997	0.932941	0.745248	-6048.692971	-6047.947723	—	-16.3
<sup>5</sup> I	0.599543	0.658343	0.659288	0.497561	-5338.750443	-5338.252882	—	0.0
<sup>5</sup> INT1	0.692514	0.760483	0.761428	0.579764	-5943.488253	-5942.908489	—	-3.2
<sup>5</sup> TS1	0.692023	0.759363	0.760308	0.581397	-5943.467505	-5942.886108	-387.76i	10.9
<sup>5</sup> INT2	0.601203	0.661056	0.662000	0.499526	-5413.904441	-5413.404915	—	4.2
<sup>5</sup> INT3-S	0.858767	0.932931	0.933875	0.744749	-6048.659251	-6047.914502	—	4.5
MECP-1	—	—	—	—	-6048.652490	—	—	—
MECP-2	—	—	—	—	-6048.690889	—	—	—
<sup>5</sup> TS2-S	0.856032	0.929342	0.930286	0.744402	-6048.645801	-6047.901399	-381.59i	12.8
<sup>5</sup> INT4-S	0.857488	0.931995	0.932939	0.744069	-6048.692364	-6047.948295	—	-16.7
<sup>5</sup> TS3-S	0.855840	0.930309	0.931253	0.741706	-6048.687297	-6047.945591	193.71i	-15.0
Pro-S	0.259735	0.274161	0.275105	0.218080	-709.980440	-709.762360	—	—
<sup>3</sup> TS2-R_sub	—	—	—	—	-634.717671	—	—	—
<sup>3</sup> TS2-S_sub	—	—	—	—	-634.722223	—	—	—
<sup>3</sup> TS2-R	0.856570	0.929584	0.930528	0.745749	-6048.651800	-6047.906051	224.57i	—
<sup>5</sup> TS2-R	0.856392	0.929599	0.930543	0.744433	-6048.642868	-6047.898435	207.81i	—
<sup>3</sup> TS4-R	0.855187	0.929260	0.930204	0.738970	-6048.639526	-6047.900556	191.71i	—
<sup>3</sup> TS4-S	0.855217	0.929282	0.930226	0.739099	-6048.639652	-6047.900553	191.50i	—
<sup>5</sup> TS4-R	0.853967	0.928244	0.929188	0.736977	-6048.631858	-6047.894881	441.79i	—
<sup>5</sup> TS4-S	0.853985	0.928240	0.929184	0.737147	-6048.632046	-6047.894899	455.00i	—
<sup>3</sup> TS5-R	0.854029	0.928305	0.929250	0.736634	-6048.639264	-6047.902630	224.61i	—
<sup>3</sup> TS5-S	0.853727	0.927995	0.928939	0.736220	-6048.638818	-6047.902598	292.91i	—

<sup>5</sup> TS5-R	0.852481	0.926982	0.927926	0.734298	-6048.632186	-6047.897888	691.90i	—
<sup>5</sup> TS5-S	0.852333	0.926803	0.927747	0.734080	-6048.631418	-6047.897338	702.65i	—
<sup>3</sup> TS6-R	0.854256	0.928089	0.929033	0.739243	-6048.642204	-6047.902961	602.45i	—
<sup>3</sup> TS6-S	0.854262	0.928089	0.929034	0.739393	-6048.642147	-6047.902754	596.12i	—
<sup>5</sup> TS6-R	0.853876	0.927815	0.928759	0.738308	-6048.633802	-6047.895494	631.60i	—
<sup>5</sup> TS6-S	0.853859	0.927810	0.928754	0.738198	-6048.633791	-6047.895593	620.31i	—
<sup>3</sup> TS7-R	0.853794	0.927837	0.928781	0.738367	-6048.640073	-6047.901706	530.39i	—
<sup>3</sup> TS7-S	0.853821	0.927854	0.928798	0.738551	-6048.640127	-6047.901576	560.49i	—
<sup>5</sup> TS7-R	0.852981	0.927171	0.928116	0.736875	-6048.632108	-6047.895233	867.52i	—
<sup>5</sup> TS7-S	0.852993	0.927183	0.928127	0.737058	-6048.631991	-6047.894933	908.08i	—
<sup>3</sup> TS8-R	0.691196	0.763921	0.764865	0.579649	-6220.172910	-6219.593261	387.62i	—
<sup>3</sup> TS8-S	0.691197	0.763921	0.764865	0.579654	-6220.172905	-6219.593251	387.62i	—
<sup>5</sup> TS8-R	0.690342	0.763138	0.764082	0.576711	-6220.167441	-6219.590730	409.32i	—
<sup>5</sup> TS8-S	0.690342	0.763138	0.764082	0.576711	-6220.167441	-6219.590730	409.31i	—
<sup>3</sup> TS9-R	0.692257	0.765053	0.765997	0.579342	-6220.178003	-6219.598661	160.40i	—
<sup>3</sup> TS9-S	0.692257	0.765053	0.765997	0.579342	-6220.178003	-6219.598661	160.41i	—
<sup>5</sup> TS9-R	0.690904	0.763914	0.764859	0.576881	-6220.164202	-6219.587321	431.52i	—
<sup>5</sup> TS9-S	0.690904	0.763914	0.764859	0.576881	-6220.164202	-6219.587321	431.52i	—

ZPVE = zero-point vibrational energy; TCE = thermal correction to energy; TCH = thermal correction to enthalpy; TCG = thermal correction to Gibbs free energy. Energies are shown in kcal mol<sup>-1</sup>.

**Table S2. The Calculated Energy (kcal/mol) of the Key Transition States using Different Basis Sets.**

Transition Structures	<sup>3</sup> TS2-S	<sup>3</sup> TS2-R	<sup>5</sup> TS2-S	<sup>5</sup> TS2-R	$\Delta\Delta G^{\ddagger a}$
def2-TZVP//6-31G(d)-LANL2DZ	7.9	9.8	12.8	14.6	1.9
def2-TZVPP//6-31G(d,p)-LANL2DZ	8.4	10.4	13.1	15.0	2.0

<sup>a</sup>  $\Delta\Delta G^{\ddagger} = \Delta G^{\ddagger}_{3TS2-R} - \Delta G^{\ddagger}_{3TS2-S}$

We conducted additional calculations on the hydrogen atom abstraction transition state structure involving the C–H breaking step at the B3LYP-D3/def2-TZVPP-SMD(Dichloromethane)//B3LYP-D3/6-31G(d,p)-LANL2DZ level. The energy ordering of the hydrogen atom abstraction transition state under the new basis set are the same. Related results have been included in Table S2 in the revised Supporting Information.

## Cartesian coordinates of the structures

(U)B3LYP-D3/def2-TZVP-SMD(Dichloromethane)//B3LYP-D3/6-31G(d)-LANL2DZ

<sup>1</sup>1

C	1.73963100	-2.17693600	-0.23882700
C	3.15892600	-2.40072400	-0.32017000
C	3.75456400	-1.18008400	-0.39583300
C	2.69767800	-0.20647600	-0.34701000
N	1.46720500	-0.82110300	-0.24241600
H	3.64269700	-3.36641100	-0.31727600
H	4.81127100	-0.96874500	-0.47820700
C	-0.07682600	3.08987100	-0.14851500
C	0.90205900	4.14291900	-0.20947500
C	2.12039300	3.54588000	-0.30483800
C	1.88993900	2.12852900	-0.30048800
N	0.54393300	1.85550300	-0.19550500
H	0.68305600	5.20004200	-0.17259400
H	3.09492700	4.00710200	-0.36956500
C	-2.55226000	-2.01751100	0.08803100
C	-2.77914500	-3.43924000	0.07024400
C	-1.56152500	-4.03343800	-0.02749000
C	-0.58208800	-2.97925400	-0.07013800
N	-1.20096100	-1.74677700	0.00094800
H	-3.74651800	-3.91739100	0.11503200
H	-1.34299600	-5.08998000	-0.07704600
C	-3.35092700	0.30961200	0.16707600
C	-4.40049000	1.28972200	0.26769700
C	-3.81054300	2.51106600	0.19156400
C	-2.39501300	2.28600400	0.05868900
N	-2.12375800	0.93155700	0.05270700
H	-5.45122200	1.06915000	0.38489100
H	-4.28894800	3.47886500	0.22139500
C	0.79125700	-3.19695200	-0.17219400
C	-1.45015400	3.30636900	-0.04049200
C	2.91991700	1.17752700	-0.37657800
C	-3.56959600	-1.06809600	0.17519800
Mn	-0.35262600	0.05042600	-0.37547800
Cl	-0.55552900	0.01724700	-2.57176400
C	-1.93477900	4.71673000	-0.02261800
C	-2.45141700	5.29453000	1.14063200

C	-1.88554200	5.51508100	-1.16958800
C	-2.90823700	6.60999800	1.16863600
F	-2.52369300	4.57346700	2.26798700
C	-2.32975500	6.83573800	-1.16413500
F	-1.39384300	5.01579900	-2.30900500
C	-2.84435600	7.38258000	0.01019200
F	-3.39965500	7.13616000	2.29568000
F	-2.26974000	7.57811700	-2.27418400
F	-3.27525400	8.64571900	0.02589200
C	-4.97519600	-1.55450700	0.28053300
C	-5.43858400	-2.19409200	1.43420100
C	-5.88230000	-1.39056200	-0.77115300
C	-6.74740400	-2.65797100	1.54313100
F	-4.61071800	-2.38146100	2.47082400
C	-7.19834400	-1.83927300	-0.68258200
F	-5.49465100	-0.78051800	-1.89716000
C	-7.62980600	-2.47692900	0.47939400
F	-7.16276500	-3.26789400	2.65827900
F	-8.04562600	-1.66756700	-1.70222200
F	-8.88740200	-2.91364200	0.57375900
C	1.27667300	-4.60632500	-0.21425100
C	1.81646800	-5.15398300	-1.38221500
C	1.21166800	-5.43118500	0.91236000
C	2.27712200	-6.46800700	-1.43139900
F	1.90600600	-4.40800100	-2.48871800
C	1.65984200	-6.74953200	0.88557900
F	0.69977200	-4.95742600	2.05690300
C	2.19607300	-7.26729000	-0.29228100
F	2.78908000	-6.96746200	-2.56041300
F	1.58403200	-7.51667100	1.97843900
F	2.63098300	-8.52849900	-0.32918700
C	4.26155000	1.65361600	-0.44650700
C	5.39712300	2.08182000	-0.44578400
C	6.73816500	2.64753500	-0.43055500
H	6.79734500	3.39545900	-1.23327400
C	7.22514900	3.28117900	0.91455700
H	6.56990800	4.04967000	1.33375200
C	7.95292000	1.67346000	-0.52593100
H	7.94243000	0.97754700	-1.36674700
C	9.11711700	2.69062300	-0.51817600
H	10.05767700	2.22826700	-0.20256800
H	9.27624600	3.10446600	-1.51949200
C	8.61977300	3.79387300	0.47928800
H	9.28999000	3.92228000	1.33557700

H	8.53470300	4.76656800	-0.01632500
C	7.44427900	2.05950800	1.84067900
H	8.18738300	2.30070900	2.60554000
C	7.94630300	0.96728400	0.84882300
H	8.93849100	0.56866900	1.08360400
C	6.17580800	1.45914300	2.51777000
H	5.27674100	2.03614800	2.27141900
H	6.27592700	1.43423100	3.60898100
C	6.93985000	-0.17442200	0.95086400
O	6.90689600	-1.16751500	0.23554700
N	6.08721600	0.10840100	1.97784600
H	5.26544100	-0.46898600	2.10305800

<sup>31</sup>

C	1.74624800	-2.17360300	-0.23545700
C	3.16620400	-2.39378900	-0.32347800
C	3.75803500	-1.17122600	-0.39588400
C	2.69791900	-0.20069800	-0.33910600
N	1.46991700	-0.81866900	-0.23002400
H	3.65291000	-3.35803300	-0.32717900
H	4.81381700	-0.95687400	-0.48206300
C	-0.08387400	3.09331900	-0.14475100
C	0.89289500	4.14859600	-0.21118300
C	2.11225100	3.55331000	-0.30311500
C	1.88392000	2.13506700	-0.29197600
N	0.53905100	1.85977800	-0.18324400
H	0.67219800	5.20559100	-0.18023700
H	3.08575900	4.01639300	-0.37021500
C	-2.54572600	-2.02283900	0.09760600
C	-2.77146200	-3.44510700	0.07381500
C	-1.55323700	-4.03742600	-0.02748500
C	-0.57522100	-2.98121200	-0.06531400
N	-1.19473000	-1.74987800	0.01403800
H	-3.73816300	-3.92486400	0.11665400
H	-1.33376600	-5.09354900	-0.08247300
C	-3.35084000	0.30482500	0.17542300
C	-4.40467300	1.28173900	0.26865600
C	-3.81867300	2.50473900	0.18910600
C	-2.40163900	2.28328200	0.06223000
N	-2.12514500	0.93015800	0.06508800
H	-5.45514000	1.05843700	0.38320100
H	-4.30073700	3.47093900	0.21287200
C	0.79905300	-3.19512500	-0.17044800
C	-1.45829000	3.30556100	-0.03922200

C	2.91528600	1.18462900	-0.36682600
C	-3.56423000	-1.07410900	0.18480300
Mn	-0.35153500	0.05105600	-0.35687600
Cl	-0.55220100	0.01621300	-2.54219900
C	-1.94713500	4.71464800	-0.02875200
C	-2.46921100	5.29533600	1.13059600
C	-1.89694100	5.50848800	-1.17875500
C	-2.93007500	6.60952100	1.15197300
F	-2.54263000	4.57854400	2.26054400
C	-2.34537900	6.82770900	-1.17996000
F	-1.40046000	5.00610900	-2.31479400
C	-2.86514800	7.37765000	-0.00936300
F	-3.42647900	7.13865300	2.27542200
F	-2.28445900	7.56577400	-2.29285000
F	-3.30000600	8.63949600	-0.00002800
C	-4.96899200	-1.56433600	0.28725000
C	-5.43275600	-2.20368900	1.44082400
C	-5.87399700	-1.40515800	-0.76686400
C	-6.74037900	-2.67148000	1.54754100
F	-4.60655900	-2.38680100	2.47946500
C	-7.18873500	-1.85810500	-0.68066500
F	-5.48555500	-0.79592900	-1.89308700
C	-7.62084500	-2.49512800	0.48142000
F	-7.15636300	-3.28091600	2.66270700
F	-8.03415200	-1.69100200	-1.70263600
F	-8.87725000	-2.93575800	0.57357300
C	1.28669700	-4.60359000	-0.22008200
C	1.82592200	-5.14483000	-1.39124700
C	1.22391000	-5.43390500	0.90260700
C	2.28824300	-6.45798000	-1.44727200
F	1.91298700	-4.39347700	-2.49435900
C	1.67402900	-6.75143700	0.86903300
F	0.71260000	-4.96632900	2.04990500
C	2.20963600	-7.26280500	-0.31189200
F	2.79951100	-6.95133600	-2.57929200
F	1.60054700	-7.52389300	1.95829100
F	2.64629000	-8.52320700	-0.35533100
C	4.25577300	1.66376300	-0.43801100
C	5.39041300	2.09457400	-0.43693700
C	6.72961400	2.66449500	-0.42067200
H	6.78465500	3.41742300	-1.21899300
C	7.21638400	3.29205300	0.92743100
H	6.55891800	4.05559800	1.35211600
C	7.94781200	1.69555200	-0.52372700

H	7.93856300	1.00451200	-1.36856700
C	9.10810800	2.71709800	-0.51200900
H	10.05098300	2.25646800	-0.20082300
H	9.26388400	3.13748400	-1.51113100
C	8.60834900	3.81251500	0.49285100
H	9.27950900	3.93829900	1.34879100
H	8.51882100	4.78783500	0.00322200
C	7.44155300	2.06575300	1.84592800
H	8.18487100	2.30530300	2.61110000
C	7.94622800	0.98136900	0.84688700
H	8.94036100	0.58527600	1.07767100
C	6.17638200	1.45652600	2.52130200
H	5.27479300	2.03171900	2.27996500
H	6.27833100	1.42535900	3.61218100
C	6.94443000	-0.16488800	0.94371500
O	6.91456800	-1.15393400	0.22274600
N	6.09191900	0.10878400	1.97329800
H	5.27239900	-0.47233500	2.09611100

**<sup>3</sup>INT1**

C	-2.40742900	-0.24443900	-1.40790100
C	-3.44974400	-1.22814900	-1.55658400
C	-2.86505200	-2.44830600	-1.39601400
C	-1.46168200	-2.21249000	-1.14802300
N	-1.21515600	-0.86080300	-1.13121000
H	-4.47564300	-1.00443300	-1.80952900
H	-3.33853300	-3.41785800	-1.45018300
C	2.73926600	-2.00646100	-0.14918100
C	1.84598900	-4.03457900	-0.55344700
C	0.84749300	-2.99406600	-0.67655700
N	1.42083200	-1.77030300	-0.43659500
H	1.67922600	-5.08904400	-0.71702300
C	0.34399200	3.07956900	-1.05719400
C	-0.57364600	4.11304700	-1.47401200
C	-1.76953300	3.50882900	-1.71634700
C	-1.58185800	2.10307800	-1.47066500
N	-0.29160700	1.85883700	-1.07404200
H	-0.33072900	5.16120900	-1.57317400
H	-2.69623200	3.95788300	-2.04335800
C	2.56980500	2.30162100	-0.28510500
C	3.91299500	2.55361800	0.19436600
C	4.48026400	1.34280200	0.42549900
C	3.48810600	0.34406700	0.08520400
N	2.33457100	0.95358800	-0.32523000

H	4.35335000	3.52914600	0.34160900
H	5.47356400	1.13816000	0.79769700
C	-2.60806300	1.14185400	-1.54528600
C	3.70376900	-1.03723900	0.14928600
C	-0.50102600	-3.22159300	-0.97848000
C	1.66405000	3.30412200	-0.65031400
Mn	0.57526600	0.04148400	-0.76256200
Cl	1.13789000	-0.08294400	-2.96477900
C	-0.88078500	-5.56865700	-0.11716600
C	-1.44031800	-5.09380400	-2.38285200
C	-1.29851600	-6.88735800	-0.27033700
C	-1.87062000	-6.40720600	-2.56135200
C	-1.79841000	-7.30808100	-1.50079700
F	-1.22598800	-7.74693000	0.75294800
F	-2.20618300	-8.56921200	-1.66251800
F	-2.34386600	-6.81090500	-3.74492600
F	-1.51855700	-4.26369800	-3.42792600
F	-0.39196200	-5.20789300	1.08431800
C	-0.94508900	-4.63365800	-1.15537200
C	2.12904600	4.71877500	-0.58137700
C	1.60411000	5.60700900	0.36264600
C	3.10449800	5.21488700	-1.45242000
C	2.02032400	6.93337000	0.44044200
F	0.66751800	5.18718700	1.22721300
C	3.54299300	6.53623700	-1.38888800
F	3.64660000	4.41299000	-2.37507900
C	2.99611400	7.39769300	-0.43973900
F	1.49792500	7.75961600	1.35483700
F	4.47746800	6.98449600	-2.23413100
F	3.40657800	8.66697200	-0.37281200
C	-3.94434500	1.63570700	-1.58996700
C	-5.04719100	2.11510600	-1.41947900
C	-6.28543300	2.78531200	-1.05077200
H	-6.50756300	3.55939400	-1.79785300
C	-7.56613700	1.93568800	-0.78300200
H	-7.89067500	1.29813500	-1.60965600
C	-6.28281900	3.41273700	0.38191100
H	-5.44743500	4.07904700	0.60509500
C	-7.68156100	4.07210300	0.39934200
H	-8.04782400	4.22990600	1.41887500
H	-7.64957100	5.05064700	-0.09052500
C	-8.56347300	3.05997100	-0.41160700
H	-9.40999900	2.67788400	0.16824700
H	-8.97133400	3.52613900	-1.31435100



C	-7.23754300	1.16265700	0.51767400
H	-8.15910800	0.91794700	1.05248500
C	-6.34754800	2.17216800	1.30745200
H	-6.74928500	2.45084500	2.28726600
C	-6.37353600	-0.11640500	0.35458100
H	-6.14823900	-0.31436600	-0.69773700
H	-6.86640000	-1.00238600	0.76985400
C	-5.02891400	1.44181000	1.54975400
O	-4.04490100	1.92042600	2.12700700
N	-5.15246000	0.17456100	1.09295500
H	-4.35634900	-0.45067400	1.06814500
C	3.01138800	-3.42539600	-0.21787000
H	3.97476300	-3.88651500	-0.05530000
C	5.05900100	-1.51338800	0.54646000
C	6.18077800	-1.29067800	-0.25967400
C	5.26086600	-2.20963900	1.74304000
C	7.45013500	-1.73308800	0.10691600
C	6.51876900	-2.66824200	2.12650800
C	7.61749700	-2.42624100	1.30420400
F	4.22494600	-2.45565700	2.55659800
F	6.05232700	-0.63285000	-1.41753000
F	6.68039300	-3.33111300	3.27795400
F	8.50505900	-1.50494400	-0.68338100
F	8.82938800	-2.85810700	1.66348800
O	0.24350700	0.10245300	1.14158300
I	-1.35836100	0.98233500	1.79234300
C	-2.16803200	-0.82386900	2.66734500
C	-1.54877600	-2.01572900	2.31729300
C	-3.25003700	-0.74235000	3.53843900
C	-2.06965400	-3.19561900	2.86012100
H	-0.69060200	-2.02363800	1.65306200
C	-3.74785200	-1.93573200	4.06935400
H	-3.70102900	0.21203800	3.78289700
C	-3.16216800	-3.15658600	3.72856000
H	-1.61333500	-4.14150400	2.59531800
H	-4.59263400	-1.90115600	4.75160700
H	-3.55468800	-4.08010200	4.14462800

**<sup>3</sup>INT2**

N	0.45944500	1.92936100	-0.29669100
N	-2.17409400	0.84094300	0.03573400
N	-1.08363400	-1.82727600	0.02653200
N	1.55009600	-0.73895900	-0.32616600
C	1.76954600	2.26405400	-0.41777000

C	1.92023700	3.69027400	-0.58571100
C	0.66644700	4.21328400	-0.57817000
C	-0.24355900	3.10679800	-0.38098300
C	-1.63120800	3.22475900	-0.27690300
C	-2.52318500	2.15651100	-0.07265000
C	-3.95327500	2.30697300	0.06575900
C	-4.46026700	1.06098700	0.25535900
C	-3.33967100	0.14953100	0.23125500
C	-3.45369800	-1.24383300	0.34406100
C	-2.39788300	-2.15788700	0.21887000
C	-2.55297700	-3.59529800	0.23519000
C	-1.31952900	-4.12194200	0.02412900
C	-0.40686300	-3.00685700	-0.09342500
C	0.97851000	-3.13374400	-0.29143100
C	1.88076500	-2.06956200	-0.38943900
C	3.31164600	-2.21773900	-0.53643400
C	3.83958800	-0.96543000	-0.55769200
C	2.72443300	-0.05580600	-0.42606400
C	2.85364900	1.35140000	-0.42044700
H	2.86315500	4.20116500	-0.71438800
H	0.37931000	5.24678400	-0.70397600
H	-4.49382000	3.24101100	0.02741400
H	-5.49548400	0.78048400	0.38141500
H	-3.48159600	-4.12697700	0.37929900
H	-1.05071300	-5.16506900	-0.05087700
H	3.84477500	-3.15405600	-0.60947800
H	4.87915900	-0.69221700	-0.66944100
Mn	-0.29823000	0.05525900	-0.00079200
Cl	-0.56607900	-0.03061800	-2.40257800
O	-0.10411600	0.11957400	1.58684900
C	-4.81994700	-1.79457300	0.57965500
C	-5.47204200	-1.59821000	1.80090400
C	-5.50150000	-2.51048400	-0.40933000
C	-6.75146300	-2.09540400	2.03681400
C	-6.78032300	-3.01944100	-0.19411600
C	-7.40581400	-2.80908700	1.03386300
C	-2.21532400	4.59283800	-0.38327200
C	-2.00227100	5.55353000	0.61008100
C	-2.99828300	4.96203000	-1.48194600
C	-2.54127800	6.83448300	0.51869300
C	-3.54976100	6.23656900	-1.59229700
C	-3.31818100	7.17479400	-0.58755000
C	1.53436800	-4.51340000	-0.39786200
C	1.56069200	-5.37311600	0.70432000

C	2.05349400	-4.99286300	-1.60487800
C	2.07830400	-6.66278400	0.61597500
C	2.57827600	-6.27873900	-1.71533500
C	2.58907200	-7.11480100	-0.59991500
F	-4.86554100	-0.91287700	2.77745700
F	-7.35203700	-1.89562200	3.21391500
F	-8.63083200	-3.29102000	1.24946500
F	-7.41068100	-3.70109800	-1.15510300
F	-4.92335000	-2.72459000	-1.59619100
F	-3.23680200	4.07927500	-2.45697300
F	-4.29340600	6.56560500	-2.65246600
F	-3.84027400	8.39856600	-0.68443400
F	-2.32245400	7.73424300	1.48285900
F	-1.26062100	5.25183400	1.68316400
F	2.05649600	-4.20929400	-2.68735500
F	1.07688000	-4.96079500	1.88318200
F	2.09258400	-7.46448900	1.68557700
F	3.08818600	-8.34810300	-0.69553400
F	3.06625300	-6.71538500	-2.87968700
C	4.15899800	1.89980800	-0.41836000
C	5.26860100	2.39004400	-0.32640800
C	6.56320200	3.03481800	-0.18955300
H	6.59374300	3.87336300	-0.89878600
C	6.94580800	3.54502100	1.24221800
H	6.21680500	4.21206100	1.70974100
C	7.85072200	2.16555700	-0.33212700
H	7.92646900	1.56997200	-1.24363000
C	8.93149400	3.25738400	-0.15794300
H	9.89117800	2.83048700	0.14937700
H	9.09793000	3.79178800	-1.09915700
C	8.31241300	4.20233700	0.92948300
H	8.93624700	4.28097500	1.82571100
H	8.17184100	5.21611100	0.54046200
C	7.22150900	2.24478400	2.03639700
H	7.91484700	2.45215100	2.85579000
C	7.84194800	1.31035300	0.95473300
H	8.85062800	0.95652900	1.19037800
C	5.97851100	1.48257500	2.58587900
H	5.04739100	2.02320100	2.37795700
H	6.04583100	1.33186100	3.66923400
C	6.91802600	0.09799900	0.87955100
O	6.98923600	-0.80462700	0.05553900
N	6.00302200	0.20518900	1.88499800
H	5.22524400	-0.44219500	1.91468700

**<sup>3</sup>INT3-S**

N	-0.37655000	1.99810200	-0.57905100
N	-2.85152500	0.58656400	-0.33345300
N	-1.44886500	-1.90556400	-0.57800700
N	1.01285300	-0.48354300	-0.81740100
C	0.81600600	2.50908600	-0.97274000
C	0.79372300	3.95106900	-0.92510600
C	-0.43473400	4.30302800	-0.46119700
C	-1.17564700	3.07234600	-0.27619200
C	-2.53456700	2.99809200	0.04198900
C	-3.32432300	1.83350700	-0.04636800
C	-4.76487400	1.80090400	0.06474100
C	-5.14910100	0.52377600	-0.20106700
C	-3.94135600	-0.23887000	-0.41907100
C	-3.89221300	-1.62894100	-0.60704600
C	-2.72091100	-2.40130800	-0.64964700
C	-2.68453400	-3.84723600	-0.66771500
C	-1.37568500	-4.20602300	-0.57383100
C	-0.61286000	-2.97879500	-0.52817800
C	0.79319900	-2.91017900	-0.50519400
C	1.54513200	-1.74284300	-0.67654400
C	2.98161600	-1.68559600	-0.84218500
C	3.29193300	-0.39896100	-1.15417700
C	2.05131800	0.33954600	-1.12113400
C	1.95420000	1.73979100	-1.31102900
H	1.62503000	4.58879100	-1.18857200
H	-0.82121500	5.29747300	-0.29135200
H	-5.39953500	2.64434400	0.29164700
H	-6.15505800	0.13261300	-0.23365500
H	-3.54627300	-4.49640000	-0.72170800
H	-0.95967500	-5.20313500	-0.56063600
H	3.66140200	-2.51452600	-0.71874000
H	4.26796300	0.03919800	-1.30415500
Mn	-0.90517700	0.03936000	-0.46805800
Cl	-1.21861600	0.11597500	-2.85061800
O	-0.77503700	-0.03994500	1.14513000
C	-5.18691100	-2.36198900	-0.71074900
C	-6.04484600	-2.49771100	0.38455400
C	-5.57466800	-2.96141800	-1.91359300
C	-7.24939900	-3.19039600	0.29144700
C	-6.77380400	-3.66168800	-2.02846000
C	-7.61279200	-3.77435200	-0.92105300
C	-3.20053500	4.27033200	0.44213200

C	-2.88131800	4.88332700	1.65836200
C	-4.13429300	4.91245000	-0.37671800
C	-3.47379400	6.07928100	2.05591500
C	-4.74104500	6.10813100	0.00105000
C	-4.40756900	6.69229700	1.22202000
C	1.53563400	-4.18778100	-0.32244000
C	1.49567900	-4.85325100	0.90624400
C	2.32019900	-4.74709800	-1.33533600
C	2.25402200	-5.99445000	1.14138800
C	3.06584200	-5.90548800	-1.12862800
C	3.03676400	-6.52358300	0.11923200
F	-5.71552600	-1.95237600	1.56302800
F	-8.05219000	-3.30445300	1.35456100
F	-8.76364300	-4.44215800	-1.02086500
F	-7.12419400	-4.22318800	-3.18929800
F	-4.78476700	-2.87297700	-2.98760900
F	-4.46580900	4.37843500	-1.55818900
F	-5.63131000	6.70087800	-0.80039400
F	-4.98156200	7.83837700	1.59202100
F	-3.15417600	6.64040100	3.22586700
F	-1.98196500	4.32069600	2.47657700
F	2.38077000	-4.16012900	-2.53602700
F	0.73363800	-4.37976600	1.89860500
F	2.28593000	-6.55268600	2.35863300
F	3.80011300	-7.59255100	0.35467000
F	3.82173100	-6.41252900	-2.10763500
C	3.08699700	2.39616300	-1.84223600
C	4.09051200	2.88211000	-2.32831000
C	5.32836100	3.35570000	-2.92667200
H	5.24325900	3.21878100	-4.01394800
C	5.82598300	4.80224400	-2.61235000
H	5.11801700	5.60314100	-2.84146100
C	6.63619500	2.68294700	-2.39951400
H	6.64932300	1.59160300	-2.42035400
C	7.68782100	3.37562000	-3.29591100
H	8.68156300	3.36141500	-2.83703500
H	7.76676800	2.86732000	-4.26249400
C	7.11906000	4.82713400	-3.46185300
H	7.81596300	5.59713400	-3.11582800
H	6.88792700	5.04341600	-4.51016600
C	6.24750000	4.73593700	-1.12316100
H	7.02712300	5.47589200	-0.92368300
C	6.76185900	3.26994300	-0.97585300
H	7.78870800	3.18376300	-0.60583300

C	5.10295200	4.87702400	-0.08252000
H	4.14503800	5.11337000	-0.56348000
H	5.31084100	5.66681300	0.64843900
C	5.81765700	2.62815500	0.03884600
O	5.79032700	1.41864800	0.31141000
N	5.02678800	3.57939700	0.56998200
H	4.18168600	3.29935700	1.09514300
C	4.66414100	-2.85334800	2.56883700
C	4.67557200	-1.53208500	2.13544000
C	3.56529900	-0.69870000	2.36033300
C	2.41814100	-1.18297600	3.02778600
C	2.41334400	-2.53200000	3.43773600
C	3.50619200	-3.35126500	3.21157700
H	5.54471200	-1.11985300	1.62871100
C	1.33443900	-0.27102800	3.26258200
H	1.53068600	-2.92364000	3.93443400
H	3.47314000	-4.38835700	3.53486300
C	1.37601900	1.03227000	2.86465600
C	2.54899600	1.51050200	2.13270600
H	0.45581100	-0.65161100	3.77395200
C	5.88310600	-3.73495000	2.38460300
H	6.68813300	-3.14609600	1.92916300
H	6.25080100	-4.04505000	3.37286700
O	2.63727200	2.67688400	1.69030400
C	0.29319500	2.05432900	3.10068200
H	0.75478600	2.93024800	3.57717600
H	-0.04772100	2.41193200	2.12393800
C	-0.90756900	1.57432800	3.91440700
H	-1.62260200	2.39377200	4.03636000
H	-1.41768000	0.75444200	3.39992300
H	-0.61196600	1.23201400	4.91409900
C	5.63053800	-4.99073800	1.53612300
H	6.55435000	-5.56519200	1.40624000
H	4.89459300	-5.65188500	2.00444100
H	5.25733100	-4.72080800	0.54156100
N	3.57256900	0.61217300	1.93702900
H	4.38313900	0.93785000	1.38849000

**<sup>3</sup>INT4-S**

N	-0.39806500	1.96676600	-0.62001000
N	-2.90923500	0.68708300	-0.37618300
N	-1.64111700	-1.79799400	-0.69581400
N	0.84798800	-0.49979800	-0.96241800
C	0.77315000	2.45106800	-1.14051900

C	0.81092400	3.87824200	-0.98141500
C	-0.32504300	4.23695300	-0.31666800
C	-1.10373300	3.03690700	-0.13035900
C	-2.43436800	3.00263300	0.30838300
C	-3.28857000	1.90923200	0.11567800
C	-4.72569300	1.92903500	0.26137800
C	-5.19210100	0.73731300	-0.20121100
C	-4.04198700	-0.06291000	-0.55405400
C	-4.06809500	-1.43052900	-0.85433400
C	-2.92607300	-2.24271100	-0.84173700
C	-2.93330900	-3.68483100	-0.76652700
C	-1.65473500	-4.07839300	-0.50339000
C	-0.84062000	-2.88788800	-0.48242500
C	0.55583000	-2.86906800	-0.38401200
C	1.34344400	-1.75139500	-0.68426200
C	2.77073600	-1.74651400	-0.89847300
C	3.10350700	-0.51273600	-1.37542100
C	1.89594900	0.27163600	-1.38239900
C	1.84116500	1.66220900	-1.60199700
H	1.62737400	4.50661700	-1.30706800
H	-0.63419100	5.22875800	-0.01925800
H	-5.30535500	2.76102400	0.63239300
H	-6.22021400	0.41262300	-0.26186900
H	-3.81285600	-4.30594800	-0.85796200
H	-1.28215300	-5.08458400	-0.37263300
H	3.43532800	-2.57429800	-0.70510500
H	4.08617800	-0.12597800	-1.60541300
Mn	-1.03191200	0.08201600	-0.65810400
Cl	-1.35014600	0.23666200	-2.95273700
O	-0.82195500	-0.08003100	1.11106500
C	-5.38124200	-2.10154200	-1.06454700
C	-6.30197400	-2.28260300	-0.02790200
C	-5.72063100	-2.61489800	-2.32127700
C	-7.52033600	-2.92658200	-0.22950200
C	-6.93050900	-3.26941100	-2.54457000
C	-7.83303300	-3.42289500	-1.49381300
C	-2.96807800	4.24341600	0.93443200
C	-2.48139800	4.66638700	2.17657600
C	-3.92670700	5.05289800	0.31709400
C	-2.93416700	5.83052300	2.79121000
C	-4.40102700	6.21873700	0.91496700
C	-3.90052200	6.60866500	2.15583500
C	1.24033600	-4.11133800	0.06239000
C	1.11030200	-4.51999000	1.39295200

C	2.08848900	-4.85941700	-0.75877900
C	1.82224900	-5.59984000	1.90219900
C	2.81189100	-5.94338300	-0.26895500
C	2.68128400	-6.30729300	1.06859600
F	-6.02301100	-1.82909200	1.20248500
F	-8.38359900	-3.08142700	0.78071700
F	-8.99613400	-4.04583300	-1.69722500
F	-7.23151500	-3.74782400	-3.75604500
F	-4.87160900	-2.48650300	-3.34541900
F	-4.41618000	4.71542800	-0.88291600
F	-5.32125700	6.97026300	0.30193300
F	-4.34506000	7.72600700	2.73476700
F	-2.45237500	6.20407800	3.98109500
F	-1.54572000	3.94236200	2.81177100
F	2.25275300	-4.51707000	-2.04323300
F	0.33601300	-3.82316300	2.23550800
F	1.75859400	-5.90020300	3.20635000
F	3.43505400	-7.29304000	1.56804800
F	3.66622200	-6.60534500	-1.05695500
C	2.96585500	2.28817700	-2.20204900
C	3.95012700	2.76043400	-2.73208400
C	5.16718800	3.24107500	-3.36912300
H	5.05251700	3.13076100	-4.45636000
C	5.67373200	4.68051400	-3.03687800
H	4.95869400	5.48568800	-3.22604300
C	6.49083700	2.55984900	-2.89820700
H	6.50483600	1.46915000	-2.94305000
C	7.51431000	3.27315000	-3.81131800
H	8.52336200	3.24777900	-3.38734900
H	7.55972200	2.78831900	-4.79201300
C	6.94149200	4.72833300	-3.92318200
H	7.64927200	5.48946900	-3.57909600
H	6.67912300	4.97102500	-4.95823700
C	6.14073500	4.58222700	-1.56310800
H	6.92384500	5.32026000	-1.36979900
C	6.66654200	3.11642100	-1.46722600
H	7.70814800	3.02977100	-1.14044200
C	5.03189400	4.69378300	-0.48039700
H	4.05357900	4.91195100	-0.92629000
H	5.25045900	5.48183800	0.24917700
C	5.77694100	2.45262400	-0.42079800
O	5.78027800	1.24048800	-0.15594600
N	5.00788200	3.38985100	0.16480900
H	4.21314400	3.09904200	0.75120800



C	5.17237800	-3.01959600	2.09750900
C	5.04063200	-1.69126500	1.69527700
C	3.93331500	-0.93105400	2.09534600
C	2.91322700	-1.49410100	2.90800000
C	3.06587900	-2.84507000	3.30767000
C	4.16569900	-3.58532100	2.91462800
H	5.79395000	-1.22485600	1.06514200
C	1.80907900	-0.68030600	3.26956800
H	2.29017200	-3.30206000	3.91482800
H	4.25344800	-4.62115000	3.23266000
C	1.70908000	0.66815300	2.87177400
C	2.77827500	1.22704100	2.00163900
H	1.01601500	-1.11775100	3.86834400
C	6.36116700	-3.84707300	1.65838300
H	7.10705000	-3.19133900	1.19401700
H	6.84229500	-4.28910900	2.54172200
O	2.74958700	2.39055400	1.56335800
C	0.65673400	1.51968900	3.21208200
H	0.69479700	2.52939500	2.81655900
H	-0.05913400	0.45207800	1.40494100
C	-0.50404300	1.11649400	4.06650100
H	-1.17946900	1.95923700	4.22673500
H	-1.07903200	0.31141600	3.58757900
H	-0.17530400	0.74259800	5.04690700
C	5.99360000	-4.97511100	0.67772900
H	6.89230200	-5.50407400	0.34130900
H	5.33337600	-5.71219000	1.14391500
H	5.48425600	-4.57907700	-0.20827000
N	3.81169000	0.38587100	1.69012000
H	4.52800300	0.74915800	1.03937500

**<sup>3</sup>TS1**

C	2.04380200	1.39046800	-1.21826300
C	2.66716200	2.68402000	-1.33442600
C	1.71384600	3.60681800	-1.02875500
C	0.49703800	2.87796200	-0.75075100
N	0.72965300	1.53190400	-0.87288900
H	3.69948100	2.84473200	-1.60975500
H	1.81143200	4.68306400	-1.02319200
C	-3.45042100	1.18143500	-0.35182900
C	-3.23494900	3.41671600	-0.15852900
C	-1.94444600	2.78646500	-0.33243900
N	-2.10684400	1.42818100	-0.43994500
H	-3.40433800	4.47716800	-0.04328100

C	0.72616200	-2.68617700	-0.60703300
C	2.01574300	-3.30904500	-0.77829500
C	2.89774100	-2.32294400	-1.09529800
C	2.15351900	-1.08770800	-1.09340900
N	0.83880300	-1.32293000	-0.77203500
H	2.21536100	-4.36683300	-0.68566400
H	3.95960000	-2.40971700	-1.27222300
C	-1.72309100	-2.78311800	-0.28065700
C	-2.96286500	-3.50690900	-0.12613700
C	-3.96339600	-2.58852100	-0.17672600
C	-3.34131500	-1.29290300	-0.32894100
N	-1.97834900	-1.43890200	-0.38665000
H	-3.05166400	-4.57678000	-0.00519800
H	-5.02631800	-2.76402000	-0.09610600
C	2.72664400	0.16874000	-1.35878200
C	-4.04518300	-0.08335800	-0.33732800
C	-0.73246900	3.47389000	-0.44405700
C	-0.45837100	-3.37695700	-0.34109800
Mn	-0.63232000	0.05386700	-0.63587700
Cl	-0.96966800	0.02194700	-2.90364800
C	1.86009300	1.79186900	2.28159600
C	2.89729900	2.71729500	2.43460400
C	4.09598400	2.34360400	3.04495800
C	4.27375000	1.03655900	3.50630600
C	3.25678100	0.08831900	3.35006800
C	2.07654900	0.50023000	2.73839500
H	0.92528300	2.06591800	1.80792800
H	2.74540400	3.72935600	2.07592000
H	4.89402300	3.07050800	3.16427400
H	5.20744100	0.73980800	3.97512200
H	3.39733600	-0.93180200	3.69454600
I	0.46867600	-0.91735100	2.47653400
O	-0.51963300	0.35041000	1.18098900
C	-0.09032000	5.51024800	0.87248900
C	-1.33554800	5.83420400	-1.13505400
C	-0.04431500	6.88409900	1.08842500
C	-1.31354200	7.21380500	-0.93671800
C	-0.66294300	7.73940500	0.17804900
F	0.58153600	7.38568400	2.15967600
F	-0.63117000	9.05959600	0.37410100
F	-1.90208300	8.03535500	-1.81167900
F	-1.96042400	5.36196900	-2.21930000
F	0.51580100	4.71175000	1.77176700
C	-0.73156300	4.94971400	-0.23626100

C	-0.36080300	-4.84750600	-0.11665900
C	0.18560100	-5.35157500	1.06649100
C	-0.79656800	-5.77493100	-1.06696500
C	0.30322400	-6.71800400	1.30379400
F	0.61753200	-4.50465900	2.01831100
C	-0.69628000	-7.14834500	-0.85100900
F	-1.33362000	-5.35041600	-2.21564300
C	-0.14157900	-7.61927500	0.33780000
F	0.83009600	-7.16938000	2.44774800
F	-1.12235900	-8.01507600	-1.77525000
F	-0.03879400	-8.93278300	0.55325800
C	4.09288500	0.21603600	-1.75663700
C	5.26229600	0.26648500	-2.07594400
C	6.67045400	0.31680200	-2.43752400
H	6.74841200	0.52923400	-3.51272800
C	7.57959500	1.30357500	-1.63593700
H	7.25600400	2.34824600	-1.64145900
C	7.53468300	-0.93023800	-2.07441100
H	7.16402400	-1.88942600	-2.44075800
C	8.90606100	-0.48970300	-2.63552400
H	9.73175200	-1.02946300	-2.16087700
H	8.96399900	-0.68438000	-3.71157900
C	8.93683600	1.04913800	-2.33536800
H	9.78139200	1.33957100	-1.70173700
H	9.00803900	1.63112200	-3.26018900
C	7.65487400	0.67076800	-0.22441600
H	8.58305000	0.97081600	0.26983600
C	7.61388800	-0.85687900	-0.53302100
H	8.48151200	-1.41295600	-0.16291100
C	6.44841700	0.93881700	0.72200400
H	5.70202000	1.59259400	0.25595900
H	6.76743300	1.41029900	1.65879100
C	6.37078200	-1.38421800	0.18282100
O	5.90241300	-2.50943700	0.07819600
N	5.88841800	-0.38153300	0.97596800
H	4.96839400	-0.48518500	1.38391100
C	-4.16606000	2.42942900	-0.19776900
H	-5.23854400	2.53047200	-0.11947000
C	-5.53386600	-0.15526700	-0.27413400
C	-6.28185500	-0.59823500	-1.36973200
C	-6.23695400	0.20098500	0.88024200
C	-7.67229400	-0.68136100	-1.32403300
C	-7.62648800	0.13406800	0.94693200
C	-8.34514500	-0.31126500	-0.16104300

F	-5.57098700	0.62787100	1.96287400
F	-5.66215800	-0.96420500	-2.49633900
F	-8.27273900	0.48487000	2.06508800
F	-8.36380400	-1.10905600	-2.38559300
F	-9.67754500	-0.38402000	-0.10740900

**<sup>3</sup>TS2-S**

N	-0.52557200	1.99182300	-0.58105500
N	-2.98198000	0.61694300	-0.38764000
N	-1.58789700	-1.83049700	-0.65634200
N	0.83954500	-0.41624900	-0.89776500
C	0.63313900	2.52554700	-1.08205000
C	0.60967000	3.95158600	-0.91606300
C	-0.55011200	4.26106600	-0.26686000
C	-1.28353000	3.03077400	-0.10039200
C	-2.61978200	2.94201100	0.31220200
C	-3.42737700	1.81866800	0.09153300
C	-4.86747400	1.77434000	0.20685600
C	-5.26712600	0.55803000	-0.25349500
C	-4.07206600	-0.19045700	-0.57486200
C	-4.02781600	-1.56323300	-0.84998800
C	-2.85278100	-2.32664200	-0.81020400
C	-2.80015800	-3.76855200	-0.73450400
C	-1.50709000	-4.10972000	-0.46989700
C	-0.74318100	-2.88601000	-0.44370400
C	0.65150800	-2.80494000	-0.34925300
C	1.38683200	-1.64927900	-0.63940100
C	2.81184900	-1.58555300	-0.86683300
C	3.09024100	-0.33583700	-1.33437000
C	1.85107000	0.39864800	-1.32241700
C	1.73775500	1.78517100	-1.53703900
H	1.40432900	4.61409300	-1.22801500
H	-0.90532600	5.23810800	0.02817600
H	-5.49263000	2.58267300	0.55575500
H	-6.27725400	0.18451500	-0.33306800
H	-3.65234400	-4.42574700	-0.83234300
H	-1.09327800	-5.10023900	-0.34306600
H	3.51176600	-2.38748600	-0.68926900
H	4.05448800	0.09103300	-1.57163100
Mn	-1.06378800	0.09247400	-0.60063400
Cl	-1.37055800	0.18001300	-2.92162000
O	-0.95954600	-0.13520100	1.10169700
C	-5.30721600	-2.29563300	-1.06732700
C	-6.22899600	-2.50789100	-0.03769900

C	-5.61055200	-2.83539300	-2.32209300
C	-7.41507500	-3.20812500	-0.24420000
C	-6.78758800	-3.54590000	-2.55013700
C	-7.69258100	-3.72995300	-1.50644300
C	-3.20627100	4.14715900	0.95859300
C	-2.75280800	4.54740600	2.22091000
C	-4.18472700	4.93897800	0.35061600
C	-3.25486400	5.67674600	2.86168800
C	-4.70751200	6.06988300	0.97462900
C	-4.23810200	6.43981400	2.23367000
C	1.39854400	-4.02164100	0.06836000
C	1.30747800	-4.46078900	1.39215700
C	2.27487300	-4.71065100	-0.77546300
C	2.07975100	-5.51178100	1.87323900
C	3.06519600	-5.75956200	-0.31206500
C	2.96904000	-6.15465400	1.01942000
F	-5.98276400	-2.03000700	1.19043500
F	-8.28053600	-3.39206300	0.75933600
F	-8.82444200	-4.40672600	-1.71460300
F	-7.05479800	-4.04915800	-3.75952300
F	-4.75787400	-2.67914300	-3.33903500
F	-4.64646300	4.61761600	-0.86486300
F	-5.64515200	6.80691800	0.37023700
F	-4.72934100	7.52388000	2.83783800
F	-2.80487900	6.03161800	4.06963500
F	-1.80470300	3.83428100	2.84908900
F	2.40256900	-4.34150200	-2.05609400
F	0.51442000	-3.81495600	2.26007700
F	2.04721200	-5.83843800	3.17253500
F	3.77952900	-7.10749400	1.49386000
F	3.94338000	-6.36133900	-1.12170300
C	2.83742500	2.45991100	-2.13149200
C	3.80046900	2.96948800	-2.66616400
C	4.98107900	3.50605500	-3.32748400
H	4.83099700	3.42206300	-4.41285200
C	5.44881000	4.95295000	-2.97251400
H	4.69906800	5.73637100	-3.11222400
C	6.34510600	2.86054000	-2.92659600
H	6.39614000	1.77268100	-3.00264200
C	7.30535300	3.63477600	-3.85855400
H	8.33160700	3.63157500	-3.47733800
H	7.32536100	3.18072300	-4.85472600
C	6.68039700	5.07209800	-3.90205900
H	7.37480900	5.84591500	-3.55892000

H	6.37190000	5.33816300	-4.91846200
C	5.97128600	4.82969800	-1.51985600
H	6.72883100	5.59448400	-1.32843100
C	6.56091800	3.38532400	-1.48841800
H	7.61868600	3.33353000	-1.20994400
C	4.89499900	4.85914600	-0.39941800
H	3.89325800	5.04464600	-0.80600000
H	5.10290600	5.63484300	0.34638000
C	5.74487000	2.65512800	-0.42726100
O	5.81893900	1.43861000	-0.19176300
N	4.95034900	3.53735400	0.20718600
H	4.17342000	3.18366600	0.78365200
C	5.46538900	-2.90449300	2.08645400
C	5.29002900	-1.58208600	1.69281700
C	4.13129900	-0.87693200	2.06433600
C	3.11568000	-1.50586500	2.82533400
C	3.32411900	-2.83932100	3.24104400
C	4.47065500	-3.52234200	2.88191100
H	6.03599000	-1.07849700	1.08299200
C	1.91422900	-0.77359400	3.07769400
H	2.55174800	-3.33549300	3.82093600
H	4.60026000	-4.55527900	3.19459700
C	1.73535200	0.51389000	2.64366800
C	2.81730800	1.17543900	1.90003600
H	1.10942700	-1.28361300	3.59958200
C	6.67869400	-3.69272500	1.64346100
H	7.42076400	-3.01061400	1.21253900
H	7.15114100	-4.15824000	2.51900600
O	2.73449200	2.34645500	1.48273300
C	0.45942800	1.25755700	2.75968200
H	0.60378000	2.32102100	2.55552200
H	-0.16954700	0.87181000	1.85112800
C	-0.42341100	0.99590800	3.97217100
H	-1.32605600	1.60946800	3.90788000
H	-0.73575200	-0.05200100	4.02701600
H	0.10234000	1.24893700	4.90167300
C	6.33488200	-4.79003100	0.61896700
H	7.24229900	-5.30268300	0.28102400
H	5.66930400	-5.54450000	1.04860300
H	5.83834700	-4.36626900	-0.26139600
N	3.94974600	0.42869200	1.67106400
H	4.65843600	0.84663400	1.04358800

C	1.71530200	-2.21109600	-0.20958100
C	3.13274800	-2.44991600	-0.27386100
C	3.74414200	-1.23772800	-0.36506000
C	2.70121800	-0.24876700	-0.34030300
N	1.46762100	-0.85280500	-0.23563900
H	3.60468700	-3.42102000	-0.24984000
H	4.80428200	-1.04051500	-0.43900600
C	-0.03534200	3.08947700	-0.13357800
C	0.95975500	4.12642500	-0.19850400
C	2.16896900	3.51290600	-0.31030200
C	1.92229700	2.09881600	-0.30860100
N	0.57378100	1.85183100	-0.19248800
H	0.75623300	5.18619200	-0.15369900
H	3.14906700	3.96084000	-0.38249100
C	-2.58593700	-1.99203900	0.06705700
C	-2.82812700	-3.41082300	0.04229800
C	-1.61680500	-4.02137400	-0.03461900
C	-0.62055000	-2.98294200	-0.06095700
N	-1.23016200	-1.74728500	0.00278600
H	-3.80219800	-3.87615800	0.06991900
H	-1.41180800	-5.08059300	-0.08182000
C	-3.35366900	0.34743700	0.15687600
C	-4.38664100	1.34333600	0.27061300
C	-3.77860200	2.55724400	0.21461600
C	-2.36610700	2.31668600	0.07814200
N	-2.12270800	0.95912600	0.05376700
H	-5.44050300	1.13635800	0.38352600
H	-4.24284500	3.53122600	0.25890400
C	0.75201100	-3.21873300	-0.14366400
C	-1.40583600	3.32438100	-0.01365200
C	2.93953900	1.13301300	-0.38702600
C	-3.59149200	-1.02815700	0.14821200
Mn	-0.35185500	0.04816500	-0.37859700
Cl	-0.57074900	0.01347400	-2.71285800
C	-1.87010700	4.74077600	0.02315100
C	-2.38048700	5.30885700	1.19416300
C	-1.80900700	5.55459700	-1.11270800
C	-2.82025200	6.62949700	1.24048200
F	-2.46360300	4.57259500	2.31108300
C	-2.23567800	6.88091800	-1.08831800
F	-1.32221600	5.06556500	-2.25787400
C	-2.74470700	7.41755900	0.09316600
F	-3.30602200	7.14578900	2.37441700
F	-2.16431700	7.63831900	-2.18714200

F	-3.15884100	8.68573200	0.12655000
C	-5.00455500	-1.49460600	0.23463000
C	-5.48664200	-2.14879200	1.37264900
C	-5.90162900	-1.29487400	-0.82001200
C	-6.80317300	-2.59396000	1.46342900
F	-4.66944400	-2.36894000	2.41154300
C	-7.22529100	-1.72418000	-0.74870400
F	-5.49690300	-0.66853000	-1.92997700
C	-7.67494200	-2.37782300	0.39741200
F	-7.23604300	-3.21856800	2.56361100
F	-8.06262600	-1.51857500	-1.76988700
F	-8.93975900	-2.79602400	0.47469600
C	1.21898400	-4.63417800	-0.16705700
C	1.78126700	-5.19542500	-1.31833400
C	1.11249300	-5.45267700	0.96141300
C	2.22390700	-6.51627700	-1.34877100
F	1.91090600	-4.45682900	-2.42497300
C	1.54162300	-6.77745100	0.95247700
F	0.57787900	-4.96583700	2.09010800
C	2.10104800	-7.30866400	-0.20853900
F	2.75809500	-7.02876600	-2.46117500
F	1.42598500	-7.53776000	2.04650900
F	2.51832200	-8.57597000	-0.22810500
C	4.28556500	1.59144800	-0.47348300
C	5.42608300	2.00582300	-0.49257700
C	6.77511100	2.55197400	-0.50756600
H	6.83823800	3.27016300	-1.33667300
C	7.28435900	3.22431900	0.81014700
H	6.64548600	4.01768400	1.20777700
C	7.97320500	1.55549000	-0.57919000
H	7.94387800	0.83111200	-1.39512800
C	9.15364700	2.55308700	-0.61676800
H	10.08932400	2.08669300	-0.29274000
H	9.31060600	2.92868700	-1.63334200
C	8.68290600	3.69871600	0.34512000
H	9.36273600	3.84648600	1.19061500
H	8.60871700	4.65451400	-0.18394200
C	7.49242500	2.03249400	1.77677400
H	8.24657800	2.28787500	2.52602400
C	7.96711100	0.89785900	0.81948200
H	8.95449400	0.49073100	1.05979700
C	6.22075400	1.47774100	2.48584200
H	5.32900600	2.06075100	2.22707400
H	6.33054100	1.48946200	3.57632600



C	6.94270100	-0.22223700	0.97034800
O	6.88583200	-1.23913500	0.29077300
N	6.10499700	0.11065100	1.99452000
H	5.27695700	-0.44994600	2.15035600

**<sup>5</sup>INT1**

C	2.07922800	1.25246100	-1.31687300
C	2.76257900	2.51296500	-1.43305400
C	1.86785600	3.48146700	-1.08966200
C	0.62297400	2.81805000	-0.78707200
N	0.78220300	1.46038000	-0.92858600
H	3.79352300	2.62378400	-1.73661400
H	2.02378900	4.55053800	-1.07084100
C	-3.39652000	1.32364000	-0.28463100
C	-3.05292600	3.54244900	-0.07849600
C	-1.80438500	2.84916400	-0.29247100
N	-2.04119700	1.50144700	-0.39870400
H	-3.16199000	4.60887200	0.05318300
C	0.56962900	-2.75042900	-0.71614300
C	1.82558400	-3.43753600	-0.89227400
C	2.75371100	-2.49955800	-1.22803000
C	2.07221300	-1.23009000	-1.23869900
N	0.75140800	-1.40142000	-0.91222200
H	1.97398200	-4.50230600	-0.78488800
H	3.81091400	-2.63522000	-1.39903500
C	-1.87980100	-2.71815500	-0.33929700
C	-3.14617700	-3.37769300	-0.12276300
C	-4.10398700	-2.41355300	-0.14157300
C	-3.42989800	-1.15053100	-0.33511100
N	-2.08254600	-1.36677800	-0.46460400
H	-3.28037700	-4.44013500	0.01928600
H	-5.16874300	-2.53635700	-0.00690100
C	2.69911900	0.00197300	-1.49813900
C	-4.06562400	0.09510400	-0.28850700
C	-0.56390600	3.47570200	-0.44198100
C	-0.64608100	-3.37330300	-0.41500600
Mn	-0.67311700	0.05171800	-0.79297700
Cl	-1.09655000	0.10055300	-3.17517000
C	0.18528400	5.49717900	0.84354700
C	-1.06417700	5.84957900	-1.15759400
C	0.29631600	6.87051200	1.03887200
C	-0.97700100	7.22939900	-0.97934900
C	-0.29174400	7.74003100	0.12171700
F	0.95457300	7.35785400	2.09700100

F	-0.19793100	9.05979600	0.29817700
F	-1.53702200	8.06473700	-1.85949900
F	-1.72257200	5.39019400	-2.22649800
F	0.76063300	4.68305700	1.74753300
C	-0.49033300	4.95205500	-0.25167600
C	-0.61613500	-4.84164300	-0.15863800
C	-0.07014400	-5.34702200	1.02405600
C	-1.11773200	-5.76636800	-1.07886400
C	-0.01449300	-6.71199900	1.28982600
F	0.42329200	-4.50272600	1.94909300
C	-1.08030600	-7.13817300	-0.83400300
F	-1.65841000	-5.34013900	-2.22463000
C	-0.52378800	-7.61051400	0.35346200
F	0.51411400	-7.16388800	2.43250700
F	-1.56832500	-8.00208500	-1.72925700
F	-0.48094300	-8.92229800	0.59615600
C	4.06206700	-0.01241500	-1.90444800
C	5.23833100	-0.02725600	-2.19976500
C	6.66345100	-0.07685100	-2.48275000
H	6.81617400	-0.00814700	-3.56843800
C	7.57241200	0.96204400	-1.74983500
H	7.30728500	2.01109700	-1.90850600
C	7.43311700	-1.30541400	-1.90545200
H	7.03522500	-2.28552600	-2.17544700
C	8.86064100	-1.00478900	-2.41718300
H	9.62258600	-1.51299300	-1.81749800
H	8.97954000	-1.34323600	-3.45179000
C	8.95447000	0.55732700	-2.31739000
H	9.77308600	0.89160200	-1.67152800
H	9.11224700	1.00754900	-3.30302500
C	7.52747200	0.51329900	-0.26759700
H	8.44329400	0.82485500	0.24233300
C	7.41268700	-1.03748200	-0.38413000
H	8.21941400	-1.58436500	0.11523500
C	6.29023200	0.96337500	0.56285600
H	5.61053200	1.59124400	-0.02577500
H	6.58247500	1.53206400	1.45286300
C	6.09789600	-1.40118300	0.30869100
O	5.56595400	-2.50307700	0.31677200
N	5.63958400	-0.28183100	0.94221200
H	4.70583900	-0.28610800	1.33094900
C	-4.03661200	2.60556700	-0.10281000
H	-5.09981100	2.76389300	0.00051700
C	-5.55237900	0.10242400	-0.18058400

C	-6.35300700	-0.30792500	-1.25220500
C	-6.20352500	0.49786200	0.99187200
C	-7.74396300	-0.32052200	-1.16619200
C	-7.59213300	0.50131700	1.09796800
C	-8.36369600	0.08801100	0.01335000
F	-5.48684800	0.89389100	2.05337600
F	-5.78549600	-0.70960500	-2.39323600
F	-8.18752400	0.88814200	2.23221200
F	-8.48618000	-0.71736300	-2.20487200
F	-9.69574900	0.08260600	0.10530900
O	-0.46273200	0.11618200	1.45201400
I	0.70904400	-1.03448700	2.45420200
C	2.27343300	0.42351900	2.79193900
C	2.05458900	1.67815800	2.24392500
C	3.40814800	0.08862300	3.52348800
C	3.04520300	2.64796000	2.42692900
H	1.14196600	1.88769800	1.69484600
C	4.38082800	1.07830300	3.70383800
H	3.55146600	-0.90521300	3.93773500
C	4.20058800	2.35010200	3.15389700
H	2.89489500	3.63518200	2.00497200
H	5.28066100	0.84302300	4.26449700
H	4.96205200	3.11137700	3.29625500

**<sup>5</sup>INT2**

N	0.50371000	1.90506800	-0.33334700
N	-2.15727000	0.87814100	0.02408700
N	-1.12550600	-1.80731500	-0.00238800
N	1.53870000	-0.77848500	-0.34740600
C	1.82029200	2.21103200	-0.47457200
C	1.99635500	3.63333700	-0.63987800
C	0.75538500	4.18377000	-0.60369400
C	-0.17616900	3.09872300	-0.39513300
C	-1.55713200	3.25206200	-0.25900900
C	-2.47141600	2.20576400	-0.05250500
C	-3.89515200	2.38925500	0.10900100
C	-4.43286800	1.15373900	0.27400000
C	-3.33854800	0.21264000	0.21742200
C	-3.48685200	-1.17743400	0.30627200
C	-2.44915600	-2.10953200	0.17871700
C	-2.63019800	-3.54285100	0.20234100
C	-1.40490300	-4.09521200	0.01509100
C	-0.46756400	-3.00160900	-0.09978200
C	0.91657000	-3.16081800	-0.27115800

C	1.84139700	-2.11767300	-0.37251400
C	3.27054800	-2.29719300	-0.49601400
C	3.82408800	-1.05765900	-0.54591200
C	2.72818300	-0.12130400	-0.45273400
C	2.88646100	1.28046400	-0.47859600
H	2.94817600	4.12312900	-0.78309600
H	0.48801700	5.22388400	-0.71656700
H	-4.40985100	3.33835100	0.09891300
H	-5.47350200	0.89689000	0.40442200
H	-3.57132600	-4.05392900	0.33860700
H	-1.15445100	-5.14367600	-0.04539600
H	3.78412300	-3.24623100	-0.53519200
H	4.87036200	-0.80776300	-0.64829300
Mn	-0.29831000	0.05136800	-0.05475800
Cl	-0.58876500	-0.02802500	-2.48178900
O	-0.09714200	0.11082300	1.58797500
C	-4.86481000	-1.70294100	0.52797000
C	-5.52192300	-1.50818000	1.74691300
C	-5.55132300	-2.39663400	-0.47355700
C	-6.81193100	-1.98463100	1.96776900
C	-6.84060300	-2.88470100	-0.27311200
C	-7.47135500	-2.67587400	0.95246900
C	-2.10618500	4.63642700	-0.33489400
C	-1.84616800	5.57669400	0.66695800
C	-2.90143400	5.04202100	-1.41172900
C	-2.35217900	6.87277500	0.60446800
C	-3.42044300	6.33228900	-1.49274100
C	-3.14257700	7.24944400	-0.48027000
C	1.44493100	-4.55308500	-0.34590400
C	1.43324200	-5.39532800	0.77009500
C	1.97561300	-5.06214600	-1.53573500
C	1.92569200	-6.69652400	0.71113000
C	2.47567800	-6.35997600	-1.61644300
C	2.44898800	-7.17808500	-0.48800600
F	-4.91073800	-0.84438100	2.73485300
F	-7.41768500	-1.78656100	3.14235800
F	-8.70631900	-3.13777100	1.15392200
F	-7.47563700	-3.54513800	-1.24561200
F	-4.96732500	-2.60972900	-1.65754100
F	-3.18401600	4.17992300	-2.39336700
F	-4.17685900	6.69620000	-2.53214700
F	-3.63323900	8.48786800	-0.54922000
F	-2.08878300	7.75254000	1.57569100
F	-1.09006300	5.24007100	1.71891700

F	2.01426600	-4.29604100	-2.62991400
F	0.93605900	-4.95477500	1.93260600
F	1.90381900	-7.48130600	1.79286400
F	2.92405500	-8.42255400	-0.55521500
F	2.97548100	-6.82492900	-2.76460300
C	4.20207300	1.80342700	-0.49520200
C	5.32145600	2.27259300	-0.41585300
C	6.63005100	2.89071200	-0.29057100
H	6.69341100	3.69214600	-1.03942700
C	7.00320500	3.46024600	1.12117400
H	6.28488500	4.16794900	1.54323300
C	7.89603800	1.98250100	-0.36875500
H	7.97050500	1.34137200	-1.24892900
C	9.00262700	3.05318300	-0.22891600
H	9.94556400	2.61709900	0.11511900
H	9.19821200	3.53654100	-1.19187700
C	8.39172300	4.06582100	0.80066700
H	9.00299700	4.17181700	1.70269100
H	8.28465500	5.06271100	0.36068900
C	7.23140200	2.19358900	1.98215800
H	7.91723500	2.42294200	2.80198700
C	7.84354800	1.19166000	0.95769600
H	8.83840600	0.82341900	1.22747900
C	5.96044000	1.49123900	2.54733600
H	5.04710500	2.04557700	2.30055200
H	6.00837600	1.38963800	3.63737300
C	6.88859400	0.00156400	0.92516800
O	6.94955600	-0.94187800	0.14707400
N	5.96021900	0.18210400	1.90711400
H	5.16629300	-0.44400300	1.95814800

**<sup>5</sup>INT3-S**

N	-0.39557900	2.00597800	-0.60353900
N	-2.87256800	0.59263100	-0.34582200
N	-1.46907400	-1.88712000	-0.61715000
N	1.00281500	-0.46649400	-0.83473400
C	0.80348600	2.51853800	-0.97929300
C	0.77968400	3.95853000	-0.91806600
C	-0.45328900	4.30707000	-0.46433500
C	-1.19697000	3.07758400	-0.29367900
C	-2.55306500	3.00395700	0.03423200
C	-3.34160000	1.84079500	-0.05008500
C	-4.77955100	1.80395800	0.08594600
C	-5.16651800	0.52723500	-0.17307200

C	-3.96303700	-0.23447200	-0.41386900
C	-3.91557400	-1.62134400	-0.61329900
C	-2.74165600	-2.38628500	-0.67372500
C	-2.69808500	-3.83051900	-0.69152200
C	-1.38758800	-4.18468300	-0.60892000
C	-0.62607300	-2.95821800	-0.56888100
C	0.77839000	-2.89199000	-0.53160900
C	1.53220100	-1.72607100	-0.69117600
C	2.97106100	-1.66839400	-0.83823000
C	3.28603000	-0.38098400	-1.13819600
C	2.04478500	0.35786700	-1.11995300
C	1.94813700	1.75655900	-1.30828500
H	1.61548700	4.59663000	-1.16540300
H	-0.84222400	5.29971500	-0.29053800
H	-5.41044100	2.64693300	0.32398700
H	-6.17174800	0.13363700	-0.18762100
H	-3.55895300	-4.48130300	-0.73568000
H	-0.96697200	-5.17973800	-0.59752700
H	3.64721500	-2.49974300	-0.71181300
H	4.26363900	0.05885400	-1.27243200
Mn	-0.93313600	0.05044000	-0.50986800
Cl	-1.21646700	0.14406300	-2.93299100
O	-0.76704500	-0.04094000	1.13630200
C	-5.20821900	-2.35758300	-0.71094100
C	-6.05859100	-2.50030400	0.38956300
C	-5.60147600	-2.95369200	-1.91385200
C	-7.26153100	-3.19641700	0.30105700
C	-6.79909100	-3.65726100	-2.02380700
C	-7.63066200	-3.77678600	-0.91147700
C	-3.21150500	4.27184500	0.45812400
C	-2.87046600	4.87156000	1.67542400
C	-4.16095100	4.92119000	-0.33657700
C	-3.45717300	6.06238300	2.09633700
C	-4.76204700	6.11184000	0.06520300
C	-4.40679100	6.68304700	1.28619100
C	1.51894700	-4.16797600	-0.33147400
C	1.47806200	-4.81598500	0.90649800
C	2.30722500	-4.73735600	-1.33557600
C	2.23610400	-5.95441400	1.15684000
C	3.05354400	-5.89217000	-1.11281600
C	3.02042600	-6.49556200	0.14218000
F	-5.72363900	-1.95843000	1.56768600
F	-8.05714900	-3.31721200	1.36857500
F	-8.77984900	-4.44773000	-1.00662800

F	-7.15496700	-4.21537600	-3.18441400
F	-4.81845200	-2.85864000	-2.99210900
F	-4.51409500	4.39858700	-1.51695800
F	-5.66765100	6.71186100	-0.71317500
F	-4.97512100	7.82420200	1.67891600
F	-3.11700100	6.61153100	3.26594900
F	-1.95578700	4.30130800	2.47005700
F	2.37158600	-4.16220600	-2.54177400
F	0.71585400	-4.32783800	1.89092700
F	2.26330100	-6.50085600	2.37924800
F	3.78263500	-7.56221400	0.39149300
F	3.81379300	-6.40973200	-2.08279300
C	3.08046100	2.41593000	-1.83540400
C	4.08310900	2.90169200	-2.32349400
C	5.31610400	3.37646900	-2.93071300
H	5.21517600	3.25550600	-4.01855000
C	5.82604700	4.81588300	-2.60323900
H	5.11942800	5.62364100	-2.81147100
C	6.62744200	2.68939600	-2.43138900
H	6.63415700	1.59840800	-2.46741700
C	7.66994100	3.38876300	-3.33315400
H	8.67011600	3.36230600	-2.88908300
H	7.73183100	2.89382600	-4.30788000
C	7.10736800	4.84564400	-3.47019600
H	7.81335000	5.60663600	-3.12267200
H	6.86311300	5.07851200	-4.51195500
C	6.26712000	4.72622500	-1.12105400
H	7.05245600	5.46002700	-0.92128300
C	6.77672100	3.25602900	-1.00163100
H	7.80835000	3.15965900	-0.64787600
C	5.13647300	4.85689200	-0.06395600
H	4.17402400	5.10692700	-0.52868700
H	5.35842200	5.63339200	0.67706600
C	5.84329300	2.60365800	0.01616100
O	5.81600100	1.39069400	0.27309900
N	5.06026300	3.54929100	0.56832700
H	4.21610800	3.26222700	1.09203800
C	4.71783400	-2.88987000	2.56415300
C	4.72692000	-1.56890100	2.12995500
C	3.62031100	-0.73347400	2.36600500
C	2.47894500	-1.21486200	3.04605600
C	2.47703000	-2.56377300	3.45760900
C	3.56591700	-3.38502100	3.22022200
H	5.59156400	-1.15864700	1.61381800

C	1.39629600	-0.30335800	3.28495500
H	1.59885200	-2.95360100	3.96367400
H	3.53519000	-4.42158900	3.54523900
C	1.43091900	0.99592400	2.87587700
C	2.59488500	1.46995800	2.13025900
H	0.51960200	-0.68355000	3.79964800
C	5.93208700	-3.77502900	2.36682500
H	6.73634400	-3.18738700	1.90841700
H	6.30555000	-4.09170300	3.35083400
O	2.67382300	2.63044500	1.66789200
C	0.33787300	2.01003200	3.09374800
H	0.78593300	2.89648400	3.56420100
H	0.00201300	2.34869200	2.10837700
C	-0.86693000	1.52485600	3.89810900
H	-1.59031300	2.33923800	4.00679400
H	-1.36089100	0.69880200	3.37803700
H	-0.58002600	1.19232700	4.90382200
C	5.66778000	-5.02560000	1.51423000
H	6.58661200	-5.60698000	1.37971800
H	4.92779900	-5.68253100	1.98202400
H	5.29426300	-4.74917800	0.52152700
N	3.62292200	0.57559800	1.93809800
H	4.42538500	0.89971900	1.37772400

**<sup>5</sup>INT4-S**

N	-0.39451400	1.96160800	-0.61594400
N	-2.91010900	0.69049300	-0.37170800
N	-1.65502000	-1.79850700	-0.69548100
N	0.84006900	-0.50963800	-0.93868500
C	0.78065200	2.43975300	-1.13079800
C	0.82913300	3.86594300	-0.96272300
C	-0.30537700	4.22864000	-0.29761100
C	-1.09306600	3.03264600	-0.12013300
C	-2.42424200	3.00328100	0.31749600
C	-3.28375200	1.91464800	0.12079100
C	-4.72118300	1.94272200	0.25919700
C	-5.19302800	0.75531600	-0.20975100
C	-4.04677500	-0.05162600	-0.55874700
C	-4.07914800	-1.41831800	-0.86353200
C	-2.94135900	-2.23657200	-0.84665600
C	-2.95655000	-3.67869300	-0.76735300
C	-1.68188300	-4.07798800	-0.49422500
C	-0.86172700	-2.89153500	-0.47183900
C	0.53378700	-2.87828600	-0.36258300



C	1.32837600	-1.76437500	-0.65910100
C	2.75517500	-1.76747400	-0.87269500
C	3.09468400	-0.53692400	-1.35438200
C	1.89230500	0.25442200	-1.36397700
C	1.84467600	1.64415700	-1.59068100
H	1.65202800	4.48979100	-1.28079100
H	-0.60744200	5.22063000	0.00638000
H	-5.29760100	2.77746700	0.62903700
H	-6.22300100	0.43792000	-0.27695200
H	-3.83886900	-4.29539200	-0.86192400
H	-1.31531000	-5.08551400	-0.35677200
H	3.41548200	-2.59787600	-0.67578600
H	4.07963900	-0.15674100	-1.58602300
Mn	-1.03772100	0.07918900	-0.65066600
Cl	-1.34350500	0.23349400	-2.94584500
O	-0.84379100	-0.07481500	1.12412500
C	-5.39460700	-2.08177100	-1.08232900
C	-6.32378800	-2.25721500	-0.05222300
C	-5.72778300	-2.59404100	-2.34122300
C	-7.54424300	-2.89447100	-0.26234200
C	-6.93965600	-3.24185300	-2.57294400
C	-7.85059400	-3.38969800	-1.52864300
C	-2.95188500	4.24432000	0.94829600
C	-2.46502300	4.65662100	2.19400200
C	-3.90353000	5.06341100	0.33311300
C	-2.91082800	5.82092000	2.81345200
C	-4.37091400	6.22942200	0.93606800
C	-3.87035400	6.60912500	2.18010800
C	1.21160800	-4.12134000	0.09205200
C	1.08243700	-4.51715000	1.42643300
C	2.05553000	-4.87926400	-0.72414400
C	1.79151700	-5.59487100	1.94406200
C	2.77533000	-5.96193600	-0.22620000
C	2.64578300	-6.31328100	1.11484700
F	-6.05110200	-1.80499400	1.18003400
F	-8.41553700	-3.04403800	0.74168900
F	-9.01563000	-4.00618300	-1.74013100
F	-7.23455800	-3.71917100	-3.78630800
F	-4.87067500	-2.47091600	-3.35927900
F	-4.39286500	4.73529100	-0.86966800
F	-5.28464900	6.99057800	0.32513000
F	-4.30833300	7.72648200	2.76397100
F	-2.42919400	6.18474700	4.00645300
F	-1.53675600	3.92193500	2.82639500

F	2.21993000	-4.54702300	-2.01125500
F	0.31260600	-3.80914400	2.26363200
F	1.73004400	-5.88271500	3.25100400
F	3.39663200	-7.29744700	1.62156000
F	3.62587800	-6.63395800	-1.00967700
C	2.96993800	2.26036100	-2.19934300
C	3.95203300	2.72048400	-2.74404400
C	5.16330000	3.18343200	-3.40496200
H	5.02970100	3.06060400	-4.48872500
C	5.68776100	4.62241800	-3.09962800
H	4.97666800	5.43145500	-3.28714700
C	6.48866600	2.49644200	-2.94747300
H	6.49245700	1.40519000	-2.97866800
C	7.50290900	3.18912800	-3.88632600
H	8.51852400	3.16034100	-3.47856800
H	7.52809300	2.69148200	-4.86131600
C	6.94075900	4.64769600	-4.00752400
H	7.66067000	5.40695700	-3.68515900
H	6.66314100	4.87937500	-5.04112300
C	6.17835400	4.53851100	-1.63275200
H	6.97092700	5.27189500	-1.46161200
C	6.69257300	3.06924200	-1.52675800
H	7.73836700	2.97698800	-1.21528800
C	5.08791500	4.67357600	-0.53421600
H	4.10473700	4.89587300	-0.96744900
H	5.32526700	5.46820600	0.18225000
C	5.81291200	2.42633200	-0.45902300
O	5.80811500	1.21736700	-0.18031800
N	5.06169500	3.37775800	0.12687000
H	4.27155200	3.10079400	0.72621600
C	5.15976300	-3.01998500	2.11005100
C	5.04503500	-1.69089300	1.70350900
C	3.94667000	-0.91626200	2.09861300
C	2.91729300	-1.46296500	2.91023200
C	3.05196000	-2.81484900	3.31360700
C	4.14397600	-3.57004200	2.92598000
H	5.80537500	-1.23590400	1.07339600
C	1.82164600	-0.63508900	3.26607000
H	2.26954300	-3.26038400	3.92073900
H	4.21823400	-4.60545800	3.24882100
C	1.73810100	0.71687400	2.86719400
C	2.81831100	1.25646300	1.99443200
H	1.02121800	-1.06604600	3.85930200
C	6.34041900	-3.86258400	1.67751200

H	7.09208700	-3.21779600	1.20712700
H	6.81829900	-4.30120100	2.56436800
O	2.80713200	2.41831200	1.55092700
C	0.70788900	1.59552900	3.20170500
H	0.76116800	2.59031000	2.77104400
H	-0.00325400	0.33384700	1.39967600
C	-0.48495500	1.25585500	4.03521100
H	-0.88449900	2.15104300	4.52061800
H	-1.28267300	0.84524500	3.39811700
H	-0.26303900	0.50934700	4.80620800
C	5.96267100	-4.99592900	0.70699000
H	6.85664400	-5.53475200	0.37355300
H	5.29768900	-5.72407400	1.18038100
H	5.45487800	-4.60349000	-0.18154500
N	3.84049100	0.40090900	1.68734900
H	4.56029800	0.75200700	1.03418600

**<sup>5</sup>TS1**

C	2.02283500	1.38259100	-1.22530900
C	2.64511900	2.67370800	-1.35110000
C	1.70157900	3.60202700	-1.03045400
C	0.48679600	2.88274000	-0.73314400
N	0.71125100	1.53475800	-0.85944500
H	3.67460800	2.82907200	-1.63924700
H	1.80476100	4.67764300	-1.02206300
C	-3.46052600	1.19094400	-0.31630200
C	-3.22826900	3.42408400	-0.09900900
C	-1.94256400	2.79623900	-0.28093400
N	-2.11101000	1.43704100	-0.39501400
H	-3.39319800	4.48384100	0.02785100
C	0.70304300	-2.68223500	-0.61578700
C	1.99269300	-3.31153800	-0.77450200
C	2.88150400	-2.33174100	-1.09433400
C	2.14046600	-1.09446800	-1.11065100
N	0.82709800	-1.32784100	-0.80330200
H	2.18688400	-4.36940100	-0.67218900
H	3.94480100	-2.42285800	-1.26067000
C	-1.75526400	-2.77000600	-0.32698400
C	-2.99599300	-3.49169500	-0.16132700
C	-3.99822900	-2.57549000	-0.20905900
C	-3.37896800	-1.27991500	-0.37161600
N	-2.02133300	-1.43042000	-0.45461500
H	-3.08263400	-4.56047700	-0.03063400
H	-5.06006900	-2.74992000	-0.11436900

C	2.70881400	0.16426700	-1.37630300
C	-4.07249100	-0.06534800	-0.34044800
C	-0.73394300	3.48428700	-0.40727300
C	-0.49061800	-3.36503200	-0.36160400
Mn	-0.66528200	0.06208600	-0.66071600
Cl	-0.96933300	0.00690100	-3.03523000
C	1.88900900	1.74867300	2.26670300
C	2.87784800	2.73412500	2.34880200
C	4.10853600	2.45512200	2.94620800
C	4.36469000	1.18474300	3.46840900
C	3.39443200	0.18021800	3.38723600
C	2.17915500	0.49375100	2.78355500
H	0.92811500	1.94317500	1.80474300
H	2.66694500	3.71856900	1.94702400
H	4.86907000	3.22801800	3.00918100
H	5.32195600	0.96184900	3.93093400
H	3.59368300	-0.81037000	3.78492700
I	0.64575300	-1.01405700	2.64704800
O	-0.49156300	0.10276700	1.27962000
C	-0.09928000	5.53622000	0.88953600
C	-1.33625400	5.83304300	-1.12856400
C	-0.05576800	6.91306700	1.08746300
C	-1.31645600	7.21507400	-0.94811700
C	-0.67120800	7.75545100	0.16288800
F	0.56358600	7.42942800	2.15494100
F	-0.64192900	9.07780100	0.34182500
F	-1.90263400	8.02448700	-1.83551100
F	-1.95728800	5.34473700	-2.20753700
F	0.50076900	4.74865700	1.80051700
C	-0.73390800	4.96189200	-0.21552400
C	-0.40242600	-4.83601900	-0.13356000
C	0.12936500	-5.34571600	1.05384900
C	-0.83275400	-5.75878600	-1.09136300
C	0.23774200	-6.71374500	1.28766900
F	0.55567900	-4.50506700	2.01225700
C	-0.74125800	-7.13317300	-0.87868100
F	-1.35584900	-5.32796900	-2.24398000
C	-0.20117800	-7.61009200	0.31453200
F	0.75046200	-7.17084200	2.43545200
F	-1.16178100	-7.99490300	-1.80988000
F	-0.10696100	-8.92448300	0.52715000
C	4.07184100	0.21468900	-1.78222400
C	5.23917000	0.26057400	-2.10936200
C	6.64366100	0.30152600	-2.48537400

H	6.71043300	0.50511000	-3.56302400
C	7.56758000	1.28886400	-1.70167500
H	7.25037200	2.33545900	-1.71165700
C	7.50386800	-0.94824200	-2.12189500
H	7.12311700	-1.90775500	-2.47685600
C	8.87161100	-0.52059000	-2.70168200
H	9.69908400	-1.06129000	-2.23127600
H	8.91673700	-0.72477400	-3.77657300
C	8.91487400	1.02052400	-2.41502700
H	9.76844400	1.31136500	-1.79384200
H	8.97847800	1.59422800	-3.34556100
C	7.65575600	0.66648600	-0.28632300
H	8.59214900	0.96385100	0.19381400
C	7.60024600	-0.86315500	-0.58224300
H	8.46787200	-1.42256800	-0.21721300
C	6.46359900	0.95042200	0.67314700
H	5.71637500	1.60730300	0.21257000
H	6.79738300	1.42547700	1.60275100
C	6.36194700	-1.37584900	0.15291400
O	5.88555700	-2.49935800	0.06315100
N	5.89624600	-0.36347000	0.94210300
H	4.98733600	-0.45891800	1.37648300
C	-4.16406100	2.43981400	-0.15115700
H	-5.23624000	2.54602400	-0.07883800
C	-5.56042700	-0.12614300	-0.27215300
C	-6.31358000	-0.56479700	-1.36656000
C	-6.25895400	0.22980700	0.88562400
C	-7.70411900	-0.64290000	-1.31666100
C	-7.64849800	0.16802300	0.95586600
C	-8.37208200	-0.27254800	-0.15089000
F	-5.58870600	0.65106900	1.96745000
F	-5.69878900	-0.93066500	-2.49548100
F	-8.28996200	0.51853000	2.07655000
F	-8.40017900	-1.06570900	-2.37683300
F	-9.70426200	-0.34034700	-0.09343200

**<sup>5</sup>TS2-s**

N	-0.53168900	1.99560700	-0.56229400
N	-3.00123800	0.61691900	-0.41993600
N	-1.60047000	-1.81118300	-0.63037700
N	0.82876600	-0.41476700	-0.90415400
C	0.63000100	2.53284800	-1.04567100
C	0.61070400	3.95706000	-0.86439800
C	-0.55871200	4.26166000	-0.22792300

C	-1.29172400	3.02843600	-0.08351800
C	-2.63844200	2.93794000	0.30527400
C	-3.44576900	1.82263400	0.06142900
C	-4.88704100	1.78103600	0.17109900
C	-5.28846900	0.56592900	-0.28851200
C	-4.09233700	-0.18532500	-0.60251100
C	-4.04367400	-1.56303000	-0.85424800
C	-2.86719800	-2.31837800	-0.78039700
C	-2.80818500	-3.75558500	-0.68048300
C	-1.51375700	-4.09019600	-0.40866100
C	-0.74943800	-2.87068100	-0.40537700
C	0.64321600	-2.79407300	-0.32846100
C	1.37983200	-1.64133400	-0.63782000
C	2.80538000	-1.57853500	-0.85972300
C	3.08433300	-0.32724000	-1.32308800
C	1.84244600	0.40446300	-1.31600400
C	1.73363400	1.79383900	-1.51083300
H	1.40936100	4.62174700	-1.16122000
H	-0.91800000	5.23626600	0.07009500
H	-5.51134200	2.59001900	0.51978800
H	-6.29878100	0.19311300	-0.36864400
H	-3.65751800	-4.41746600	-0.77143500
H	-1.10072400	-5.07864500	-0.26495300
H	3.50592600	-2.37836600	-0.67532100
H	4.04965600	0.10258100	-1.55104000
Mn	-1.09033500	0.08222100	-0.63970300
Cl	-1.34056300	0.25633700	-2.95120700
O	-0.98703200	-0.11163400	1.11706500
C	-5.31770800	-2.30385700	-1.07248400
C	-6.25150200	-2.49945700	-0.05034200
C	-5.60438000	-2.86792100	-2.32050400
C	-7.43345800	-3.20626300	-0.25842900
C	-6.77684900	-3.58539200	-2.54985100
C	-7.69427200	-3.75209000	-1.51406600
C	-3.22898400	4.13736900	0.95887600
C	-2.78445000	4.52334000	2.22900300
C	-4.20028200	4.93796500	0.35099600
C	-3.28952000	5.64710200	2.87724800
C	-4.72549000	6.06357100	0.98241000
C	-4.26578300	6.41903000	2.24916100
C	1.39213200	-4.01051500	0.08576700
C	1.31097800	-4.45198700	1.40947600
C	2.26224300	-4.69846600	-0.76575100
C	2.08614600	-5.50473400	1.88231900

C	3.05593900	-5.74816400	-0.31034400
C	2.96959600	-6.14567300	1.02112100
F	-6.02127400	-1.99861600	1.17158900
F	-8.31067200	-3.37371100	0.73761100
F	-8.82184300	-4.43542800	-1.72345900
F	-7.02781600	-4.11191100	-3.75274100
F	-4.73911200	-2.72896100	-3.32956900
F	-4.65262200	4.63069200	-0.87176500
F	-5.65622500	6.80927800	0.37787300
F	-4.75954400	7.49789000	2.86056700
F	-2.84872300	5.98850900	4.09238700
F	-1.84269400	3.80219100	2.85644000
F	2.37906400	-4.32823100	-2.04706400
F	0.52481300	-3.80806100	2.28477400
F	2.06311200	-5.83394700	3.18110800
F	3.78344000	-7.09935400	1.48790600
F	3.92718700	-6.34915000	-1.12795000
C	2.83212200	2.47209200	-2.10239600
C	3.79113100	2.98322800	-2.64327500
C	4.96307700	3.51921300	-3.32023100
H	4.79406600	3.43962100	-4.40319200
C	5.44156100	4.96326300	-2.96831800
H	4.69213200	5.74959900	-3.09235400
C	6.33161500	2.86764700	-2.94542000
H	6.37754700	1.77991800	-3.02620500
C	7.27811100	3.64214500	-3.89104900
H	8.31076800	3.63411100	-3.52762800
H	7.27936300	3.19171300	-4.88906200
C	6.65736100	5.08167800	-3.91848400
H	7.36015900	5.85188000	-3.58443600
H	6.33236400	5.35260700	-4.92843700
C	5.98823200	4.83284500	-1.52530900
H	6.75120700	5.59459800	-1.34365700
C	6.57368000	3.38644500	-1.50927500
H	7.63574100	3.32999000	-1.24870500
C	4.93050900	4.86116400	-0.38733000
H	3.92292700	5.05257700	-0.77653100
H	5.15358500	5.63243700	0.35866300
C	5.77225400	2.65439500	-0.43834600
O	5.84565700	1.43649100	-0.20961500
N	4.99034200	3.53623000	0.21191300
H	4.22021900	3.18207200	0.79733700
C	5.49841800	-2.91777200	2.05758900
C	5.32484500	-1.59310700	1.67009000

C	4.17070800	-0.88591400	2.05114100
C	3.15662300	-1.51522700	2.81474600
C	3.36469600	-2.85046100	3.22582900
C	4.50718200	-3.53524200	2.85799400
H	6.06881900	-1.08965100	1.05771600
C	1.95788300	-0.78248800	3.07431400
H	2.59497500	-3.34561100	3.81007300
H	4.63630400	-4.56935100	3.16704300
C	1.77938800	0.50929600	2.64887200
C	2.86321300	1.17219900	1.90724300
H	1.15346700	-1.29321000	3.59598100
C	6.70506100	-3.70910900	1.60264700
H	7.44656000	-3.02873200	1.16803800
H	7.18239000	-4.17972300	2.47281400
O	2.78564700	2.34759800	1.50200200
C	0.50711000	1.25517000	2.77560700
H	0.65791200	2.31992800	2.58203300
H	-0.12846500	0.87757000	1.87447100
C	-0.36455100	0.99114800	3.99751700
H	-1.26719100	1.60579300	3.94166100
H	-0.68025100	-0.05582100	4.05048700
H	0.16791500	1.23991600	4.92441600
C	6.34784200	-4.80141300	0.57726700
H	7.25000400	-5.31752400	0.23063000
H	5.68168700	-5.55381100	1.00967000
H	5.84654600	-4.37223500	-0.29773300
N	3.99135300	0.42253000	1.66664900
H	4.69780300	0.84201700	1.03790400

**<sup>5</sup>TS3-S**

N	-0.55998700	2.06683000	-0.84111900
N	-2.94959300	0.58694200	-0.45270500
N	-1.48850900	-1.80015800	-0.70593800
N	0.87786600	-0.33179700	-1.18650000
C	0.58282200	2.62683700	-1.33348200
C	0.54110900	4.05187800	-1.13330000
C	-0.61011300	4.32477300	-0.45528700
C	-1.31583400	3.07436900	-0.30223200
C	-2.62447900	2.94270800	0.17562100
C	-3.40513100	1.79172300	0.01338800
C	-4.83478500	1.71356000	0.19921600
C	-5.22357300	0.47133300	-0.20156400
C	-4.02687800	-0.25270000	-0.56145300
C	-3.94949300	-1.62981600	-0.80224700



C	-2.74633000	-2.34676300	-0.80966100
C	-2.63612600	-3.78199400	-0.76397000
C	-1.31639900	-4.08116300	-0.58921200
C	-0.59460700	-2.83551300	-0.58756400
C	0.80316600	-2.71739400	-0.59404200
C	1.47996500	-1.54224700	-0.94217100
C	2.89373100	-1.42818700	-1.21882800
C	3.11222100	-0.16875200	-1.68396100
C	1.84905000	0.52507100	-1.62191500
C	1.70197900	1.91412400	-1.80092700
H	1.31695200	4.73554100	-1.44689100
H	-0.97592900	5.28700900	-0.12595100
H	-5.46288000	2.51785200	0.55339300
H	-6.22529700	0.06790400	-0.21824300
H	-3.46750700	-4.46955500	-0.82527000
H	-0.86233400	-5.05885000	-0.51212300
H	3.62584200	-2.20584300	-1.07131700
H	4.05282600	0.28882600	-1.94875000
Mn	-1.03466700	0.13566500	-0.80765600
Cl	-1.47335500	0.15545300	-3.11159300
O	-0.70530800	0.19340500	1.00309300
C	-5.21271300	-2.40762900	-0.93978700
C	-6.07076600	-2.62636600	0.14193700
C	-5.56852800	-2.97727500	-2.16714500
C	-7.24569100	-3.36279900	0.01331700
C	-6.73518900	-3.72473500	-2.31786800
C	-7.57630600	-3.91499400	-1.22300800
C	-3.21857900	4.12117200	0.86492200
C	-2.78343100	4.46347100	2.14948600
C	-4.19486900	4.93094400	0.27983400
C	-3.29441100	5.56529800	2.83031400
C	-4.72596000	6.03542600	0.94330400
C	-4.27016300	6.35343000	2.22157800
C	1.59996000	-3.91404600	-0.21360500
C	1.50618200	-4.41729500	1.08876600
C	2.50326500	-4.54617200	-1.07529800
C	2.29761500	-5.47089800	1.53173500
C	3.32994900	-5.58022400	-0.64311700
C	3.23259100	-6.03437700	0.66981600
F	-5.77133000	-2.11788000	1.34670600
F	-8.04948400	-3.55198300	1.06596000
F	-8.69758900	-4.62688300	-1.35729200
F	-7.05340100	-4.25719400	-3.50191100
F	-4.77746700	-2.81554700	-3.23161600

F	-4.64820900	4.64845200	-0.94806700
F	-5.66093600	6.79381800	0.36159900
F	-4.77009100	7.41106300	2.86458200
F	-2.86244700	5.86865000	4.05892200
F	-1.85087000	3.71689900	2.76179900
F	2.61468700	-4.14286900	-2.34785200
F	0.66825400	-3.84963800	1.96904300
F	2.21871900	-5.89361300	2.79983900
F	4.06459600	-6.98267100	1.11338400
F	4.22046200	-6.13278700	-1.47415700
C	2.81170500	2.63387000	-2.32056800
C	3.81181800	3.18916400	-2.72498400
C	5.06629700	3.77705700	-3.16831900
H	5.06620600	3.82156400	-4.26613000
C	5.48572800	5.16352900	-2.58377100
H	4.76580000	5.97293600	-2.73229500
C	6.35846400	3.06196000	-2.65954300
H	6.41609000	1.98944800	-2.85578000
C	7.44262800	3.91908900	-3.35302400
H	8.40549000	3.85201300	-2.83639800
H	7.60016200	3.58226600	-4.38294000
C	6.83497200	5.36409100	-3.31504700
H	7.47792900	6.07974700	-2.79238600
H	6.67159500	5.75054700	-4.32653300
C	5.80275500	4.86320000	-1.09748800
H	6.53274900	5.58432900	-0.71985700
C	6.37478900	3.41287400	-1.15379100
H	7.38553700	3.31074400	-0.74477600
C	4.58799300	4.78939000	-0.13050100
H	3.64856800	5.03307100	-0.64151500
H	4.69747100	5.47869900	0.71458400
C	5.42622500	2.58521700	-0.28971500
O	5.46726800	1.35096400	-0.17505900
N	4.56363700	3.41075800	0.33279000
H	3.73921200	3.01579200	0.80730400
C	5.10442200	-3.07243900	2.03107400
C	4.85919700	-1.77753800	1.57557700
C	3.76659100	-1.04667600	2.06432900
C	2.88032800	-1.61243200	3.02073200
C	3.17240800	-2.91089900	3.50181800
C	4.25881700	-3.61860400	3.02244000
H	5.50169200	-1.32075200	0.82661200
C	1.73143300	-0.87090600	3.40180900
H	2.50009900	-3.36497000	4.22434200

H	4.44071400	-4.62954100	3.37693800
C	1.44511200	0.39047600	2.86508800
C	2.42873400	1.00109000	1.93474300
H	1.04063100	-1.32505800	4.10687000
C	6.25882300	-3.88911000	1.49425400
H	5.92696200	-4.92452700	1.33501500
H	6.56159900	-3.50203100	0.51355700
O	2.30053900	2.14642700	1.46896400
C	0.26948700	1.11743800	3.07664100
H	0.20912200	2.08456800	2.59273600
H	-0.98145200	-0.65286100	1.39791100
C	-0.85953200	0.73099800	3.97250000
H	-0.96605200	-0.35365100	4.08744200
H	-0.72452000	1.15266700	4.98103700
H	-1.79732500	1.13393800	3.57833200
C	7.47152100	-3.88739000	2.44241200
H	7.19862500	-4.29060100	3.42420400
H	8.28742700	-4.49676300	2.03740400
H	7.84402400	-2.86796400	2.59234700
N	3.51579500	0.23326200	1.60511300
H	4.18141100	0.64225200	0.93013900

**MECP-1**

N	-0.37258500	1.99876100	-0.56975700
N	-2.84707500	0.58760300	-0.34627500
N	-1.44712400	-1.90851600	-0.56612300
N	1.00583000	-0.48278200	-0.82504500
C	0.81752100	2.51114800	-0.96889400
C	0.79411300	3.95350600	-0.92631500
C	-0.43396200	4.30515600	-0.46188800
C	-1.17257400	3.07334900	-0.27301600
C	-2.53276300	2.99864500	0.03935900
C	-3.32094800	1.83395000	-0.05573700
C	-4.76101900	1.79961100	0.05887400
C	-5.14435500	0.52236600	-0.20665800
C	-3.93645300	-0.23908300	-0.42768200
C	-3.88893300	-1.63002300	-0.60826100
C	-2.71880600	-2.40358100	-0.64434500
C	-2.68431100	-3.84992300	-0.66825900
C	-1.37616200	-4.21038500	-0.57472800
C	-0.61351000	-2.98278000	-0.52366800
C	0.79208300	-2.91189500	-0.50685000
C	1.53976400	-1.74289800	-0.68420700
C	2.97551000	-1.68435300	-0.84704000

C	3.28587400	-0.39734600	-1.15873900
C	2.04588100	0.34053500	-1.12699800
C	1.95277500	1.74159100	-1.31215500
H	1.62419900	4.59110300	-1.19400100
H	-0.82275300	5.29924600	-0.29536300
H	-5.39591800	2.64139300	0.29126500
H	-6.14969000	0.12928400	-0.23349800
H	-3.54698500	-4.49745400	-0.72650300
H	-0.96060000	-5.20778000	-0.56557400
H	3.65586200	-2.51209300	-0.71860900
H	4.26246100	0.04128500	-1.30429200
Mn	-0.89826300	0.03848400	-0.44306900
Cl	-1.23021400	0.11577400	-2.83488300
O	-0.79290700	-0.03026300	1.13772100
C	-5.18473200	-2.36210400	-0.71188700
C	-6.04264800	-2.49800900	0.38340800
C	-5.57310400	-2.96113400	-1.91465300
C	-7.24746000	-3.19039600	0.29033200
C	-6.77227700	-3.66146500	-2.02944100
C	-7.61117400	-3.77429500	-0.92203800
C	-3.20028900	4.26989000	0.44004400
C	-2.88128400	4.88291300	1.65640800
C	-4.13468200	4.91190500	-0.37825600
C	-3.47417200	6.07853000	2.05442000
C	-4.74166000	6.10742200	-0.00018200
C	-4.40814500	6.69157000	1.22076900
C	1.53686900	-4.18775000	-0.32403800
C	1.49637100	-4.85318300	0.90466400
C	2.32150000	-4.74717900	-1.33676500
C	2.25449600	-5.99442300	1.14007000
C	3.06689700	-5.90565800	-1.12985300
C	3.03745000	-6.52364800	0.11808200
F	-5.71376100	-1.95242400	1.56197400
F	-8.05032600	-3.30408900	1.35347500
F	-8.76207700	-4.44207200	-1.02175600
F	-7.12263600	-4.22299000	-3.19029000
F	-4.78346400	-2.87306200	-2.98894700
F	-4.46630100	4.37832100	-1.55987100
F	-5.63197900	6.70022500	-0.80153400
F	-4.98213800	7.83757000	1.59094100
F	-3.15463400	6.63945400	3.22451500
F	-1.98179800	4.32054700	2.47477500
F	2.38172800	-4.16058600	-2.53767300
F	0.73417700	-4.37950400	1.89688700

F	2.28598600	-6.55266400	2.35732100
F	3.80064900	-7.59260100	0.35382000
F	3.82267100	-6.41299700	-2.10878700
C	3.08643700	2.39683400	-1.84338300
C	4.09007200	2.88260800	-2.32922000
C	5.32793200	3.35615800	-2.92776100
H	5.24298100	3.21922700	-4.01504000
C	5.82560900	4.80264800	-2.61346400
H	5.11758800	5.60350800	-2.84251800
C	6.63580700	2.68339500	-2.40060700
H	6.64897900	1.59205400	-2.42154200
C	7.68747600	3.37613600	-3.29696000
H	8.68121700	3.36200900	-2.83806800
H	7.76645900	2.86781100	-4.26353100
C	7.11866100	4.82761600	-3.46296400
H	7.81551000	5.59768100	-3.11696300
H	6.88749500	5.04384200	-4.51128600
C	6.24709100	4.73632700	-1.12425900
H	7.02673300	5.47625900	-0.92474400
C	6.76142400	3.27031400	-0.97693100
H	7.78827900	3.18415700	-0.60690300
C	5.10250800	4.87744000	-0.08367000
H	4.14453800	5.11346900	-0.56464500
H	5.31027800	5.66735600	0.64717200
C	5.81724900	2.62859500	0.03788100
O	5.78989700	1.41905900	0.31054600
N	5.02659400	3.57988900	0.56905100
H	4.18161400	3.30003100	1.09451300
C	4.66446500	-2.85314700	2.56760500
C	4.67557600	-1.53195900	2.13391200
C	3.56503400	-0.69885500	2.35851000
C	2.41808300	-1.18342600	3.02615700
C	2.41367000	-2.53226400	3.43639900
C	3.50664000	-3.35124900	3.21036400
H	5.54482300	-1.11945000	1.62761100
C	1.33424500	-0.27139800	3.26125800
H	1.53107100	-2.92394600	3.93331000
H	3.47381100	-4.38828500	3.53388300
C	1.37566200	1.03150400	2.86337800
C	2.54884700	1.51061600	2.13180700
H	0.45628700	-0.65198300	3.77425700
C	5.88361900	-3.73448800	2.38354400
H	6.68855600	-3.14548800	1.92815500
H	6.25130600	-4.04458600	3.37181300

O	2.63728400	2.67744100	1.69122400
C	0.29263100	2.05329300	3.09865600
H	0.75363200	2.92934600	3.57541000
H	-0.04724300	2.41072700	2.12151200
C	-0.90819600	1.57353000	3.91252400
H	-1.62323300	2.39295800	4.03436500
H	-1.41942900	0.75297500	3.40013300
H	-0.61203800	1.23171900	4.91217600
C	5.63110000	-4.99021800	1.53502800
H	6.55487500	-5.56469600	1.40511700
H	4.89512600	-5.65131600	2.00336800
H	5.25784000	-4.72023600	0.54049700
N	3.57215600	0.61215700	1.93545800
H	4.38302100	0.93825600	1.38745600

**MECP-2**

N	-0.32337000	1.92911800	-0.54749300
N	-2.87580600	0.71873200	-0.31852200
N	-1.69362200	-1.80256400	-0.74048700
N	0.84137100	-0.57457600	-0.91642700
C	0.86997800	2.37839500	-1.04746600
C	0.95849900	3.80181200	-0.86959300
C	-0.17618200	4.19393800	-0.22417800
C	-1.00012800	3.01944400	-0.06377400
C	-2.33799600	3.02917600	0.35332500
C	-3.21905100	1.95552000	0.16755300
C	-4.65423200	2.01851700	0.30959500
C	-5.15665900	0.84311300	-0.15632200
C	-4.03342500	0.00800900	-0.51078700
C	-4.10852600	-1.34995800	-0.84576800
C	-2.99366700	-2.19958700	-0.87438400
C	-3.05150000	-3.64251900	-0.81783600
C	-1.78653000	-4.08301400	-0.56680600
C	-0.93201600	-2.92109000	-0.53379800
C	0.46120600	-2.94868100	-0.40648200
C	1.29106400	-1.85053200	-0.66209500
C	2.71984500	-1.88701800	-0.85151300
C	3.10052400	-0.65579800	-1.30009800
C	1.92093700	0.16812000	-1.31093000
C	1.91516000	1.56225200	-1.51272800
H	1.80570600	4.40235400	-1.16755000
H	-0.45307100	5.19256200	0.08102500
H	-5.20866600	2.86628500	0.68296100
H	-6.19462600	0.55333600	-0.22190600

H	-3.95324800	-4.23079900	-0.90845700
H	-1.44769900	-5.10258600	-0.44761800
H	3.35416300	-2.73829600	-0.65912600
H	4.09932900	-0.29790600	-1.50803300
Mn	-1.02392500	0.06065100	-0.62499900
Cl	-1.31964600	0.28964200	-2.91701800
O	-0.84495800	-0.19830200	1.14759700
C	-5.44541500	-1.97350800	-1.05138800
C	-6.37269200	-2.11377600	-0.01361800
C	-5.80346100	-2.48638600	-2.30354400
C	-7.61465100	-2.71215000	-0.21091200
C	-7.03610600	-3.09870700	-2.52181500
C	-7.94500600	-3.20817600	-1.47075200
C	-2.85325600	4.30414700	0.92577800
C	-2.35679400	4.78349200	2.14342200
C	-3.79653100	5.10130700	0.26819400
C	-2.78604700	5.98597900	2.69799800
C	-4.24795400	6.30480000	0.80634500
C	-3.73885800	6.74874000	2.02535600
C	1.09902600	-4.21095300	0.05337100
C	0.93677200	-4.60253600	1.38571900
C	1.94852400	-4.98222100	-0.74391900
C	1.62153000	-5.68692400	1.92109600
C	2.64292300	-6.07347900	-0.22862100
C	2.48207000	-6.41928800	1.11041100
F	-6.07797300	-1.66396300	1.21446100
F	-8.48330500	-2.82542400	0.80016000
F	-9.13002300	-3.78972300	-1.66944400
F	-7.35306800	-3.57872300	-3.72855000
F	-4.94977400	-2.39969700	-3.32854500
F	-4.29068600	4.71830400	-0.91609300
F	-5.15355700	7.04175700	0.15508700
F	-4.16031300	7.90291400	2.54595300
F	-2.29215000	6.41056600	3.86560100
F	-1.42579500	4.08349900	2.80898800
F	2.14786600	-4.65213500	-2.02653300
F	0.16103800	-3.88080500	2.20565200
F	1.53297300	-5.96633100	3.22808900
F	3.21082900	-7.41054400	1.63456900
F	3.50214700	-6.75715000	-0.99216400
C	3.05510500	2.15692900	-2.11703200
C	4.03831800	2.60212000	-2.67273600
C	5.24303600	3.03758200	-3.36550000
H	5.08447400	2.89223200	-4.44326400

C	5.79480000	4.47602300	-3.10660900
H	5.09117400	5.29109400	-3.29645600
C	6.56832300	2.34257600	-2.92096700
H	6.55629500	1.25090300	-2.92767800
C	7.57176400	2.99907900	-3.89713400
H	8.59550000	2.96622100	-3.51033400
H	7.56943600	2.47810600	-4.86002600
C	7.02694100	4.46198500	-4.04240600
H	7.76381600	5.21848200	-3.75351500
H	6.73040900	4.67295500	-5.07508100
C	6.31988700	4.42031400	-1.65071100
H	7.13021900	5.14212600	-1.51761300
C	6.80839300	2.94420200	-1.51826100
H	7.85715800	2.83876900	-1.22173500
C	5.25775900	4.60591100	-0.53345900
H	4.27144800	4.84297100	-0.95209900
H	5.52850000	5.41028400	0.15999100
C	5.93353200	2.34476400	-0.42090900
O	5.90536400	1.14267300	-0.11513100
N	5.21498800	3.32610900	0.15598500
H	4.43207600	3.08440300	0.78025100
C	5.02773200	-3.07571700	2.12145000
C	4.98631000	-1.73619500	1.73443200
C	3.90747200	-0.92151900	2.10192800
C	2.82274400	-1.43848500	2.85786400
C	2.88117700	-2.80127600	3.23936700
C	3.95737200	-3.59533900	2.88495200
H	5.79074400	-1.30429100	1.14370300
C	1.75366100	-0.56557300	3.19489500
H	2.05675600	-3.22227700	3.80734300
H	3.97810600	-4.63618800	3.19783200
C	1.75913300	0.80312000	2.84675500
C	2.89640600	1.31163700	2.03254100
H	0.91644700	-0.97216900	3.75394600
C	6.19258300	-3.95934400	1.72886500
H	6.97541600	-3.34348400	1.27084900
H	6.63352900	-4.39951000	2.63427000
O	2.96522100	2.48796800	1.63611500
C	0.76461600	1.72116000	3.18485600
H	0.88822600	2.73274700	2.81307800
H	0.08297200	-0.04656600	1.40460300
C	-0.51180700	1.36770200	3.86436700
H	-0.97929200	2.24533900	4.31598600
H	-1.21421000	0.95945300	3.11555700



H	-0.38622900	0.59789400	4.63511200
C	5.80582000	-5.09393500	0.76336200
H	6.69240400	-5.65247000	0.44301400
H	5.12315100	-5.80654200	1.23537400
H	5.31451500	-4.69975500	-0.13365500
N	3.87550900	0.40838000	1.71748100
H	4.63003800	0.73707400	1.09238200

**PhI**

C	0.58219200	-0.00001800	0.00000200
C	1.26536100	1.21608700	0.00000000
C	2.66286600	1.20738800	0.00000200
C	3.36346000	0.00000600	-0.00000200
C	2.66290000	-1.20737200	-0.00000100
C	1.26537100	-1.21608800	0.00000300
H	0.72349600	2.15553800	0.00000500
H	3.19999000	2.15209500	-0.00000200
H	4.44969700	0.00003200	-0.00000100
H	3.20000600	-2.15208900	-0.00000600
H	0.72355100	-2.15556600	0.00000600
I	-1.56810600	0.00000000	0.00000000

**PhIO**

O	-1.76020300	1.60692500	0.00039000
I	-1.41347100	-0.27171000	-0.00007800
C	0.76484300	-0.15350900	0.00009200
C	1.24666100	1.14447500	-0.00005100
C	1.57971100	-1.27762100	0.00018300
C	2.63248600	1.32538600	-0.00013000
H	0.54066000	1.97488000	-0.00013100
C	2.96427600	-1.07631900	0.00012800
H	1.16737100	-2.28303700	0.00053900
C	3.48734000	0.21946900	-0.00009100
H	3.04274200	2.33161500	-0.00012100
H	3.62922700	-1.93574700	0.00022100
H	4.56368600	0.36623000	-0.00031100

**Pro-S**

O	4.13714500	-0.10802100	1.24830000
C	-3.05226500	0.06632100	-0.34245000
C	-2.01906900	-0.86622000	-0.36400000
C	-0.68762000	-0.45942300	-0.18863400
C	-0.37160600	0.90513100	0.01195400
C	-1.42825900	1.83627300	0.03050300

C	-2.73980100	1.42810300	-0.14255300
H	-2.24044700	-1.92047400	-0.51790400
C	1.01147700	1.26240100	0.17941100
H	-1.19543900	2.88765000	0.18001500
H	-3.54292400	2.16033500	-0.12771500
C	2.01546800	0.34713000	0.14853200
C	1.70010300	-1.07316900	-0.04507200
H	1.25023400	2.31406300	0.33158900
C	-4.49362700	-0.37257000	-0.47626700
H	-5.04562900	0.36173400	-1.07677200
H	-4.54384300	-1.32409900	-1.01960200
O	2.53993300	-1.98313100	-0.06932400
C	3.48725600	0.70587700	0.28248300
H	3.55500200	1.73051500	0.66829300
H	3.98175200	-1.02667700	0.95468600
C	4.19929500	0.63728100	-1.07823100
H	4.12471700	-0.37527300	-1.48771000
H	3.75848300	1.33918200	-1.79611100
H	5.25770400	0.88263100	-0.94373700
C	-5.18055200	-0.52784900	0.89330300
H	-5.16415600	0.41745200	1.44726900
H	-6.22509800	-0.83702000	0.77450100
H	-4.66651500	-1.27938500	1.50286900
N	0.35419500	-1.36889800	-0.20578700
H	0.15537900	-2.35485100	-0.33484300

**Sub**

C	-2.72354000	-0.12933100	-0.33217200
C	-1.77519400	0.88840500	-0.27318800
C	-0.40862600	0.58698000	-0.16537500
C	0.02908100	-0.75743400	-0.11514800
C	-0.94216700	-1.77465200	-0.17674200
C	-2.28958200	-1.47053400	-0.28286600
H	-2.09097300	1.92920600	-0.31162000
C	1.44264800	-1.01223200	-0.00759000
H	-0.61527900	-2.81123400	-0.14348400
H	-3.02499300	-2.26955200	-0.33155000
C	2.36644100	-0.01654700	0.04851000
C	1.92779600	1.38997200	-0.00225700
H	1.75910000	-2.05176500	0.02893100
C	-4.20047000	0.19281100	-0.39279300
H	-4.34733700	1.18233000	-0.84301500
H	-4.70653100	-0.52825900	-1.04748200
O	2.68716600	2.35566300	0.04229900

C	3.85689600	-0.21209600	0.16214000
H	4.33111500	0.31211700	-0.67880500
H	4.20233400	0.33586200	1.04942400
C	4.33286700	-1.66399300	0.21754900
H	3.91461100	-2.19286400	1.08241400
H	4.04707600	-2.21701700	-0.68528700
H	5.42395300	-1.70311400	0.29980500
C	-4.85748300	0.16189800	0.99959800
H	-4.39011800	0.89585200	1.66565500
H	-5.92762200	0.38913100	0.93400600
H	-4.74455900	-0.82532600	1.46164000
N	0.55045200	1.57966600	-0.10788900
H	0.26671800	2.55219200	-0.14179900

**<sup>3</sup>INT4-R**

N	-0.58686700	1.98851900	-0.54539700
N	-2.98812200	0.49383100	-0.32163100
N	-1.52700400	-1.88290200	-0.62918200
N	0.86469800	-0.38481400	-0.81459300
C	0.57120900	2.55634200	-1.00218300
C	0.50772100	3.98207800	-0.82551100
C	-0.68122300	4.25637800	-0.21589500
C	-1.38688700	3.00479900	-0.08374800
C	-2.72281100	2.86446500	0.30301300
C	-3.47397600	1.69995400	0.10822800
C	-4.91423800	1.63230000	0.17089000
C	-5.27618200	0.39552700	-0.26936000
C	-4.05908000	-0.33446200	-0.53601800
C	-3.97530800	-1.70311300	-0.81885200
C	-2.77419000	-2.42301500	-0.78287100
C	-2.67442000	-3.86273900	-0.71490800
C	-1.37109800	-4.16187600	-0.45604500
C	-0.64859200	-2.91285600	-0.42421400
C	0.74190900	-2.79355600	-0.32676600
C	1.44478500	-1.61151800	-0.58790200
C	2.86553500	-1.50627300	-0.81278600
C	3.11318500	-0.23795300	-1.24867500
C	1.85831400	0.46532900	-1.22390000
C	1.71036600	1.85007500	-1.42766600
H	1.29804000	4.66596900	-1.10028900
H	-1.06235900	5.22001100	0.08945300
H	-5.56006500	2.44575000	0.46956800
H	-6.27567700	0.00132300	-0.37838900
H	-3.50555000	-4.54655700	-0.81081700

H	-0.92432700	-5.13821000	-0.33239400
H	3.58449200	-2.29460900	-0.65194500
H	4.06685100	0.21753100	-1.47545700
Mn	-1.06509500	0.04842600	-0.56380100
Cl	-1.33541000	0.16425800	-2.86821100
O	-0.90549500	-0.07778900	1.21352600
C	-5.22919800	-2.47158800	-1.05245500
C	-6.17245800	-2.68556400	-0.04227700
C	-5.48863900	-3.04278400	-2.30353300
C	-7.33635900	-3.41743600	-0.26489400
C	-6.64241700	-3.78521400	-2.54694700
C	-7.56949400	-3.97018600	-1.52292600
C	-3.42030800	4.04998000	0.87637200
C	-3.68492600	4.11569900	2.24718300
C	-3.83955800	5.12366700	0.08680300
C	-4.33796700	5.20521500	2.81865300
C	-4.49254800	6.22573500	0.63524800
C	-4.74400900	6.26254100	2.00591300
C	1.52440700	-4.00263100	0.04656800
C	1.46950200	-4.48091200	1.35823400
C	2.39124700	-4.65143100	-0.83753400
C	2.26689600	-5.53511000	1.78911000
C	3.20338200	-5.70454100	-0.42556200
C	3.14416200	-6.13949800	0.89566500
F	-5.96926400	-2.17956800	1.18210100
F	-8.22247200	-3.60240900	0.72001500
F	-8.67963400	-4.67726200	-1.74594200
F	-6.86693900	-4.31739900	-3.75259900
F	-4.61458000	-2.88565800	-3.30256300
F	-3.60853100	5.11180200	-1.23171600
F	-4.88276300	7.24198100	-0.14130100
F	-5.37018000	7.31297800	2.54106500
F	-4.57499500	5.24532000	4.13381400
F	-3.29764000	3.11419700	3.05065800
F	2.48592600	-4.23841700	-2.10780300
F	0.68427000	-3.87516000	2.26001900
F	2.26916800	-5.90146100	3.07788800
F	3.98015500	-7.09263600	1.32235100
F	4.07078700	-6.26895300	-1.27285900
C	2.79766300	2.56129400	-2.00243100
C	3.74548300	3.10889300	-2.52653900
C	4.90996200	3.68673600	-3.18147400
H	4.75642000	3.62175600	-4.26764600
C	5.34704200	5.13636800	-2.79916600

H	4.57971200	5.90570700	-2.92039300
C	6.28885000	3.06330300	-2.79846200
H	6.36314300	1.97859200	-2.89706000
C	7.22914000	3.87733200	-3.71681600
H	8.25602100	3.89008600	-3.33750400
H	7.25734400	3.44340400	-4.72169900
C	6.57164000	5.30067900	-3.73113000
H	7.24974500	6.08366900	-3.37645700
H	6.25270300	5.57832500	-4.74118900
C	5.87925200	4.99607500	-1.35166400
H	6.62352000	5.77115500	-1.15003000
C	6.49636200	3.56278800	-1.35072700
H	7.55529400	3.52625500	-1.07408100
C	4.80988900	4.98508900	-0.22425500
H	3.80185400	5.15610300	-0.62222400
H	5.00609800	5.75263600	0.53301200
C	5.69856500	2.79704000	-0.30055700
O	5.79135500	1.57745100	-0.09101000
N	4.89790100	3.65497500	0.35878900
H	4.15287000	3.28460300	0.96452400
C	5.55630200	-2.82994900	1.94733400
C	5.32896600	-1.49148100	1.62791100
C	4.18571900	-0.83192400	2.09844900
C	3.22406400	-1.50895400	2.89433500
C	3.48103400	-2.86355500	3.22239900
C	4.61639400	-3.50389500	2.76203000
H	6.03076400	-0.94221200	1.00505700
C	2.06572900	-0.80153800	3.29656100
H	2.75557000	-3.40344200	3.82347500
H	4.78195800	-4.54735200	3.01855500
C	1.84168800	0.55474300	2.96544200
C	2.87333300	1.24215700	2.14391900
H	1.31077600	-1.32654700	3.87674000
C	6.77002600	-3.56046700	1.41534700
H	7.45980900	-2.83848000	0.96267900
H	7.31041700	-4.02673400	2.25064100
O	2.78211200	2.43036800	1.78762800
C	0.67951800	1.21678200	3.37312300
H	-0.03782100	0.25395200	1.50943800
C	6.41799000	-4.64717900	0.38310300
H	7.32632000	-5.11129000	-0.01718600
H	5.81111500	-5.44101400	0.82852700
H	5.85542700	-4.22618900	-0.45803100
N	3.96195300	0.49446500	1.77940500

H	4.63583500	0.94775100	1.13982000
C	0.25847800	2.62639100	3.09473000
H	0.79772800	3.33466600	3.74188400
H	0.48335300	2.92860600	2.07045400
H	-0.81318200	2.74164500	3.28006000
H	-0.00522800	0.61980700	3.97298000

**<sup>5</sup>INT4-R**

N	-0.62481200	2.00670800	-0.58456700
N	-3.00000100	0.47530000	-0.33759700
N	-1.50408100	-1.88314000	-0.62931900
N	0.86424200	-0.35031900	-0.82088300
C	0.52923100	2.58713600	-1.03168400
C	0.45234700	4.01181500	-0.84606300
C	-0.73939800	4.27060200	-0.23588700
C	-1.43325700	3.01097200	-0.11292300
C	-2.76581000	2.85223700	0.27862200
C	-3.50127800	1.67693900	0.08754300
C	-4.94008400	1.58921900	0.15335900
C	-5.28582700	0.34490200	-0.27925900
C	-4.05948300	-0.36960800	-0.54390300
C	-3.95595600	-1.73928000	-0.81531100
C	-2.74455800	-2.44140900	-0.77510500
C	-2.62512100	-3.87913400	-0.69698500
C	-1.31711400	-4.15889200	-0.44090900
C	-0.61131400	-2.90000900	-0.42057600
C	0.77789300	-2.76133400	-0.33043000
C	1.46227000	-1.56992100	-0.59826200
C	2.87912700	-1.44712100	-0.83518400
C	3.10723500	-0.17633100	-1.27451400
C	1.84435500	0.51148900	-1.24126300
C	1.67888800	1.89335100	-1.45009700
H	1.23638700	4.70496100	-1.11551500
H	-1.12956700	5.22855100	0.07575100
H	-5.59673600	2.39523300	0.44855300
H	-6.28000200	-0.06368100	-0.38392700
H	-3.44732800	-4.57470800	-0.78478400
H	-0.85694500	-5.12821900	-0.31159100
H	3.60910100	-2.22634300	-0.67963300
H	4.05339000	0.28991000	-1.51006300
Mn	-1.07380500	0.05748900	-0.58241200
Cl	-1.34174700	0.14671000	-2.88895500
O	-0.92231400	-0.02013100	1.20107700
C	-5.19912400	-2.52765200	-1.03999700

C	-6.13699400	-2.74697900	-0.02594800
C	-5.45310300	-3.11241200	-2.28590400
C	-7.29079900	-3.49714700	-0.24005300
C	-6.59668300	-3.87316200	-2.52073900
C	-7.51876200	-4.06317300	-1.49312600
C	-3.47644100	4.02421300	0.86271600
C	-3.75620600	4.06457700	2.23181500
C	-3.89367400	5.10904600	0.08737800
C	-4.42194600	5.14032100	2.81458400
C	-4.55863900	6.19785100	0.64770500
C	-4.82504100	6.20947900	2.01596100
C	1.57987100	-3.96075800	0.03382400
C	1.54433600	-4.44481900	1.34407400
C	2.44196200	-4.59875500	-0.86288500
C	2.35215000	-5.49728800	1.75996500
C	3.26679700	-5.64744900	-0.46512400
C	3.22454700	-6.09014900	0.85413000
F	-5.93830800	-2.22841400	1.19388700
F	-8.17198700	-3.68690400	0.74833800
F	-8.61914200	-4.78779500	-1.70793900
F	-6.81621100	-4.41811500	-3.72157700
F	-4.58351100	-2.95083200	-3.28809700
F	-3.64943800	5.12126600	-1.22888900
F	-4.94655100	7.22507800	-0.11548800
F	-5.46304800	7.24692000	2.56237600
F	-4.67369300	5.15632300	4.12752500
F	-3.37305700	3.05120800	3.02176500
F	2.51810400	-4.18016500	-2.13254400
F	0.76491400	-3.84906200	2.25768600
F	2.36709800	-5.87518200	3.04532000
F	4.07067300	-7.04068100	1.26637900
F	4.12863700	-6.20132300	-1.32494800
C	2.76121500	2.61973700	-2.01506800
C	3.70637400	3.18792200	-2.52154700
C	4.87085000	3.79701200	-3.14695100
H	4.73325500	3.75834700	-4.23648100
C	5.28107100	5.24235200	-2.72034900
H	4.50420800	6.00345300	-2.83257600
C	6.25316300	3.18361500	-2.76026500
H	6.34494900	2.10303900	-2.88590900
C	7.19404300	4.03487100	-3.64364800
H	8.21540900	4.05207900	-3.24991500
H	7.24211800	3.62815200	-4.65910900
C	6.51622100	5.44871000	-3.62981400

H	7.17789700	6.23140500	-3.24475700
H	6.20757200	5.74866200	-4.63668000
C	5.79472700	5.07150400	-1.26934100
H	6.52435700	5.85186000	-1.03688500
C	6.43356500	3.64816600	-1.29725300
H	7.48930100	3.62048300	-1.00766500
C	4.71066200	5.01483300	-0.15718900
H	3.70538200	5.18064300	-0.56401300
H	4.88499200	5.76540500	0.62212700
C	5.63519100	2.84358800	-0.27693100
O	5.74651700	1.62100200	-0.09583700
N	4.81202400	3.67159400	0.39275800
H	4.06808200	3.27492400	0.98310400
C	5.63567900	-2.80747600	1.90995800
C	5.36927200	-1.47442200	1.59717200
C	4.22025700	-0.84361100	2.09225100
C	3.29359900	-1.54443900	2.90864300
C	3.59169400	-2.89145200	3.23183600
C	4.73134200	-3.50421900	2.74518300
H	6.04399100	-0.90789200	0.95997300
C	2.12288400	-0.86915500	3.32969700
H	2.89238000	-3.44912000	3.84748000
H	4.92664000	-4.54436400	2.99446900
C	1.84927100	0.47581200	2.99126000
C	2.84823000	1.19136000	2.15316100
H	1.39425500	-1.41394200	3.92509400
C	6.85081300	-3.51072500	1.34578600
H	7.52084700	-2.77217400	0.89014100
H	7.41379600	-3.98047000	2.16394900
O	2.71620000	2.37500300	1.79389800
C	0.67003900	1.10190100	3.40717500
H	-0.01645600	0.20635300	1.47895400
C	6.49399100	-4.58796700	0.30515700
H	7.40042600	-5.03775200	-0.11531600
H	5.90154500	-5.39305000	0.75002700
H	5.91396500	-4.16194000	-0.52144200
N	3.95446400	0.47605900	1.77686100
H	4.60677800	0.94844000	1.12904300
C	0.19244000	2.48843300	3.10409200
H	0.71801200	3.23162900	3.72229100
H	0.38668700	2.77191600	2.06805500
H	-0.87946800	2.56994400	3.30432800
H	0.01326300	0.48935300	4.02207500



**<sup>3</sup>TS2-R\_sub**

C	2.77615500	0.02792500	-0.35597200
C	1.72727900	-0.88691100	-0.32411500
C	0.40341300	-0.44807200	-0.16431700
C	0.11322200	0.92950600	-0.03623800
C	1.18461600	1.84269000	-0.07070400
C	2.48885500	1.40363200	-0.22662400
H	1.92964100	-1.95155000	-0.42329700
C	-1.26313600	1.31472400	0.11226300
H	0.97018900	2.90460000	0.02268800
H	3.30460400	2.12152700	-0.25378800
C	-2.30254100	0.43288900	0.11876800
C	-2.00646800	-1.01166900	0.06764500
H	-1.47485600	2.37959300	0.20379100
C	4.20919400	-0.44273400	-0.47233500
H	4.24058900	-1.42015600	-0.96929300
H	4.77249700	0.25156500	-1.10900000
O	-2.82049700	-1.92623800	0.18325200
C	-3.71941700	0.92070000	0.36307400
H	-3.87111000	0.96476400	1.45285900
H	-3.78122100	1.95873500	0.01233900
C	-4.87129600	0.10001900	-0.23723200
H	-4.75052500	-0.01970700	-1.32030100
H	-4.91833900	-0.89515700	0.20186300
H	-5.81960400	0.62088100	-0.06028300
C	4.89858200	-0.54462200	0.90091100
H	4.37293400	-1.25634100	1.54733800
H	5.93711000	-0.87823100	0.79486000
H	4.90097200	0.42643800	1.40873100
N	-0.65719400	-1.32852600	-0.12336500
H	-0.47929900	-2.32583700	-0.16171800

**<sup>3</sup>TS2-S\_sub**

C	-2.71911200	-0.15098900	-0.34892500
C	-1.76709200	0.86494500	-0.33476200
C	-0.40632400	0.56661800	-0.16365200
C	0.02123600	-0.77221600	-0.00280700
C	-0.95356300	-1.78792200	-0.01978400
C	-2.29511200	-1.48693500	-0.18892900
H	-2.07530500	1.90135500	-0.45834000
C	1.42866100	-1.02071900	0.16716900
H	-0.63398700	-2.82052200	0.09869400
H	-3.03371000	-2.28436800	-0.20211600
C	2.36064700	-0.03018500	0.17416400

C	1.92976800	1.37282000	0.02202300
H	1.73895700	-2.05630300	0.28881700
C	-4.19154200	0.17135300	-0.47836300
H	-4.31870300	1.12603600	-1.00352700
H	-4.68164000	-0.59356700	-1.09427800
O	2.68270600	2.34472800	0.03439600
C	3.84117600	-0.24983900	0.38336900
H	4.36434000	0.61052300	-0.04585500
H	4.05721700	-0.21093800	1.46141600
C	4.39366000	-1.55082300	-0.21083500
H	3.96699200	-2.44024100	0.26769500
H	4.17980800	-1.61307400	-1.28379400
H	5.47963000	-1.59945900	-0.07607900
C	-4.89084800	0.24424700	0.89168500
H	-4.43961300	1.02289100	1.51685700
H	-5.95706500	0.47024000	0.77670000
H	-4.79816700	-0.70719300	1.42742700
N	0.55717900	1.55568200	-0.14812500
H	0.28002200	2.52489100	-0.25402100

**<sup>3</sup>TS2-R**

N	-0.60919800	1.97718500	-0.48778800
N	-2.99865700	0.47171300	-0.33079400
N	-1.49006600	-1.90044600	-0.63965600
N	0.87332600	-0.36531500	-0.82834300
C	0.53402500	2.56740900	-0.95976400
C	0.44635500	3.98969100	-0.77815600
C	-0.74112800	4.24307000	-0.15643100
C	-1.42718200	2.98163100	-0.02534600
C	-2.76767100	2.82612100	0.34008800
C	-3.50768200	1.65988800	0.11174100
C	-4.94861400	1.56822100	0.16372700
C	-5.28456000	0.32885000	-0.28756200
C	-4.05037800	-0.37722900	-0.55220200
C	-3.94109400	-1.74525100	-0.83290100
C	-2.73173100	-2.45262500	-0.79396900
C	-2.61302300	-3.89155500	-0.73409400
C	-1.30478600	-4.17629400	-0.48004400
C	-0.59769100	-2.91896900	-0.44162300
C	0.79179100	-2.77620100	-0.34815300
C	1.47335800	-1.58168800	-0.60940100
C	2.89265900	-1.45238800	-0.84404000
C	3.11584600	-0.17955300	-1.27700500
C	1.84766800	0.50204500	-1.23690800

C	1.67475700	1.88631100	-1.41809500
H	1.22044900	4.68825300	-1.06190700
H	-1.13704000	5.19996300	0.15130700
H	-5.61034700	2.36748900	0.46608100
H	-6.27578600	-0.08335500	-0.40540600
H	-3.43478600	-4.58587500	-0.83534400
H	-0.84565000	-5.14825300	-0.36644800
H	3.62615100	-2.22973300	-0.69487700
H	4.05964500	0.29316300	-1.50928600
Mn	-1.05378700	0.04697000	-0.53475800
Cl	-1.35190000	0.16429600	-2.85774700
O	-0.96405900	-0.23571400	1.15749400
C	-5.18356600	-2.53253000	-1.06852400
C	-6.12054000	-2.76690000	-0.05717600
C	-5.43692400	-3.10091100	-2.32201300
C	-7.27326000	-3.51596500	-0.28067200
C	-6.57958500	-3.86016100	-2.56647000
C	-7.50089700	-4.06538600	-1.54114800
C	-3.48389200	3.99831600	0.91808000
C	-3.75639400	4.05112200	2.28766600
C	-3.91626900	5.07003300	0.13301100
C	-4.42929900	5.12638300	2.86295000
C	-4.58940200	6.15810100	0.68518900
C	-4.84817000	6.18217700	2.05475700
C	1.59716100	-3.96932700	0.02874800
C	1.54706700	-4.44642000	1.34137700
C	2.48746200	-4.59793800	-0.84705000
C	2.36955200	-5.47750000	1.78096900
C	3.32921900	-5.62400100	-0.42479400
C	3.27143100	-6.05845400	0.89657300
F	-5.92205500	-2.26423900	1.16943800
F	-8.15382500	-3.72039300	0.70555100
F	-8.60035900	-4.78886900	-1.76521300
F	-6.79884300	-4.38954200	-3.77440100
F	-4.56794700	-2.92506200	-3.32205000
F	-3.67821100	5.07041300	-1.18416800
F	-4.99168100	7.17314900	-0.08681200
F	-5.49361100	7.21917700	2.59338500
F	-4.67364000	5.15419600	4.17714500
F	-3.35702400	3.05034400	3.08651700
F	2.57819000	-4.18937500	-2.11873200
F	0.74283000	-3.85751500	2.23894000
F	2.37073300	-5.84206000	3.07069100
F	4.12892500	-6.98844000	1.33239300

F	4.21896600	-6.16561800	-1.26379300
C	2.74473600	2.62233500	-1.99433100
C	3.68343600	3.18735200	-2.51643100
C	4.83765000	3.79335100	-3.16447800
H	4.68523200	3.74000500	-4.25144000
C	5.24781500	5.24555000	-2.76262300
H	4.46595300	6.00180700	-2.87281700
C	6.22904100	3.19132300	-2.79121600
H	6.32415900	2.10965600	-2.90424700
C	7.15195400	4.03526400	-3.70001000
H	8.17956600	4.06113300	-3.32332200
H	7.18503500	3.61632800	-4.71110400
C	6.46870000	5.44643900	-3.69219600
H	7.13273200	6.23598800	-3.32554800
H	6.14433000	5.73389700	-4.69775700
C	5.78220600	5.09489800	-1.31694100
H	6.50859300	5.88331100	-1.10208100
C	6.43089700	3.67573200	-1.33687600
H	7.49132700	3.65810300	-1.06433500
C	4.71074800	5.04184700	-0.19273600
H	3.70033800	5.19817500	-0.58994500
H	4.88935900	5.80035900	0.57790400
C	5.65064500	2.87709900	-0.29867100
O	5.77414200	1.65719700	-0.10537400
N	4.82429800	3.70400400	0.36919800
H	4.06313800	3.29667100	0.93021300
C	5.65732100	-2.75181400	2.02760100
C	5.41199000	-1.42839100	1.67802600
C	4.22664400	-0.79343100	2.09113300
C	3.25890900	-1.49388300	2.85047800
C	3.53913400	-2.82687900	3.22422100
C	4.70961800	-3.44131500	2.82285700
H	6.12010500	-0.87116200	1.06986200
C	2.03236800	-0.82563400	3.14314500
H	2.80278900	-3.37684800	3.80231300
H	4.89514500	-4.47595400	3.09962000
C	1.76993800	0.46399800	2.75002900
C	2.79870600	1.19350900	1.99688600
H	1.26206500	-1.38389800	3.67076100
C	6.89506400	-3.46913500	1.53500300
H	7.59681800	-2.74064800	1.11260400
H	7.40590300	-3.94168200	2.38481100
O	2.66280400	2.36190400	1.58684600
C	0.41446500	1.04170300	2.94887500

H	-0.18570000	0.69979400	2.00243400
C	6.57720300	-4.54627500	0.48093500
H	7.49848100	-5.00757800	0.10837200
H	5.95332500	-5.34256100	0.89762700
H	6.04474700	-4.11559100	-0.37471400
N	3.96790100	0.50964800	1.74070900
H	4.64255900	0.98086300	1.11325400
C	0.19765300	2.54116800	3.12550800
H	0.54073000	3.10402600	2.25869700
H	-0.86806800	2.73345500	3.28450600
H	0.74894900	2.90678500	4.00207700
H	-0.11034600	0.47492400	3.72657800

**<sup>5</sup>TS2-R**

N	-0.61049100	1.97845800	-0.46587000
N	-3.01810400	0.47603400	-0.35916500
N	-1.51494400	-1.87995100	-0.60971300
N	0.85689000	-0.37073600	-0.83512300
C	0.53391500	2.56902300	-0.92631800
C	0.45231500	3.99063100	-0.73463900
C	-0.74108600	4.24221700	-0.12083800
C	-1.42557200	2.97865300	-0.00326300
C	-2.77525700	2.82413000	0.34226300
C	-3.52020300	1.67012900	0.09085500
C	-4.96207900	1.58651300	0.14220500
C	-5.30653900	0.35072800	-0.31041300
C	-4.07536500	-0.36280200	-0.57357000
C	-3.96746800	-1.73593200	-0.83308300
C	-2.75957800	-2.43975200	-0.76114200
C	-2.63873300	-3.87425000	-0.67678600
C	-1.33038000	-4.15638800	-0.41460100
C	-0.61854400	-2.90540900	-0.39927900
C	0.76919500	-2.77110300	-0.32332300
C	1.45677500	-1.58143400	-0.60569300
C	2.87712300	-1.45815300	-0.83453900
C	3.10467400	-0.18486700	-1.26500400
C	1.83573100	0.49760700	-1.23126100
C	1.67088500	1.88483500	-1.39548200
H	1.22929400	4.68961100	-1.00952500
H	-1.14016200	5.19746900	0.18825100
H	-5.61835700	2.38846100	0.44928000
H	-6.30007700	-0.05635100	-0.42634900
H	-3.45947800	-4.57075000	-0.77126800
H	-0.87516700	-5.12789000	-0.28340600

H	3.60887500	-2.23554000	-0.67719200
H	4.05099200	0.28746400	-1.48833500
Mn	-1.08502600	0.03457300	-0.57417700
Cl	-1.32502800	0.24872600	-2.88590100
O	-0.99009200	-0.20562100	1.17351100
C	-5.20719800	-2.52673300	-1.06885700
C	-6.15697100	-2.74200400	-0.06516500
C	-5.44575000	-3.11743600	-2.31497500
C	-7.30813700	-3.49318300	-0.28983000
C	-6.58642400	-3.87925400	-2.56029600
C	-7.52091900	-4.06464800	-1.54308800
C	-3.48701800	3.99662700	0.92702100
C	-3.71203100	4.06952800	2.30397600
C	-3.95346800	5.05137300	0.13902800
C	-4.37404700	5.14941900	2.88364500
C	-4.61756800	6.14283900	0.69543400
C	-4.82926900	6.18782800	2.07260000
C	1.57264100	-3.96548900	0.05291100
C	1.53321200	-4.43952400	1.36705000
C	2.45325000	-4.59864500	-0.82973600
C	2.35574600	-5.47337600	1.80038900
C	3.29520400	-5.62683200	-0.41357000
C	3.24790100	-6.05867900	0.90911200
F	-5.97265900	-2.21832000	1.15474300
F	-8.20113400	-3.67879400	0.68872300
F	-8.61852600	-4.79045700	-1.76797000
F	-6.79117100	-4.43003500	-3.76109400
F	-4.56347800	-2.96117400	-3.30686100
F	-3.75789900	5.03087900	-1.18486200
F	-5.05414300	7.14182600	-0.07890100
F	-5.46516400	7.22844800	2.61564900
F	-4.57444700	5.19755200	4.20461600
F	-3.27812600	3.08525900	3.10447200
F	2.53267800	-4.19333700	-2.10317500
F	0.73969800	-3.84648400	2.27099500
F	2.36739800	-5.83592500	3.09052300
F	4.10594500	-6.99087500	1.33882700
F	4.17456600	-6.17365000	-1.26001600
C	2.74023200	2.61950200	-1.97311100
C	3.67506800	3.18168000	-2.50566800
C	4.82033700	3.78131400	-3.17508300
H	4.64419600	3.72954600	-4.25858100
C	5.24865200	5.23044900	-2.78160100
H	4.46972300	5.99198400	-2.87475800

C	6.21528000	3.16951700	-2.83224600
H	6.30042800	2.08730500	-2.94779600
C	7.12400300	4.00779900	-3.76028500
H	8.15961700	4.02635300	-3.40576200
H	7.13244800	3.58936100	-4.77209000
C	6.45074300	5.42358100	-3.73695000
H	7.12778700	6.20826100	-3.38394800
H	6.10701000	5.71410900	-4.73517200
C	5.81255200	5.07509600	-1.34774700
H	6.54833400	5.85863000	-1.14754900
C	6.45128000	3.65161800	-1.38231500
H	7.51701200	3.62645700	-1.13204600
C	4.76407000	5.02795300	-0.20188800
H	3.74682000	5.19270100	-0.57788100
H	4.96410300	5.78360000	0.56628600
C	5.68663700	2.85689800	-0.32957200
O	5.80530300	1.63575600	-0.14076800
N	4.87885000	3.68818300	0.35508200
H	4.12487900	3.28467200	0.92882600
C	5.68216500	-2.77933200	1.99261500
C	5.44418400	-1.45311900	1.64786300
C	4.26826600	-0.80938900	2.07364000
C	3.30162400	-1.50360000	2.84063500
C	3.57536600	-2.83927800	3.21004000
C	4.73695300	-3.46236000	2.79655400
H	6.15104600	-0.90061400	1.03392200
C	2.08322200	-0.82685600	3.14588300
H	2.84085900	-3.38355900	3.79583200
H	4.91730800	-4.49870400	3.07043900
C	1.82597300	0.46661200	2.75968100
C	2.85569100	1.18956500	2.00040600
H	1.31343700	-1.38041600	3.67913200
C	6.90850600	-3.50630700	1.48613600
H	7.61160800	-2.78345700	1.05635800
H	7.42473800	-3.98370800	2.32997300
O	2.72769100	2.36111000	1.59691700
C	0.47591700	1.05451300	2.97304400
H	-0.13352600	0.72586000	2.04311700
C	6.56976800	-4.58012700	0.43514100
H	7.48277300	-5.04973500	0.05268700
H	5.94301400	-5.37073800	0.85828000
H	6.03216100	-4.14427900	-0.41463400
N	4.01682700	0.49700400	1.73048400
H	4.68839300	0.96471200	1.09755300

C	0.27877200	2.55764500	3.15945400
H	0.84115100	2.91783200	4.03111100
H	0.61580400	3.11944500	2.28964300
H	-0.78380900	2.75959700	3.32876200
H	-0.03569900	0.49519400	3.76522400

**<sup>3</sup>TS4-R**

N	-0.02939000	1.99987300	0.49815200
N	2.53165500	0.72575100	0.46838000
N	1.24029900	-1.82491200	0.52901500
N	-1.30066300	-0.52094800	0.54500700
C	-1.28235700	2.44428800	0.85232400
C	-1.27578800	3.88399800	0.91231000
C	-0.03115600	4.29496000	0.54685200
C	0.75845000	3.11072900	0.32040900
C	2.13761800	3.12487600	0.08817000
C	2.95857800	1.99957900	0.18724800
C	4.40176500	2.01842300	0.13122600
C	4.83248700	0.76215800	0.42367300
C	3.65080700	-0.04761700	0.60505600
C	3.67306400	-1.44261800	0.77195500
C	2.52722400	-2.25564200	0.68639800
C	2.56500000	-3.69628500	0.64742100
C	1.29001600	-4.12009400	0.43965200
C	0.45702600	-2.94223500	0.38671200
C	-0.93687400	-2.95604200	0.29954700
C	-1.73990000	-1.81784700	0.40407400
C	-3.17478300	-1.84783700	0.53317500
C	-3.58219300	-0.57864000	0.80134600
C	-2.40295700	0.25066500	0.81587300
H	-2.11912800	4.50079400	1.18388700
H	0.33872700	5.30770500	0.47960700
H	5.00868800	2.88604900	-0.08207000
H	5.85395200	0.41353500	0.48268800
H	3.46487500	-4.28525100	0.74705300
H	0.93602900	-5.13578700	0.33929500
H	-3.78942900	-2.73174700	0.44804300
H	-4.59437000	-0.22636400	0.93246500
Mn	0.60591300	0.09958000	0.46441900
Cl	0.67069900	0.10759500	2.80482800
O	0.73562600	0.01641200	-1.24168100
C	2.77735800	4.44694100	-0.16654900
C	2.56663400	5.13420000	-1.36544300
C	3.59195800	5.06328900	0.78969400



C	3.14187900	6.37809500	-1.61379900
C	4.18301800	6.30415000	0.56216400
C	3.95425900	6.96337400	-0.64454300
C	-1.62278500	-4.28180900	0.26447800
C	-2.30621200	-4.74308300	-0.86287400
C	-1.63548300	-5.10656700	1.39594400
C	-2.98176700	-5.96114000	-0.87308200
C	-2.29253700	-6.33517900	1.40658900
C	-2.97154900	-6.76194200	0.26661100
F	3.82073700	4.45875100	1.96062900
F	4.95687100	6.86983500	1.49355400
F	4.51212700	8.15436300	-0.87145600
F	2.92320300	7.00948300	-2.77224400
F	1.79109000	4.59921700	-2.32019900
F	-1.00408100	-4.72040200	2.50933700
F	-2.33252200	-4.00531000	-1.98324000
F	-3.63400200	-6.36466300	-1.97012500
F	-3.61072800	-7.93373500	0.26720700
F	-2.28515100	-7.10053200	2.50238400
C	5.99335900	-2.67809000	0.96711500
C	7.23870300	-3.42980100	0.99814200
H	7.26591200	-4.00872900	1.93163200
C	7.51599200	-4.37497000	-0.21752000
H	6.72950500	-5.10381000	-0.43211700
C	8.57618000	-2.64701700	0.82098400
H	8.73321600	-1.80895500	1.50247400
C	9.58911300	-3.80787900	0.94894900
H	10.55118800	-3.55930400	0.48984800
H	9.77982500	-4.04099600	2.00184600
C	8.86265200	-4.99592900	0.22754900
H	9.43136800	-5.38446800	-0.62367700
H	8.69262000	-5.83160100	0.91443600
C	7.81323200	-3.39983700	-1.38380500
H	8.44788500	-3.89122500	-2.12627200
C	8.54164400	-2.22435200	-0.66536400
H	9.55338500	-2.02918400	-1.03529600
C	6.58292100	-2.75848700	-2.09353500
H	5.63831300	-3.13742800	-1.68641400
H	6.59200700	-2.95689900	-3.17140600
C	7.69081900	-0.98701500	-0.93573600
O	7.85563400	0.11808400	-0.43449000
N	6.72235600	-1.33117900	-1.83238800
H	5.97491900	-0.67513200	-2.02132100
C	-7.12443600	-0.77135800	-1.53008900

C	-6.01545000	-1.47888000	-1.98657700
C	-4.81922400	-0.81327500	-2.29647100
C	-4.72265700	0.59306800	-2.14597800
C	-5.86153100	1.29866100	-1.70226700
C	-7.03444700	0.63228000	-1.39405300
H	-6.06871800	-2.55995700	-2.09975600
C	-3.45585800	1.21568600	-2.38811800
H	-5.79888100	2.37689800	-1.59040300
H	-7.89904500	1.18906900	-1.04196600
C	-2.34597700	0.50860200	-2.75700300
C	-2.44305100	-0.94971000	-2.96867900
H	-3.38558300	2.28613700	-2.24478200
C	-8.42679800	-1.48105900	-1.23571600
H	-8.23069000	-2.53136500	-0.98757100
H	-8.89759400	-1.03100100	-0.35229400
O	-1.51183900	-1.66096200	-3.32826600
C	-0.99806700	1.08938400	-2.91284600
H	-0.34284300	0.61922100	-2.05769400
C	-9.40468600	-1.40961300	-2.42355100
H	-10.34439400	-1.92113500	-2.18722400
H	-9.63536900	-0.36878200	-2.67659800
H	-8.97053000	-1.88025300	-3.31261800
N	-3.70480000	-1.49828700	-2.72687800
H	-3.73664500	-2.50797300	-2.80345600
C	-0.85115800	2.59959700	-2.83859600
H	-1.35987600	3.08572000	-3.68177200
H	-1.26924000	3.00617200	-1.91247100
H	0.20399900	2.87806400	-2.87118400
H	-0.48418200	0.64644200	-3.77334100
C	-2.40589300	1.63433800	1.03288500
C	-3.69497200	2.24839700	1.45559300
C	-4.30210400	1.86279500	2.65989600
C	-4.39603700	3.16941700	0.67339100
C	-5.55237000	2.34122000	3.04610600
C	-5.65109900	3.65119600	1.02983300
C	-6.23482800	3.23534800	2.22299900
C	4.93245900	-2.09128500	0.91352800
F	-3.88656500	3.60454100	-0.49470600
F	-6.30852200	4.47890200	0.20719100
F	-7.44084400	3.68618200	2.57389300
F	-6.10381200	1.94463700	4.19676300
F	-3.69052500	0.99129600	3.46660300

<sup>3</sup>TS4-S

N	0.32211200	2.17449300	0.46445200
N	-2.42559600	1.37308400	0.42741100
N	-1.60564400	-1.36548300	0.54224600
N	1.12583400	-0.53155900	0.55827400
C	1.63214300	2.39421200	0.82201600
C	1.87983000	3.81235600	0.87196200
C	0.72787900	4.43397800	0.49978500
C	-0.25715600	3.40627800	0.27682700
C	-1.61084100	3.66196300	0.03524900
C	-2.61809200	2.69874100	0.12964300
C	-4.03418700	2.96818100	0.04245400
C	-4.67761700	1.80456100	0.32664600
C	-3.66162800	0.80483400	0.54389100
C	-3.93368200	-0.56175700	0.74116200
C	-2.94980400	-1.56429100	0.70259200
C	-3.24081100	-2.97815400	0.70182000
C	-2.05784500	-3.61825800	0.50271200
C	-1.03103500	-2.60604800	0.42584500
C	0.33818000	-2.86650700	0.34115600
C	1.32920800	-1.88681000	0.43419700
C	2.73647800	-2.16851700	0.56711800
C	3.36168300	-0.98831400	0.82031400
C	2.34747900	0.03700100	0.82073800
H	2.81794500	4.27253600	1.14329100
H	0.54335500	5.49579700	0.42572200
H	-4.47218900	3.92804900	-0.18898900
H	-5.73981500	1.61286600	0.36784700
H	-4.21895800	-3.42336400	0.81560500
H	-1.89238300	-4.68306800	0.42790500
H	3.18455500	-3.14841700	0.49398300
H	4.42019700	-0.81868400	0.94915000
Mn	-0.63946100	0.41302600	0.45251200
Cl	-0.71852100	0.47736200	2.79140300
O	-0.77143100	0.31927500	-1.25240900
C	-2.00557400	5.07448200	-0.23028000
C	-1.64849400	5.71530400	-1.42060700
C	-2.72543200	5.82369000	0.70720700
C	-1.99302900	7.04011100	-1.67812200
C	-3.08734700	7.14784200	0.46968400
C	-2.71695600	7.75755000	-0.72777300
C	0.77971600	-4.29266400	0.31976500
C	1.35491600	-4.88086800	-0.80855100
C	0.66255200	-5.09148500	1.46350000
C	1.80552800	-6.19867500	-0.80845900

C	1.09384100	-6.41623100	1.48506100
C	1.67083900	-6.97018800	0.34352400
F	-3.08684200	5.26917500	1.86995800
F	-3.77713200	7.83850100	1.38321100
F	-3.05558700	9.02670500	-0.96413500
F	-1.63901900	7.62363100	-2.82803700
F	-0.95271400	5.05487900	-2.35753000
F	0.12505600	-4.58468800	2.57738100
F	1.49451000	-4.17229900	-1.94002100
F	2.36196300	-6.72449700	-1.90657300
F	2.09533100	-8.23554200	0.35455600
F	0.96925200	-7.15376900	2.59235000
C	6.78940100	-1.86318000	-1.48321500
C	5.57235700	-2.36037200	-1.94183700
C	4.52108000	-1.49009000	-2.26971700
C	4.68426000	-0.08815800	-2.13595400
C	5.93052100	0.40157800	-1.69010100
C	6.95858300	-0.46524900	-1.36387000
H	5.42630900	-3.43414700	-2.04192600
C	3.55495000	0.75372600	-2.39409900
H	6.06641100	1.47439100	-1.59102500
H	7.90857700	-0.07286000	-1.01027200
C	2.33592400	0.25822300	-2.76309300
C	2.16431800	-1.19558000	-2.95896400
H	3.68178700	1.82042400	-2.26198400
C	7.93649000	-2.79664900	-1.16815400
H	7.54831600	-3.78959300	-0.91025200
H	8.47527400	-2.42969500	-0.28514500
O	1.12042600	-1.72743700	-3.31882100
C	1.11790100	1.07457100	-2.93204300
H	0.38664000	0.74052100	-2.07494000
C	8.91998100	-2.92168600	-2.34689500
H	9.74744600	-3.59443700	-2.09542000
H	9.34049300	-1.94446800	-2.60922500
H	8.41348500	-3.31574700	-3.23492500
N	3.30213500	-1.96395600	-2.70086700
H	3.14751200	-2.96323600	-2.76464200
C	1.25040200	2.58692600	-2.87505900
H	1.84490900	2.96113900	-3.71922800
H	1.73035800	2.92114300	-1.95000700
H	0.26456400	3.05402400	-2.91962300
H	0.53418100	0.72334500	-3.79033400
C	2.59497100	1.40040500	1.01775900
C	3.97152900	1.78339800	1.43685200

C	4.49999400	1.31381600	2.64838600
C	4.82422200	2.55648300	0.64503300
C	5.81418600	1.57118400	3.03302800
C	6.14375700	2.81582000	0.99982700
C	6.64383800	2.32066400	2.20075100
F	4.40028000	3.05811000	-0.53057900
F	6.93716700	3.50433700	0.16890100
F	7.90962400	2.55822600	2.55033700
F	6.28589500	1.10015900	4.19100000
F	3.74391500	0.57443600	3.46438800
C	-6.47110800	-1.26082000	0.88751700
C	-7.89091000	-1.57854500	0.88077800
H	-8.36418400	-1.04557400	1.71696900
C	-8.66879800	-1.27838300	-0.44345700
H	-8.58642300	-0.25195200	-0.81155600
C	-8.31247000	-3.08013100	0.90376000
H	-7.89107900	-3.68259500	1.71053900
C	-9.85101800	-2.92908400	0.91975600
H	-10.35129500	-3.83517700	0.56360900
H	-10.21050600	-2.73500200	1.93583600
C	-10.09739700	-1.69393900	-0.01467400
H	-10.72574400	-1.93612200	-0.87811500
H	-10.58870400	-0.87915900	0.52738700
C	-8.14610400	-2.35108800	-1.43100200
H	-8.89929200	-2.54722100	-2.19897100
C	-7.91135200	-3.58035500	-0.50262400
H	-8.49103700	-4.46772400	-0.77667700
C	-6.77138900	-2.07111400	-2.10982400
H	-6.36951800	-1.09314300	-1.82033700
H	-6.85025000	-2.09599800	-3.20273500
C	-6.43042000	-3.92141600	-0.63835300
O	-5.82305200	-4.74894900	0.02948600
N	-5.91016600	-3.14544500	-1.63196100
H	-4.90727100	-3.13257300	-1.77004600
C	-5.29775100	-0.95200800	0.86043000

**<sup>5</sup>TS4-R**

N	-0.02208500	2.01352100	0.49919600
N	2.53298300	0.71246800	0.48489300
N	1.24550800	-1.81365200	0.56118200
N	-1.30288200	-0.51610900	0.54953900
C	-1.27799300	2.46015000	0.83204500
C	-1.27268800	3.90192800	0.88909000
C	-0.02147800	4.30876400	0.54153900

C	0.76262200	3.11692000	0.32606500
C	2.14868600	3.11943500	0.09770800
C	2.96205700	1.99427200	0.19783300
C	4.40438700	2.00870800	0.13237000
C	4.83640600	0.75457400	0.42859900
C	3.65596900	-0.05444500	0.62115800
C	3.67744900	-1.44792200	0.80082200
C	2.52842600	-2.25625000	0.71954100
C	2.55849800	-3.69703400	0.68343900
C	1.28225000	-4.11442400	0.47427200
C	0.45334000	-2.93439100	0.41895900
C	-0.93602700	-2.94650300	0.32367300
C	-1.74550700	-1.80565500	0.41728200
C	-3.18130600	-1.83748100	0.53847400
C	-3.58801000	-0.56298400	0.78758900
C	-2.40387600	0.26125700	0.79941300
H	-2.11826100	4.52166600	1.14674700
H	0.35290600	5.31998200	0.47670600
H	5.01147300	2.87366500	-0.09059700
H	5.85822100	0.40609400	0.48293100
H	3.45513600	-4.29056400	0.78542300
H	0.92458000	-5.12876600	0.37358500
H	-3.79661700	-2.72162700	0.46035500
H	-4.60025300	-0.20720800	0.90851700
Mn	0.63333100	0.09053400	0.50061900
Cl	0.57237200	0.17919000	2.84364600
O	0.71406300	0.04089900	-1.23773500
C	2.79340700	4.43785200	-0.16340200
C	2.57217700	5.12535100	-1.36044800
C	3.61846200	5.05254000	0.78487800
C	3.14839800	6.36746100	-1.61494800
C	4.21025300	6.29188700	0.55100400
C	3.97160700	6.95107000	-0.65376100
C	-1.62371800	-4.27075600	0.27601300
C	-2.29137500	-4.72242200	-0.86442600
C	-1.65814800	-5.10014900	1.40319700
C	-2.97451300	-5.93574300	-0.89130100
C	-2.32354100	-6.32444700	1.39759100
C	-2.98751000	-6.74139200	0.24512200
F	3.85706600	4.44835100	1.95404900
F	4.99442600	6.85599800	1.47469100
F	4.53040300	8.14044000	-0.88665600
F	2.92025900	6.99898200	-2.77141800
F	1.78525000	4.59191600	-2.30624600

F	-1.04102600	-4.72307700	2.52750400
F	-2.29223600	-3.97890500	-1.98157300
F	-3.61183400	-6.33009800	-2.00038000
F	-3.63422800	-7.90890300	0.23036100
F	-2.33813600	-7.09511300	2.48950700
C	-7.09221500	-0.82243500	-1.47930200
C	-5.98656500	-1.51910500	-1.95819900
C	-4.80280500	-0.84210400	-2.29167900
C	-4.71562800	0.56670100	-2.14119100
C	-5.85506900	1.26143100	-1.67722600
C	-7.01379500	0.58370800	-1.34637700
H	-6.03175500	-2.60049400	-2.07118700
C	-3.46244300	1.20101300	-2.40341800
H	-5.80183200	2.34062200	-1.57119000
H	-7.87768100	1.13146200	-0.97880400
C	-2.34959200	0.50585300	-2.79891700
C	-2.44403700	-0.95301500	-3.02507700
H	-3.39782800	2.27106800	-2.25585600
C	-8.38129000	-1.54338900	-1.15685800
H	-8.17198000	-2.59480200	-0.92511900
H	-8.83022600	-1.10511900	-0.25625600
O	-1.52192300	-1.65499100	-3.42170900
C	-1.01125000	1.09330900	-2.95474000
H	-0.35594200	0.62471100	-2.09117500
C	-9.39210400	-1.46569800	-2.31660300
H	-10.32183100	-1.98505600	-2.05910500
H	-9.63584600	-0.42387600	-2.55269400
H	-8.98025100	-1.92509600	-3.22196700
N	-3.69419900	-1.51449600	-2.75080700
H	-3.71889400	-2.52401200	-2.83247700
C	-0.87006000	2.60440900	-2.87351400
H	-1.37796000	3.09890800	-3.71261500
H	-1.28760900	3.00352300	-1.94362200
H	0.18504500	2.88447300	-2.90172700
H	-0.49183800	0.65193600	-3.81278500
C	-2.40373200	1.64948000	1.00236200
C	-3.69261100	2.26743800	1.42111700
C	-4.29948400	1.88736700	2.62760600
C	-4.39002500	3.19044500	0.63823900
C	-5.54647200	2.37328400	3.01487100
C	-5.64231200	3.67886900	0.99571200
C	-6.22601100	3.26874000	2.19077600
F	-3.88182300	3.61932300	-0.53267000
F	-6.29764700	4.50662200	0.17149900

F	-7.42932300	3.72603400	2.54247900
F	-6.09765200	1.98265700	4.16760100
F	-3.69028000	1.01688400	3.43649300
C	5.99504300	-2.68791100	0.98789900
C	7.23912400	-3.44154600	1.01209600
H	7.27430600	-4.01389400	1.94938200
C	7.50244300	-4.39606100	-0.19958600
H	6.71248900	-5.12489700	-0.40098500
C	8.57612600	-2.66247100	0.81580700
H	8.74145500	-1.81978900	1.48958900
C	9.58811600	-3.82433500	0.94213800
H	10.54595300	-3.58091200	0.47159100
H	9.78898800	-4.05009900	1.99474500
C	8.85229600	-5.01626800	0.23680500
H	9.41174300	-5.41213000	-0.61716300
H	8.68754700	-5.84653100	0.93148700
C	7.79000700	-3.42998600	-1.37579800
H	8.41664200	-3.92807400	-2.12058800
C	8.52731800	-2.25053400	-0.67313400
H	9.53560000	-2.05962200	-1.05452300
C	6.55414900	-2.79168700	-2.07859100
H	5.61264600	-3.16670800	-1.66072000
H	6.55320800	-2.99711700	-3.15515900
C	7.67573100	-1.01373600	-0.94401000
O	7.84754000	0.09463100	-0.45232200
N	6.69767400	-1.36295500	-1.82798100
H	5.95053000	-0.70662900	-2.01718000
C	4.93496300	-2.09867800	0.93936400

**<sup>5</sup>TS4-S**

N	0.31627600	2.18706100	0.45721700
N	-2.42987900	1.35356000	0.44176800
N	-1.60300100	-1.35764200	0.56779300
N	1.13277800	-0.52748800	0.56671100
C	1.62828200	2.41184900	0.79486800
C	1.87485200	3.83226300	0.83873800
C	0.71465500	4.44812400	0.48211800
C	-0.26418000	3.40966700	0.27239100
C	-1.62764400	3.65211300	0.03893800
C	-2.62596500	2.68621100	0.14026600
C	-4.04299700	2.95032100	0.05149400
C	-4.68451300	1.78805200	0.34117000
C	-3.66692700	0.79043200	0.56253800
C	-3.93499300	-0.57574500	0.76774000



C	-2.94527900	-1.57215800	0.72721000
C	-3.22558700	-2.98783800	0.72382900
C	-2.03865500	-3.61913300	0.52296400
C	-1.01725900	-2.60258000	0.44892600
C	0.34818800	-2.85772200	0.36100000
C	1.34415100	-1.87496800	0.45012700
C	2.75220200	-2.15608500	0.57896400
C	3.37458800	-0.96957600	0.81502100
C	2.35245200	0.04975700	0.81019400
H	2.81438100	4.29741800	1.09636900
H	0.52328100	5.50873700	0.40836200
H	-4.48342200	3.90753700	-0.18586300
H	-5.74648500	1.59527200	0.38374300
H	-4.20054900	-3.44034400	0.83667600
H	-1.86722000	-4.68277700	0.44509300
H	3.20297500	-3.13529000	0.51265100
H	4.43319000	-0.79433900	0.93568100
Mn	-0.66570300	0.40371400	0.48474800
Cl	-0.61293900	0.53762400	2.82642200
O	-0.73648400	0.32721300	-1.25169900
C	-2.03171800	5.06097700	-0.23277200
C	-1.67758700	5.69743800	-1.42638400
C	-2.75313200	5.81171600	0.70219300
C	-2.02727600	7.01971000	-1.68965200
C	-3.11954000	7.13361300	0.45900200
C	-2.75255100	7.73900500	-0.74166100
C	0.79441500	-4.28194500	0.32495200
C	1.35329800	-4.85640000	-0.81827500
C	0.70242200	-5.08985900	1.46410000
C	1.81493500	-6.17004000	-0.83687300
C	1.14552100	-6.41101900	1.46751800
C	1.70728200	-6.95107100	0.31172700
F	-3.11179200	5.26130400	1.86772000
F	-3.81080000	7.82605200	1.37006700
F	-3.09595000	9.00581900	-0.98352600
F	-1.67684600	7.59917400	-2.84263900
F	-0.98065500	5.03468800	-2.36033300
F	0.17926700	-4.59591100	2.59032600
F	1.46331800	-4.13709000	-1.94663400
F	2.35601300	-6.68275800	-1.94876600
F	2.14259200	-8.21274100	0.30559100
F	1.04626500	-7.15842500	2.57066200
C	6.74030300	-1.90531600	-1.42850300
C	5.52890900	-2.39082200	-1.91182200

C	4.49361400	-1.51029400	-2.26382400
C	4.66786000	-0.10790300	-2.12827200
C	5.91245300	0.36933900	-1.65943100
C	6.92269000	-0.50730500	-1.31016500
H	5.37374600	-3.46310100	-2.01334100
C	3.55611700	0.74429200	-2.40834100
H	6.05884400	1.44099700	-1.56467200
H	7.87012900	-0.12506500	-0.93913900
C	2.33659000	0.26277700	-2.80746000
C	2.16103400	-1.19098900	-3.01915100
H	3.68966100	1.80931700	-2.27115900
C	7.87077700	-2.84853900	-1.08537300
H	7.46844900	-3.84049400	-0.84646100
H	8.38472900	-2.49095700	-0.18387000
O	1.12870600	-1.71456000	-3.41932200
C	1.13088200	1.08578100	-2.97756100
H	0.39975200	0.75217000	-2.11126600
C	8.88911300	-2.97171600	-2.23455600
H	9.70422300	-3.65122300	-1.96204100
H	9.32364800	-1.99559900	-2.47734000
H	8.40770800	-3.35694300	-3.14019300
N	3.28331100	-1.97121300	-2.72631700
H	3.12051800	-2.96878100	-2.79657300
C	1.27185700	2.59774700	-2.91414700
H	1.86931800	2.97862300	-3.75357800
H	1.74906500	2.92436200	-1.98470600
H	0.28747200	3.06857200	-2.95635400
H	0.54134600	0.73741000	-3.83307600
C	2.59471600	1.41872900	0.98777500
C	3.96979100	1.80977000	1.40539100
C	4.49689600	1.34982400	2.62156200
C	4.81961000	2.58577800	0.61347600
C	5.80746600	1.61933500	3.01009500
C	6.13591100	2.85631900	0.97217800
C	6.63487700	2.37086400	2.17744200
F	4.39801100	3.07741200	-0.56718700
F	6.92768500	3.54573400	0.14051400
F	7.89748000	2.61940900	2.53074200
F	6.27789800	1.15812000	4.17243700
F	3.74306100	0.61121600	3.43960800
C	-6.46862600	-1.28588500	0.91126900
C	-7.88639700	-1.61152600	0.90114800
H	-8.36388700	-1.08388900	1.73833900
C	-8.66382400	-1.31105700	-0.42347100

H	-8.58668000	-0.28287400	-0.78774300
C	-8.29925100	-3.11563300	0.91805400
H	-7.87572300	-3.71849500	1.72341400
C	-9.83866200	-2.97343900	0.93201200
H	-10.33306300	-3.88107800	0.57165700
H	-10.20095800	-2.78523800	1.94819700
C	-10.09063500	-1.73625400	0.00178900
H	-10.71627300	-1.97876100	-0.86350600
H	-10.58731000	-0.92625200	0.54610100
C	-8.13349200	-2.37733700	-1.41389700
H	-8.88457700	-2.57517300	-2.18346600
C	-7.89274700	-3.60838300	-0.48941500
H	-8.46653100	-4.49831500	-0.76751100
C	-6.75963200	-2.08703200	-2.09004700
H	-6.36412900	-1.10732300	-1.79761200
H	-6.83671500	-2.10950600	-3.18310500
C	-6.40947700	-3.93994400	-0.62393200
O	-5.79829700	-4.76616100	0.04215100
N	-5.89242100	-3.15718700	-1.61370200
H	-4.88966400	-3.13878200	-1.75220800
C	-5.29641100	-0.97160500	0.88648200

**<sup>3</sup>TS6-R**

N	-0.40586700	2.26465200	-0.44372900
N	-2.60203800	0.44124000	-0.43047100
N	-0.78751500	-1.71942400	-0.78151800
N	1.39270000	0.11693600	-0.80162000
C	0.69173700	3.01252400	-0.80395800
C	0.35297800	4.41166300	-0.73610400
C	-0.92710700	4.49424900	-0.28119300
C	-1.41160900	3.14629500	-0.12794000
C	-2.73657000	2.82035500	0.17497300
C	-3.28813100	1.54993000	-0.00376300
C	-4.69457700	1.23701400	0.08947100
C	-4.84971200	-0.04637700	-0.33510100
C	-3.52851000	-0.54465500	-0.63456200
C	-3.24727000	-1.87959700	-0.97205500
C	-1.94569200	-2.41494000	-0.99269200
C	-1.64938300	-3.81867100	-1.11735500
C	-0.30650000	-3.95790800	-0.94274600
C	0.23351900	-2.63380000	-0.74885700
C	1.59798300	-2.33825400	-0.65090000
C	2.12268100	-1.04586700	-0.71217400
C	3.52725300	-0.73182700	-0.80979900

C	3.62390400	0.60858800	-1.00910600
C	2.28324500	1.14120000	-0.99135100
H	1.01531400	5.22596100	-0.98911400
H	-1.51258100	5.38516500	-0.10581700
H	-5.46723600	1.92031500	0.41066100
H	-5.77055000	-0.60758600	-0.41280900
H	-2.38973800	-4.58436600	-1.29750500
H	0.27724100	-4.86637600	-0.97466100
H	4.33250500	-1.44672100	-0.72983500
H	4.52360500	1.19642900	-1.11101800
Mn	-0.59273600	0.27830100	-0.57407600
Cl	-0.81425600	0.46726900	-2.89094900
O	-0.51468100	0.00946800	1.13359700
C	-3.63859200	3.92957400	0.59760800
C	-3.55186300	4.48297200	1.87755000
C	-4.59028800	4.47097800	-0.27268800
C	-4.37313400	5.53160300	2.28473100
C	-5.42660200	5.51663100	0.11256900
C	-5.31416000	6.04872800	1.39622800
C	2.53930200	-3.48942200	-0.55513200
C	2.57669900	-4.28751500	0.59046100
C	3.40089900	-3.84241100	-1.59764700
C	3.42673600	-5.37847300	0.71993900
C	4.27177200	-4.92579100	-1.49263500
C	4.28172900	-5.69716800	-0.33262100
F	-4.71367000	3.98267000	-1.51146200
F	-6.32679400	6.01702100	-0.73890400
F	-6.10788000	7.05244300	1.77477000
F	-4.26852400	6.03894600	3.51752800
F	-2.66310500	4.00063400	2.76038200
F	3.40878200	-3.12866200	-2.73121000
F	1.80488700	-3.96393100	1.65420700
F	3.43809800	-6.09849900	1.83982200
F	5.11613900	-6.73026200	-0.22582800
F	5.09059000	-5.23420300	-2.50401700
C	-5.23701200	-3.57379000	-1.31608300
C	-6.28645000	-4.57231300	-1.45246700
H	-6.21012800	-5.01269700	-2.45620000
C	-6.31860900	-5.70941500	-0.37833400
H	-5.38651600	-6.26923200	-0.26162300
C	-7.75780400	-4.13431800	-1.17620400
H	-8.11184800	-3.26807900	-1.73805300
C	-8.49526400	-5.46198200	-1.46506900
H	-9.47593700	-5.49522300	-0.98001800

H	-8.65805700	-5.58818600	-2.54060900
C	-7.50777500	-6.54639800	-0.90970700
H	-7.95518100	-7.16146700	-0.12201400
H	-7.17673300	-7.22403000	-1.70356400
C	-6.79155500	-4.98861600	0.90852800
H	-7.28381700	-5.70207900	1.57491300
C	-7.77757400	-3.91676800	0.35392000
H	-8.79741500	-3.99993800	0.74320100
C	-5.71236300	-4.19327900	1.70310300
H	-4.71941600	-4.29714600	1.25015500
H	-5.64852700	-4.53186100	2.74361700
C	-7.21041400	-2.57028000	0.79318100
O	-7.62392200	-1.47122500	0.44624000
N	-6.16735400	-2.80996000	1.63932700
H	-5.57635100	-2.03648900	1.91685900
C	6.52602300	-1.87663500	1.93030300
C	6.28018900	-0.53777300	1.96718400
C	4.97426900	0.00575500	2.21479000
C	5.42652700	-2.82654000	2.17281300
H	7.09544900	0.16090700	1.78520900
C	3.39063700	1.84546500	2.36172600
H	3.43606200	-2.90745300	2.60271600
C	2.32655900	0.94083800	2.58823400
C	2.60361600	-0.43110600	2.62956700
H	3.19616000	2.90847600	2.32213900
C	7.88274600	-2.47369000	1.66874300
H	7.77702700	-3.26672300	0.91867500
H	8.54334500	-1.70543700	1.24922900
C	0.91905200	1.38888700	2.75195400
H	0.30118600	0.87386500	1.84742200
C	8.51420700	-3.07839800	2.93702600
H	9.49400400	-3.51209800	2.70836600
H	8.64972100	-2.31314100	3.70985600
H	7.87169700	-3.86816900	3.33558900
C	0.61071200	2.87379800	2.76579100
H	1.04455300	3.34919800	3.65647000
H	1.01135800	3.38328100	1.88654800
H	-0.46832800	3.03919200	2.78751700
H	0.42709500	0.85684800	3.57539700
C	1.96541200	2.50220500	-1.07022900
C	3.06856300	3.44641300	-1.39791700
C	3.72136500	3.37429100	-2.63607100
C	3.52633500	4.41739300	-0.50081900
C	4.77868000	4.22021900	-2.96462300

C	4.57697800	5.27761400	-0.80746200
C	5.20689800	5.17692400	-2.04624200
C	-4.33322900	-2.77436100	-1.18611200
F	2.94993800	4.55318800	0.70819300
F	4.98689100	6.19096000	0.07972200
F	6.21702400	5.99368000	-2.35081700
F	5.38049700	4.12363800	-4.15337900
F	3.33969900	2.46671500	-3.53906900
C	3.90684300	-0.89772400	2.44398200
H	1.78962700	-1.14100300	2.75355000
C	4.68366100	1.38306900	2.19071500
H	5.49519900	2.08621400	2.01899400
N	4.19135800	-2.25044300	2.44341100
O	5.55036400	-4.05276500	2.13795800

**<sup>3</sup>TS6-S**

N	-0.22226200	2.48084800	0.41719100
N	-2.64216800	0.96608000	0.34824300
N	-1.13938700	-1.41794100	0.73105500
N	1.26646600	0.10986100	0.79660500
C	0.95837800	3.07314400	0.80191700
C	0.81061400	4.50508900	0.74391000
C	-0.44045500	4.76155400	0.27298600
C	-1.09720900	3.49174700	0.09726500
C	-2.44808600	3.34788000	-0.23174100
C	-3.16563100	2.15839900	-0.08331000
C	-4.59648800	2.03031700	-0.22448000
C	-4.92211800	0.77000800	0.17146000
C	-3.68971500	0.10392000	0.50954600
C	-3.59900500	-1.25686600	0.85829200
C	-2.38289200	-1.95723500	0.92758000
C	-2.27713400	-3.38816300	1.07139000
C	-0.96163300	-3.69973400	0.90994900
C	-0.24847700	-2.45981900	0.71601400
C	1.14410700	-2.34931300	0.63319500
C	1.83597100	-1.13906700	0.70823600
C	3.26881400	-1.01569400	0.82522200
C	3.54059600	0.29848300	1.03551300
C	2.28311900	1.00578500	1.00373900
H	1.57151600	5.22160700	1.01502100
H	-0.89890000	5.72454300	0.10054800
H	-5.26123200	2.81303300	-0.56002600
H	-5.89719800	0.30742300	0.21751400
H	-3.09628500	-4.06900400	1.25601000

H	-0.50773000	-4.67884900	0.95739600
H	3.97211600	-1.83158500	0.75063600
H	4.50906300	0.76067500	1.15335300
Mn	-0.67353700	0.53354500	0.53379900
Cl	-0.91692100	0.75155000	2.84572400
O	-0.59852700	0.25906600	-1.17288000
C	-3.18564400	4.57180100	-0.65584100
C	-2.96939100	5.14730000	-1.91103000
C	-4.10309500	5.20510900	0.18928700
C	-3.63322600	6.30229900	-2.31770700
C	-4.78397200	6.35770600	-0.19677500
C	-4.54470600	6.90821000	-1.45494500
C	1.92212300	-3.61639500	0.53805900
C	1.86101300	-4.40461900	-0.61325000
C	2.71631500	-4.09076000	1.58560400
C	2.55422500	-5.60111100	-0.74347800
C	3.43088800	-5.28302500	1.48034800
C	3.34649800	-6.04106900	0.31458700
F	-4.34667600	4.70282500	1.40495900
F	-5.65599200	6.94199000	0.63081800
F	-5.18927500	8.01355100	-1.83387400
F	-3.40715100	6.82720500	-3.52650100
F	-2.10546400	4.58452100	-2.76983200
F	2.81097600	-3.39123200	2.72419400
F	1.15307600	-3.96986100	-1.68218600
F	2.47934700	-6.30725900	-1.86961800
F	4.03292200	-7.17752700	0.20708700
F	4.19013500	-5.70679100	2.49633800
C	6.13471600	-2.57183400	-1.88558900
C	6.07428900	-1.21177200	-1.91262700
C	4.85826800	-0.49323200	-2.17217700
C	4.91938700	-3.36106300	-2.15149200
H	6.97455100	-0.63229800	-1.71349600
C	3.54346700	1.54718300	-2.32488800
H	2.94260300	-3.16642800	-2.60747600
C	2.36944200	0.79816000	-2.57487200
C	2.45669300	-0.59862800	-2.62315700
H	3.49566100	2.62660200	-2.27840200
C	7.39348800	-3.35056100	-1.61256100
H	7.17031400	-4.12696100	-0.87091400
H	8.14717300	-2.68279900	-1.17822100
C	1.03950400	1.43532100	-2.75812100
H	0.34138300	1.00621700	-1.86784900
C	7.95330800	-4.02707000	-2.87826900

H	8.86165100	-4.59198500	-2.64132300
H	8.20218300	-3.28219700	-3.64279500
H	7.21441600	-4.71903200	-3.29129100
C	0.93569700	2.94839700	-2.76529700
H	1.44540600	3.36619700	-3.64457500
H	1.38554000	3.39377300	-1.87516500
H	-0.11070200	3.25788900	-2.80324300
H	0.49387800	0.97966200	-3.59347400
C	2.14876000	2.39581600	1.08480100
C	3.36279400	3.18320300	1.43389100
C	3.97982000	3.02229200	2.68196500
C	3.96086900	4.08541400	0.54769400
C	5.13530300	3.71871600	3.03040800
C	5.11201600	4.79683700	0.87409800
C	5.70247900	4.61090900	2.12245800
F	3.42788400	4.29783800	-0.67019700
F	5.65503000	5.64829200	-0.00314100
F	6.80770600	5.28467300	2.44610600
F	5.69937600	3.54076800	4.22819900
F	3.46544200	2.17264300	3.57533400
C	3.68086700	-1.24078400	-2.42382300
H	1.55538900	-1.18969500	-2.76505000
C	4.75826600	0.91069900	-2.13967200
H	5.65581800	1.49474500	-1.95047000
N	3.77795400	-2.61960300	-2.43209100
O	4.87466200	-4.59267100	-2.12754700
C	-5.86337900	-2.58498300	1.09903300
C	-7.14730600	-3.26734900	1.15487500
H	-7.76357100	-2.77022800	1.91664600
C	-7.94823600	-3.36996000	-0.18549400
H	-8.13409200	-2.41935200	-0.69309300
C	-7.15474200	-4.80912200	1.39182700
H	-6.60571800	-5.16063800	2.26724600
C	-8.67796300	-5.07254100	1.41134100
H	-8.91161900	-6.11915300	1.19209800
H	-9.09781400	-4.84327900	2.39643000
C	-9.22368200	-4.08829600	0.31912700
H	-9.74573700	-4.60554300	-0.49259100
H	-9.92591300	-3.36753600	0.75085800
C	-7.13766600	-4.38945000	-1.02350700
H	-7.79395300	-4.88249100	-1.74577700
C	-6.60473800	-5.37260100	0.06176300
H	-6.92130500	-6.41117100	-0.07830500
C	-5.87251900	-3.84780000	-1.75481900



H	-5.75227300	-2.76820100	-1.60676900
H	-5.91828400	-4.04021100	-2.83292600
C	-5.08414100	-5.32131400	-0.04823200
O	-4.29235300	-5.85518800	0.71806800
N	-4.76726500	-4.57888600	-1.14817300
H	-3.80129700	-4.31562300	-1.29782900
C	-4.81361200	-1.98046400	1.02392400

**<sup>5</sup>TS6-R**

N	-0.39609800	2.26266000	-0.43151200
N	-2.60343900	0.43967600	-0.44512700
N	-0.80896500	-1.71356000	-0.76603200
N	1.38966100	0.09711500	-0.79020200
C	0.70560900	3.00282100	-0.78682400
C	0.37652700	4.40563100	-0.72208200
C	-0.90579400	4.49488400	-0.27377800
C	-1.39265400	3.14656000	-0.12123500
C	-2.72502800	2.82237000	0.17261200
C	-3.28267400	1.56014000	-0.01611700
C	-4.69160200	1.25788200	0.07334900
C	-4.85853700	-0.02224200	-0.35469000
C	-3.54113500	-0.53306200	-0.65066000
C	-3.26729200	-1.87205300	-0.97840400
C	-1.96871200	-2.41211200	-0.97511400
C	-1.67641500	-3.81725200	-1.07464500
C	-0.33542500	-3.96025500	-0.88756800
C	0.21301200	-2.63898400	-0.71432500
C	1.57627300	-2.35412700	-0.62264400
C	2.11381400	-1.06372500	-0.69798400
C	3.52028500	-0.76264900	-0.80456900
C	3.62375400	0.57780800	-1.00417500
C	2.28473200	1.11684800	-0.98105900
H	1.04386200	5.21643500	-0.97306700
H	-1.48865700	5.38821200	-0.10220100
H	-5.45867300	1.94665100	0.39603000
H	-5.78442700	-0.57491400	-0.43471400
H	-2.41846300	-4.58257900	-1.24946900
H	0.24232800	-4.87294400	-0.90001100
H	4.32120000	-1.48260000	-0.72661400
H	4.52657800	1.16028800	-1.10886300
Mn	-0.61310500	0.25655400	-0.59551100
Cl	-0.75810700	0.54093900	-2.90379400
O	-0.52465000	0.03266400	1.15336700
C	-3.62091600	3.93496200	0.59983500

C	-3.52975900	4.48104900	1.88267700
C	-4.56661200	4.48929600	-0.26871900
C	-4.34205700	5.53488600	2.29438900
C	-5.39359700	5.54064700	0.12111000
C	-5.27745600	6.06508300	1.40758400
C	2.51031600	-3.51107400	-0.52279500
C	2.55809200	-4.29479500	0.63207600
C	3.35639800	-3.88116200	-1.57199700
C	3.40405900	-5.38873800	0.76364500
C	4.22218400	-4.96838800	-1.46540900
C	4.24294800	-5.72549800	-0.29616500
F	-4.69325200	4.00838200	-1.51015400
F	-6.28840400	6.05354200	-0.72862500
F	-6.06248100	7.07391700	1.79055600
F	-4.23431700	6.03490900	3.52980800
F	-2.64629500	3.98570900	2.76296100
F	3.35305200	-3.18066800	-2.71377700
F	1.80192300	-3.95393400	1.70134500
F	3.42719300	-6.09426000	1.89254600
F	5.07306700	-6.76178000	-0.18736400
F	5.02584700	-5.29385500	-2.48351200
C	6.53479600	-1.87804900	1.87916300
C	6.29478500	-0.53744000	1.91407100
C	4.99671700	0.01189800	2.18302400
C	5.43618400	-2.82217100	2.14703500
H	7.10960000	0.15689800	1.71434300
C	3.42599500	1.86009700	2.35932400
H	3.45335800	-2.89286700	2.61248100
C	2.35960300	0.96096800	2.60341100
C	2.63188700	-0.41328300	2.64049300
H	3.23572800	2.92397000	2.32588400
C	7.88428200	-2.48142500	1.59672900
H	7.76215100	-3.27922000	0.85423900
H	8.53969800	-1.71832100	1.16007900
C	0.95612800	1.41269800	2.77979800
H	0.33475300	0.90301700	1.89022700
C	8.53683300	-3.07989000	2.85744000
H	9.51084000	-3.51837000	2.61370600
H	8.68894900	-2.30998100	3.62249900
H	7.89905700	-3.86478400	3.27285000
C	0.65527600	2.90075100	2.79257700
H	1.09464600	3.38226200	3.67724300
H	1.04994500	3.40401200	1.90693800
H	-0.42353600	3.06921600	2.81868300

H	0.47901800	0.89018800	3.61844800
C	1.97544000	2.48096600	-1.05566100
C	3.08285600	3.41622700	-1.39575900
C	3.72797600	3.32907900	-2.63726700
C	3.55046500	4.39397800	-0.51109300
C	4.78786200	4.16606000	-2.97995300
C	4.60466400	5.24468400	-0.83191700
C	5.22703700	5.12872200	-2.07310700
F	2.98161200	4.54642900	0.69911900
F	5.02459100	6.16412500	0.04415500
F	6.24001900	5.93669400	-2.39110500
F	5.38183300	4.05501700	-4.17136500
F	3.33579400	2.41628600	-3.53025600
C	3.92897400	-0.88604500	2.43508000
H	1.81593900	-1.11846200	2.77797800
C	4.71222600	1.39190800	2.16363300
H	5.52470000	2.09060400	1.97839900
N	4.20814800	-2.24004300	2.43470300
O	5.55580300	-4.04913300	2.11841700
C	-5.26326800	-3.55810200	-1.32242800
C	-6.31835800	-4.55075100	-1.45708800
H	-6.24049200	-4.99806200	-2.45763700
C	-6.36262500	-5.68069800	-0.37577700
H	-5.43477300	-6.24589600	-0.25142600
C	-7.78795400	-4.10121800	-1.18995200
H	-8.13380600	-3.23629300	-1.75887800
C	-8.53289500	-5.42583900	-1.47356600
H	-9.51577300	-5.44951600	-0.99246200
H	-8.69201900	-5.55778900	-2.54896100
C	-7.55494100	-6.51318800	-0.90718900
H	-8.00972900	-7.12037500	-0.11763300
H	-7.22491100	-7.19790200	-1.69536700
C	-6.83653100	-4.94871100	0.90439900
H	-7.33666900	-5.65476400	1.57278700
C	-7.81274400	-3.87371100	0.33863800
H	-8.83479100	-3.94740400	0.72400300
C	-5.75580300	-4.15579400	1.69926400
H	-4.76133600	-4.26930800	1.25194700
H	-5.69929700	-4.48813000	2.74218500
C	-7.23829300	-2.52835500	0.77200000
O	-7.64266100	-1.42873500	0.41603700
N	-6.20089000	-2.76986100	1.62438400
H	-5.60695600	-1.99876800	1.90230500
C	-4.35575700	-2.76264900	-1.19310000

**<sup>5</sup>TS6-S**

N	-0.19592500	2.47500700	0.40137100
N	-2.63514200	0.97431500	0.36631400
N	-1.15983900	-1.40697100	0.71585000
N	1.26788200	0.08178000	0.78676000
C	0.99111200	3.05410700	0.77880300
C	0.85955700	4.48885800	0.72530800
C	-0.39297300	4.75807200	0.26461100
C	-1.05837300	3.49145100	0.09081500
C	-2.41805300	3.35732700	-0.22344700
C	-3.14586500	2.17967700	-0.06319400
C	-4.57928200	2.07023200	-0.19541800
C	-4.92100400	0.81555100	0.20234700
C	-3.69576700	0.13123900	0.53096000
C	-3.61816900	-1.23336000	0.86639000
C	-2.40787700	-1.94392000	0.90908700
C	-2.31197700	-3.37604700	1.02796200
C	-0.99958300	-3.69679000	0.85640000
C	-0.27309900	-2.46451500	0.68357400
C	1.11717000	-2.37062600	0.60895400
C	1.82641000	-1.16687400	0.69633900
C	3.26015900	-1.06254400	0.81851800
C	3.54495800	0.24990200	1.02496600
C	2.29279900	0.96876400	0.98989400
H	1.62867800	5.19769800	0.99323700
H	-0.84480800	5.72519300	0.09811200
H	-5.23477300	2.86168700	-0.52845700
H	-5.90220100	0.36659400	0.25357100
H	-3.13581200	-4.05338600	1.20502700
H	-0.55658700	-4.68151600	0.88537500
H	3.95472800	-1.88596900	0.74529500
H	4.51807900	0.70254600	1.14126100
Mn	-0.68843300	0.51372800	0.55588900
Cl	-0.84239400	0.82014000	2.86034400
O	-0.59447900	0.27272800	-1.19070200
C	-3.14569800	4.58795500	-0.64597200
C	-2.93396600	5.15452000	-1.90599700
C	-4.04487500	5.23791900	0.20598200
C	-3.58543900	6.31721100	-2.31081100
C	-4.71274200	6.39877100	-0.17801400
C	-4.47870600	6.94016900	-1.44111500
C	1.88199400	-3.64596600	0.51445600
C	1.82812100	-4.42759600	-0.64151400

C	2.65815800	-4.13269400	1.56987800
C	2.51198200	-5.62985000	-0.76850700
C	3.36209100	-5.33145300	1.46838600
C	3.28543200	-6.08288100	0.29781800
F	-4.28307600	4.74417400	1.42627700
F	-5.56746000	6.99926200	0.65602300
F	-5.11119600	8.05305200	-1.81824800
F	-3.36498300	6.83338200	-3.52430400
F	-2.08805000	4.57474100	-2.77076800
F	2.74428700	-3.43912100	2.71276900
F	1.13770500	-3.98113600	-1.71680600
F	2.44654800	-6.32930900	-1.89933500
F	3.96239800	-7.22536200	0.19342100
F	4.10361000	-5.76766200	2.49211700
C	6.11899600	-2.59103500	-1.84078300
C	6.07099700	-1.22996000	-1.87303900
C	4.86615600	-0.50236200	-2.15262100
C	4.90071800	-3.37015900	-2.12249000
H	6.97366900	-0.65801600	-1.66331100
C	3.57497800	1.55015200	-2.34055700
H	2.93170000	-3.15942600	-2.60408100
C	2.39490900	0.81120400	-2.59817000
C	2.46989300	-0.58782800	-2.63453100
H	3.53714600	2.63028500	-2.30659200
C	7.36694700	-3.37962500	-1.54826300
H	7.12632700	-4.15372800	-0.80967800
H	8.11952800	-2.71772500	-1.10319800
C	1.07167000	1.45704400	-2.79072500
H	0.37331500	1.03470000	-1.91296900
C	7.94013500	-4.06177900	-2.80510100
H	8.84010800	-4.63391500	-2.55400200
H	8.20661800	-3.31960400	-3.56628600
H	7.20178100	-4.74792000	-3.22863100
C	0.98314500	2.97253600	-2.79744300
H	1.49890800	3.39222500	-3.67230900
H	1.43112800	3.41076000	-1.90266200
H	-0.06087900	3.29068000	-2.83727100
H	0.53778500	1.01057500	-3.63905700
C	2.17382500	2.36117400	1.06339800
C	3.39473100	3.13466400	1.42065600
C	4.00541100	2.95840100	2.67010500
C	4.00391700	4.03957300	0.54468100
C	5.16578800	3.64134100	3.02860900
C	5.16078400	4.73689400	0.88128100

C	5.74500000	4.53523700	2.13006500
F	3.47744900	4.26932500	-0.67245000
F	5.71474700	5.59057600	0.01314200
F	6.85526800	5.19584300	2.46324600
F	5.72316400	3.44865500	4.22724200
F	3.47964100	2.10767500	3.55562800
C	3.68475700	-1.24000900	-2.41742400
H	1.56369000	-1.17005200	-2.78167900
C	4.77965400	0.90404100	-2.13238500
H	5.68108800	1.48022000	-1.93731600
N	3.76944400	-2.61980000	-2.41804500
O	4.84642300	-4.60158300	-2.09877800
C	-5.89283800	-2.54143800	1.11493500
C	-7.18161400	-3.21368100	1.17929000
H	-7.78064000	-2.72600400	1.96066400
C	-8.00619700	-3.28487500	-0.14874700
H	-8.19305500	-2.32352600	-0.63529200
C	-7.19720900	-4.75957000	1.38747300
H	-6.63619800	-5.13157700	2.24667800
C	-8.72190000	-5.01189400	1.42805600
H	-8.96738600	-6.05224100	1.19257400
H	-9.12307800	-4.79880400	2.42448000
C	-9.27850300	-4.00250500	0.36464800
H	-9.81907900	-4.49982200	-0.44737600
H	-9.96693400	-3.28454000	0.82246000
C	-7.21858500	-4.29485700	-1.01956500
H	-7.89144800	-4.76968000	-1.73875600
C	-6.67402400	-5.30168200	0.03789500
H	-7.00010400	-6.33534200	-0.11601900
C	-5.96267500	-3.74915600	-1.76349600
H	-5.83161700	-2.67332000	-1.59812900
H	-6.02875300	-3.92157000	-2.84388700
C	-5.15519800	-5.25855100	-0.09773400
O	-4.35383300	-5.81121200	0.64511700
N	-4.85244100	-4.49898500	-1.18972000
H	-3.88728800	-4.24180300	-1.35424900
C	-4.83771800	-1.94674100	1.03535600

**<sup>3</sup>TS5-R**

N	0.61971800	-1.29390700	-0.15656900
N	-2.18569800	-1.49744800	0.07351500
N	-2.35858400	1.31641800	0.19744400
N	0.43816200	1.49952600	-0.03259800
C	1.93017500	-1.05803600	0.16492600

C	2.68392700	-2.27512900	0.03047100
C	1.82088300	-3.22905200	-0.42420500
C	0.51245500	-2.62526900	-0.48281100
C	-0.69196300	-3.31696100	-0.64719600
C	-1.94126600	-2.79029200	-0.30271500
C	-3.14265900	-3.57134600	-0.12149100
C	-4.08236400	-2.74034900	0.40598100
C	-3.49093600	-1.42349700	0.48351400
C	-4.17806800	-0.24083700	0.78046500
C	-3.64724900	1.03742900	0.56205700
C	-4.42221100	2.25602500	0.52096000
C	-3.59649200	3.24093800	0.07106600
C	-2.29165400	2.65037300	-0.10922600
C	-1.12269100	3.36267900	-0.39885100
C	0.16127400	2.82410300	-0.26456500
C	1.38082800	3.58502600	-0.14312800
C	2.35782800	2.71682800	0.24603100
C	1.76698900	1.40601900	0.27420200
C	2.47436400	0.20505600	0.45604000
H	3.73115800	-2.37128500	0.26853600
H	2.03582200	-4.26779000	-0.62797400
H	-3.23132300	-4.62833500	-0.32841900
H	-5.09394400	-2.98660200	0.69280900
H	-5.47149400	2.33161500	0.76750800
H	-3.83216000	4.28314800	-0.09032200
H	1.46535600	4.64951300	-0.30131700
H	3.40003100	2.91607000	0.45140000
Mn	-0.86777900	0.00591900	-0.03520400
Cl	-0.64868600	-0.09864500	2.33909600
O	-1.16435000	0.08402500	-1.71999100
C	-5.59246300	-0.32469600	1.23962500
C	-6.62247500	-0.76967400	0.40489300
C	-5.94359300	0.07934600	2.53263200
C	-7.94504800	-0.83230800	0.83711600
C	-7.26099300	0.03249700	2.98412000
C	-8.26354200	-0.42735800	2.13218500
C	-0.63984500	-4.73615000	-1.09984900
C	-0.99651200	-5.07239200	-2.40861300
C	-0.25664900	-5.77488000	-0.24703300
C	-0.96998300	-6.38936600	-2.86153700
C	-0.21905800	-7.09953100	-0.67847700
C	-0.57964400	-7.40485100	-1.99005400
C	-1.26305200	4.79663900	-0.77596200
C	-1.76069800	5.14239600	-2.03686300

C	-0.92937100	5.83862700	0.09302200
C	-1.91178600	6.47208200	-2.42480500
C	-1.06527400	7.17485900	-0.27600000
C	-1.56044400	7.49005900	-1.54007000
F	-6.34923000	-1.15194700	-0.85031500
F	-8.90890500	-1.26606200	0.01739300
F	-9.52849600	-0.47899400	2.55547300
F	-7.56873300	0.42190700	4.22545400
F	-5.00316600	0.52977100	3.36899700
F	0.09111400	-5.50593300	1.01578100
F	0.15289200	-8.07679400	0.15435700
F	-0.54870900	-8.67075900	-2.41267600
F	-1.31226700	-6.68462400	-4.12009800
F	-1.37272900	-4.11268400	-3.26553000
F	-0.45640500	5.56395300	1.31709000
F	-2.11146100	4.18528300	-2.90049600
F	-2.38879300	6.77790900	-3.63571000
F	-1.69870400	8.76771700	-1.90267900
F	-0.73287900	8.15322800	0.57417400
C	3.79939600	0.27455600	0.95164400
C	4.84027000	0.29838000	1.57226400
C	5.97456700	0.26386600	2.47392900
H	6.87612100	0.62166200	1.95834500
C	5.78955300	1.01910400	3.83256600
H	5.54871700	2.08227000	3.74677600
C	6.24066200	-1.11088900	3.16228300
H	6.37422400	-1.96063200	2.48955300
C	7.46866100	-0.74805100	4.02922600
H	7.58788700	-1.43585500	4.87236500
H	8.38945000	-0.79417000	3.43717400
C	7.16190400	0.72112200	4.48534100
H	7.12551300	0.82657900	5.57444200
H	7.92343200	1.41645700	4.11579300
C	4.72404900	0.18200400	4.58848600
H	4.86941700	0.29895000	5.66601000
C	5.02761100	-1.26669600	4.10661900
H	5.26287600	-1.96492300	4.91692600
C	3.22418700	0.42866500	4.24178400
H	3.10272400	1.22774300	3.50023800
H	2.64722900	0.70820300	5.13018900
C	3.73583200	-1.75475400	3.43941300
O	3.62001300	-2.79623100	2.80577700
N	2.75873400	-0.84418800	3.70778000
H	1.84185800	-0.92562200	3.27530900



C	6.82581100	0.77452800	-1.33486100
C	5.84300400	1.67771100	-1.72872000
C	4.62033600	1.22143100	-2.24309800
C	4.37365900	-0.16639700	-2.38464200
C	5.38810400	-1.06698900	-1.99987600
C	6.58547300	-0.60955000	-1.48127300
H	6.01031800	2.74722500	-1.61788600
C	3.08618500	-0.58527600	-2.84993700
H	5.19993300	-2.13316700	-2.09361200
H	7.34963200	-1.31723600	-1.17086200
C	2.08215200	0.29732400	-3.14278300
C	2.32330500	1.74709800	-2.99728500
H	2.90494400	-1.65260400	-2.93043200
C	8.15139700	1.26137600	-0.79383100
H	8.02739800	2.25475400	-0.34505400
H	8.48487200	0.59196700	0.01014200
O	1.48304900	2.62140300	-3.19459700
C	0.71503500	-0.09302700	-3.54128700
H	0.02030700	0.08741800	-2.61219700
C	9.23726700	1.32268800	-1.88401300
H	10.19057700	1.66828800	-1.46883400
H	9.39603900	0.33512600	-2.33119200
H	8.94256000	2.00816800	-2.68631000
N	3.61408300	2.09445600	-2.60013100
H	3.74504700	3.08945200	-2.46107000
C	0.46878200	-1.52911000	-3.97557900
H	0.75578500	-2.24439100	-3.19896400
H	-0.59477300	-1.68267100	-4.17367800
H	1.03083400	-1.76831500	-4.88772800
H	0.29173100	0.64392400	-4.23205100

**<sup>3</sup>TS5-S**

N	0.24496600	1.62866800	-0.01792800
N	-2.52629800	1.15109800	0.17943900
N	-2.04774600	-1.62582200	0.00053300
N	0.71857400	-1.12363500	-0.20667800
C	1.57842200	1.66482400	0.27875400
C	2.03908300	3.02411700	0.24318500
C	0.97228000	3.79854300	-0.11926500
C	-0.16693700	2.92268700	-0.22914900
C	-1.50169200	3.32965900	-0.34176600
C	-2.59065400	2.49769900	-0.06478100
C	-3.93857400	2.95749300	0.17327200
C	-4.65699000	1.88297600	0.59979600

C	-3.77642300	0.73779800	0.55441300
C	-4.17265800	-0.59718900	0.70932600
C	-3.36456900	-1.68733600	0.36623400
C	-3.84075200	-3.04101000	0.18564800
C	-2.81340100	-3.76048500	-0.34142200
C	-1.67677900	-2.87316200	-0.42933100
C	-0.37444100	-3.26249200	-0.75193000
C	0.74711700	-2.45369100	-0.53878400
C	2.09763400	-2.94371100	-0.40733700
C	2.85213000	-1.92002500	0.08223800
C	1.98905800	-0.77060000	0.16954100
C	2.39987900	0.53728400	0.47140700
H	3.05991000	3.32421600	0.43169100
H	0.94822700	4.87042300	-0.25241000
H	-4.27139500	3.98078000	0.07225900
H	-5.69623400	1.85873900	0.89242300
H	-4.84533900	-3.37721700	0.39838100
H	-2.80807400	-4.80407600	-0.62123000
H	2.40394900	-3.96124800	-0.60111300
H	3.88907900	-1.92557600	0.37880800
Mn	-0.89770000	0.00829000	-0.06775900
Cl	-0.67985400	-0.12923400	2.30585100
O	-1.17312800	0.07212800	-1.75801600
C	-5.56648300	-0.88800600	1.14686200
C	-6.67429500	-0.60644900	0.34118900
C	-5.81046400	-1.49266100	2.38509900
C	-7.97428700	-0.89274500	0.75085900
C	-7.10188900	-1.79495600	2.81258000
C	-8.18639400	-1.49110800	1.99169600
C	-1.78602800	4.75215400	-0.68096900
C	-2.27555800	5.08676900	-1.94734700
C	-1.59601300	5.79309700	0.23158800
C	-2.56297500	6.40349000	-2.29973000
C	-1.87173300	7.11820600	-0.09919500
C	-2.35946700	7.42145800	-1.36938800
C	-0.13776300	-4.66369900	-1.20071200
C	0.12758700	-4.94664500	-2.54411300
C	-0.14779200	-5.73192600	-0.29958900
C	0.38263200	-6.24774000	-2.97561600
C	0.10030000	-7.03932100	-0.71084500
C	0.36904900	-7.29373900	-2.05496200
F	-6.50058500	-0.04382500	-0.86296100
F	-9.01514000	-0.60845600	-0.03980900
F	-9.42792900	-1.77361000	2.39273200

F	-7.30753000	-2.36984400	4.00181600
F	-4.78881300	-1.79938500	3.19029300
F	-1.13061200	5.52828700	1.45916100
F	-1.67805700	8.09660700	0.79163700
F	-2.62849300	8.68745600	-1.69571900
F	-3.02668200	6.69698400	-3.51876100
F	-2.47597600	4.12693400	-2.86038400
F	-0.40166800	-5.50754100	0.99556400
F	0.12846200	-3.96564100	-3.44675100
F	0.63159700	-6.50031400	-4.26531200
F	0.60925900	-8.54322600	-2.46119100
F	0.08682100	-8.04651400	0.16950300
C	3.70102000	0.74135100	0.99201600
C	4.72551200	0.88192600	1.62417200
C	5.85470300	0.98054800	2.52745000
H	6.70118700	1.45739700	2.01501900
C	6.29921000	-0.35505200	3.20007300
H	6.53991200	-1.17346700	2.51814700
C	5.57666100	1.69065400	3.89421400
H	5.20026200	2.71456200	3.82006200
C	6.97718500	1.56550400	4.54339900
H	6.92877000	1.65047500	5.63382700
H	7.64090900	2.35930200	4.18385300
C	7.47269500	0.15524800	4.06764500
H	7.68594600	-0.52111900	4.90143500
H	8.38805300	0.23816500	3.47119800
C	5.11972500	-0.67736100	4.14525500
H	5.44672100	-1.34609700	4.94852000
C	4.62924000	0.71458800	4.64009000
H	4.75631200	0.83906800	5.71908300
N	2.81653700	-0.54863100	3.73931500
H	1.92115700	-0.74214400	3.29800100
C	6.77395800	0.93218200	-1.22439800
C	5.98019300	-0.10250400	-1.71013800
C	4.70642200	0.16122200	-2.23392700
C	4.20867600	1.48750400	-2.28179400
C	5.03777800	2.52685400	-1.81212300
C	6.29107500	2.25771700	-1.29233400
H	6.33474500	-1.12991700	-1.66054800
C	2.86705600	1.69540900	-2.73652000
H	4.66167300	3.54628200	-1.84294600
H	6.91049700	3.06853500	-0.91785400
C	2.04676300	0.66686800	-3.11602000
C	2.56192000	-0.71806600	-3.09537300

H	2.48865900	2.71306200	-2.73502100
C	8.15019400	0.64686700	-0.66630000
H	8.16542100	-0.35250800	-0.21387900
H	8.37347800	1.35868500	0.13903800
O	1.90819500	-1.71194700	-3.39765600
C	0.62979900	0.82022500	-3.49616000
H	-0.02002100	0.40696500	-2.59861200
C	9.24601900	0.74045300	-1.74402800
H	10.23425400	0.53653600	-1.31694500
H	9.26576300	1.73957200	-2.19348600
H	9.06283800	0.01768800	-2.54682600
N	3.88884000	-0.85057800	-2.68846500
H	4.19845100	-1.81252500	-2.61397200
C	0.09965600	2.21552300	-3.78356100
H	0.26237900	2.89334700	-2.93980400
H	-0.97794600	2.17830200	-3.96088300
H	0.58382600	2.64726800	-4.66929300
H	0.35398100	0.08624400	-4.26069900
C	3.90365900	-1.32475100	3.47266000
O	3.92604500	-2.37014300	2.83488000
C	3.11073300	0.76757400	4.29057300
H	2.50043300	0.95768900	5.18035300
H	2.88727400	1.55289200	3.55843800

**<sup>5</sup>TS5-R**

N	0.60922800	-1.29716900	-0.21614800
N	-2.21294300	-1.53779200	-0.03261000
N	-2.42950000	1.26922700	0.16010100
N	0.37946000	1.51300400	-0.00456000
C	1.91413200	-1.04120300	0.10411700
C	2.69037900	-2.24730800	-0.00701100
C	1.83806800	-3.22331400	-0.43347900
C	0.52582100	-2.62920900	-0.51697800
C	-0.66826800	-3.35172000	-0.67881300
C	-1.93416200	-2.83834600	-0.39608500
C	-3.14376200	-3.62230900	-0.30796200
C	-4.12057000	-2.80304100	0.16046000
C	-3.54314000	-1.48537100	0.29526100
C	-4.25963100	-0.32066800	0.58992900
C	-3.73377300	0.96832300	0.44808200
C	-4.52019200	2.17980700	0.43033100
C	-3.68532600	3.19219600	0.07284800
C	-2.36660800	2.62457800	-0.07482300
C	-1.20476200	3.36513900	-0.29382600

C	0.08896600	2.83967000	-0.16951000
C	1.29464400	3.61615800	-0.01520700
C	2.28782700	2.74265100	0.31764400
C	1.71039100	1.42581300	0.28324500
C	2.43669600	0.22734100	0.41601800
H	3.73719700	-2.32617700	0.23876000
H	2.06043500	-4.26717600	-0.60021100
H	-3.22415500	-4.67227200	-0.54728600
H	-5.14852900	-3.05732600	0.37118900
H	-5.58066800	2.23328700	0.62976800
H	-3.92517800	4.23877600	-0.04829500
H	1.36288300	4.68798800	-0.12281200
H	3.32913200	2.94562000	0.52266900
Mn	-0.93233400	-0.01534000	-0.05263400
Cl	-0.64572500	-0.18415900	2.31510500
O	-1.13357300	0.10759900	-1.77453200
C	-5.69569700	-0.43555200	0.96857100
C	-6.67330500	-0.85699100	0.06188900
C	-6.12103200	-0.08610500	2.25502000
C	-8.01672200	-0.94829200	0.41794500
C	-7.46041300	-0.16264200	2.63143200
C	-8.40981500	-0.59747100	1.70835300
C	-0.54348900	-4.79534800	-1.02901800
C	-0.11290800	-5.19657400	-2.29704600
C	-0.80430400	-5.80330100	-0.09408600
C	0.04409100	-6.53909100	-2.63263900
C	-0.66167000	-7.15296600	-0.40849400
C	-0.23373300	-7.52040400	-1.68305600
C	-1.35632000	4.81559600	-0.59849800
C	-1.82725800	5.22400600	-1.85070700
C	-1.05301600	5.81184600	0.33294700
C	-1.98277700	6.57125200	-2.17019300
C	-1.19449000	7.16470500	0.03318800
C	-1.66297400	7.54308100	-1.22375200
F	-6.32647400	-1.18954200	-1.18915500
F	-8.92936900	-1.35863400	-0.46949600
F	-9.69522700	-0.67706000	2.05919900
F	-7.83967100	0.17473700	3.86810100
F	-5.23231200	0.34006800	3.15817000
F	-1.20471700	-5.48165300	1.14120600
F	-0.92242600	-8.09450700	0.50367200
F	-0.09043800	-8.81033100	-1.99398700
F	0.45468100	-6.89043700	-3.85595400
F	0.16553300	-4.27819900	-3.23390200

F	-0.60523200	5.47516100	1.55067300
F	-2.14762700	4.31153600	-2.77263400
F	-2.43421400	6.93758900	-3.37401400
F	-1.80607300	8.83705600	-1.52040500
F	-0.89218100	8.09876500	0.94225500
C	3.75983400	0.30619500	0.90956300
C	4.79969500	0.33821300	1.53258000
C	5.93820100	0.31616400	2.42759700
H	6.82842500	0.69565400	1.90769300
C	5.74585500	1.05904400	3.79231500
H	5.48403500	2.11781500	3.71449500
C	6.23528000	-1.05765000	3.10485200
H	6.38146100	-1.90003500	2.42554700
C	7.46126100	-0.67581900	3.96630400
H	7.60033800	-1.36722600	4.80337700
H	8.37877300	-0.69847700	3.36776300
C	7.12740700	0.78330700	4.43537000
H	7.09441000	0.87954600	5.52540000
H	7.87285400	1.49669100	4.06747600
C	4.70048200	0.19616000	4.54706300
H	4.84748100	0.30990700	5.62468300
C	5.03115200	-1.24330200	4.05544100
H	5.28557100	-1.94110500	4.86023800
N	2.75370000	-0.86226700	3.66219800
H	1.83453900	-0.96025000	3.23714700
C	6.89632600	0.83888200	-1.29109600
C	5.94153600	1.78412400	-1.65541500
C	4.70098200	1.38204000	-2.17171800
C	4.40594900	0.00582900	-2.34448000
C	5.39129500	-0.93795500	-1.98355000
C	6.60680200	-0.53310200	-1.46461100
H	6.14689400	2.84446700	-1.52281500
C	3.10939700	-0.35802100	-2.82120200
H	5.16550000	-1.99437900	-2.10018100
H	7.34870400	-1.27300900	-1.17614500
C	2.13503300	0.56540100	-3.11191700
C	2.42459400	2.00325000	-2.92183600
H	2.89064100	-1.41662500	-2.92372700
C	8.24348800	1.26721700	-0.75387800
H	8.16182600	2.25948400	-0.29309200
H	8.55608000	0.57577000	0.03985200
O	1.61913600	2.91222500	-3.10192300
C	0.77723400	0.22474800	-3.55438000
H	0.05306000	0.29451900	-2.60932400

H	0.35846500	1.02770400	-4.16923800
C	0.52857400	-1.16653300	-4.11593800
H	1.12541900	-1.34741500	-5.01973300
H	0.76560300	-1.94740800	-3.38830100
H	-0.52889500	-1.27750900	-4.37049900
C	9.32349900	1.29859000	-1.85128900
H	9.05061500	2.00460700	-2.64337900
H	10.29234300	1.60145000	-1.43880000
H	9.44022600	0.31088600	-2.31085500
N	3.72299900	2.29576300	-2.50341500
H	3.88932900	3.28312300	-2.34763800
C	3.74618300	-1.75458900	3.39197700
C	3.19472700	0.41468900	4.20668700
H	2.61478200	0.67422600	5.09917000
H	3.05383400	1.21820300	3.47330400
O	3.64934600	-2.79811400	2.75809700

**<sup>5</sup>TS5-S**

N	0.24287400	1.63432100	0.00609200
N	-2.54440000	1.16042700	0.18208800
N	-2.08833100	-1.60979500	0.00109900
N	0.69719300	-1.14317100	-0.18880100
C	1.57922400	1.65848400	0.27419800
C	2.05265400	3.01509700	0.26133100
C	0.98342800	3.80316000	-0.06178500
C	-0.15828200	2.93008000	-0.17655400
C	-1.49389400	3.34494700	-0.28695300
C	-2.58946300	2.51822700	-0.04157100
C	-3.93936900	2.98731600	0.16189800
C	-4.68236900	1.91537600	0.54671900
C	-3.81323200	0.76156500	0.51081000
C	-4.22750000	-0.56894900	0.64430800
C	-3.41837200	-1.66398800	0.32268900
C	-3.89987000	-3.01428100	0.13722400
C	-2.86150400	-3.74751700	-0.34381200
C	-1.71310700	-2.87416900	-0.39994900
C	-0.41255300	-3.28092900	-0.69003300
C	0.71928800	-2.47376600	-0.49483400
C	2.06853500	-2.97192000	-0.38066500
C	2.83809000	-1.93902500	0.06461200
C	1.97558700	-0.78803200	0.14897200
C	2.39769400	0.52077900	0.43573600
H	3.07837300	3.30497800	0.43889500
H	0.96126600	4.87775200	-0.17139100

H	-4.25842100	4.01535200	0.06575500
H	-5.73019800	1.89820600	0.80711600
H	-4.91443100	-3.33957000	0.31650400
H	-2.85915600	-4.79263100	-0.61686100
H	2.36671500	-3.99504800	-0.55616300
H	3.88207300	-1.94099100	0.33503100
Mn	-0.94024400	0.00366000	-0.02930500
Cl	-0.63466900	-0.11943800	2.33779300
O	-1.14790700	0.09597300	-1.75491200
C	-5.63731100	-0.84824900	1.03499100
C	-6.71571700	-0.54515500	0.19778700
C	-5.92723500	-1.46234900	2.25858000
C	-8.03121000	-0.81997100	0.56358200
C	-7.23479700	-1.75333900	2.64225700
C	-8.28927600	-1.42814400	1.79087200
C	-1.76386000	4.77541600	-0.60613600
C	-2.21604400	5.13760200	-1.87857600
C	-1.58971600	5.79615500	0.33166500
C	-2.48440100	6.46332400	-2.21203100
C	-1.84764100	7.12950500	0.02023500
C	-2.29895000	7.46111300	-1.25635800
C	-0.18046600	-4.69522900	-1.09806700
C	0.18328600	-5.00841000	-2.41175900
C	-0.28452400	-5.74777400	-0.18386000
C	0.43924900	-6.32218000	-2.80190300
C	-0.03801800	-7.06740900	-0.55467200
C	0.32809000	-7.35173000	-1.86940900
F	-6.49734400	0.02798900	-0.99380200
F	-9.04314700	-0.51506800	-0.25616300
F	-9.54592700	-1.69966200	2.14978400
F	-7.48441900	-2.33760500	3.81832900
F	-4.93468100	-1.78975800	3.09178600
F	-1.15732000	5.50278100	1.56464600
F	-1.67061900	8.08883800	0.93492100
F	-2.55042700	8.73525300	-1.56454400
F	-2.91296400	6.78450200	-3.43688800
F	-2.39769400	4.19734900	-2.81503800
F	-0.63077000	-5.49703900	1.08486300
F	0.28288300	-4.04289100	-3.32538600
F	0.78255700	-6.60212600	-4.06390700
F	0.56837200	-8.61319500	-2.23612700
F	-0.14377800	-8.05810500	0.33788600
C	3.70851000	0.71626600	0.92939500
C	4.74298500	0.85384000	1.54678500



C	5.88861800	0.95034900	2.42763700
H	6.72883200	1.41320200	1.89243200
C	6.33142500	-0.38197600	3.10766000
H	6.55137900	-1.21045300	2.43096000
C	5.64216500	1.67954900	3.79075000
H	5.27518500	2.70640500	3.71079500
C	7.05284600	1.54701900	4.41590200
H	7.02467400	1.64489900	5.50593200
H	7.71798500	2.32980200	4.03544600
C	7.52545000	0.12638100	3.94782000
H	7.74701200	-0.54249600	4.78543200
H	8.43057000	0.19310700	3.33393700
C	5.16523100	-0.68060000	4.07679700
H	5.49888400	-1.34384900	4.88182000
C	4.69798200	0.72199200	4.56408500
H	4.84531100	0.85755000	5.63913700
C	3.93068200	-1.32234500	3.43214400
N	2.85691900	-0.53100800	3.70676500
H	1.95000800	-0.72087200	3.28716200
C	6.84730500	0.86874900	-1.26993800
C	6.03819100	-0.15504100	-1.75453500
C	4.75628700	0.12241700	-2.25032300
C	4.26369100	1.45262700	-2.26834900
C	5.10664500	2.48043200	-1.79530300
C	6.36890800	2.19740900	-1.30589300
H	6.38952000	-1.18445100	-1.72957600
C	2.91977100	1.67533300	-2.70212700
H	4.73493900	3.50187500	-1.80294300
H	6.99999000	2.99943300	-0.93188100
C	2.08754500	0.65889800	-3.10158300
C	2.59681700	-0.73052600	-3.10490400
H	2.54585700	2.69428300	-2.67664900
C	8.23469000	0.56955100	-0.74793800
H	8.25967500	-0.44145700	-0.32271800
H	8.47478900	1.25999900	0.07115600
O	1.93803700	-1.71633100	-3.41837300
C	0.67878200	0.83115800	-3.47900300
H	0.00901300	0.41507400	-2.57962900
H	0.39301100	0.10636900	-4.24860500
C	0.15975200	2.23518400	-3.74575000
H	0.65285700	2.68648600	-4.61711300
H	0.31509700	2.89493000	-2.88587800
H	-0.91650600	2.20561100	-3.93269100
C	9.30794800	0.69254200	-1.84537400

H	9.10833700	-0.00894600	-2.66295700
H	10.30478800	0.47824200	-1.44420500
H	9.31812500	1.70320000	-2.26853500
N	3.92623900	-0.87694400	-2.70870000
H	4.23153100	-1.84184700	-2.65644800
C	3.17421500	0.78705800	4.24012400
H	2.58127000	0.99232900	5.13818900
H	2.94581100	1.56796000	3.50456300
O	3.93212600	-2.37527100	2.80645400

**<sup>3</sup>TS7-R**

N	0.87482500	2.11821400	0.23471000
N	-1.15930300	0.15673300	0.09311300
N	0.79270400	-1.85061200	-0.12551900
N	2.83572400	0.07524900	0.08350100
C	1.95518900	2.88321700	0.59033700
C	1.55017600	4.26991700	0.65317400
C	0.24595300	4.32542200	0.27022000
C	-0.18449300	2.96711700	0.04089300
C	-1.50819300	2.57933300	-0.17127900
C	-1.95909900	1.26166200	-0.04530800
C	-3.33964200	0.88109000	0.14284500
C	-3.34800200	-0.44439700	0.45201200
C	-1.98195600	-0.89825400	0.38534200
C	-1.56762200	-2.23402300	0.48912300
C	-0.26944600	-2.66670200	0.15694100
C	0.11273900	-4.03390200	-0.04986300
C	1.40493400	-4.02600300	-0.49788900
C	1.84233000	-2.65523500	-0.50274200
C	3.16035100	-2.22865100	-0.70768300
C	3.62305600	-0.95514000	-0.36425800
C	5.00786200	-0.55027400	-0.31226400
C	5.03563700	0.70617800	0.20926300
C	3.66395200	1.11093200	0.41712100
H	2.19077300	5.09288300	0.93344200
H	-0.38971400	5.19596100	0.19193400
H	-4.18230700	1.55420500	0.08189700
H	-4.18825100	-1.06953600	0.70610200
H	-0.54260000	-4.87915500	0.10552900
H	2.02437300	-4.87432300	-0.75229800
H	5.84833500	-1.15999200	-0.60984500
H	5.90003500	1.32680900	0.39620600
Mn	0.83240300	0.12157400	0.01879700
Cl	0.80349500	-0.08200500	2.38936500

O	0.88550200	0.37054800	-1.68614200
C	-2.54465800	3.62141200	-0.42505900
C	-2.96713500	3.89687200	-1.72428100
C	-3.19834100	4.28860500	0.61356700
C	-4.02277200	4.75578900	-2.00340200
C	-4.24610800	5.17311200	0.36450400
C	-4.66127800	5.40156600	-0.94716500
C	4.12106100	-3.22611600	-1.25320600
C	4.01374900	-3.65346400	-2.58077500
C	5.13816500	-3.79233400	-0.47903600
C	4.87862100	-4.59941400	-3.12422000
C	6.02079400	-4.73548500	-1.00179600
C	5.88735800	-5.14096000	-2.32874000
F	-2.83109400	4.06783100	1.88098600
F	-4.85897000	5.79976200	1.37342900
F	-5.66896100	6.24083600	-1.18896800
F	-4.41371300	4.96586600	-3.25977400
F	-2.36400000	3.27843300	-2.76807100
F	5.28421700	-3.42893600	0.80102300
F	3.05481600	-3.14645100	-3.37361700
F	4.75216300	-4.98610500	-4.39765500
F	6.72474500	-6.04644600	-2.83781300
F	6.98509800	-5.25968900	-0.23911400
C	-3.18970300	-3.93277800	1.63912700
C	-3.94480400	-4.71356900	2.60173300
H	-4.48340100	-5.52431000	2.09281600
C	-4.91311800	-3.90324500	3.52004000
H	-5.65217700	-3.28560800	3.00555000
C	-3.12378200	-5.28493100	3.80727900
H	-2.28134100	-5.92689400	3.53556600
C	-4.25956100	-6.00479300	4.57591600
H	-4.00338300	-6.15711300	5.62935800
H	-4.45402200	-6.99137200	4.14163700
C	-5.48910700	-5.04966300	4.38386800
H	-5.88823000	-4.67947700	5.33348500
H	-6.30693200	-5.55760900	3.86124900
C	-3.94986100	-3.08590500	4.40842400
H	-4.45119000	-2.78255400	5.33367700
C	-2.73205600	-4.02944800	4.63005300
H	-2.61105800	-4.30934300	5.68021900
C	-3.37444600	-1.81942600	3.76345500
N	-2.01659300	-1.90221600	3.82511600
H	-1.42999200	-1.19691800	3.38612400
C	-6.06440000	-0.19143500	-2.18849800

C	-5.42098600	-1.38843700	-2.27150300
C	-4.03536200	-1.49823100	-2.64039100
C	-5.33673000	1.05005400	-2.51252900
H	-5.94292400	-2.30622500	-2.01303100
C	-1.94615700	-2.72166400	-2.83528800
H	-3.54352300	1.73489600	-3.17572800
C	-1.25607900	-1.53170100	-3.16583900
C	-1.97204000	-0.33447200	-3.25564500
H	-1.38767400	-3.64850400	-2.74637000
C	-7.48862100	0.00270600	-1.73766100
H	-8.02743300	0.53674000	-2.53267600
H	-7.47812300	0.71058000	-0.89783000
C	0.21980900	-1.52150500	-3.30600900
H	0.66971300	-2.48727000	-3.06457800
H	0.58981000	-0.77236100	-2.43602000
C	0.82695100	-0.90663100	-4.56035700
H	1.91828600	-0.90332300	-4.48452200
H	0.48916200	0.12326000	-4.71114800
H	0.54385800	-1.49089200	-5.44589000
C	-8.24018200	-1.27012500	-1.34779000
H	-9.26021700	-1.02689700	-1.03370900
H	-7.74932500	-1.78650200	-0.51408800
H	-8.30870600	-1.97258700	-2.18707600
C	-2.49126200	-3.19500200	0.97569300
C	3.26503700	2.41559500	0.73811700
C	4.32859300	3.37371100	1.14956900
C	4.98081600	3.22618400	2.37893300
C	4.74192000	4.42621700	0.32668800
C	5.99353900	4.09450700	2.78155500
C	5.74655800	5.31075600	0.71131600
C	6.37479700	5.14123200	1.94397700
F	4.16611400	4.60549300	-0.87055900
F	6.11863100	6.31032100	-0.09577500
F	7.34196200	5.98027800	2.32085900
F	6.59836800	3.93264900	3.96251200
F	4.63910200	2.22784400	3.19936900
C	-3.34165000	-0.31203700	-2.98723500
C	-3.30929500	-2.70455200	-2.59507900
H	-3.82791200	-3.61869900	-2.31841800
H	-1.44832000	0.59927300	-3.43720600
N	-4.04401900	0.87529300	-2.98195000
O	-5.80581700	2.18298400	-2.38068200
C	-1.48610600	-3.21351400	4.16942000
H	-0.74148400	-3.13102800	4.96886900

H	-0.99429300	-3.67329500	3.30298400
O	-4.03772400	-0.89734000	3.30608100

**<sup>3</sup>TS7-S**

N	-0.67918000	2.23053500	0.30653400
N	1.27734000	0.19854500	0.16965400
N	-0.74686300	-1.72312700	-0.17190600
N	-2.72245800	0.28159600	0.02509400
C	-1.74508200	3.03221600	0.61009700
C	-1.30648700	4.40808200	0.65424400
C	0.01592700	4.41859500	0.32909700
C	0.41375500	3.04562600	0.14066800
C	1.72929900	2.61152600	-0.02258000
C	2.12386800	1.27476300	0.08840600
C	3.48213500	0.83053500	0.29127700
C	3.42737500	-0.50888200	0.54088000
C	2.04624400	-0.89900200	0.43512000
C	1.57813500	-2.22285800	0.48407200
C	0.27440200	-2.59320000	0.11491600
C	-0.16231600	-3.94019900	-0.12794200
C	-1.43580700	-3.86586800	-0.61170500
C	-1.81840300	-2.47755000	-0.59043100
C	-3.11558300	-1.99903000	-0.80301200
C	-3.53869200	-0.71822300	-0.43211700
C	-4.91382300	-0.28270400	-0.35086900
C	-4.90618300	0.95950400	0.20137400
C	-3.52240500	1.33390800	0.38932000
H	-1.94214000	5.25352600	0.87464800
H	0.67927700	5.26902800	0.25771400
H	4.35460000	1.46691700	0.25162600
H	4.24211300	-1.19179900	0.73091400
H	0.43154500	-4.81788400	0.07342000
H	-2.08860300	-4.68340300	-0.88120900
H	-5.77238400	-0.86874700	-0.64336000
H	-5.75697100	1.58336000	0.43166400
Mn	-0.71840000	0.24049900	0.02935600
Cl	-0.78960600	-0.04023400	2.38904700
O	-0.69752700	0.54967200	-1.66713600
C	2.81050000	3.61916800	-0.22449000
C	3.23759000	3.95333100	-1.50831800
C	3.49632900	4.19723100	0.84613000
C	4.32307200	4.78786700	-1.74393200
C	4.57601800	5.05418700	0.64216500
C	4.99096800	5.34630800	-0.65674600

C	-4.10293900	-2.95041100	-1.38285100
C	-3.99450300	-3.34507800	-2.72016000
C	-5.14205500	-3.50860500	-0.63266800
C	-4.87929100	-4.25200600	-3.29654400
C	-6.04519000	-4.41261800	-1.18865400
C	-5.90996400	-4.78631800	-2.52467500
F	3.13207000	3.91147200	2.10241600
F	5.21961100	5.59349600	1.68244600
F	6.02927100	6.15886400	-0.85621100
F	4.71789400	5.05404100	-2.98832300
F	2.61316700	3.41210800	-2.58147300
F	-5.29157900	-3.17329300	0.65413500
F	-3.01245600	-2.84497500	-3.48972000
F	-4.75104200	-4.60820300	-4.57886900
F	-6.76746600	-5.65380300	-3.06564700
F	-7.03195400	-4.92851700	-0.44978800
C	3.09379000	-4.02740000	1.61577500
C	3.71194800	-4.92959500	2.56969000
H	4.57699500	-5.43112700	2.11539200
C	4.11555500	-4.29522700	3.94388400
H	4.80953900	-3.45241800	3.88325100
C	2.75122200	-5.97247400	3.22332200
H	2.20203400	-6.61315600	2.53032100
C	3.74089800	-6.70212100	4.16177200
H	3.22302400	-7.20076300	4.98719600
H	4.30073200	-7.46931100	3.61595900
C	4.68683200	-5.54979700	4.64973000
H	4.68893000	-5.43712700	5.73868500
H	5.72151500	-5.72970000	4.33852700
C	2.76068400	-3.96059500	4.62190100
H	2.88342200	-3.99198000	5.70806800
C	1.83163700	-5.09604700	4.10146200
H	1.37901300	-5.69823000	4.89653500
N	0.79222600	-3.05261700	3.63100000
H	0.17133900	-2.38183000	3.18485400
C	6.18634100	-0.22877700	-2.08532400
C	5.51076400	-1.40305700	-2.22246800
C	4.12406100	-1.45861100	-2.59960300
C	5.49242600	1.04546600	-2.34956100
H	6.00806400	-2.34580900	-2.00867600
C	2.00419000	-2.61457900	-2.86529300
H	3.72299500	1.80761100	-2.99490300
C	1.35249600	-1.39374700	-3.15759800
C	2.10092200	-0.21380300	-3.18758500

H	1.41917400	-3.52799100	-2.81823300
C	7.61757200	-0.09396400	-1.63381800
H	8.16524100	0.46668500	-2.40395100
H	7.63137500	0.57029900	-0.75892100
C	-0.12029900	-1.33447400	-3.32177000
H	-0.60550000	-2.28942700	-3.10805700
H	-0.47564900	-0.58883900	-2.44056600
C	-0.68505800	-0.67279100	-4.57178300
H	-1.77671000	-0.63328800	-4.51356200
H	-0.30833700	0.34719900	-4.69571300
H	-0.40775800	-1.24884600	-5.46457700
C	8.33972400	-1.40369700	-1.31723000
H	9.36758200	-1.20303300	-0.99853200
H	7.84162900	-1.95312800	-0.50915800
H	8.38517700	-2.06176900	-2.19308700
C	2.45883500	-3.22888500	0.95905800
C	-3.07789900	2.61574800	0.72683400
C	-4.08139100	3.64160600	1.12829700
C	-4.10877100	4.13485400	2.43731400
C	-5.00337100	4.17432500	0.22219200
C	-5.02188300	5.10938300	2.83533900
C	-5.93013500	5.14326300	0.59907800
C	-5.93632900	5.61245200	1.91159200
F	-5.01259000	3.75062800	-1.04962800
F	-6.80326800	5.63160800	-0.28871400
F	-6.81721800	6.54395900	2.28281600
F	-5.02839000	5.56203700	4.09297700
F	-3.23885300	3.67406100	3.34143500
C	3.46632500	-0.24007300	-2.90004100
C	3.36461500	-2.64516500	-2.61046400
H	3.85470500	-3.58438900	-2.36784300
H	1.60386800	0.74008900	-3.33603300
N	4.19883300	0.92766100	-2.83216500
O	5.99070100	2.15797800	-2.15830500
C	0.69105100	-4.38375800	3.36318900
C	2.05278200	-2.63016400	4.22420700
H	1.87439600	-1.99236000	5.09686600
H	2.64557900	-2.05104800	3.50479500
O	-0.16556500	-4.93600500	2.68383000

**<sup>5</sup>TS7-R**

N	0.90307100	2.09932100	0.25509600
N	-1.15755600	0.17028400	0.12002000
N	0.77777200	-1.86369700	-0.13485200

N	2.84593900	0.05466300	0.12947000
C	1.99343500	2.86571500	0.59171600
C	1.59938300	4.25487800	0.63570000
C	0.29220200	4.31774400	0.26456100
C	-0.15705100	2.96405500	0.06265200
C	-1.48414900	2.59373100	-0.12562700
C	-1.95010700	1.27765100	0.00282700
C	-3.33370100	0.90946600	0.18500800
C	-3.35391500	-0.42416100	0.45791100
C	-1.99000900	-0.88689800	0.38027000
C	-1.59313500	-2.22902400	0.43947300
C	-0.29449000	-2.67203300	0.10689300
C	0.07300900	-4.04189500	-0.11750700
C	1.37556000	-4.03918900	-0.53332500
C	1.82246000	-2.66975500	-0.50450600
C	3.14974300	-2.25175500	-0.67572800
C	3.62309900	-0.98900400	-0.31211000
C	5.01338800	-0.60134600	-0.25394100
C	5.05561000	0.65750500	0.25879200
C	3.68733600	1.07945000	0.45592300
H	2.24846800	5.07621000	0.90061800
H	-0.33473400	5.19393000	0.17984200
H	-4.16973600	1.59187100	0.13872700
H	-4.19967400	-1.04902200	0.69341800
H	-0.59445100	-4.88244100	0.00876300
H	1.99338500	-4.88888800	-0.78702300
H	5.84742600	-1.22252900	-0.54553700
H	5.92657500	1.26924300	0.44438800
Mn	0.84591500	0.13331500	0.06676400
Cl	0.78885100	-0.19299300	2.42039700
O	0.92102900	0.34443000	-1.67445700
C	-2.51004900	3.64913000	-0.36749600
C	-2.91209300	3.96229400	-1.66459900
C	-3.17195400	4.29445600	0.67970000
C	-3.95482600	4.83971400	-1.93467600
C	-4.20782300	5.19543600	0.44013300
C	-4.60170300	5.46358600	-0.87052700
C	4.10522800	-3.24951900	-1.23046200
C	3.99759900	-3.65556100	-2.56492500
C	5.11384400	-3.83707600	-0.46149500
C	4.85584900	-4.60096600	-3.11972100
C	5.98921600	-4.78054300	-0.99571300
C	5.85662600	-5.16417300	-2.32919000
F	-2.82476300	4.03599600	1.94561700



F	-4.82874600	5.80086200	1.45701700
F	-5.59813900	6.31853600	-1.10364500
F	-4.32778400	5.08529600	-3.19009300
F	-2.30488600	3.36116800	-2.71586900
F	5.25880300	-3.49471300	0.82458100
F	3.04566000	-3.12812200	-3.35195700
F	4.73031900	-4.96732900	-4.39927000
F	6.68726600	-6.06972900	-2.84930100
F	6.94576100	-5.32572900	-0.23782100
C	-3.24143500	-3.94631300	1.52221500
C	-4.01063500	-4.75053400	2.45353900
H	-4.55788400	-5.53510600	1.91376100
C	-4.97106400	-3.96020400	3.39715700
H	-5.69959300	-3.31428500	2.90274500
C	-3.20192800	-5.37621300	3.64046800
H	-2.36741200	-6.01955100	3.34840200
C	-4.35058600	-6.10739400	4.37866000
H	-4.10042300	-6.30149500	5.42664700
H	-4.55721100	-7.07468800	3.90813400
C	-5.56593600	-5.12863800	4.21760000
H	-5.96283600	-4.78708300	5.17879000
H	-6.38913400	-5.60588300	3.67487200
C	-3.99960500	-3.18853600	4.31682900
H	-4.49999100	-2.91057400	5.25051600
C	-2.79612600	-4.15664800	4.50909900
H	-2.68357100	-4.47571800	5.54896500
C	-3.40349600	-1.90873600	3.71828200
N	-2.04752300	-2.01273300	3.78186200
H	-1.44852000	-1.30069000	3.37095000
C	-6.07036600	-0.04398400	-2.16225900
C	-5.45083600	-1.25378500	-2.24840900
C	-4.06977400	-1.39005800	-2.62059800
C	-5.31725700	1.18327800	-2.48388200
H	-5.99046300	-2.16152900	-1.99103900
C	-2.01081500	-2.65837900	-2.83560800
H	-3.51079600	1.83471100	-3.14743900
C	-1.29441500	-1.48248700	-3.17430200
C	-1.98652700	-0.26843000	-3.25177400
H	-1.47151600	-3.59711700	-2.75476700
C	-7.48981300	0.17723500	-1.70997100
H	-8.01900900	0.72192900	-2.50425600
H	-7.46472700	0.88469300	-0.87006800
C	0.17507900	-1.50651800	-3.32903200
H	0.60197700	-2.48961100	-3.11574700

H	0.56527300	-0.77666400	-2.44320000
C	0.79065800	-0.87608400	-4.57360500
H	1.88186300	-0.89639700	-4.49792800
H	0.47759000	0.16491000	-4.69880400
H	0.49613000	-1.43211100	-5.47365500
C	-8.26522300	-1.08106700	-1.31961900
H	-9.27986000	-0.81811000	-1.00410500
H	-7.78338000	-1.60699900	-0.48666600
H	-8.34862000	-1.78165900	-2.15909100
C	-2.53122900	-3.19345200	0.88851200
C	3.29823800	2.39245400	0.75449500
C	4.36780900	3.34905100	1.15281900
C	5.01916000	3.21361800	2.38406600
C	4.78988900	4.38621700	0.31495800
C	6.03930100	4.07891900	2.77414200
C	5.80194800	5.26770900	0.68688100
C	6.42919800	5.11035300	1.92166500
F	4.21454300	4.55373000	-0.88418000
F	6.18191000	6.25267400	-0.13425900
F	7.40339000	5.94652200	2.28646200
F	6.64285800	3.92887300	3.95724600
F	4.66896400	2.23008100	3.21879400
C	-3.35085000	-0.21655000	-2.96901900
C	-3.37011600	-2.61315400	-2.58536300
H	-3.90654500	-3.51628600	-2.30685300
H	-1.44376400	0.65338200	-3.43780500
N	-4.02819000	0.98489700	-2.95408000
O	-5.76502900	2.32423000	-2.34916400
C	-1.53694500	-3.34253100	4.08253300
H	-0.79492000	-3.29834500	4.88736900
H	-1.04731000	-3.77863700	3.20269800
O	-4.05240800	-0.96240400	3.29026000

**<sup>5</sup>TS7-s**

N	-0.70715500	2.20949100	0.31784600
N	1.27384700	0.20566400	0.20125900
N	-0.73786000	-1.74117600	-0.17242100
N	-2.73781900	0.25903200	0.08558200
C	-1.78117100	3.01636400	0.60121000
C	-1.34974200	4.39309300	0.61945900
C	-0.02450800	4.40709000	0.30617100
C	0.38858600	3.03728900	0.15185700
C	1.70763800	2.61788000	0.01806700
C	2.11459100	1.28248900	0.13690500

C	3.47695200	0.84752900	0.32771500
C	3.43294600	-0.49854200	0.54002700
C	2.05273200	-0.89499400	0.42971300
C	1.60143100	-2.22416200	0.43496600
C	0.29498400	-2.60364000	0.07069400
C	-0.12942600	-3.95361200	-0.18345700
C	-1.41780200	-3.88443100	-0.62615700
C	-1.80821300	-2.49713400	-0.57369800
C	-3.11667500	-2.02745700	-0.74528000
C	-3.54763600	-0.75578200	-0.35693300
C	-4.92740800	-0.33485600	-0.26634400
C	-4.92972600	0.91425100	0.26857600
C	-3.54785000	1.30455300	0.43746700
H	-1.99157800	5.23877600	0.82011600
H	0.63211200	5.26167900	0.22434100
H	4.34401300	1.49164400	0.29761800
H	4.25343100	-1.18063800	0.70640000
H	0.47804300	-4.82814900	-0.01128200
H	-2.07165800	-4.70398900	-0.88666400
H	-5.78188600	-0.93303000	-0.54561400
H	-5.78486400	1.53292400	0.49659100
Mn	-0.73436000	0.24778400	0.08429400
Cl	-0.78024000	-0.15352700	2.42234600
O	-0.74148800	0.51604800	-1.65305200
C	2.77869700	3.63762300	-0.17641100
C	3.16753700	4.02398300	-1.45776000
C	3.48899700	4.18055700	0.89666900
C	4.23665600	4.88038000	-1.68969300
C	4.55424500	5.05616500	0.69680400
C	4.92869300	5.40412000	-0.60056400
C	-4.10352200	-2.98063900	-1.32361200
C	-4.00336700	-3.36029600	-2.66614400
C	-5.13067700	-3.55525100	-0.56973000
C	-4.88649200	-4.26802300	-3.24382700
C	-6.03134200	-4.46088000	-1.12701200
C	-5.90550900	-4.81903700	-2.46817700
F	3.16274100	3.84208100	2.15042100
F	5.22126800	5.56163600	1.73931500
F	5.95324500	6.23469300	-0.79688100
F	4.59666700	5.19604000	-2.93316200
F	2.52595100	3.50940900	-2.53356000
F	-5.27090400	-3.23485000	0.72201900
F	-3.03220200	-2.84454300	-3.43821900
F	-4.76744300	-4.60982100	-4.53094700

F	-6.76094200	-5.68781900	-3.01049200
F	-7.00682300	-4.99300700	-0.38453900
C	3.15501600	-4.04008600	1.49392900
C	3.80254600	-4.95602100	2.41438300
H	4.66651200	-5.43280100	1.93217100
C	4.22220600	-4.34784200	3.79569500
H	4.90178200	-3.49288200	3.74229200
C	2.87060800	-6.02935300	3.06037100
H	2.31808900	-6.66186300	2.36255700
C	3.88968300	-6.76523400	3.96179000
H	3.39570500	-7.29224800	4.78420300
H	4.45119700	-7.50958400	3.38684300
C	4.82626000	-5.60967900	4.46024400
H	4.84678600	-5.52313900	5.55138500
H	5.85769600	-5.76519600	4.12597800
C	2.87536500	-4.05104700	4.50621400
H	3.01923300	-4.10510800	5.58887300
C	1.95475100	-5.18915300	3.97691700
H	1.52755900	-5.81736600	4.76585000
N	0.87564600	-3.15241000	3.57022800
H	0.23440700	-2.48158200	3.15371300
C	6.16919600	-0.07536400	-2.08448800
C	5.52175700	-1.26560500	-2.22275800
C	4.13698600	-1.35340100	-2.59639700
C	5.44268800	1.18229200	-2.34173400
H	6.04252200	-2.19665800	-2.01380200
C	2.04939300	-2.56283900	-2.87060800
H	3.65136800	1.90456400	-2.97577300
C	1.36469600	-1.35810900	-3.16743100
C	2.08400900	-0.15805700	-3.18778100
H	1.48756600	-3.49084800	-2.82823300
C	7.59841500	0.09278200	-1.63871500
H	8.12918000	0.66810600	-2.40987400
H	7.59994000	0.75553800	-0.76253200
C	-0.10410600	-1.33771000	-3.33904500
H	-0.56271700	-2.31069600	-3.14728300
H	-0.47530800	-0.60879900	-2.44306300
C	-0.68501100	-0.66694000	-4.57872900
H	-1.77710700	-0.65303100	-4.51580400
H	-0.33531700	0.36468400	-4.68354000
H	-0.39862800	-1.21818300	-5.48443100
C	8.35307400	-1.19989500	-1.32790800
H	9.37698100	-0.97506700	-1.01276000
H	7.87161000	-1.76279900	-0.51904700

H	8.41103600	-1.85476100	-2.20540100
C	2.49935600	-3.23295800	0.86843000
C	-3.10902100	2.59738900	0.74096700
C	-4.11514600	3.62624700	1.12695800
C	-4.13152500	4.15383500	2.42274200
C	-5.05310600	4.12625200	0.21848400
C	-5.04901300	5.12985200	2.80643200
C	-5.98452800	5.09614400	0.58139200
C	-5.97948000	5.59967800	1.88110900
F	-5.07348400	3.66950600	-1.04144000
F	-6.87287700	5.55277000	-0.30801500
F	-6.86462600	6.53242500	2.23854900
F	-5.04445500	5.61554000	4.05166700
F	-3.24572300	3.72550900	3.32780700
C	3.44659300	-0.14959200	-2.89295500
C	3.40860400	-2.55990500	-2.61341100
H	3.92230900	-3.48668000	-2.37203700
H	1.56206700	0.78238900	-3.33631700
N	4.14916900	1.03589800	-2.81693100
O	5.91720600	2.30494200	-2.15044500
C	0.78861300	-4.47925300	3.27726200
C	2.13905600	-2.72351700	4.15230100
H	1.96540700	-2.10969500	5.04294500
H	2.71004900	-2.11731200	3.43745400
O	-0.07298200	-5.03095200	2.60403400

**<sup>3</sup>TS8-R**

N	1.00021300	-1.83700800	0.35587000
N	2.71213000	0.39574900	0.23165000
N	0.47503100	2.07557600	0.63241000
N	-1.19225400	-0.20120900	0.82055500
C	0.14951200	-2.80678400	0.82043300
C	0.70856600	-4.09993000	0.52159300
C	1.87428800	-3.89229200	-0.15203200
C	2.08181600	-2.46670700	-0.20992600
C	3.27350600	-1.84394000	-0.60043200
C	3.58629200	-0.51072600	-0.30039000
C	4.89552400	0.09502400	-0.39051500
C	4.79281300	1.34624300	0.13394300
C	3.40230100	1.55376700	0.47280100
C	2.82566200	2.78705200	0.80347700
C	1.44479500	3.02598700	0.79128900
C	0.82649800	4.33193400	0.75952500
C	-0.50041900	4.14210000	0.51294400

C	-0.72057500	2.71604600	0.45887200
C	-1.97316700	2.09356300	0.39602800
C	-2.18171800	0.73615100	0.68030100
C	-3.44523600	0.14165300	1.05153400
C	-3.17929300	-1.11718700	1.49745300
C	-1.76965100	-1.35249400	1.29645700
C	-1.11753400	-2.58772800	1.37944700
H	0.23630900	-5.04367700	0.75121400
H	2.55870700	-4.63506400	-0.53569900
H	5.78384000	-0.38804300	-0.76906900
H	5.57822300	2.07874700	0.24654700
H	1.35220100	5.26922700	0.87267800
H	-1.27314500	4.89219800	0.42037900
H	-4.40550500	0.63162600	1.01489500
H	-3.88694300	-1.83861800	1.87540100
Mn	0.75035300	0.10747900	0.47578400
Cl	1.12091100	0.04225100	2.78733200
O	0.51975600	0.37125200	-1.20710700
C	3.71560000	3.95503400	1.05603000
C	4.47745200	4.54572600	0.04322100
C	3.78562700	4.52877300	2.33041800
C	5.29401500	5.64786600	0.28435400
C	4.59025100	5.63581100	2.59330600
C	5.34777200	6.19447800	1.56544900
C	4.27744500	-2.68648800	-1.30581600
C	4.01084500	-3.15316800	-2.59785800
C	5.48853900	-3.07239100	-0.72404200
C	4.90973400	-3.95805800	-3.29227400
C	6.40738400	-3.87159400	-1.40115500
C	6.11426100	-4.31688200	-2.68898700
C	-3.14425100	2.92998900	0.01777400
C	-3.25258700	3.38461800	-1.30037800
C	-4.19237600	3.24137300	0.88843800
C	-4.36848200	4.08128300	-1.74963800
C	-5.32524200	3.92687000	0.45675600
C	-5.41208800	4.34301100	-0.86891500
F	4.43442800	4.05105700	-1.20208200
F	6.01477500	6.18971900	-0.70357900
F	6.12348600	7.25344700	1.80673600
F	4.64147700	6.16305700	3.82038900
F	3.06480300	4.01692300	3.33243300
F	5.79318700	-2.67038500	0.51661000
F	7.55961400	-4.22183600	-0.82130800
F	6.98586700	-5.08579700	-3.34424000

F	4.62856300	-4.38459600	-4.52737000
F	2.85734300	-2.82709700	-3.20262400
F	-4.14395100	2.84527800	2.16766000
F	-2.29180600	3.09589600	-2.18992300
F	-4.48381400	4.41898100	-3.04103800
F	-6.52653400	4.93576300	-1.31130300
F	-6.34487300	4.15275100	1.29200500
C	-6.39569300	0.41539300	-2.05652500
C	-5.68002200	-0.71629600	-1.67506400
C	-4.35188500	-0.89977500	-2.09316400
C	-3.70975500	0.07514700	-2.89511700
C	-4.45498200	1.20593900	-3.28978000
C	-5.76643100	1.37401800	-2.88211800
H	-6.14683400	-1.46941100	-1.04382400
C	-2.32727100	-0.11681500	-3.21885100
H	-3.97121800	1.96740100	-3.89378500
H	-6.31276100	2.26407700	-3.18282500
C	-1.62043300	-1.21431000	-2.80965400
C	-2.29038000	-2.25630900	-2.00865900
H	-1.82848400	0.66734100	-3.78120000
C	-7.81130300	0.63904400	-1.57065100
H	-8.20139700	-0.28953900	-1.13730000
H	-8.45589700	0.87905100	-2.42666500
O	-1.74141900	-3.27499100	-1.58901700
C	-0.16043300	-1.37878200	-2.98708700
H	0.13763800	-2.42153200	-2.85181800
H	0.27983500	-0.83480800	-2.05015800
C	0.50735600	-0.70724500	-4.17788300
H	1.57969200	-0.91894400	-4.16564200
H	0.38140000	0.38012800	-4.15079800
H	0.09236400	-1.07988400	-5.12304700
C	-7.91709300	1.77171200	-0.53276400
H	-8.94503200	1.86563900	-0.16581600
H	-7.62952100	2.73573700	-0.96228900
H	-7.26687600	1.58007000	0.32850700
N	-3.63162200	-2.01529000	-1.72772000
H	-4.05754100	-2.70416200	-1.12110400
C	-1.77113600	-3.74814600	2.04549600
C	-2.96591700	-4.34701500	1.63352800
C	-1.14282500	-4.31780700	3.16547300
C	-3.51811900	-5.44151300	2.29452200
C	-1.67126700	-5.41706500	3.83762200
C	-2.86668300	-5.98235700	3.39957300
F	-3.65399000	-3.87652800	0.57754600

F	0.00551700	-3.80636300	3.61730200
F	-1.04229000	-5.92897400	4.89925200
F	-3.38653000	-7.03326200	4.03611000
F	-4.66707300	-5.97719400	1.86647900

**<sup>3</sup>TS8-S**

N	-1.00029100	-1.83699500	0.35583100
N	-2.71212300	0.39583100	0.23164900
N	-0.47496100	2.07556500	0.63244400
N	1.19223900	-0.20128900	0.82055100
C	-0.14962400	-2.80681400	0.82036500
C	-0.70872400	-4.09993200	0.52148700
C	-1.87443700	-3.89223300	-0.15213600
C	-2.08191400	-2.46663800	-0.20998800
C	-3.27357600	-1.84381600	-0.60049000
C	-3.58631600	-0.51060000	-0.30041400
C	-4.89552400	0.09520300	-0.39053800
C	-4.79276900	1.34640700	0.13394700
C	-3.40225100	1.55387100	0.47281700
C	-2.82556600	2.78712700	0.80351900
C	-1.44469000	3.02601000	0.79133900
C	-0.82634300	4.33193400	0.75960700
C	0.50056800	4.14205500	0.51303300
C	0.72067000	2.71599400	0.45892900
C	1.97324000	2.09346600	0.39608400
C	2.18173800	0.73603700	0.68032000
C	3.44523500	0.14148300	1.05153800
C	3.17924600	-1.11736000	1.49742000
C	1.76959400	-1.35260700	1.29642300
C	1.11743200	-2.58782000	1.37937800
H	-0.23650000	-5.04370200	0.75107900
H	-2.55888100	-4.63496900	-0.53582800
H	-5.78385600	-0.38782200	-0.76911000
H	-5.57815100	2.07893900	0.24655900
H	-1.35201100	5.26924400	0.87277900
H	1.27332400	4.89212600	0.42049200
H	4.40552200	0.63142100	1.01491200
H	3.88687000	-1.83882800	1.87534600
Mn	-0.75035800	0.10748000	0.47578500
Cl	-1.12092300	0.04222800	2.78733300
O	-0.51975000	0.37124600	-1.20709900
C	-3.71545900	3.95513800	1.05609300
C	-4.47728700	4.54587900	0.04329400
C	-3.78546800	4.52885300	2.33049300



C	-5.29380900	5.64804400	0.28444800
C	-4.59005200	5.63591500	2.59340100
C	-5.34755000	6.19463200	1.56555400
C	-4.27752800	-2.68630200	-1.30592800
C	-4.01091800	-3.15292700	-2.59798800
C	-5.48864400	-3.07219700	-0.72419500
C	-4.90981800	-3.95775700	-3.29245900
C	-6.40750000	-3.87134000	-1.40136300
C	-6.11436600	-4.31657500	-2.68921100
C	3.14436100	2.92986600	0.01789000
C	3.25274500	3.38454900	-1.30023900
C	4.19247200	3.24118300	0.88859600
C	4.36867300	4.08120000	-1.74943900
C	5.32537100	3.92666400	0.45697400
C	5.41226600	4.34285500	-0.86867800
F	-4.43427900	4.05123300	-1.20201900
F	-6.01454700	6.18994400	-0.70347500
F	-6.12322500	7.25362500	1.80686100
F	-4.64126100	6.16313900	3.82049500
F	-3.06466600	4.01695600	3.33249900
F	-5.79330300	-2.67024000	0.51647100
F	-7.55975100	-4.22157700	-0.82155500
F	-6.98598300	-5.08543300	-3.34451700
F	-4.62863800	-4.38424200	-4.52757100
F	-2.85739700	-2.82685600	-3.20271900
F	4.14399900	2.84503900	2.16780100
F	2.29197900	3.09589300	-2.18982200
F	4.48405000	4.41894900	-3.04082200
F	6.52674300	4.93558700	-1.31101300
F	6.34498500	4.15248100	1.29226000
C	6.39564400	0.41541200	-2.05663700
C	5.67995900	-0.71616700	-1.67487500
C	4.35183200	-0.89975800	-2.09295900
C	3.70972600	0.07494500	-2.89519700
C	4.45497000	1.20562000	-3.29016300
C	5.76641000	1.37380500	-2.88251800
H	6.14675100	-1.46910700	-1.04341200
C	2.32724900	-0.11709800	-3.21890900
H	3.97122500	1.96691400	-3.89439600
H	6.31275300	2.26377500	-3.18346500
C	1.62040200	-1.21448800	-2.80944800
C	2.29032500	-2.25627100	-2.00815100
H	1.82848000	0.66690400	-3.78148700
C	7.81124200	0.63919600	-1.57078700

H	8.20131800	-0.28926100	-1.13715100
H	8.45586300	0.87894700	-2.42685300
O	1.74134600	-3.27482700	-1.58822800
C	0.16040700	-1.37901300	-2.98688800
H	-0.13764400	-2.42174500	-2.85143200
H	-0.27989500	-0.83488900	-2.05006200
C	-0.50736000	-0.70772200	-4.17783600
H	-1.57968800	-0.91946000	-4.16559300
H	-0.38144700	0.37966000	-4.15094800
H	-0.09232000	-1.08052200	-5.12291600
C	7.91700700	1.77217200	-0.53323300
H	8.94493400	1.86619900	-0.16627800
H	7.62945800	2.73607200	-0.96305600
H	7.26675800	1.58079100	0.32807100
N	3.63155800	-2.01517200	-1.72723000
H	4.05745700	-2.70387600	-1.12040900
C	1.77099800	-3.74828300	2.04538500
C	2.96575200	-4.34718200	1.63338400
C	1.14268000	-4.31795700	3.16535100
C	3.51792200	-5.44172200	2.29433500
C	1.67108900	-5.41725700	3.83745800
C	2.86648000	-5.98257700	3.39937700
F	3.65382700	-3.87668500	0.57740800
F	-0.00563900	-3.80648600	3.61721000
F	1.04210700	-5.92917700	4.89907800
F	3.38629600	-7.03352200	4.03587300
F	4.66685100	-5.97743100	1.86626000

**<sup>5</sup>TS8-R**

C	-2.04887500	0.47932100	0.84358000
C	-3.26885500	-0.25110500	1.08893300
C	-2.91164400	-1.51689700	1.43520000
C	-1.47253300	-1.59578900	1.34426200
N	-0.97870800	-0.36417600	0.99941200
H	-4.26643700	0.15362500	1.01324500
H	-3.56107100	-2.34988900	1.65524100
C	2.52631600	-2.40950900	0.06352100
C	2.52316300	-3.82969600	0.31835500
C	1.35890500	-4.11513700	0.96102100
C	0.60640900	-2.88625000	1.04379800
N	1.35985800	-1.86355000	0.52030900
H	3.33109000	-4.50535400	0.07765200
H	1.02862200	-5.07394200	1.33063100
C	1.39089700	3.06975300	0.72090000

C	0.66212700	4.31354300	0.78210200
C	-0.65943500	4.00855200	0.67020500
C	-0.75940900	2.57141700	0.59930600
N	0.50282300	2.02993200	0.63652300
H	1.11237400	5.29230800	0.86342800
H	-1.49818800	4.68949700	0.67420300
C	3.42567300	1.77811500	0.23585200
C	4.79587100	1.67962600	-0.20864400
C	4.99032500	0.40121500	-0.62730600
C	3.76794600	-0.32123800	-0.36628200
N	2.82839200	0.54670200	0.13792600
H	5.50535700	2.49339100	-0.22538600
H	5.89191400	-0.02627400	-1.03992800
C	-1.96007900	1.85639900	0.59499800
C	3.62069800	-1.70584900	-0.45812300
C	-0.73110600	-2.78150000	1.44109000
C	2.77926700	2.96476200	0.59082500
Mn	0.92954000	0.09584100	0.56717100
Cl	1.41600900	0.08937600	2.84216500
O	0.54310700	0.11022300	-1.16427300
C	3.58072800	4.21290700	0.72836800
C	4.17648400	4.83923100	-0.37048300
C	3.73560100	4.82328500	1.97780500
C	4.91400400	6.01319200	-0.23776600
C	4.46225700	6.00212100	2.13346000
C	5.05451200	6.59633100	1.02044300
C	4.71291800	-2.51263100	-1.06940700
C	4.49452500	-3.19027500	-2.27400400
C	5.96729100	-2.66045300	-0.46962500
C	5.48097200	-3.97316700	-2.86827000
C	6.97204200	-3.43303800	-1.04816100
C	6.72522700	-4.09246700	-2.25112500
C	-1.45713900	-4.01310000	1.85126800
C	-1.61637400	-5.10645000	0.98951600
C	-2.06328700	-4.09907500	3.11061800
C	-2.34815100	-6.23104500	1.36127400
C	-2.80167700	-5.21320200	3.50040800
C	-2.94335900	-6.28359600	2.61971500
C	-3.19898600	2.63169400	0.31667200
C	-3.35269400	3.24818300	-0.93055900
C	-4.23137600	2.80744600	1.24361900
C	-4.48009000	3.99377000	-1.25392400
C	-5.37893300	3.53654700	0.93628000
C	-5.49555200	4.13894800	-0.31412700

F	-4.13861500	2.26401400	2.46389000
F	-6.35965000	3.67272200	1.83424500
F	-6.59692900	4.83221400	-0.62422500
F	3.17224400	4.27782200	3.06021100
F	6.22926400	-2.04889200	0.69250600
F	8.16343000	-3.55395300	-0.45406000
F	7.67954000	-4.83769200	-2.81181800
F	-1.95368000	-3.08213300	3.97471800
F	-3.36970800	-5.26405600	4.71063200
F	-3.64632400	-7.35941200	2.98267700
F	-2.48417300	-7.26012300	0.51788300
F	-1.05222100	-5.10855900	-0.22216300
F	-2.40250100	3.10808000	-1.86769600
F	-4.60976300	4.53749400	-2.47070200
F	3.30652900	-3.09796200	-2.88892800
F	5.24511100	-4.60589400	-4.02183300
F	4.04863300	4.30671300	-1.59408900
F	5.47681800	6.58754000	-1.30649600
F	5.75503800	7.72390900	1.15857000
F	4.59646300	6.56393100	3.33869900
C	-6.77654400	0.92863000	-2.71405100
C	-6.37599500	-0.28870100	-2.16788400
C	-5.02632500	-0.66679500	-2.18054100
C	-4.04128100	0.18336100	-2.74486200
C	-4.46654100	1.40715400	-3.30361200
C	-5.80150700	1.77318200	-3.28719800
H	-7.11394900	-0.95550300	-1.72619000
C	-2.67447400	-0.24236100	-2.70347200
H	-3.72298000	2.07596300	-3.72469900
H	-6.10163500	2.73113000	-3.70118400
C	-2.28360200	-1.44100700	-2.16377900
C	-3.29980600	-2.32593600	-1.55906000
H	-1.91586600	0.43254400	-3.09308200
C	-8.22451300	1.35733100	-2.63803300
H	-8.87350400	0.47736500	-2.72818200
H	-8.45998100	2.01130100	-3.48635400
O	-3.07192000	-3.40011900	-1.00480100
C	-0.86736900	-1.87412000	-2.10934500
H	-0.76088100	-2.78108700	-1.51122900
C	-8.54523600	2.09218800	-1.32228600
H	-9.60747800	2.35632800	-1.27489700
H	-7.96411100	3.01396600	-1.23151500
H	-8.31258200	1.46076900	-0.45693800
N	-4.61015900	-1.86529500	-1.64192000

H	-5.29180200	-2.48638600	-1.22101500
C	-0.11313400	-1.96404600	-3.43462100
H	-0.16705000	-1.02333900	-3.99268900
H	-0.53552700	-2.75908700	-4.06267000
H	0.94124900	-2.18957600	-3.24999300
H	-0.27835300	-1.02373600	-1.52690700

**<sup>5</sup>TS8-S**

C	2.04887500	0.47932100	0.84358000
C	3.26885500	-0.25110500	1.08893300
C	2.91164400	-1.51689700	1.43520000
C	1.47253300	-1.59578900	1.34426200
N	0.97870800	-0.36417600	0.99941200
H	4.26643700	0.15362500	1.01324500
H	3.56107100	-2.34988900	1.65524100
C	-2.52631600	-2.40950900	0.06352100
C	-2.52316300	-3.82969600	0.31835500
C	-1.35890500	-4.11513700	0.96102100
C	-0.60640900	-2.88625000	1.04379800
N	-1.35985800	-1.86355000	0.52030900
H	-3.33109000	-4.50535400	0.07765200
H	-1.02862200	-5.07394200	1.33063100
C	-1.39089700	3.06975300	0.72090000
C	-0.66212700	4.31354300	0.78210200
C	0.65943500	4.00855200	0.67020500
C	0.75940900	2.57141700	0.59930600
N	-0.50282300	2.02993200	0.63652300
H	-1.11237400	5.29230800	0.86342800
H	1.49818800	4.68949700	0.67420300
C	-3.42567300	1.77811500	0.23585200
C	-4.79587100	1.67962600	-0.20864400
C	-4.99032500	0.40121500	-0.62730600
C	-3.76794600	-0.32123800	-0.36628200
N	-2.82839200	0.54670200	0.13792600
H	-5.50535700	2.49339100	-0.22538600
H	-5.89191400	-0.02627400	-1.03992800
C	1.96007900	1.85639900	0.59499800
C	-3.62069800	-1.70584900	-0.45812300
C	0.73110600	-2.78150000	1.44109000
C	-2.77926700	2.96476200	0.59082500
Mn	-0.92954000	0.09584100	0.56717100
Cl	-1.41600900	0.08937600	2.84216500
O	-0.54310700	0.11022300	-1.16427300
C	-3.58072800	4.21290700	0.72836800

C	-4.17648400	4.83923100	-0.37048300
C	-3.73560100	4.82328500	1.97780500
C	-4.91400400	6.01319200	-0.23776600
C	-4.46225700	6.00212100	2.13346000
C	-5.05451200	6.59633100	1.02044300
C	-4.71291800	-2.51263100	-1.06940700
C	-4.49452500	-3.19027500	-2.27400400
C	-5.96729100	-2.66045300	-0.46962500
C	-5.48097200	-3.97316700	-2.86827000
C	-6.97204200	-3.43303800	-1.04816100
C	-6.72522700	-4.09246700	-2.25112500
C	1.45713900	-4.01310000	1.85126800
C	1.61637400	-5.10645000	0.98951600
C	2.06328700	-4.09907500	3.11061800
C	2.34815100	-6.23104500	1.36127400
C	2.80167700	-5.21320200	3.50040800
C	2.94335900	-6.28359600	2.61971500
C	3.19898600	2.63169400	0.31667200
C	3.35269400	3.24818300	-0.93055900
C	4.23137600	2.80744600	1.24361900
C	4.48009000	3.99377000	-1.25392400
C	5.37893300	3.53654700	0.93628000
C	5.49555200	4.13894800	-0.31412700
F	4.13861500	2.26401400	2.46389000
F	6.35965000	3.67272200	1.83424500
F	6.59692900	4.83221400	-0.62422500
F	-3.17224400	4.27782200	3.06021100
F	-6.22926400	-2.04889200	0.69250600
F	-8.16343000	-3.55395300	-0.45406000
F	-7.67954000	-4.83769200	-2.81181800
F	1.95368000	-3.08213300	3.97471800
F	3.36970800	-5.26405600	4.71063200
F	3.64632400	-7.35941200	2.98267700
F	2.48417300	-7.26012300	0.51788300
F	1.05222100	-5.10855900	-0.22216300
F	2.40250100	3.10808000	-1.86769600
F	4.60976300	4.53749400	-2.47070200
F	-3.30652900	-3.09796200	-2.88892800
F	-5.24511100	-4.60589400	-4.02183300
F	-4.04863300	4.30671300	-1.59408900
F	-5.47681800	6.58754000	-1.30649600
F	-5.75503800	7.72390900	1.15857000
F	-4.59646300	6.56393100	3.33869900
C	6.77654400	0.92863000	-2.71405100

C	6.37599500	-0.28870100	-2.16788400
C	5.02632500	-0.66679500	-2.18054100
C	4.04128100	0.18336100	-2.74486200
C	4.46654100	1.40715400	-3.30361200
C	5.80150700	1.77318200	-3.28719800
H	7.11394900	-0.95550300	-1.72619000
C	2.67447400	-0.24236100	-2.70347200
H	3.72298000	2.07596300	-3.72469900
H	6.10163500	2.73113000	-3.70118400
C	2.28360200	-1.44100700	-2.16377900
C	3.29980600	-2.32593600	-1.55906000
H	1.91586600	0.43254400	-3.09308200
C	8.22451300	1.35733100	-2.63803300
H	8.87350400	0.47736500	-2.72818200
H	8.45998100	2.01130100	-3.48635400
O	3.07192000	-3.40011900	-1.00480100
C	0.86736900	-1.87412000	-2.10934500
H	0.76088100	-2.78108700	-1.51122900
C	8.54523600	2.09218800	-1.32228600
H	9.60747800	2.35632800	-1.27489700
H	7.96411100	3.01396600	-1.23151500
H	8.31258200	1.46076900	-0.45693800
N	4.61015900	-1.86529500	-1.64192000
H	5.29180200	-2.48638600	-1.22101500
C	0.11313400	-1.96404600	-3.43462100
H	0.16705000	-1.02333900	-3.99268900
H	0.53552700	-2.75908700	-4.06267000
H	-0.94124900	-2.18957600	-3.24999300
H	0.27835300	-1.02373600	-1.52690700

**<sup>3</sup>TS9-R**

N	-0.12838000	1.97187500	-0.67641000
N	0.94837200	-0.63934100	-1.00712800
N	-1.58224000	-1.74944300	-0.37769800
N	-2.68357500	0.85540700	-0.13769700
C	-0.85348900	3.13326200	-0.74370800
C	0.05401900	4.25199200	-0.85847400
C	1.31577800	3.75136700	-0.79666500
C	1.19758000	2.31356500	-0.71354700
C	2.27595300	1.43110000	-0.83095500
C	2.12506400	0.06110900	-1.08164200
C	3.17060500	-0.81538600	-1.55763500
C	2.60022100	-2.03047100	-1.78572400
C	1.21402400	-1.92809200	-1.39891100

C	0.32934300	-3.00426400	-1.30141300
C	-0.95964400	-2.90800900	-0.77036700
C	-1.80411200	-4.03163200	-0.45303300
C	-2.92142300	-3.53681000	0.14829600
C	-2.79067200	-2.10129400	0.17176700
C	-3.79814100	-1.21880300	0.57664100
C	-3.75054300	0.16207300	0.37154200
C	-4.85410900	1.07144500	0.57801000
C	-4.44591300	2.29542700	0.15179100
C	-3.06968900	2.16148800	-0.26945400
H	-0.24193900	5.28569800	-0.95734400
H	2.24882000	4.29260400	-0.85546000
H	4.19321000	-0.52426100	-1.74473700
H	3.07358700	-2.92192000	-2.17143900
H	-1.56072800	-5.06524600	-0.65212400
H	-3.77742500	-4.08703700	0.51107800
H	-5.81833400	0.79924600	0.98124400
H	-5.00534000	3.21952100	0.15560500
Mn	-0.85647300	0.10346800	-0.51013500
Cl	-1.38349000	0.16280800	-2.78452700
O	-0.49661700	0.18275000	1.16700600
C	3.64686800	2.00153500	-0.70751100
C	4.06604700	2.52459300	0.52200100
C	4.55894100	2.05472700	-1.76581500
C	5.33319300	3.07252700	0.69283500
C	5.84533300	2.56374500	-1.60755200
C	6.22972500	3.07720800	-0.37205800
C	-5.02903500	-1.80871000	1.17504500
C	-5.00864700	-2.36420300	2.45769700
C	-6.23938600	-1.85394900	0.47581800
C	-6.14001000	-2.94084400	3.02955700
C	-7.38683000	-2.41795200	1.02954300
C	-7.33405700	-2.96516400	2.31064800
F	4.20918700	1.59036000	-2.97464600
F	6.69977200	2.57687200	-2.63245800
F	7.46241300	3.55968900	-0.19994100
F	5.70627500	3.56243200	1.88123700
F	3.24114100	2.49903100	1.57706700
F	-6.31624300	-1.34134400	-0.75783000
F	-3.87462700	-2.35200700	3.17406300
F	-6.08969500	-3.46323200	4.25887900
F	-8.42576500	-3.51111700	2.84877500
F	-8.53115500	-2.44521700	0.34022500
C	6.41899300	0.61923100	2.39831600



C	5.44157700	0.66891200	3.34614000
C	4.19077600	-0.02457700	3.21098700
C	6.19052900	-0.14322300	1.15801700
H	5.59461700	1.27359800	4.23805800
C	1.92928100	-0.57889900	3.91773500
H	4.86721700	-1.41443500	0.28130200
C	1.74567300	-1.38497800	2.76933000
C	2.80272000	-1.52210500	1.86646700
H	1.11795300	-0.45783400	4.62703300
C	7.73660400	1.33743000	2.51802200
H	7.68831800	2.04155300	3.35631200
H	7.90743100	1.92606900	1.61067800
C	0.42937500	-1.97943000	2.40725900
H	0.55424700	-2.79930800	1.69154900
H	-0.07118300	-1.13809100	1.77836400
C	-0.55689800	-2.33598300	3.51165900
H	-1.47536900	-2.74060100	3.07921100
H	-0.83455900	-1.46114000	4.10813600
H	-0.13151000	-3.08834400	4.18807700
C	8.91647000	0.36603300	2.70301400
H	9.85947300	0.91843500	2.78061600
H	8.98415900	-0.31038100	1.84624900
H	8.79430500	-0.23281400	3.61283000
C	-2.24135600	3.23566800	-0.61194700
C	-2.87654500	4.57650900	-0.74902400
C	-3.73354400	4.85204100	-1.82026400
C	-2.67070600	5.59410400	0.18766600
C	-4.35457100	6.09132200	-1.96258400
C	-3.27477000	6.84266000	0.06184900
C	-4.12125500	7.08935000	-1.01789700
F	-1.86967500	5.38088900	1.24090600
F	-3.05678100	7.79840800	0.97122700
F	-4.70863400	8.28049000	-1.14598300
F	-5.16746800	6.32947800	-2.99598800
F	-3.97889900	3.91027100	-2.73634700
C	4.00114700	-0.83475600	2.06581100
C	3.13069000	0.07227500	4.13564400
H	3.26419300	0.69192500	5.01868500
H	2.68061600	-2.14093700	0.98458600
N	5.02226100	-0.89394000	1.13633800
O	6.94105400	-0.13398000	0.17987000
C	0.82589700	-4.35968800	-1.66823900
C	1.75691100	-5.02837300	-0.86886200
C	0.36302700	-5.02178100	-2.80902500

C	2.22908800	-6.29776400	-1.18921900
C	0.81604600	-6.29570400	-3.14877000
C	1.75351900	-6.93215200	-2.33664000
F	2.21653900	-4.44426600	0.25271200
F	-0.53955800	-4.43448300	-3.59966500
F	3.12044200	-6.91232100	-0.40571700
F	2.19408600	-8.15016000	-2.65450600
F	0.36139800	-6.90811400	-4.24512600

**<sup>3</sup>TS9-s**

N	0.12838000	1.97187500	-0.67641000
N	-0.94837200	-0.63934100	-1.00712800
N	1.58224000	-1.74944300	-0.37769800
N	2.68357500	0.85540700	-0.13769700
C	0.85348900	3.13326200	-0.74370800
C	-0.05401900	4.25199200	-0.85847400
C	-1.31577800	3.75136700	-0.79666500
C	-1.19758000	2.31356500	-0.71354700
C	-2.27595300	1.43110000	-0.83095500
C	-2.12506400	0.06110900	-1.08164200
C	-3.17060500	-0.81538600	-1.55763500
C	-2.60022100	-2.03047100	-1.78572400
C	-1.21402400	-1.92809200	-1.39891100
C	-0.32934300	-3.00426400	-1.30141300
C	0.95964400	-2.90800900	-0.77036700
C	1.80411200	-4.03163200	-0.45303300
C	2.92142300	-3.53681000	0.14829600
C	2.79067200	-2.10129400	0.17176700
C	3.79814100	-1.21880300	0.57664100
C	3.75054300	0.16207300	0.37154200
C	4.85410900	1.07144500	0.57801000
C	4.44591300	2.29542700	0.15179100
C	3.06968900	2.16148800	-0.26945400
H	0.24193900	5.28569800	-0.95734400
H	-2.24882000	4.29260400	-0.85546000
H	-4.19321000	-0.52426100	-1.74473700
H	-3.07358700	-2.92192000	-2.17143900
H	1.56072800	-5.06524600	-0.65212400
H	3.77742500	-4.08703700	0.51107800
H	5.81833400	0.79924600	0.98124400
H	5.00534000	3.21952100	0.15560500
Mn	0.85647300	0.10346800	-0.51013500
Cl	1.38349000	0.16280800	-2.78452700
O	0.49661700	0.18275000	1.16700600

C	-3.64686800	2.00153500	-0.70751100
C	-4.06604700	2.52459300	0.52200100
C	-4.55894100	2.05472700	-1.76581500
C	-5.33319300	3.07252700	0.69283500
C	-5.84533300	2.56374500	-1.60755200
C	-6.22972500	3.07720800	-0.37205800
C	5.02903500	-1.80871000	1.17504500
C	5.00864700	-2.36420300	2.45769700
C	6.23938600	-1.85394900	0.47581800
C	6.14001000	-2.94084400	3.02955700
C	7.38683000	-2.41795200	1.02954300
C	7.33405700	-2.96516400	2.31064800
F	-4.20918700	1.59036000	-2.97464600
F	-6.69977200	2.57687200	-2.63245800
F	-7.46241300	3.55968900	-0.19994100
F	-5.70627500	3.56243200	1.88123700
F	-3.24114100	2.49903100	1.57706700
F	6.31624300	-1.34134400	-0.75783000
F	3.87462700	-2.35200700	3.17406300
F	6.08969500	-3.46323200	4.25887900
F	8.42576500	-3.51111700	2.84877500
F	8.53115500	-2.44521700	0.34022500
C	-6.41899300	0.61923100	2.39831600
C	-5.44157700	0.66891200	3.34614000
C	-4.19077600	-0.02457700	3.21098700
C	-6.19052900	-0.14322300	1.15801700
H	-5.59461700	1.27359800	4.23805800
C	-1.92928100	-0.57889900	3.91773500
H	-4.86721700	-1.41443500	0.28130200
C	-1.74567300	-1.38497800	2.76933000
C	-2.80272000	-1.52210500	1.86646700
H	-1.11795300	-0.45783400	4.62703300
C	-7.73660400	1.33743000	2.51802200
H	-7.68831800	2.04155300	3.35631200
H	-7.90743100	1.92606900	1.61067800
C	-0.42937500	-1.97943000	2.40725900
H	-0.55424700	-2.79930800	1.69154900
H	0.07118300	-1.13809100	1.77836400
C	0.55689800	-2.33598300	3.51165900
H	1.47536900	-2.74060100	3.07921100
H	0.83455900	-1.46114000	4.10813600
H	0.13151000	-3.08834400	4.18807700
C	-8.91647000	0.36603300	2.70301400
H	-9.85947300	0.91843500	2.78061600

H	-8.98415900	-0.31038100	1.84624900
H	-8.79430500	-0.23281400	3.61283000
C	2.24135600	3.23566800	-0.61194700
C	2.87654500	4.57650900	-0.74902400
C	3.73354400	4.85204100	-1.82026400
C	2.67070600	5.59410400	0.18766600
C	4.35457100	6.09132200	-1.96258400
C	3.27477000	6.84266000	0.06184900
C	4.12125500	7.08935000	-1.01789700
F	1.86967500	5.38088900	1.24090600
F	3.05678100	7.79840800	0.97122700
F	4.70863400	8.28049000	-1.14598300
F	5.16746800	6.32947800	-2.99598800
F	3.97889900	3.91027100	-2.73634700
C	-4.00114700	-0.83475600	2.06581100
C	-3.13069000	0.07227500	4.13564400
H	-3.26419300	0.69192500	5.01868500
H	-2.68061600	-2.14093700	0.98458600
N	-5.02226100	-0.89394000	1.13633800
O	-6.94105400	-0.13398000	0.17987000
C	-0.82589700	-4.35968800	-1.66823900
C	-1.75691100	-5.02837300	-0.86886200
C	-0.36302700	-5.02178100	-2.80902500
C	-2.22908800	-6.29776400	-1.18921900
C	-0.81604600	-6.29570400	-3.14877000
C	-1.75351900	-6.93215200	-2.33664000
F	-2.21653900	-4.44426600	0.25271200
F	0.53955800	-4.43448300	-3.59966500
F	-3.12044200	-6.91232100	-0.40571700
F	-2.19408600	-8.15016000	-2.65450600
F	-0.36139800	-6.90811400	-4.24512600

**<sup>5</sup>TS9-R**

N	0.47977400	-1.88210500	0.43094200
N	2.80065200	-0.22928500	0.25281800
N	1.09871300	2.05903100	0.23000600
N	-1.16392300	0.40614200	0.56332200
C	-0.65168200	-2.50576600	0.89992000
C	-0.43345000	-3.92877300	0.92976100
C	0.82088700	-4.15150800	0.44591900
C	1.40563000	-2.86066200	0.18004500
C	2.76298400	-2.66176400	-0.11177600
C	3.40965000	-1.42656900	-0.01621200
C	4.84024900	-1.22425800	-0.09882700

C	5.07179200	0.08854400	0.15862000
C	3.78048400	0.71903800	0.32970400
C	3.56745600	2.10081100	0.39827500
C	2.31270400	2.70442500	0.27925500
C	2.10418400	4.11668200	0.08044600
C	0.77136900	4.30475200	-0.12273100
C	0.13485400	3.01954300	0.00378700
C	-1.24406900	2.80503300	0.01423600
C	-1.83417600	1.57696400	0.33830700
C	-3.24026200	1.38973200	0.61996900
C	-3.39207500	0.11379900	1.06143100
C	-2.08888500	-0.50816600	1.00055200
H	-1.14864000	-4.66371100	1.26761500
H	1.32817800	-5.09898400	0.33624500
H	5.56950000	-1.99384400	-0.30307100
H	6.02414300	0.59587800	0.19766600
H	2.88617300	4.86192000	0.06891300
H	0.25894200	5.23514600	-0.31825700
H	-4.00500300	2.14452400	0.51396200
H	-4.31066200	-0.38309400	1.33931400
Mn	0.81666200	0.10648000	0.36131800
Cl	1.01294500	0.10695400	2.68248700
O	0.77231400	0.15042300	-1.39908000
C	3.56441500	-3.86816500	-0.45928500
C	3.32701900	-4.55802400	-1.65269900
C	4.55085800	-4.38237800	0.38884100
C	4.04199300	-5.70013100	-2.00249500
C	5.28463500	-5.51992000	0.05860800
C	5.02675900	-6.18127900	-1.14106000
C	-2.16236400	3.95531100	-0.21906300
C	-3.00693800	3.97922100	-1.33239500
C	-2.28084900	5.01303600	0.68895500
C	-3.94502500	4.98636600	-1.53389800
C	-3.19543600	6.04749800	0.49788900
C	-4.03549000	6.03017900	-0.61507200
F	4.81320700	-3.77748900	1.55359100
F	6.22356800	-5.98597800	0.88723600
F	5.72100800	-7.27335800	-1.46451000
F	3.79287000	-6.33318600	-3.15294400
F	2.38127800	-4.12240000	-2.50148500
F	-1.50829700	5.04665100	1.78086100
F	-2.94056500	2.99480600	-2.24002900
F	-4.75255300	4.95241300	-2.60135300
F	-4.92269700	7.00921100	-0.79852300

F	-3.28403500	7.04575100	1.38169000
C	-5.89502400	0.32827800	-1.73248700
C	-4.97484400	0.78409700	-2.62973400
C	-3.75778300	0.07955800	-2.91367000
C	-5.66689100	-0.95183600	-1.03977000
H	-5.12821000	1.74770800	-3.11148300
C	-1.53105300	-0.07424000	-3.87238500
H	-4.37405400	-2.51946400	-0.95739600
C	-1.27628100	-1.26251500	-3.13980800
C	-2.30194700	-1.80879400	-2.36334100
H	-0.74645100	0.35785300	-4.48280400
C	-7.15025500	1.07569400	-1.37290000
H	-7.08088100	2.10409200	-1.74808400
H	-7.22488600	1.12463700	-0.27931100
C	0.09399200	-1.80863100	-3.00810400
H	0.09938600	-2.81122500	-2.56852500
H	0.52052600	-1.10977200	-2.16028000
C	1.06842400	-1.68724700	-4.17306000
H	2.03327800	-2.11681800	-3.89201800
H	1.23646300	-0.64381500	-4.45648600
H	0.69789900	-2.22683300	-5.05426500
C	-8.42018900	0.39690800	-1.91966000
H	-9.31334500	0.96103800	-1.62909800
H	-8.50530000	-0.61621000	-1.51715200
H	-8.39216600	0.33846000	-3.01365000
C	-1.85107800	-1.86412300	1.23627100
C	-2.95508400	-2.64397700	1.86361000
C	-3.38014300	-2.33073100	3.16232700
C	-3.64737800	-3.66578600	1.21277800
C	-4.44362300	-2.99521700	3.76974400
C	-4.71700100	-4.34068700	1.78897500
C	-5.11355300	-4.00513100	3.08153500
F	-3.31663900	-4.00306300	-0.05900300
F	-5.35980100	-5.29560700	1.11253200
F	-6.13166800	-4.64508300	3.65571700
F	-4.82200000	-2.67313400	5.00873600
F	-2.76976900	-1.36098900	3.84774900
C	-3.52732700	-1.14913300	-2.24619500
C	-2.74406700	0.57358900	-3.76263600
H	-2.91440500	1.50835700	-4.28782300
H	-2.12207600	-2.70980200	-1.78554800
N	-4.52555000	-1.63646300	-1.42746000
O	-6.39483100	-1.41192600	-0.15558200
C	4.75140700	3.00037600	0.50449500

C	4.98655400	3.73404500	1.67222200
C	5.65012700	3.16959300	-0.55299600
C	6.07643900	4.59428800	1.79091300
C	6.75020800	4.01804100	-0.45472000
C	6.96115500	4.73359600	0.72285200
F	4.14928700	3.62370400	2.70827100
F	6.27955600	5.28282500	2.91798400
F	8.00947100	5.55264100	0.82657200
F	7.59596300	4.15718800	-1.48121600
F	5.46575200	2.50099000	-1.70002900

**<sup>5</sup>TS9-S**

N	-0.47977400	-1.88210500	0.43094200
N	-2.80065200	-0.22928500	0.25281800
N	-1.09871300	2.05903100	0.23000600
N	1.16392300	0.40614200	0.56332200
C	0.65168200	-2.50576600	0.89992000
C	0.43345000	-3.92877300	0.92976100
C	-0.82088700	-4.15150800	0.44591900
C	-1.40563000	-2.86066200	0.18004500
C	-2.76298400	-2.66176400	-0.11177600
C	-3.40965000	-1.42656900	-0.01621200
C	-4.84024900	-1.22425800	-0.09882700
C	-5.07179200	0.08854400	0.15862000
C	-3.78048400	0.71903800	0.32970400
C	-3.56745600	2.10081100	0.39827500
C	-2.31270400	2.70442500	0.27925500
C	-2.10418400	4.11668200	0.08044600
C	-0.77136900	4.30475200	-0.12273100
C	-0.13485400	3.01954300	0.00378700
C	1.24406900	2.80503300	0.01423600
C	1.83417600	1.57696400	0.33830700
C	3.24026200	1.38973200	0.61996900
C	3.39207500	0.11379900	1.06143100
C	2.08888500	-0.50816600	1.00055200
H	1.14864000	-4.66371100	1.26761500
H	-1.32817800	-5.09898400	0.33624500
H	-5.56950000	-1.99384400	-0.30307100
H	-6.02414300	0.59587800	0.19766600
H	-2.88617300	4.86192000	0.06891300
H	-0.25894200	5.23514600	-0.31825700
H	4.00500300	2.14452400	0.51396200
H	4.31066200	-0.38309400	1.33931400
Mn	-0.81666200	0.10648000	0.36131800

C1	-1.01294500	0.10695400	2.68248700
O	-0.77231400	0.15042300	-1.39908000
C	-3.56441500	-3.86816500	-0.45928500
C	-3.32701900	-4.55802400	-1.65269900
C	-4.55085800	-4.38237800	0.38884100
C	-4.04199300	-5.70013100	-2.00249500
C	-5.28463500	-5.51992000	0.05860800
C	-5.02675900	-6.18127900	-1.14106000
C	2.16236400	3.95531100	-0.21906300
C	3.00693800	3.97922100	-1.33239500
C	2.28084900	5.01303600	0.68895500
C	3.94502500	4.98636600	-1.53389800
C	3.19543600	6.04749800	0.49788900
C	4.03549000	6.03017900	-0.61507200
F	-4.81320700	-3.77748900	1.55359100
F	-6.22356800	-5.98597800	0.88723600
F	-5.72100800	-7.27335800	-1.46451000
F	-3.79287000	-6.33318600	-3.15294400
F	-2.38127800	-4.12240000	-2.50148500
F	1.50829700	5.04665100	1.78086100
F	2.94056500	2.99480600	-2.24002900
F	4.75255300	4.95241300	-2.60135300
F	4.92269700	7.00921100	-0.79852300
F	3.28403500	7.04575100	1.38169000
C	5.89502400	0.32827800	-1.73248700
C	4.97484400	0.78409700	-2.62973400
C	3.75778300	0.07955800	-2.91367000
C	5.66689100	-0.95183600	-1.03977000
H	5.12821000	1.74770800	-3.11148300
C	1.53105300	-0.07424000	-3.87238500
H	4.37405400	-2.51946400	-0.95739600
C	1.27628100	-1.26251500	-3.13980800
C	2.30194700	-1.80879400	-2.36334100
H	0.74645100	0.35785300	-4.48280400
C	7.15025500	1.07569400	-1.37290000
H	7.08088100	2.10409200	-1.74808400
H	7.22488600	1.12463700	-0.27931100
C	-0.09399200	-1.80863100	-3.00810400
H	-0.09938600	-2.81122500	-2.56852500
H	-0.52052600	-1.10977200	-2.16028000
C	-1.06842400	-1.68724700	-4.17306000
H	-2.03327800	-2.11681800	-3.89201800
H	-1.23646300	-0.64381500	-4.45648600
H	-0.69789900	-2.22683300	-5.05426500



C	8.42018900	0.39690800	-1.91966000
H	9.31334500	0.96103800	-1.62909800
H	8.50530000	-0.61621000	-1.51715200
H	8.39216600	0.33846000	-3.01365000
C	1.85107800	-1.86412300	1.23627100
C	2.95508400	-2.64397700	1.86361000
C	3.38014300	-2.33073100	3.16232700
C	3.64737800	-3.66578600	1.21277800
C	4.44362300	-2.99521700	3.76974400
C	4.71700100	-4.34068700	1.78897500
C	5.11355300	-4.00513100	3.08153500
F	3.31663900	-4.00306300	-0.05900300
F	5.35980100	-5.29560700	1.11253200
F	6.13166800	-4.64508300	3.65571700
F	4.82200000	-2.67313400	5.00873600
F	2.76976900	-1.36098900	3.84774900
C	3.52732700	-1.14913300	-2.24619500
C	2.74406700	0.57358900	-3.76263600
H	2.91440500	1.50835700	-4.28782300
H	2.12207600	-2.70980200	-1.78554800
N	4.52555000	-1.63646300	-1.42746000
O	6.39483100	-1.41192600	-0.15558200
C	-4.75140700	3.00037600	0.50449500
C	-4.98655400	3.73404500	1.67222200
C	-5.65012700	3.16959300	-0.55299600
C	-6.07643900	4.59428800	1.79091300
C	-6.75020800	4.01804100	-0.45472000
C	-6.96115500	4.73359600	0.72285200
F	-4.14928700	3.62370400	2.70827100
F	-6.27955600	5.28282500	2.91798400
F	-8.00947100	5.55264100	0.82657200
F	-7.59596300	4.15718800	-1.48121600
F	-5.46575200	2.50099000	-1.70002900

**(U)B3LYP-D3/def2-TZVPP-SMD(Dichloromethane)//B3LYP-D3/6-31G(d,p)-LANL2DZ**

**PhIO**

O	-1.75350300	1.60836900	0.00000200
I	-1.41343800	-0.27155500	0.00010100
C	0.76438200	-0.15417000	-0.00003300
C	1.24499900	1.14382100	-0.00019600
C	1.57892500	-1.27834700	0.00003800
C	2.63077900	1.32492900	-0.00029300
H	0.53654000	1.97215800	-0.00024800
C	2.96316800	-1.07651200	-0.00005400

H	1.16664600	-2.28324400	0.00015600
C	3.48549400	0.21936300	-0.00022100
H	3.04065900	2.33079100	-0.00042900
H	3.62854900	-1.93499200	-0.00000100
H	4.56135100	0.36623800	-0.00028500

**PhI**

C	0.58219200	-0.00001800	0.00000200
C	1.26536100	1.21608700	0.00000000
C	2.66286600	1.20738800	0.00000200
C	3.36346000	0.00000600	-0.00000200
C	2.66290000	-1.20737200	-0.00000100
C	1.26537100	-1.21608800	0.00000300
H	0.72349600	2.15553800	0.00000500
H	3.19999000	2.15209500	-0.00000200
H	4.44969700	0.00003200	-0.00000100
H	3.20000600	-2.15208900	-0.00000600
H	0.72355100	-2.15556600	0.00000600
I	-1.56810600	0.00000000	0.00000000

**Sub**

C	-2.72290900	-0.12919200	-0.33217300
C	-1.77478800	0.88860200	-0.27288000
C	-0.40839400	0.58699200	-0.16525600
C	0.02905900	-0.75754400	-0.11513600
C	-0.94209900	-1.77461900	-0.17677100
C	-2.28927100	-1.47035400	-0.28282300
H	-2.09029800	1.92900200	-0.31107600
C	1.44245800	-1.01284800	-0.00763100
H	-0.61536300	-2.81077000	-0.14352300
H	-3.02456000	-2.26884300	-0.33151900
C	2.36582300	-0.01704300	0.04847400
C	1.92719600	1.38949600	-0.00217200
H	1.75912100	-2.05190300	0.02882000
C	-4.19937700	0.19279200	-0.39262300
H	-4.34544100	1.18113900	-0.84362200
H	-4.70383500	-0.52815900	-1.04727700
O	2.68701100	2.35481600	0.04245000
C	3.85549100	-0.21194300	0.16196400
H	4.32767300	0.31367700	-0.67822900
H	4.19907700	0.33721800	1.04826000
C	4.33251100	-1.66305400	0.21727500
H	3.91503600	-2.19193700	1.08122800
H	4.04728600	-2.21588500	-0.68463100

H	5.42249200	-1.70236000	0.29940000
C	-4.85697800	0.16223100	0.99927900
H	-4.39059900	0.89584200	1.66467900
H	-5.92626600	0.38845100	0.93431300
H	-4.74351300	-0.82363400	1.46158700
N	0.55039700	1.57959400	-0.10767700
H	0.26800600	2.55137500	-0.14142800

**<sup>3</sup>Cat1**

C	1.73706700	-2.17775100	-0.22863100
C	3.15579100	-2.40605100	-0.31617200
C	3.75440000	-1.18730000	-0.39492300
C	2.69953000	-0.21096700	-0.34091900
N	1.46822500	-0.82143700	-0.22840700
H	3.63655400	-3.37267800	-0.31518500
H	4.81104700	-0.97926800	-0.48250600
C	-0.06925300	3.09002100	-0.13966300
C	0.91012300	4.14281600	-0.20733000
C	2.12745100	3.54458200	-0.30548600
C	1.89519600	2.12711000	-0.29526400
N	0.55024100	1.85501900	-0.18229300
H	0.69207100	5.19969500	-0.17294700
H	3.10188300	4.00417600	-0.37556500
C	-2.55741700	-2.01340400	0.09218800
C	-2.78675400	-3.43494400	0.06831600
C	-1.56948700	-4.03017400	-0.02596700
C	-0.58879700	-2.97632600	-0.06110200
N	-1.20564000	-1.74357500	0.01410900
H	-3.75458900	-3.91163200	0.10642100
H	-1.35197700	-5.08625900	-0.07872700
C	-3.35265300	0.31653500	0.17101500
C	-4.40088300	1.29911000	0.26547000
C	-3.80719900	2.51873000	0.19254900
C	-2.39134700	2.28919100	0.06679500
N	-2.12307100	0.93456500	0.06522100
H	-5.45230900	1.08134900	0.37691900
H	-4.28283200	3.48742400	0.21927000
C	0.78511400	-3.19478800	-0.16196900
C	-1.44275400	3.30697800	-0.03155700
C	2.92323600	1.17326000	-0.37258500
C	-3.57298400	-1.06132800	0.17677700
Mn	-0.35126400	0.05198200	-0.35639600
Cl	-0.55165100	0.01841000	-2.54197700
C	-1.92572600	4.71811300	-0.01680100

C	-2.44083700	5.29858000	1.14572300
C	-1.87711400	5.51373700	-1.16557900
C	-2.89643000	6.61452400	1.17138600
F	-2.51239600	4.57989300	2.27458200
C	-2.32042100	6.83468700	-1.16257300
F	-1.38730900	5.01136600	-2.30451600
C	-2.83324400	7.38448200	0.01115800
F	-3.38619900	7.14355800	2.29779800
F	-2.26118300	7.57456600	-2.27435900
F	-3.26313000	8.64801100	0.02455700
C	-4.97993300	-1.54547200	0.27429300
C	-5.44936900	-2.18724500	1.42426400
C	-5.88188300	-1.37753300	-0.78112500
C	-6.75945700	-2.64912400	1.52616700
F	-4.62654000	-2.37820300	2.46417500
C	-7.19896000	-1.82447300	-0.69966200
F	-5.48796600	-0.76583400	-1.90411600
C	-7.63670100	-2.46415000	0.45884900
F	-7.18088900	-3.26097700	2.63796200
F	-8.04126800	-1.64917000	-1.72282400
F	-8.89541700	-2.89907800	0.54645000
C	1.26713100	-4.60539300	-0.20719200
C	1.80291600	-5.15302600	-1.37691600
C	1.20168300	-5.43136500	0.91849900
C	2.25959700	-6.46831700	-1.42866400
F	1.89196100	-4.40596900	-2.48278700
C	1.64623600	-6.75088900	0.88926600
F	0.69335000	-4.95742600	2.06450600
C	2.17859900	-7.26871300	-0.29031600
F	2.76773300	-6.96791900	-2.55936700
F	1.57045400	-7.51915900	1.98133300
F	2.60988200	-8.53111700	-0.32963500
C	4.26519200	1.64706100	-0.44768700
C	5.40170500	2.07294500	-0.45055400
C	6.74342900	2.63596500	-0.43940600
H	6.79866700	3.38463300	-1.24095100
C	7.23693400	3.26668300	0.90464000
H	6.58507100	4.03512900	1.32764900
C	7.95641600	1.66060300	-0.54167100
H	7.94145800	0.96606500	-1.38286000
C	9.12228400	2.67554200	-0.53631300
H	10.06261700	2.21121800	-0.22577000
H	9.27822300	3.09100500	-1.53655100
C	8.63072500	3.77756200	0.46517000

H	9.30379400	3.90322400	1.31859300
H	8.54580200	4.75064500	-0.02787500
C	7.45711800	2.04278400	1.82751300
H	8.20303100	2.28142100	2.58964500
C	7.95314000	0.95183800	0.83164100
H	8.94418200	0.54937300	1.06187600
C	6.19048400	1.44316300	2.50835400
H	5.29291200	2.02431900	2.26793100
H	6.29559800	1.41586800	3.59863200
C	6.94519200	-0.18794100	0.93542000
O	6.90896200	-1.18009500	0.21882300
N	6.09551700	0.09468900	1.96416400
H	5.27760200	-0.48472600	2.09497400

<sup>3</sup>Cat2

N	-2.13034700	0.18265000	0.30391500
N	-0.30493200	-1.89341800	0.90424500
N	1.81391800	-0.02277000	0.91632000
N	-0.01013900	2.05233500	0.30325600
C	-2.86718000	1.29699800	-0.04075800
C	-4.26970800	0.97694800	-0.08369500
C	-4.38552500	-0.33770500	0.24076800
C	-3.05305300	-0.83538000	0.45968600
C	-2.75474400	-2.16458900	0.75819200
C	-1.45894100	-2.65311100	0.93092000
C	-1.13482500	-4.04458000	1.10157700
C	0.22348600	-4.13318500	1.13980100
C	0.72731600	-2.79453300	1.02100200
C	2.09446000	-2.47329400	1.02323500
C	2.58423300	-1.16057200	1.02555300
C	3.97681100	-0.82709000	1.14042800
C	4.05476100	0.52921000	1.11845100
C	2.71427800	1.02529100	0.94612100
C	2.39879100	2.37005300	0.75006400
C	1.12278200	2.83279400	0.42774900
C	0.81447900	4.20914000	0.13784900
C	-0.50054000	4.25921900	-0.19828800
C	-1.01539900	2.91981700	-0.07876800
H	-5.06160600	1.67596000	-0.30721900
H	-5.29096200	-0.91875900	0.33020000
H	-1.85332900	-4.84821900	1.16288200
H	0.84153400	-5.01173500	1.25127700
H	4.77767200	-1.54699400	1.19260800
H	4.94403300	1.13911700	1.16240200

H	1.51592000	5.02828300	0.18295200
H	-1.07454600	5.12547600	-0.49011500
Mn	-0.11606100	0.03705000	0.33712100
Cl	0.27424500	-0.38418200	-1.80935000
C	-3.88170300	-3.13519100	0.85989800
C	-4.22724500	-3.71461900	2.08459500
C	-4.62597400	-3.51265900	-0.26218400
C	-5.26967600	-4.63169300	2.19627600
C	-5.67702200	-4.42280800	-0.17400500
C	-5.99729800	-4.98450600	1.06088600
C	3.50971700	3.36053400	0.83844700
C	4.11831500	3.65272800	2.06255000
C	3.99858700	4.01597600	-0.29577000
C	5.16994600	4.56036000	2.16251700
C	5.04475600	4.93274900	-0.21951700
C	5.63242100	5.20286300	1.01524600
F	-4.33754400	-2.99145500	-1.46078100
F	-6.37353100	-4.76497900	-1.26259800
F	-7.00009900	-5.85988800	1.15613500
F	-5.57854500	-5.16999400	3.38053000
F	-3.54288900	-3.39402200	3.19049300
F	3.45282300	3.77398300	-1.49345200
F	3.69449400	3.04580200	3.17910000
F	5.73318400	4.82178900	3.34675300
F	6.63678000	6.07773700	1.09940100
F	5.49054200	5.54902800	-1.31876700
C	3.77316500	-4.41037800	0.50019800
C	4.63213300	-5.37954600	-0.15400300
H	5.01778200	-6.09760200	0.58123400
C	3.99954900	-6.13588700	-1.37045100
H	3.08343700	-6.68999000	-1.15090200
C	5.79716200	-4.78391500	-1.00535600
H	6.47338300	-4.10762100	-0.47973000
C	6.43885200	-6.08637700	-1.53739700
H	7.02039900	-5.90903200	-2.44664600
H	7.11755900	-6.51645300	-0.79427900
C	5.20237200	-7.01979100	-1.78245500
H	5.12379700	-7.35306600	-2.82150000
H	5.25406800	-7.91578200	-1.15614300
C	3.83842900	-5.03914300	-2.45588300
H	3.88335200	-5.50077400	-3.44551900
C	5.05790800	-4.11105000	-2.18279100
H	5.72992300	-3.99734200	-3.03929100
N	3.13355200	-2.77877800	-2.18361500

H	2.53577100	-1.98172400	-1.99354100
C	3.02539800	-3.54014200	0.89413000
C	-2.35360100	2.57595400	-0.26565100
C	-3.30767200	3.64048300	-0.68903700
C	-3.88850700	3.62125000	-1.96117000
C	-3.67136600	4.68381600	0.16739300
C	-4.79186500	4.59977400	-2.37059400
C	-4.56673500	5.67710600	-0.22192700
C	-5.12943100	5.63171500	-1.49644700
F	-3.14823200	4.74886300	1.39956300
F	-4.89422800	6.66511500	0.61752200
F	-5.99148500	6.57585500	-1.87908500
F	-5.33266500	4.55782200	-3.59220300
F	-3.58492400	2.63951300	-2.81755100
C	4.46319800	-2.72991700	-1.88679800
C	2.58619600	-4.11384200	-2.37876600
H	1.99636200	-4.16039400	-3.30053600
H	1.92648900	-4.39095500	-1.54710500
O	5.09023500	-1.75873300	-1.48568100

**<sup>3</sup>Cat3**

C	2.72637300	1.35797400	-0.03705200
C	4.13513300	1.07034000	0.04647000
C	4.26327400	-0.28161900	0.04640600
C	2.93361800	-0.82852300	-0.03765200
N	1.99921000	0.18596400	-0.09165700
H	4.92002300	1.80870300	0.10966000
H	5.17284100	-0.85950400	0.10968200
C	-0.82241300	-2.92946800	-0.14719700
C	-0.27677000	-4.26239100	-0.13563400
C	1.07515700	-4.13607100	-0.11711800
C	1.36413900	-2.72527300	-0.10165100
N	0.19333500	-1.99476800	-0.13418100
H	-0.85502800	-5.17381100	-0.14056700
H	1.81275600	-4.92421200	-0.11797400
C	-1.35658400	2.72655500	-0.14303200
C	-1.06681600	4.13724600	-0.12894700
C	0.28517800	4.26279700	-0.11065600
C	0.83005800	2.92963800	-0.09744700
N	-0.18570100	1.99546300	-0.13102300
H	-1.80365800	4.92602100	-0.13202400
H	0.86436500	5.17369600	-0.11023300
C	-2.92523300	0.82947900	-0.20645500
C	-4.25483100	0.28253000	-0.29099900

C	-4.12657600	-1.06949300	-0.29195500
C	-2.71784900	-1.35706500	-0.20786500
N	-1.98981400	-0.18489800	-0.17397100
H	-5.16390600	0.86099900	-0.35690700
H	-4.91073000	-1.80839900	-0.35897200
C	2.19525600	2.64773200	-0.04800000
C	-2.18795200	-2.64715300	-0.18103800
C	2.65321100	-2.19482700	-0.05072300
C	-2.64600000	2.19584100	-0.17833400
Mn	-0.00209600	-0.00038800	0.13919800
Cl	-0.03261500	-0.00601500	2.33092900
C	3.80114000	-3.14538700	-0.00114600
C	4.67344700	-3.28731200	-1.08445200
C	4.04883900	-3.92802700	1.13091100
C	5.75241200	-4.16743400	-1.04922500
C	5.11737100	-4.82026900	1.18683000
C	5.97216700	-4.93738100	0.09189600
C	3.14608000	3.79560500	0.00230900
C	3.24726300	4.60720800	1.13648900
C	3.97305200	4.10083300	-1.08280600
C	4.13110200	5.68270300	1.19282700
C	4.86929000	5.16644300	-1.04728200
C	4.94551600	5.96035000	0.09604300
C	-3.79666900	3.14423400	-0.19137400
C	-4.64862900	3.26570600	0.91092800
C	-4.06907600	3.94325300	-1.30571000
C	-5.72999300	4.14426000	0.90921700
C	-5.13977500	4.83369700	-1.32813900
C	-5.97346400	4.93149100	-0.21516000
C	-3.14205000	-3.79329500	-0.19200900
C	-3.26615900	-4.62726600	-1.30704100
C	-3.95135700	-4.07274900	0.91366300
C	-4.15273500	-5.70124600	-1.32705500
C	-4.85047100	-5.13707400	0.91448500
C	-4.94851500	-5.95408100	-0.21074300
F	4.48466400	-2.55762400	-2.19194100
F	6.57165900	-4.28181200	-2.09935300
F	7.00041800	-5.78643300	0.13584600
F	5.33044100	-5.55826300	2.28054000
F	3.24234100	-3.83561100	2.19469800
F	2.47536300	4.36298500	2.20191900
F	3.91986100	3.35205200	-2.19236300
F	4.20654200	6.44413800	2.28863100
F	5.79775500	6.98597000	0.14031300



F	5.64949100	5.43461500	-2.09913800
F	-3.87828800	-3.30214300	2.00475300
F	-2.51205800	-4.40552400	-2.39230800
F	-4.24918700	-6.48390700	-2.40663300
F	-5.80406100	-6.97784500	-0.21969000
F	-5.61368400	-5.38157100	1.98388500
F	-4.43831700	2.51950700	2.00120100
F	-3.28251700	3.86812300	-2.38797900
F	-5.37547500	5.58734600	-2.40692400
F	-7.00442100	5.77830900	-0.22650500
F	-6.52985800	4.24002900	1.97549100

**<sup>5</sup>Cat1**

C	1.71514700	-2.21084300	-0.20966500
C	3.13246900	-2.44999300	-0.27374800
C	3.74412300	-1.23802800	-0.36469000
C	2.70125100	-0.24898900	-0.33998200
N	1.46758300	-0.85268200	-0.23565200
H	3.60354700	-3.42093400	-0.24928700
H	4.80407200	-1.04112000	-0.43792200
C	-0.03492200	3.08923200	-0.13332100
C	0.96008400	4.12617000	-0.19793700
C	2.16918000	3.51261100	-0.30969900
C	1.92234400	2.09862400	-0.30830000
N	0.57395100	1.85162600	-0.19241500
H	0.75622200	5.18531600	-0.15252300
H	3.14927500	3.95946300	-0.38154400
C	-2.58579200	-1.99166500	0.06653000
C	-2.82820100	-3.41032600	0.04139900
C	-1.61699100	-4.02090700	-0.03550800
C	-0.62081300	-2.98250000	-0.06148900
N	-1.23015100	-1.74690200	0.00241600
H	-3.80206900	-3.87491700	0.06836200
H	-1.41168600	-5.07951100	-0.08331800
C	-3.35334800	0.34782900	0.15654500
C	-4.38629300	1.34366600	0.27003000
C	-3.77818600	2.55744800	0.21399700
C	-2.36580200	2.31664400	0.07769900
N	-2.12240900	0.95923800	0.05342100
H	-5.43954700	1.13639500	0.38308200
H	-4.24172800	3.53120600	0.25782800
C	0.75176000	-3.21841000	-0.14403500
C	-1.40542000	3.32429100	-0.01369300
C	2.93966700	1.13282200	-0.38674400

C	-3.59131400	-1.02775500	0.14782400
Mn	-0.35172000	0.04829500	-0.37879800
Cl	-0.57021000	0.01363400	-2.71308900
C	-1.86952300	4.74063300	0.02339900
C	-2.37958300	5.30851200	1.19465500
C	-1.80851500	5.55462800	-1.11233000
C	-2.81916400	6.62919100	1.24130100
F	-2.46228000	4.57210200	2.31150200
C	-2.23505100	6.88097800	-1.08760800
F	-1.32216200	5.06565400	-2.25770900
C	-2.74377300	7.41743400	0.09409400
F	-3.30457900	7.14538200	2.37543800
F	-2.16388500	7.63858200	-2.18630800
F	-3.15776300	8.68565500	0.12780000
C	-5.00429900	-1.49411300	0.23436600
C	-5.48633800	-2.14788300	1.37265000
C	-5.90132500	-1.29475000	-0.82038000
C	-6.80287200	-2.59298400	1.46357500
F	-4.66918800	-2.36738400	2.41170600
C	-7.22497600	-1.72404600	-0.74892600
F	-5.49647700	-0.66903500	-1.93065800
C	-7.67461000	-2.37724900	0.39744900
F	-7.23580900	-3.21712500	2.56400400
F	-8.06230600	-1.51890100	-1.77020800
F	-8.93943600	-2.79542600	0.47488600
C	1.21851300	-4.63382900	-0.16747000
C	1.78052700	-5.19516600	-1.31882700
C	1.11201900	-5.45224400	0.96106300
C	2.22293800	-6.51608500	-1.34928300
F	1.90989200	-4.45666100	-2.42556200
C	1.54095800	-6.77707100	0.95210400
F	0.57784800	-4.96517600	2.08986500
C	2.10012000	-7.30839300	-0.20899000
F	2.75683000	-7.02873900	-2.46176000
F	1.42542900	-7.53733400	2.04618700
F	2.51719400	-8.57577700	-0.22857300
C	4.28563700	1.59122300	-0.47296200
C	5.42640300	2.00493700	-0.49222500
C	6.77541400	2.55013500	-0.50772100
H	6.83698500	3.26681000	-1.33754000
C	7.28581300	3.22354100	0.80886100
H	6.64824900	4.01750500	1.20584000
C	7.97282900	1.55303400	-0.57909900
H	7.94264900	0.82783800	-1.39356800

C	9.15426900	2.54909600	-0.61727900
H	10.08878200	2.08221000	-0.29329900
H	9.31165900	2.92363300	-1.63329000
C	8.68473600	3.69594800	0.34353300
H	9.36413300	3.84394300	1.18830800
H	8.61176800	4.65059400	-0.18608700
C	7.49248600	2.03227400	1.77645100
H	8.24666000	2.28756900	2.52490900
C	7.96522600	0.89649300	0.81994800
H	8.95066500	0.48644900	1.06063700
C	6.22064300	1.47954100	2.48644200
H	5.33093700	2.06529200	2.22834100
H	6.33147200	1.49220700	3.57640000
C	6.93931600	-0.22157500	0.97184700
O	6.88181200	-1.23933700	0.29340800
N	6.10142900	0.11298300	1.99464600
H	5.27685400	-0.44935900	2.15436900

**<sup>5</sup>Cat2**

N	-2.10666500	0.39780200	0.26077100
N	-0.54787500	-1.87592000	0.89491100
N	1.78087500	-0.27291300	0.92106400
N	0.22432400	2.00701800	0.28636800
C	-2.68419400	1.57488800	-0.16044200
C	-4.11588600	1.43568700	-0.17851900
C	-4.40122600	0.17981900	0.25932500
C	-3.14662200	-0.47880500	0.50697600
C	-3.01653600	-1.81819000	0.87583200
C	-1.78696000	-2.47051400	1.00434600
C	-1.62959400	-3.89133200	1.16121600
C	-0.29377700	-4.15597600	1.09038300
C	0.37186200	-2.89580600	0.93701300
C	1.76780500	-2.74285500	0.87992200
C	2.40985300	-1.49764500	0.95015700
C	3.82599300	-1.32543200	1.10673600
C	4.05063500	0.01329400	1.20386600
C	2.78037200	0.66915700	1.04452100
C	2.61835600	2.05014400	0.90540800
C	1.42264000	2.65421300	0.51396800
C	1.28139700	4.05338600	0.20722300
C	0.01531000	4.23847400	-0.25130900
C	-0.65339900	2.96614300	-0.17501500
H	-4.81052800	2.21437600	-0.45567100
H	-5.37480300	-0.26472000	0.39963800

H	-2.43962000	-4.59555300	1.27879100
H	0.21195900	-5.10811400	1.15481600
H	4.54283200	-2.13052300	1.10994600
H	4.99939500	0.51619100	1.31210000
H	2.05806000	4.79481800	0.31594700
H	-0.43478700	5.15878500	-0.59046900
Mn	-0.12163600	0.01536500	0.32055000
Cl	0.29189400	-0.52025600	-1.97141700
C	-4.25159700	-2.62507700	1.08274100
C	-4.58650800	-3.11122700	2.35076400
C	-5.10762700	-2.94795000	0.02468300
C	-5.72570500	-3.88313500	2.56567100
C	-6.25651800	-3.71221000	0.21683700
C	-6.56377100	-4.18225200	1.49268100
C	3.81968400	2.90752000	1.11027400
C	4.37771400	3.06507500	2.38269900
C	4.45232600	3.55724100	0.04556900
C	5.51514300	3.83976700	2.59606900
C	5.58655900	4.34348700	0.23593300
C	6.11947400	4.48194600	1.51651300
F	-4.83389900	-2.51582300	-1.21197600
F	-7.05877600	-4.00370700	-0.81177000
F	-7.65973600	-4.91808000	1.68685600
F	-6.02172400	-4.33316000	3.78918300
F	-3.79716200	-2.83984900	3.39834700
F	3.96437900	3.43769000	-1.19447100
F	3.81766100	2.45510600	3.43580000
F	6.02616300	3.97461900	3.82417900
F	7.20706700	5.23059100	1.70940500
F	6.16883500	4.95828000	-0.79808500
C	3.21042300	-4.81314900	0.19409900
C	3.97174400	-5.81838100	-0.52286000
H	4.23768500	-6.63958300	0.15540100
C	3.30547200	-6.38425000	-1.82252100
H	2.32123000	-6.83828000	-1.68277000
C	5.23411600	-5.29806000	-1.27978200
H	5.96325200	-4.75739500	-0.67388300
C	5.73824900	-6.61915800	-1.90611000
H	6.37332500	-6.43656600	-2.77772600
H	6.33038500	-7.19058200	-1.18440200
C	4.41110800	-7.37105900	-2.27166000
H	4.33739700	-7.60404300	-3.33800200
H	4.32965300	-8.31595900	-1.72536000
C	3.32354400	-5.18823500	-2.80989000

H	3.35703100	-5.56682200	-3.83467700
C	4.63046500	-4.44151700	-2.41385300
H	5.34801600	-4.33591700	-3.23372200
N	2.87787200	-2.89299000	-2.34804300
H	2.36090700	-2.04184400	-2.14405700
C	2.56047900	-3.90012900	0.65881600
C	-2.01087700	2.76937300	-0.43322300
C	-2.81531100	3.91055000	-0.95331500
C	-3.34389200	3.88002000	-2.24841700
C	-3.09705400	5.03459400	-0.17095600
C	-4.11428700	4.92669200	-2.75108800
C	-3.85803200	6.09599000	-0.65447500
C	-4.36927700	6.03858400	-1.95007200
F	-2.62480700	5.11202000	1.08145700
F	-4.10806400	7.16025600	0.11557800
F	-5.10348300	7.04767300	-2.42244100
F	-4.60678600	4.87325000	-3.99213900
F	-3.11945600	2.82261700	-3.03454300
C	4.18879100	-3.02827900	-2.01430100
C	2.18842900	-4.12730100	-2.69119200
H	1.64026500	-4.01599300	-3.63262300
H	1.46120400	-4.39522300	-1.91450100
O	4.91481100	-2.17873400	-1.51121900

**<sup>5</sup>Cat3**

C	-2.84651500	-1.10171600	-0.03407100
C	-4.22044700	-0.67912400	0.04274500
C	-4.22044000	0.67921200	0.04261200
C	-2.84650200	1.10177400	-0.03425100
N	-2.01917600	0.00002100	-0.08293400
H	-5.07170800	-1.33992500	0.10189000
H	-5.07169400	1.34003300	0.10163200
C	1.09788600	2.84475700	-0.13943600
C	0.67450700	4.22069600	-0.13624100
C	-0.68365400	4.21997300	-0.11874800
C	-1.10536500	2.84383300	-0.09473100
N	-0.00335900	2.01557800	-0.11908200
H	1.33449800	5.07449700	-0.14628400
H	-1.34517000	5.07273400	-0.12557500
C	1.09784400	-2.84474100	-0.13963200
C	0.67445200	-4.22067500	-0.13638600
C	-0.68370700	-4.21993800	-0.11863500
C	-1.10539900	-2.84379300	-0.09455800
N	-0.00338700	-2.01555100	-0.11908800

H	1.33443300	-5.07448200	-0.14655400
H	-1.34523600	-5.07269000	-0.12534500
C	2.83750200	-1.10180100	-0.19879900
C	4.21028500	-0.67922800	-0.29399500
C	4.21029700	0.67921600	-0.29386900
C	2.83752000	1.10179500	-0.19860900
N	2.01009900	0.00000100	-0.15522800
H	5.05992200	-1.34078500	-0.36806200
H	5.05994400	1.34077400	-0.36781600
C	-2.43918500	-2.43640700	-0.04574900
C	2.43191300	2.43681000	-0.17419300
C	-2.43916100	2.43646000	-0.04605700
C	2.43187500	-2.43681100	-0.17452300
Mn	0.00143600	0.00001200	0.16538500
Cl	0.02166500	0.00001500	2.50754700
C	-3.49263200	3.49027500	-0.00234400
C	-4.35010300	3.70546400	-1.08571300
C	-3.66348400	4.30121500	1.12448700
C	-5.34247000	4.68215400	-1.05545600
C	-4.64415800	5.28970100	1.17468200
C	-5.48690700	5.47763000	0.08023300
C	-3.49264800	-3.49022100	-0.00180500
C	-3.66334700	-4.30104700	1.12513100
C	-4.35023500	-3.70555000	-1.08505300
C	-4.64399700	-5.28954600	1.17554900
C	-5.34258000	-4.68225500	-1.05457400
C	-5.48686900	-5.47761100	0.08121800
C	3.48873900	-3.48783100	-0.19645800
C	4.33491100	-3.68752000	0.89937200
C	3.67732200	-4.30856400	-1.31264700
C	5.33019500	-4.66263100	0.88904300
C	4.66017400	-5.29472000	-1.34295200
C	5.49019700	-5.46929500	-0.23656800
C	3.48880500	3.48780800	-0.19588900
C	3.67755200	4.30866100	-1.31196200
C	4.33485400	3.68733900	0.90006500
C	4.66044100	5.29478700	-1.34203400
C	5.33017200	4.66241800	0.88996900
C	5.49033600	5.46920800	-0.23553000
F	-4.23232400	2.95335200	-2.18828000
F	-6.14955400	4.86462300	-2.10529300
F	-6.43132200	6.41895600	0.11917900
F	-4.78487400	6.05269300	2.26252800
F	-2.86657700	4.14269900	2.18667600

F	-2.86631500	-4.14240400	2.18720700
F	-4.23259500	-2.95356100	-2.18772000
F	-4.78456800	-6.05242500	2.26349200
F	-6.43126100	-6.41895100	0.12037600
F	-6.14978000	-4.86485800	-2.10429900
F	4.20421100	2.92435600	1.99020900
F	2.89301700	4.16065400	-2.38844600
F	4.81660200	6.06689200	-2.42212700
F	6.43806000	6.40780200	-0.25445100
F	6.12653400	4.83150100	1.94933100
F	4.20442200	-2.92466000	1.98962200
F	2.89266000	-4.16040900	-2.38901800
F	4.81617900	-6.06670500	-2.42315200
F	6.43788800	-6.40791900	-0.25571200
F	6.12667900	-4.83186200	1.94829000

**<sup>3</sup>TS2-s**

N	-0.52077900	1.99602800	-0.60322600
N	-2.97756800	0.62779600	-0.39940700
N	-1.58983600	-1.82160800	-0.65947800
N	0.83884300	-0.41471600	-0.91835800
C	0.63746800	2.52661900	-1.10828400
C	0.61768300	3.95253900	-0.94262100
C	-0.53807200	4.26464900	-0.28751500
C	-1.27340900	3.03651300	-0.11758300
C	-2.60729700	2.95056700	0.30281800
C	-3.41868500	1.82981500	0.08300700
C	-4.85827100	1.78914400	0.20195400
C	-5.26232400	0.57436200	-0.25866200
C	-4.07029200	-0.17702200	-0.58326200
C	-4.02957800	-1.55062100	-0.85452600
C	-2.85600400	-2.31607400	-0.81197000
C	-2.80514900	-3.75712300	-0.73231800
C	-1.51229600	-4.09978100	-0.46730600
C	-0.74622700	-2.87815200	-0.44462900
C	0.64892400	-2.79928200	-0.35306400
C	1.38521400	-1.64637500	-0.65103600
C	2.81032400	-1.58493800	-0.87717700
C	3.09041200	-0.33801600	-1.35071200
C	1.85162900	0.39724900	-1.34489300
C	1.74024300	1.78344400	-1.56339900
H	1.41152100	4.61260400	-1.25981500
H	-0.88966500	5.24163600	0.01007500
H	-5.47970500	2.59873500	0.55284600

H	-6.27302000	0.20354100	-0.33614300
H	-3.65806200	-4.41271200	-0.82877600
H	-1.10012600	-5.09000000	-0.33768700
H	3.50905100	-2.38519800	-0.69113100
H	4.05511300	0.08785100	-1.58592300
Mn	-1.06176100	0.09923000	-0.61912600
Cl	-1.37529700	0.17695500	-2.93629900
O	-0.94869000	-0.12727800	1.08082500
C	-5.31033300	-2.28143000	-1.06835600
C	-6.23245100	-2.48744400	-0.03775200
C	-5.61439700	-2.82651300	-2.32065100
C	-7.41976400	-3.18646200	-0.24119700
C	-6.79267600	-3.53588800	-2.54558600
C	-7.69810000	-3.71348900	-1.50111500
C	-3.18574500	4.15432900	0.95857100
C	-2.72180300	4.54650000	2.21974800
C	-4.16646300	4.95172200	0.36179700
C	-3.21597500	5.67410300	2.86969400
C	-4.68125800	6.08103300	0.99516400
C	-4.20141800	6.44322700	2.25254500
C	1.39238500	-4.01617800	0.06956700
C	1.29303500	-4.45427700	1.39321200
C	2.26936200	-4.70957300	-0.77001600
C	2.05723400	-5.50944300	1.87789800
C	3.05129100	-5.76302200	-0.30292100
C	2.94650400	-6.15761000	1.02809000
F	-5.98522200	-2.00473000	1.18829000
F	-8.28553900	-3.36430300	0.76305600
F	-8.83110300	-4.38909400	-1.70630000
F	-7.06060300	-4.04421700	-3.75261800
F	-4.76102500	-2.67665400	-3.33800600
F	-4.63848100	4.63710600	-0.85163000
F	-5.62124800	6.82368100	0.40144000
F	-4.68502600	7.52563000	2.86565100
F	-2.75646800	6.02153500	4.07609700
F	-1.77206000	3.82687300	2.83741700
F	2.40425600	-4.34193000	-2.05044200
F	0.49890900	-3.80465500	2.25697200
F	2.01642500	-5.83600400	3.17676000
F	3.74885500	-7.11541300	1.50611100
F	3.92942200	-6.37005900	-1.10869200
C	2.84196000	2.45623200	-2.15556700
C	3.80884400	2.96604000	-2.68291900
C	4.99772000	3.50173900	-3.32884300



H	4.85689300	3.42515700	-4.41542600
C	5.46837600	4.94390600	-2.95907200
H	4.72426200	5.73147200	-3.10112400
C	6.35444100	2.84710700	-2.91811600
H	6.40144200	1.76011000	-3.00085700
C	7.32848000	3.62345400	-3.83356900
H	8.34955100	3.61288500	-3.44107700
H	7.35801500	3.17668900	-4.83188900
C	6.71037100	5.06368500	-3.87432000
H	7.40372200	5.83181100	-3.51907600
H	6.41445800	5.33740500	-4.89156200
C	5.97469900	4.80808700	-1.50173400
H	6.73379200	5.56735800	-1.29802800
C	6.55576800	3.36051300	-1.47391300
H	7.60893000	3.29976000	-1.18238500
C	4.88811100	4.83565600	-0.39143500
H	3.89291400	5.03403800	-0.80689700
H	5.09448400	5.60400200	0.36182400
C	5.72368300	2.62862300	-0.42679100
O	5.79022000	1.40942300	-0.19901500
N	4.92588000	3.50843300	0.20398600
H	4.14307800	3.15414100	0.77517300
C	5.44340200	-2.92357500	2.08769400
C	5.26979000	-1.60335500	1.68658600
C	4.11480100	-0.89239400	2.05940400
C	3.10154600	-1.51269900	2.82938900
C	3.30663000	-2.84452200	3.24967800
C	4.44940800	-3.53375900	2.88911000
H	6.01443700	-1.10478100	1.07172000
C	1.90578000	-0.77090400	3.09054700
H	2.53461100	-3.33565300	3.83374800
H	4.57604500	-4.56537100	3.20599300
C	1.73165800	0.51356200	2.65278900
C	2.80899400	1.16203500	1.89357700
H	1.10582100	-1.27136900	3.62807000
C	6.65543200	-3.71591000	1.64893100
H	7.39629800	-3.03716600	1.21269100
H	7.12827300	-4.17223500	2.52812200
O	2.72510600	2.33112200	1.46641200
C	0.46328300	1.27877900	2.78483900
H	0.64652400	2.34819800	2.65590200
H	-0.14491200	0.97746200	1.86139100
C	-0.43101700	0.96974900	3.97847400
H	-1.31022900	1.61796100	3.95579500

H	-0.78290100	-0.06596900	3.95818800
H	0.09831100	1.13703700	4.92368600
C	6.31239400	-4.82241300	0.63493500
H	7.21844300	-5.33831500	0.30165900
H	5.64757800	-5.57237900	1.07092900
H	5.81655500	-4.40778800	-0.24883300
N	3.93592300	0.41122900	1.65855400
H	4.64273300	0.82351500	1.02374300

**<sup>3</sup>TS2-R**

N	-0.58333900	1.97388000	-0.51507700
N	-2.98351200	0.49479200	-0.34632400
N	-1.49987200	-1.89051400	-0.65612400
N	0.87438700	-0.38021900	-0.86816900
C	0.56167900	2.55384700	-0.99496900
C	0.49175600	3.97555400	-0.80353900
C	-0.68505000	4.23835300	-0.16584900
C	-1.38461500	2.98459700	-0.03610700
C	-2.72406000	2.84203600	0.33786100
C	-3.47816800	1.68530900	0.10554100
C	-4.91933300	1.60788700	0.16423500
C	-5.27011000	0.37405500	-0.29128900
C	-4.04477800	-0.34331700	-0.56491100
C	-3.94975700	-1.71250100	-0.84540200
C	-2.74719100	-2.43166100	-0.80689800
C	-2.64064400	-3.87052700	-0.74181900
C	-1.33444100	-4.16611100	-0.48709600
C	-0.61580100	-2.91616800	-0.45407300
C	0.77524700	-2.78460800	-0.36253900
C	1.46599700	-1.59820400	-0.63561900
C	2.88663000	-1.48013400	-0.86794000
C	3.11918200	-0.21267200	-1.31130000
C	1.85511400	0.47742600	-1.27984800
C	1.69261800	1.86293200	-1.46307900
H	1.27001700	4.66643900	-1.09226400
H	-1.06590400	5.19685700	0.15362700
H	-5.57067800	2.41184100	0.47471200
H	-6.26543900	-0.02769100	-0.40560600
H	-3.46824400	-4.55742700	-0.84061000
H	-0.88410200	-5.14110300	-0.36958300
H	3.61428000	-2.25987100	-0.70725200
H	4.06633300	0.25311300	-1.54181400
Mn	-1.04621900	0.05148800	-0.56545500
Cl	-1.35660400	0.16525500	-2.88323700

O	-0.94053700	-0.24377800	1.12167500
C	-5.19993600	-2.48858600	-1.07659300
C	-6.13686500	-2.71254300	-0.06284000
C	-5.46054800	-3.05756500	-2.32833200
C	-7.29662900	-3.45176400	-0.28257400
C	-6.61042800	-3.80700900	-2.56902800
C	-7.53157800	-4.00174700	-1.54148500
C	-3.42410300	4.01838100	0.92670000
C	-3.69252900	4.06423400	2.29733200
C	-3.84558700	5.10094500	0.15056900
C	-4.35035700	5.14354100	2.88233700
C	-4.50370900	6.19311200	0.71255800
C	-4.75838900	6.21029200	2.08301900
C	1.56822600	-3.98031000	0.03092200
C	1.50162700	-4.44515600	1.34743000
C	2.46017500	-4.62497200	-0.83134700
C	2.30955600	-5.48063000	1.80317900
C	3.28674900	-5.65646800	-0.39288600
C	3.21234300	-6.07912700	0.93151100
F	-5.93123600	-2.20951200	1.16244700
F	-8.17697100	-3.64631400	0.70573500
F	-8.63783500	-4.71576400	-1.76191200
F	-6.83663800	-4.33701300	-3.77532300
F	-4.59165300	-2.89178500	-3.33016300
F	-3.61156700	5.10771600	-1.16736600
F	-4.89574800	7.21851100	-0.05092000
F	-5.38952200	7.25112400	2.63095700
F	-4.59077000	5.16468100	4.19728500
F	-3.30310700	3.05283900	3.08748500
F	2.56621700	-4.22844900	-2.10582400
F	0.69477200	-3.84118000	2.23202200
F	2.29495800	-5.83445100	3.09557700
F	4.05522700	-7.01508800	1.38251900
F	4.17790400	-6.21479700	-1.21936600
C	2.76778600	2.59075300	-2.03908400
C	3.71354400	3.15076200	-2.55365900
C	4.88191600	3.74869800	-3.18231700
H	4.74554400	3.69816200	-4.27096000
C	5.29787300	5.19636700	-2.77029700
H	4.52507200	5.95937100	-2.89168700
C	6.26155900	3.13381600	-2.78689000
H	6.34935800	2.05215600	-2.90056900
C	7.20766200	3.97200800	-3.67667100
H	8.22763100	3.98853000	-3.28149600

H	7.25600500	3.55534300	-4.68719000
C	6.53594600	5.38861900	-3.67840000
H	7.19936200	6.17186600	-3.29976200
H	6.23156200	5.67971500	-4.68827600
C	5.80659900	5.03792700	-1.31604300
H	6.53684100	5.81847300	-1.08871100
C	6.44054100	3.61241900	-1.32782100
H	7.49442400	3.58180600	-1.03418500
C	4.71753600	4.99390100	-0.20873700
H	3.71681100	5.16785800	-0.62172200
H	4.89423600	5.74714800	0.56697600
C	5.63230900	2.82041900	-0.30631800
O	5.74002400	1.59799200	-0.11528200
N	4.80222100	3.65214700	0.34835800
H	4.02754100	3.25048900	0.89781000
C	5.59664900	-2.78265000	2.05278900
C	5.35958200	-1.46281900	1.68516200
C	4.17919500	-0.81392600	2.09139700
C	3.20901300	-1.49551000	2.86333900
C	3.47823100	-2.82615600	3.25068500
C	4.64357600	-3.45504900	2.85530700
H	6.07069700	-0.91790100	1.07005000
C	1.99122800	-0.80866900	3.15891500
H	2.73787300	-3.36418700	3.83431200
H	4.82048000	-4.48754000	3.14391600
C	1.74127800	0.47672400	2.75287800
C	2.76762500	1.18029700	1.97462200
H	1.22131100	-1.35019800	3.70353700
C	6.83305900	-3.51201400	1.57487800
H	7.53759200	-2.79215100	1.14445700
H	7.33905600	-3.97023200	2.43438200
O	2.63393600	2.34128100	1.53800800
C	0.39309700	1.08481200	2.95732800
H	-0.19508500	0.80538700	2.01282600
C	6.51834800	-4.60593200	0.53813900
H	7.43897600	-5.07529700	0.17725800
H	5.89208400	-5.39345200	0.96497200
H	5.99111200	-4.18979500	-0.32654300
N	3.92913700	0.48537800	1.72109300
H	4.60606100	0.94215700	1.08399100
C	0.23666900	2.58508400	3.19999500
H	0.60671100	3.16721100	2.35785900
H	-0.82025100	2.81396200	3.36348700
H	0.79610600	2.89033200	4.09276000

H	-0.14111300	0.51163300	3.72269100
<b><sup>5</sup>TS2-S</b>			
N	-0.52216100	1.99847700	-0.57936900
N	-2.99758000	0.63076900	-0.43776200
N	-1.60184400	-1.80043500	-0.63497400
N	0.82925100	-0.41538600	-0.92938700
C	0.63948600	2.53293200	-1.06537100
C	0.62462100	3.95655800	-0.88430800
C	-0.54264700	4.26416400	-0.24465200
C	-1.27782100	3.03327100	-0.09851600
C	-2.62459000	2.94775200	0.29268900
C	-3.43720000	1.83726100	0.04608100
C	-4.87825200	1.80031200	0.15979000
C	-5.28454900	0.58613400	-0.29749400
C	-4.09116100	-0.16849700	-0.61383500
C	-4.04588700	-1.54813900	-0.85729100
C	-2.87149100	-2.30549600	-0.77855000
C	-2.81536500	-3.74160400	-0.67178800
C	-1.52089900	-4.07884000	-0.40279700
C	-0.75250000	-2.86287800	-0.40822500
C	0.64019500	-2.79038800	-0.33803600
C	1.37867900	-1.64073900	-0.65630500
C	2.80455400	-1.58133900	-0.87573900
C	3.08672500	-0.33183600	-1.34147000
C	1.84562900	0.40132200	-1.33964800
C	1.74072200	1.79101000	-1.53300500
H	1.42309800	4.61873700	-1.18506700
H	-0.89910200	5.23895600	0.05419900
H	-5.49839200	2.61120000	0.50972800
H	-6.29545000	0.21581900	-0.37414700
H	-3.66634500	-4.40111700	-0.75819000
H	-1.11060900	-5.06729500	-0.25564500
H	3.50310400	-2.38032700	-0.68376100
H	4.05304400	0.09705600	-1.56489300
Mn	-1.08833300	0.08812300	-0.66307400
Cl	-1.34553700	0.26285100	-2.97106100
O	-0.98438300	-0.11116500	1.09218200
C	-5.32162500	-2.28780900	-1.06887700
C	-6.25497600	-2.47394800	-0.04456400
C	-5.61019300	-2.86063300	-2.31246700
C	-7.43857100	-3.17973800	-0.24665500
C	-6.78436300	-3.57716400	-2.53575400
C	-7.70143500	-3.73417200	-1.49810600

C	-3.20700100	4.14641600	0.95450500
C	-2.75305100	4.52482700	2.22373400
C	-4.17942600	4.95289400	0.35634900
C	-3.25030200	5.64738800	2.88007000
C	-4.69659200	6.07750900	0.99599300
C	-4.22764700	6.42559800	2.26142700
C	1.38498500	-4.00750700	0.08068700
C	1.29493000	-4.44879900	1.40403200
C	2.25611000	-4.69949500	-0.76659900
C	2.06189500	-5.50594300	1.88027000
C	3.04140000	-5.75383800	-0.30762800
C	2.94585300	-6.15160300	1.02317000
F	-6.02257300	-1.96489700	1.17352900
F	-8.31534000	-3.33799500	0.75115700
F	-8.83054300	-4.41654500	-1.70169500
F	-7.03719500	-4.11207700	-3.73446400
F	-4.74490600	-2.73134800	-3.32282700
F	-4.64078600	4.65230800	-0.86480200
F	-5.62847000	6.82911300	0.40066700
F	-4.71378600	7.50334900	2.88068700
F	-2.80106400	5.98167100	4.09397100
F	-1.81070000	3.79707100	2.84208600
F	2.38045300	-4.33032100	-2.04760600
F	0.50698200	-3.80194000	2.27519800
F	2.02991400	-5.83581200	3.17848400
F	3.75138000	-7.11049600	1.49341300
F	3.91298700	-6.35962100	-1.12131700
C	2.84159000	2.46789900	-2.12066500
C	3.80480100	2.97997800	-2.65308900
C	4.98570600	3.51554600	-3.31345100
H	4.82670600	3.44381500	-4.39790500
C	5.46696000	4.95464500	-2.94571600
H	4.72316700	5.74512400	-3.07231400
C	6.34684000	2.85472300	-2.92800300
H	6.38875400	1.76794500	-3.01596700
C	7.30811600	3.63182500	-3.85613600
H	8.33541100	3.61638200	-3.48042500
H	7.31987600	3.18912000	-4.85662600
C	6.69407900	5.07415900	-3.88081400
H	7.39563000	5.83859400	-3.53384000
H	6.38237700	5.35305400	-4.89191200
C	5.99647800	4.81099000	-1.49747700
H	6.76111100	5.56702400	-1.30271200
C	6.57310200	3.36135300	-1.48513900

H	7.63042600	3.29556400	-1.21033700
C	4.92741000	4.83712500	-0.37031100
H	3.92672500	5.04240900	-0.76906500
H	5.14885900	5.60024500	0.38396900
C	5.75392000	2.62715300	-0.42952800
O	5.81881300	1.40639900	-0.20953800
N	4.96818100	3.50634700	0.21689500
H	4.19089900	3.15138500	0.79541400
C	5.47247100	-2.93926200	2.06041100
C	5.30127500	-1.61648400	1.66599200
C	4.15009000	-0.90391100	2.04652000
C	3.13679400	-1.52540500	2.81636200
C	3.34095600	-2.85921800	3.23175300
C	4.48058900	-3.54972700	2.86449100
H	6.04508400	-1.11752500	1.05041500
C	1.94287600	-0.78383600	3.08184500
H	2.57049500	-3.34986400	3.81823200
H	4.60632500	-4.58267700	3.17739000
C	1.77000100	0.50553400	2.65344000
C	2.85149500	1.15687000	1.90053100
H	1.14160300	-1.28601600	3.61567600
C	6.67861200	-3.73438400	1.61118300
H	7.41995700	-3.05695900	1.17373300
H	7.15442700	-4.19721400	2.48536200
O	2.77496100	2.33138000	1.48782800
C	0.50406200	1.27003900	2.79179800
H	0.68793800	2.33875100	2.65827900
H	-0.11348200	0.95703200	1.87890200
C	-0.37738100	0.96825400	3.99835100
H	-1.25954800	1.61265800	3.97684600
H	-0.72763000	-0.06812000	3.98962300
H	0.15836400	1.14562600	4.93824800
C	6.32394300	-4.83437400	0.59394600
H	7.22532600	-5.35331900	0.25283800
H	5.65774600	-5.58287100	1.03038700
H	5.82491500	-4.41290900	-0.28476300
N	3.97425400	0.40294800	1.65531200
H	4.68053000	0.81749100	1.02162400

**<sup>5</sup>TS2-R**

N	-0.58546200	1.97552100	-0.48589400
N	-3.00666800	0.49805600	-0.38157200
N	-1.51943800	-1.86848900	-0.62437100
N	0.85965200	-0.38253300	-0.87848400

C	0.56033400	2.55905700	-0.95095100
C	0.49335000	3.97933800	-0.74939500
C	-0.69335900	4.23780000	-0.12510100
C	-1.38874000	2.98043800	-0.01204100
C	-2.73970500	2.83815300	0.33393800
C	-3.49701400	1.69377900	0.07495800
C	-4.93938500	1.62210000	0.13190200
C	-5.29559100	0.38972000	-0.32065600
C	-4.07077800	-0.33259100	-0.58960200
C	-3.97292100	-1.70820600	-0.84200300
C	-2.77034000	-2.42016300	-0.76707800
C	-2.65889100	-3.85391700	-0.67488100
C	-1.35126200	-4.14477100	-0.41624000
C	-0.62923200	-2.90093300	-0.41165300
C	0.75961100	-2.77675200	-0.34361100
C	1.45371100	-1.59390400	-0.63931700
C	2.87511400	-1.47904600	-0.86590800
C	3.11009300	-0.20922600	-1.30174100
C	1.84409800	0.47950800	-1.27393100
C	1.68878700	1.86821400	-1.43250700
H	1.27380000	4.67248300	-1.02674300
H	-1.08148200	5.19396400	0.19297100
H	-5.58701500	2.42822400	0.44449600
H	-6.29204200	-0.01000600	-0.43188200
H	-3.48459500	-4.54448600	-0.76360000
H	-0.90341900	-5.11854000	-0.28118800
H	3.60232000	-2.25789800	-0.69910100
H	4.05902700	0.25878900	-1.52085800
Mn	-1.07726900	0.03861400	-0.60810200
Cl	-1.33276700	0.26103800	-2.91381100
O	-0.97708000	-0.21915600	1.13743600
C	-5.21844500	-2.49213000	-1.06969800
C	-6.16717400	-2.69484600	-0.06241400
C	-5.46358000	-3.08917600	-2.31150800
C	-7.32381000	-3.43972700	-0.27982600
C	-6.60989900	-3.84474700	-2.54955400
C	-7.54328700	-4.01746500	-1.52906700
C	-3.43876300	4.01395100	0.92715500
C	-3.66348000	4.07927900	2.30450400
C	-3.89408400	5.07889200	0.14638800
C	-4.31401800	5.16207500	2.89165000
C	-4.54673700	6.17333600	0.71035900
C	-4.75815600	6.21085600	2.08781200
C	1.55320800	-3.97315100	0.04544500



C	1.49799400	-4.43999200	1.36186400
C	2.43658800	-4.61801600	-0.82591300
C	2.30770000	-5.47851300	1.80776400
C	3.26540000	-5.65151900	-0.39699700
C	3.20211500	-6.07650700	0.92727300
F	-5.97629300	-2.16519100	1.15386200
F	-8.21566300	-3.61334500	0.70184900
F	-8.64616400	-4.73723400	-1.74694200
F	-6.82096800	-4.40169100	-3.74633200
F	-4.58214900	-2.94532400	-3.30604100
F	-3.69859800	5.06537100	-1.17763600
F	-4.97272000	7.18217200	-0.05701000
F	-5.38314900	7.25423400	2.63803100
F	-4.51422600	5.20298700	4.21280800
F	-3.24010800	3.08477700	3.09779000
F	2.53017100	-4.22076300	-2.10109600
F	0.70034500	-3.83693400	2.25502900
F	2.30386100	-5.83509700	3.09938700
F	4.04714100	-7.01482500	1.36900500
F	4.14716100	-6.21055400	-1.23291000
C	2.76225800	2.59859900	-2.00675700
C	3.70352800	3.15942000	-2.52924900
C	4.86252200	3.75550700	-3.17662600
H	4.70296800	3.71028000	-4.26239900
C	5.29388200	5.19930100	-2.76730300
H	4.52239000	5.96645300	-2.86918400
C	6.24715700	3.13213000	-2.81315100
H	6.32713600	2.05059300	-2.93339500
C	7.17827300	3.96985300	-3.71895600
H	8.20633800	3.97969400	-3.34514100
H	7.20343600	3.55751600	-4.73208900
C	6.51357500	5.38962200	-3.70034000
H	7.18851400	6.16796900	-3.33215500
H	6.18956300	5.68675900	-4.70232000
C	5.83194800	5.03178100	-1.32475200
H	6.57026500	5.80797200	-1.10893600
C	6.45867600	3.60328200	-1.35604500
H	7.51809900	3.56596700	-1.08400900
C	4.76514400	4.98752900	-0.19606900
H	3.75726800	5.16994700	-0.58767700
H	4.96185500	5.73503000	0.58037500
C	5.66640900	2.80990500	-0.32313300
O	5.77107700	1.58576000	-0.14120700
N	4.85273800	3.64195300	0.35116500

H	4.08496600	3.24050600	0.91087400
C	5.62862900	-2.80801900	2.01513300
C	5.39582000	-1.48515000	1.65493100
C	4.22243800	-0.83169900	2.07323600
C	3.25371900	-1.51172700	2.84894400
C	3.51983700	-2.84497000	3.22999800
C	4.67885600	-3.47825000	2.82345600
H	6.10521100	-0.94160100	1.03659400
C	2.04130400	-0.82111400	3.15512300
H	2.78182900	-3.38068900	3.81869900
H	4.85310500	-4.51254200	3.10727900
C	1.79368300	0.46885500	2.75875900
C	2.82166900	1.17178600	1.98053100
H	1.27205400	-1.36183000	3.70140900
C	6.85604700	-3.54290300	1.52309900
H	7.56130600	-2.82584000	1.08921300
H	7.36684600	-4.00822400	2.37592900
O	2.69526100	2.33793500	1.55607700
C	0.45000000	1.08109700	2.97660100
H	-0.15055600	0.80044900	2.04519400
C	6.52417200	-4.63023300	0.48469500
H	7.43801000	-5.10523300	0.11403900
H	5.89541700	-5.41451100	0.91385100
H	5.99268400	-4.20654400	-0.37367400
N	3.97693000	0.47131800	1.71326200
H	4.65120600	0.92851600	1.07411100
C	0.30217900	2.58343300	3.21946100
H	0.86711000	2.89127900	4.10790700
H	0.66638200	3.16318400	2.37332200
H	-0.75332000	2.81576700	3.38831500
H	-0.07108600	0.51385700	3.75574600

**<sup>3</sup>TS4-S**

N	0.30874400	2.16201900	0.44534300
N	-2.43244100	1.35358300	0.40870300
N	-1.60693700	-1.37551700	0.51430300
N	1.11954700	-0.53428100	0.54979800
C	1.61156900	2.38847600	0.82701200
C	1.85149400	3.80753700	0.87413900
C	0.70548800	4.42254900	0.47245300
C	-0.27183200	3.39051000	0.23955400
C	-1.62509600	3.63974600	-0.00979700
C	-2.62992000	2.67634400	0.10115600
C	-4.04668800	2.94504800	0.03557100

C	-4.68529000	1.78417000	0.34285700
C	-3.66647200	0.78594900	0.55080100
C	-3.93378000	-0.58085600	0.75418800
C	-2.94860100	-1.58112900	0.69025100
C	-3.23334900	-2.99526200	0.67018200
C	-2.05069100	-3.62759600	0.44201900
C	-1.02788900	-2.61244900	0.36976000
C	0.34213300	-2.86590700	0.27842300
C	1.32944300	-1.88499800	0.39932100
C	2.73637100	-2.16312200	0.54126800
C	3.35407200	-0.98549900	0.82373900
C	2.33570100	0.03563000	0.83099000
H	2.78267600	4.27218600	1.15894400
H	0.51838700	5.48233600	0.38414500
H	-4.48712700	3.90296400	-0.19727500
H	-5.74603800	1.59250200	0.40433700
H	-4.20775400	-3.44676400	0.79001000
H	-1.88282600	-4.68987500	0.34706700
H	3.18960400	-3.13856600	0.45108200
H	4.41031200	-0.81349800	0.96309200
Mn	-0.64546400	0.40179000	0.44008800
Cl	-0.73185500	0.46251800	2.77404000
O	-0.76175900	0.28019800	-1.26041500
C	-2.02519400	5.04916000	-0.28496600
C	-1.71891800	5.66591000	-1.50124300
C	-2.70093100	5.81631300	0.67019400
C	-2.06777100	6.98849300	-1.76553300
C	-3.06553500	7.13863800	0.42704100
C	-2.74447100	7.72589300	-0.79580600
C	0.79054400	-4.28865700	0.22096000
C	1.36801200	-4.84253200	-0.92355500
C	0.68119400	-5.11725900	1.34388700
C	1.82828100	-6.15658000	-0.95823300
C	1.12216600	-6.43885400	1.33035700
C	1.70108000	-6.95857500	0.17373100
F	-3.01480600	5.28050500	1.85528500
F	-3.71155600	7.84840200	1.35766900
F	-3.08655600	8.99286400	-1.03830500
F	-1.76399500	7.55024400	-2.94012100
F	-1.07589800	4.98262800	-2.45857700
F	0.14261600	-4.64268500	2.47162900
F	1.50037300	-4.10302400	-2.03559300
F	2.38649000	-6.64983400	-2.07008800
F	2.13455200	-8.22059800	0.15132100

F	1.00502300	-7.20574700	2.41830500
C	6.80358900	-1.85859300	-1.36742400
C	5.59061100	-2.32903800	-1.86377800
C	4.56948800	-1.43568900	-2.22393100
C	4.76115500	-0.03859600	-2.09059800
C	6.00094500	0.42362600	-1.60382100
C	6.99909200	-0.46550200	-1.24257100
H	5.42307800	-3.39907700	-1.96653100
C	3.65827400	0.83007700	-2.38832900
H	6.15603100	1.49326700	-1.49905100
H	7.94474900	-0.09369400	-0.85760600
C	2.43770900	0.36239900	-2.77199200
C	2.23529700	-1.08666000	-2.96092700
H	3.81135400	1.89403300	-2.26435300
C	7.91895300	-2.81745200	-1.01679300
H	7.49917600	-3.79673200	-0.75914500
H	8.44401900	-2.45599100	-0.12429000
O	1.18425100	-1.59608600	-3.33509600
C	1.23008400	1.21005000	-2.96830700
H	0.48682700	0.88463400	-2.17968700
C	8.92724200	-2.97901300	-2.16922200
H	9.73093000	-3.66918000	-1.89329400
H	9.37771500	-2.01594500	-2.42993700
H	8.43283200	-3.36771300	-3.06518000
N	3.35001000	-1.88165300	-2.68316900
H	3.17322900	-2.87578200	-2.75366300
C	1.42278900	2.71816100	-2.88358400
H	2.08063400	3.07997100	-3.68296400
H	1.86070900	3.01766100	-1.92704300
H	0.46315900	3.22884600	-2.97682800
H	0.71243600	0.90593200	-3.88532900
C	2.57478100	1.39868600	1.04122300
C	3.94282800	1.78130100	1.48681500
C	4.45111500	1.29535100	2.70070700
C	4.80926500	2.56242400	0.71789500
C	5.75911500	1.54553800	3.10980500
C	6.12323600	2.81479900	1.09777400
C	6.60330400	2.30333400	2.29997800
F	4.40490200	3.08086400	-0.45631700
F	6.93114800	3.51232300	0.28885000
F	7.86352100	2.53425300	2.67281800
F	6.21119600	1.05928100	4.26929600
F	3.68060800	0.54703100	3.49507700
C	-6.46613500	-1.28350200	0.95570500

C	-7.88422600	-1.60551500	0.98681600
H	-8.33152000	-1.08458600	1.84390000
C	-8.70372700	-1.29152400	-0.30859000
H	-8.63685400	-0.26074900	-0.66582100
C	-8.29942700	-3.10881900	1.00362200
H	-7.85127200	-3.71963700	1.78866900
C	-9.83721300	-2.96509400	1.06765100
H	-10.34379800	-3.86802500	0.71493400
H	-10.16670700	-2.78643700	2.09574200
C	-10.11677400	-1.71866400	0.15805500
H	-10.77000600	-1.95134700	-0.68831600
H	-10.59393600	-0.91399200	0.72555500
C	-8.20709100	-2.34918500	-1.32534000
H	-8.98247100	-2.53887000	-2.07170600
C	-7.93797000	-3.58856100	-0.42036800
H	-8.51905300	-4.47608400	-0.68846800
C	-6.85566000	-2.05407700	-2.04292200
H	-6.45211500	-1.07675800	-1.75466000
H	-6.96864300	-2.06625200	-3.13261100
C	-6.46046400	-3.91943500	-0.60550500
O	-5.82880900	-4.75230400	0.03279600
N	-5.97407800	-3.12801600	-1.60319000
H	-4.97836800	-3.11524300	-1.77848400
C	-5.29416600	-0.97309300	0.90087100

**<sup>3</sup>TS4-R**

N	-0.02475300	1.98746000	0.48069200
N	2.53334900	0.71451500	0.45291000
N	1.24557100	-1.82891100	0.50486500
N	-1.29330200	-0.52633100	0.53490100
C	-1.27140400	2.43357600	0.85648000
C	-1.26143500	3.87306600	0.91231900
C	-0.02446400	4.28202000	0.51828700
C	0.76059100	3.09687900	0.28400900
C	2.13826000	3.10821200	0.04437500
C	2.96032900	1.98625500	0.16249100
C	4.40355900	2.00975000	0.13028900
C	4.83396200	0.75830300	0.44510100
C	3.65280700	-0.05417600	0.61514500
C	3.67445400	-1.44872900	0.78661800
C	2.53019600	-2.26170600	0.67776500
C	2.56680900	-3.70091300	0.62160800
C	1.29494100	-4.12142900	0.38597600
C	0.46261200	-2.94407500	0.33612400

C	-0.93076900	-2.95536100	0.24133200
C	-1.73366300	-1.81929200	0.37062700
C	-3.16747100	-1.85057800	0.50843000
C	-3.57245400	-0.58637700	0.80310200
C	-2.39277200	0.24204900	0.82343500
H	-2.09946700	4.49074500	1.19569400
H	0.34477900	5.29338500	0.43588100
H	5.00934600	2.87791900	-0.08198400
H	5.85548200	0.41468500	0.52523400
H	3.46439200	-4.29111800	0.72925400
H	0.94257900	-5.13508500	0.26700700
H	-3.78319800	-2.73143000	0.40827300
H	-4.58330400	-0.23560100	0.94364800
Mn	0.60986400	0.09153200	0.45300300
Cl	0.67841900	0.09567900	2.78902100
O	0.72524000	-0.00840400	-1.24940100
C	2.77899900	4.42730200	-0.22471700
C	2.62678600	5.06810400	-1.45697800
C	3.53825600	5.08215300	0.75059000
C	3.20285100	6.30937000	-1.71762000
C	4.12814500	6.32147500	0.51215000
C	3.95641100	6.93647500	-0.72714300
C	-1.61841300	-4.27862800	0.17243900
C	-2.29475700	-4.71078000	-0.97069500
C	-1.64261400	-5.12856900	1.28470300
C	-2.97476400	-5.92567200	-1.01377000
C	-2.30430700	-6.35446900	1.26226900
C	-2.97606100	-6.75224600	0.10754000
F	3.71241000	4.51621000	1.94988000
F	4.84764600	6.92681800	1.46194300
F	4.51431500	8.12514800	-0.96541100
F	3.04217000	6.89757200	-2.90759200
F	1.91577500	4.48659500	-2.43396900
F	-1.01864100	-4.76956900	2.41156600
F	-2.30940400	-3.94683100	-2.07331800
F	-3.61997100	-6.30172700	-2.12425600
F	-3.61937700	-7.92121200	0.07654000
F	-2.30824100	-7.14465200	2.34027400
C	5.99191400	-2.68183900	1.02239900
C	7.23843600	-3.42937200	1.07848800
H	7.24647000	-4.00709500	2.01242300
C	7.54494400	-4.37394900	-0.13047400
H	6.76662600	-5.10572500	-0.36130900
C	8.57643000	-2.64176700	0.92953000

H	8.71579300	-1.80301100	1.61313800
C	9.59104400	-3.79837800	1.07849800
H	10.56071800	-3.54608300	0.63983200
H	9.76086000	-4.03059200	2.13428600
C	8.88442000	-4.98930800	0.34261800
H	9.47157800	-5.37584500	-0.49584700
H	8.70374300	-5.82480500	1.02565500
C	7.86235300	-3.39777600	-1.29047100
H	8.51397900	-3.88670000	-2.01887700
C	8.57033200	-2.21930600	-0.55713000
H	9.58761500	-2.01816300	-0.90629800
C	6.64498200	-2.76168100	-2.02634200
H	5.69462500	-3.14639000	-1.63931200
H	6.67790400	-2.96080400	-3.10317300
C	7.72044300	-0.98600800	-0.84605800
O	7.87082400	0.12025900	-0.34247100
N	6.77172700	-1.33408300	-1.76114600
H	6.03221700	-0.67831600	-1.97375000
C	-7.13356700	-0.78602900	-1.41726900
C	-6.02034400	-1.46376200	-1.90761900
C	-4.85100600	-0.76665500	-2.24982600
C	-4.78838200	0.64088700	-2.10387700
C	-5.92949900	1.31544000	-1.62352300
C	-7.07550600	0.61834900	-1.28013900
H	-6.04789900	-2.54554600	-2.01990400
C	-3.54408300	1.29843600	-2.38438200
H	-5.89002900	2.39447400	-1.50897800
H	-7.94229200	1.15185400	-0.89966000
C	-2.42411200	0.62102800	-2.76288000
C	-2.48485100	-0.83915200	-2.96368100
H	-3.50378700	2.37157800	-2.25215500
C	-8.40737100	-1.53038500	-1.08606800
H	-8.17415700	-2.57153100	-0.83458400
H	-8.86773100	-1.08736200	-0.19461200
O	-1.53893000	-1.52735300	-3.33245000
C	-1.08235500	1.23827300	-2.94214700
H	-0.41466900	0.77613900	-2.15126800
C	-9.41623900	-1.49742400	-2.24881100
H	-10.33429900	-2.03306500	-1.98681700
H	-9.68241900	-0.46664700	-2.50380300
H	-8.99098700	-1.96171000	-3.14428700
N	-3.72779600	-1.42161800	-2.70413500
H	-3.73322800	-2.43059200	-2.78338100
C	-0.99941400	2.75521400	-2.84161200

H	-1.56998700	3.23774300	-3.64432100
H	-1.38919100	3.11961000	-1.88681100
H	0.03790400	3.08480100	-2.91744100
H	-0.61832700	0.85323800	-3.85741200
C	-2.39244600	1.62386600	1.05333600
C	-3.67597400	2.23189100	1.50014900
C	-4.26649000	1.82621100	2.70628300
C	-4.39091400	3.16010100	0.73905500
C	-5.51376500	2.29322500	3.11489100
C	-5.64352100	3.63076500	1.11850600
C	-6.21062000	3.19512600	2.31258300
C	4.93125600	-2.09661200	0.94954200
F	-3.89766000	3.61528300	-0.42740500
F	-6.31500500	4.46703100	0.31633900
F	-7.41403600	3.63531800	2.68476800
F	-6.04882900	1.87791600	4.26666700
F	-3.64074200	0.94616300	3.49287600

**<sup>5</sup>TS4-S**

N	-0.32868100	2.18410000	-0.46368300
N	2.42609500	1.36678500	-0.45496600
N	1.61509900	-1.35221200	-0.58845300
N	-1.12829800	-0.54025100	-0.58054500
C	-1.64495700	2.39965700	-0.78865500
C	-1.90140800	3.81818500	-0.83954000
C	-0.74090900	4.44293300	-0.50112900
C	0.24472100	3.41023100	-0.29316000
C	1.60918700	3.66211500	-0.06662000
C	2.61385900	2.70287200	-0.16147800
C	4.02925300	2.97565400	-0.06563900
C	4.67830800	1.81504400	-0.34205200
C	3.66638900	0.81119300	-0.56414700
C	3.94300300	-0.55485800	-0.76483400
C	2.95931700	-1.55839500	-0.73680400
C	3.24940000	-2.97252300	-0.74029800
C	2.06521100	-3.61238800	-0.55488100
C	1.03695500	-2.60219600	-0.48174600
C	-0.32654700	-2.86527000	-0.39607100
C	-1.33067300	-1.88818400	-0.47408100
C	-2.73802200	-2.17901200	-0.59063400
C	-3.37095800	-0.99431800	-0.80551800
C	-2.35424300	0.03066800	-0.80326000
H	-2.84589400	4.27557900	-1.09030100
H	-0.55429400	5.50444500	-0.43749700



H	4.46274800	3.93605400	0.16882800
H	5.74086700	1.62692400	-0.37667300
H	4.22773100	-3.41809200	-0.84775000
H	1.89976900	-4.67695600	-0.48506400
H	-3.18087000	-3.16149100	-0.52923300
H	-4.43159800	-0.82431000	-0.90939700
Mn	0.66808900	0.40298400	-0.49047500
Cl	0.60206500	0.55324400	-2.84037300
O	0.73685300	0.32167800	1.23140000
C	2.00347100	5.07465100	0.19902500
C	1.63124700	5.71737800	1.38398800
C	2.73208700	5.82272500	-0.73253000
C	1.97176500	7.04282000	1.64273100
C	3.08904600	7.14796900	-0.49360400
C	2.70509600	7.75929500	0.69870400
C	-0.76406300	-4.29187000	-0.35912900
C	-1.32241500	-4.86517000	0.78505100
C	-0.66393600	-5.10283800	-1.49517800
C	-1.77571500	-6.18151500	0.80746500
C	-1.09917200	-6.42663800	-1.49473400
C	-1.66039900	-6.96584900	-0.33828700
F	3.10641100	5.26706300	-1.89057300
F	3.78743600	7.83782700	-1.40107300
F	3.03962900	9.02917400	0.93629800
F	1.60463300	7.62823800	2.78734600
F	0.92476400	5.05756800	2.31258600
F	-0.14075600	-4.60954100	-2.62167900
F	-1.43861200	-4.14162300	1.91010800
F	-2.31588000	-6.69382300	1.91978500
F	-2.08775900	-8.23012100	-0.32861400
F	-0.99259200	-7.17741300	-2.59482200
C	-6.72014400	-1.91962900	1.43114000
C	-5.50300100	-2.40260200	1.90230500
C	-4.47245400	-1.51924000	2.26081000
C	-4.65755600	-0.11658900	2.14561000
C	-5.90786900	0.35736200	1.69008000
C	-6.91341200	-0.52181100	1.33328200
H	-5.33916300	-3.47449700	1.98821400
C	-3.55044800	0.74086800	2.43196800
H	-6.06243100	1.42874500	1.61129400
H	-7.86511600	-0.14163100	0.97239000
C	-2.32528000	0.26324800	2.81583800
C	-2.13914200	-1.19234000	3.00687300
H	-3.69354000	1.80653800	2.31209200

C	-7.84491500	-2.86636000	1.08024800
H	-7.43537500	-3.84927400	0.82075700
H	-8.36694400	-2.49746400	0.18898000
O	-1.10079800	-1.71389500	3.39487700
C	-1.12128300	1.09106900	2.98864900
H	-0.39329600	0.76096200	2.13182900
C	-8.85404100	-3.01862400	2.23358600
H	-9.66514700	-3.69921300	1.95607500
H	-9.29414700	-2.05142800	2.49659300
H	-8.36346400	-3.41496100	3.12822300
N	-3.25627400	-1.97726000	2.70996700
H	-3.08529400	-2.97330100	2.76815100
C	-1.27568500	2.60234700	2.93011200
H	-1.88343600	2.97757100	3.76331800
H	-1.74688700	2.92664900	1.99754400
H	-0.29698000	3.08215600	2.98151500
H	-0.54079600	0.74520100	3.85095000
C	-2.60688700	1.39962700	-0.97071600
C	-3.98824200	1.78337400	-1.37385800
C	-4.52714100	1.31746000	-2.58273800
C	-4.83158300	2.55990000	-0.57539200
C	-5.84283000	1.58086600	-2.95745000
C	-6.15272200	2.82434900	-0.92063500
C	-6.66364500	2.33213600	-2.11803300
F	-4.39841600	3.05848200	0.59758800
F	-6.93757400	3.51402400	-0.08280300
F	-7.93098600	2.57460800	-2.45789000
F	-6.32431400	1.11425800	-4.11305200
F	-3.77942600	0.58044200	-3.40781900
C	6.48098800	-1.25253500	-0.87837900
C	7.89936800	-1.57177900	-0.85130100
H	8.38283000	-1.03537700	-1.67873000
C	8.65847200	-1.27582700	0.48504000
H	8.57159200	-0.25100100	0.85473300
C	8.32049100	-3.07343900	-0.87289900
H	7.91026800	-3.67324100	-1.68665200
C	9.85898300	-2.92345100	-0.86590200
H	10.35290000	-3.83040000	-0.50567900
H	10.23332500	-2.72669600	-1.87517200
C	10.09255200	-1.69136800	0.07557900
H	10.70758300	-1.93607300	0.94679400
H	10.59205200	-0.87610000	-0.45646800
C	8.12033000	-2.35103900	1.46138100
H	8.86205900	-2.54965500	2.23896700

C	7.89774100	-3.57684500	0.52586600
H	8.47023200	-4.46631800	0.80567300
C	6.73654200	-2.07218700	2.12150400
H	6.34277000	-1.09113500	1.83248400
H	6.79993400	-2.10281000	3.21481500
C	6.41481000	-3.91640800	0.63891400
O	5.81739500	-4.74269400	-0.03961200
N	5.87970400	-3.14079800	1.62384400
H	4.87708400	-3.13448900	1.75499900
C	5.30701500	-0.94297300	-0.86832500

**<sup>5</sup>TS4-R**

N	0.02719500	2.00897200	-0.50225300
N	-2.53400800	0.71172700	-0.49669700
N	-1.24957800	-1.81915100	-0.57883200
N	1.30403200	-0.52770200	-0.56351200
C	1.28663900	2.45292500	-0.82422400
C	1.28494800	3.89445000	-0.88839800
C	0.03047100	4.30432800	-0.55782400
C	-0.75581900	3.11347500	-0.34341000
C	-2.14488700	3.11922900	-0.12286100
C	-2.96100000	1.99638600	-0.21784100
C	-4.40370400	2.01368800	-0.14687900
C	-4.83814800	0.75832700	-0.43070200
C	-3.65829900	-0.05285400	-0.62275800
C	-3.68191400	-1.44773600	-0.79828200
C	-2.53386900	-2.25937400	-0.72727600
C	-2.56739300	-3.70048500	-0.69632300
C	-1.29065900	-4.12138200	-0.50058100
C	-0.45901400	-2.94295200	-0.44688800
C	0.92998400	-2.95722000	-0.35430400
C	1.74360300	-1.81727200	-0.43955200
C	3.18047800	-1.85248100	-0.54915700
C	3.59199300	-0.57611400	-0.77890300
C	2.40850300	0.24939400	-0.79345600
H	2.13373200	4.51118600	-1.14005800
H	-0.34381200	5.31554100	-0.50288100
H	-5.00829300	2.88048100	0.07285600
H	-5.86028700	0.41092500	-0.47841900
H	-3.46602500	-4.29086700	-0.79329300
H	-0.93439500	-5.13622800	-0.40646100
H	3.79258300	-2.73846800	-0.47496400
H	4.60544400	-0.22047100	-0.88380900
Mn	-0.63486300	0.08252500	-0.50427300

C1	-0.56534200	0.19124800	-2.85579300
O	-0.70928400	0.02382200	1.21941400
C	-2.78635500	4.44035400	0.13111600
C	-2.55320800	5.13840900	1.31997000
C	-3.61896000	5.04749200	-0.81548300
C	-3.12636600	6.38297900	1.56874200
C	-4.20741500	6.28944100	-0.58712400
C	-3.95774600	6.95877500	0.60977500
C	1.61516800	-4.28235100	-0.30353900
C	2.28289800	-4.72892100	0.83896800
C	1.64683100	-5.11706800	-1.42660800
C	2.96358700	-5.94334100	0.87165400
C	2.31033800	-6.34237200	-1.41516900
C	2.97428900	-6.75456800	-0.26097200
F	-3.86763200	4.43408700	-1.97766800
F	-4.99889100	6.84629100	-1.50887600
F	-4.51352800	8.15049700	0.83720500
F	-2.88737100	7.02448300	2.71736800
F	-1.75705200	4.61285900	2.26222400
F	1.02922700	-4.74435300	-2.55211600
F	2.28481800	-3.97908800	1.95188700
F	3.60060700	-6.33359400	1.98213600
F	3.61876200	-7.92313600	-0.24075800
F	2.32280500	-7.11857500	-2.50309900
C	7.07861600	-0.81295600	1.47768400
C	5.97027700	-1.51214500	1.94652200
C	4.78850100	-0.83562700	2.28762100
C	4.70618500	0.57522200	2.15640100
C	5.84847300	1.27188500	1.70373000
C	7.00525000	0.59486000	1.36431900
H	6.01126700	-2.59470100	2.04462800
C	3.45435100	1.21104800	2.42562700
H	5.79884600	2.35220800	1.61281500
H	7.87101000	1.14448300	1.00524800
C	2.33846400	0.51458900	2.80773200
C	2.42909500	-0.94761000	3.01508900
H	3.39453600	2.28330000	2.29428300
C	8.36500900	-1.53395600	1.14609000
H	8.15060700	-2.57888500	0.89430300
H	8.81686700	-1.08170000	0.25489100
O	1.50424200	-1.65192200	3.40195900
C	0.99860500	1.10195700	2.96629100
H	0.34732800	0.63361500	2.11305300
C	9.37346800	-1.48242000	2.30886600

H	10.30105900	-2.00034500	2.04529900
H	9.62067400	-0.44714800	2.56462300
H	8.95769800	-1.95573700	3.20399500
N	3.67689100	-1.51021500	2.73545800
H	3.69730100	-2.51972700	2.80608600
C	0.86497700	2.61436800	2.88870100
H	1.38323400	3.10781300	3.72070300
H	1.27461800	3.01067200	1.95486200
H	-0.18728300	2.90065700	2.92694800
H	0.48989500	0.66367600	3.83191500
C	2.41225100	1.63982200	-0.98586900
C	3.70517800	2.25736800	-1.39224800
C	4.32436800	1.87546700	-2.59207400
C	4.39346000	3.18320700	-0.60447000
C	5.57476000	2.36145800	-2.96762300
C	5.64891000	3.67170100	-0.95061600
C	6.24536200	3.25889400	-2.13835000
F	3.87273700	3.61539000	0.55915800
F	6.29514000	4.50188600	-0.12183100
F	7.45185400	3.71608200	-2.47866500
F	6.13754400	1.96925200	-4.11414600
F	3.72326700	1.00458500	-3.40658000
C	-6.00296000	-2.68333900	-0.96146700
C	-7.24809100	-3.43435000	-0.97337500
H	-7.28604900	-4.01307700	-1.90599900
C	-7.50751800	-4.37952700	0.24654000
H	-6.71824100	-5.10762600	0.44998400
C	-8.58325900	-2.65224000	-0.77760600
H	-8.75023300	-1.81450300	-1.45624900
C	-9.59731600	-3.81341600	-0.89028900
H	-10.55205500	-3.56494200	-0.41802700
H	-9.80307200	-4.04713300	-1.93933800
C	-8.86015700	-5.00078800	-0.17900100
H	-9.41570500	-5.38904100	0.67993200
H	-8.70009700	-5.83609300	-0.86738800
C	-7.78802700	-3.40370300	1.41630500
H	-8.41152300	-3.89509000	2.16731100
C	-8.52634000	-2.22876700	0.70768900
H	-9.53143200	-2.03133600	1.09240400
C	-6.54822400	-2.76193300	2.10853800
H	-5.61019500	-3.14509100	1.69108000
H	-6.54397800	-2.95810200	3.18639100
C	-7.67149900	-0.99167100	0.96478900
O	-7.84510000	0.11330800	0.46595100

N	-6.68801600	-1.33550800	1.84386900
H	-5.94419900	-0.67672000	2.03078300
C	-4.94088900	-2.09629500	-0.92445500

**<sup>3</sup>TS5-S**

N	0.21545500	1.63524600	-0.00667800
N	-2.55110300	1.14048800	0.19054900
N	-2.05716400	-1.62979800	-0.00174900
N	0.70413200	-1.11011300	-0.20897800
C	1.54900100	1.67896100	0.28737600
C	2.00235300	3.04040400	0.24800600
C	0.93094000	3.80821600	-0.11445500
C	-0.20350300	2.92605900	-0.22169300
C	-1.54060300	3.32453800	-0.33586000
C	-2.62411100	2.48665500	-0.05536400
C	-3.97340100	2.93816100	0.18721400
C	-4.68395200	1.85983300	0.61800700
C	-3.79768200	0.71976900	0.56991100
C	-4.18550600	-0.61808400	0.72171900
C	-3.37251700	-1.70133800	0.36826900
C	-3.84176100	-3.05543400	0.17687900
C	-2.81287000	-3.76458100	-0.36141100
C	-1.68104500	-2.87147100	-0.44490000
C	-0.37684000	-3.25071400	-0.77227200
C	0.74019300	-2.43723300	-0.55127100
C	2.09220900	-2.92146200	-0.41874200
C	2.84044100	-1.89776800	0.08053900
C	1.97202500	-0.75322400	0.17279400
C	2.37618700	0.55563900	0.48011900
H	3.02189400	3.34525000	0.43310900
H	0.90103300	4.87874600	-0.25234300
H	-4.31210600	3.95891700	0.08579700
H	-5.72131500	1.82975600	0.91470100
H	-4.84336900	-3.39837400	0.39027500
H	-2.80388300	-4.80453300	-0.65221300
H	2.40385400	-3.93524200	-0.62040200
H	3.87588100	-1.90079600	0.38100600
Mn	-0.91651000	0.00987100	-0.05983000
Cl	-0.69540300	-0.13927900	2.30873100
O	-1.19747100	0.08285000	-1.74574300
C	-5.57548100	-0.91972400	1.16350300
C	-6.68893000	-0.63887200	0.36534800
C	-5.80962100	-1.53527100	2.39831100
C	-7.98512200	-0.93582500	0.77940200

C	-7.09705600	-1.84822700	2.83001700
C	-8.18744200	-1.54458400	2.01683900
C	-1.83402200	4.74271700	-0.68406700
C	-2.32731800	5.06401100	-1.95252500
C	-1.64781800	5.79179800	0.21977200
C	-2.62189400	6.37636000	-2.31510200
C	-1.93093700	7.11267100	-0.12137700
C	-2.42210900	7.40288200	-1.39331700
C	-0.13119200	-4.64599300	-1.23356100
C	0.15872000	-4.91155200	-2.57560400
C	-0.15431500	-5.72543400	-0.34604900
C	0.42382000	-6.20674200	-3.01863800
C	0.10330400	-7.02709700	-0.76916600
C	0.39605500	-7.26420400	-2.11145400
F	-6.52450900	-0.06696600	-0.83574600
F	-9.03148600	-0.65196100	-0.00394900
F	-9.42516800	-1.83731000	2.42194700
F	-7.29327600	-2.43317300	4.01584300
F	-4.78200400	-1.84218900	3.19582000
F	-1.17915100	5.53905800	1.44875600
F	-1.74110700	8.09926200	0.76115600
F	-2.69827600	8.66469500	-1.72945700
F	-3.08918800	6.65762200	-3.53550400
F	-2.52452700	4.09541600	-2.85667100
F	-0.43026800	-5.51767700	0.94756700
F	0.17395400	-3.91925000	-3.46529600
F	0.69580400	-6.44277100	-4.30665100
F	0.64563200	-8.50803300	-2.52888800
F	0.07670100	-8.04508300	0.09833000
C	3.67634900	0.76560300	0.99978600
C	4.70468600	0.90895900	1.62497700
C	5.84602000	1.01080300	2.51171700
H	6.67234400	1.51225200	1.99164400
C	6.32728100	-0.32799800	3.15128800
H	6.56941100	-1.12928300	2.45067300
C	5.58053600	1.69087500	3.89583300
H	5.18513300	2.70851500	3.84753500
C	6.99410400	1.57899300	4.51826500
H	6.96332000	1.64229900	5.61000900
H	7.63647000	2.39099900	4.16327300
C	7.50684800	0.18776500	4.00667700
H	7.74862500	-0.49962400	4.82241900
H	8.40815400	0.29939500	3.39526100
C	5.17082000	-0.68882900	4.11113600

H	5.52288700	-1.36613400	4.89553100
C	4.66322500	0.68463500	4.63877800
H	4.80453700	0.79245200	5.71721300
N	2.86021200	-0.59342700	3.73887600
H	1.96374500	-0.79656300	3.30765300
C	6.80869800	0.94329000	-1.15244900
C	6.01377300	-0.08490600	-1.65040100
C	4.74942200	0.18921500	-2.19108900
C	4.26251700	1.51863600	-2.24512700
C	5.09144800	2.55025500	-1.76163000
C	6.33605300	2.27149300	-1.22435200
H	6.35969800	-1.11469100	-1.59765200
C	2.92727600	1.73691600	-2.72069900
H	4.72401500	3.57235300	-1.79691000
H	6.95574400	3.07730300	-0.84075400
C	2.10550200	0.71632800	-3.10655100
C	2.60928500	-0.67126100	-3.07929000
H	2.55739800	2.75743600	-2.72520800
C	8.17591400	0.64527200	-0.57909400
H	8.16676800	-0.34065300	-0.09939400
H	8.40921200	1.37332800	0.20747000
O	1.94996200	-1.66016400	-3.38886100
C	0.68362200	0.87548900	-3.50023800
H	0.04712500	0.43639300	-2.65182100
C	9.27946800	0.68559800	-1.65166400
H	10.26028600	0.47205500	-1.21492700
H	9.32302200	1.67052700	-2.12747800
H	9.08480400	-0.05342900	-2.43535600
N	3.92948200	-0.81584100	-2.65657600
H	4.22969800	-1.77956400	-2.58172400
C	0.17314000	2.28537900	-3.76109500
H	0.32167900	2.93554800	-2.89414200
H	-0.89955000	2.26610800	-3.96441000
H	0.68148800	2.73967400	-4.61990000
H	0.44258300	0.18197800	-4.31294700
C	3.95652700	-1.34682600	3.44745200
O	3.98724500	-2.38270700	2.79450400
C	3.13911500	0.71659100	4.31275700
H	2.53974200	0.87888600	5.21488700
H	2.89210800	1.51254100	3.60069000

**<sup>3</sup>TS5-R**

N	0.61630200	-1.26954000	-0.15586300
N	-2.18292500	-1.51933200	0.07418200



N	-2.40274200	1.28712500	0.18620600
N	0.38676200	1.51681600	-0.04903700
C	1.92162800	-1.01165600	0.16880300
C	2.69533100	-2.21639900	0.03788500
C	1.84944200	-3.18405200	-0.41983600
C	0.53194800	-2.60166400	-0.48446000
C	-0.66067500	-3.31203800	-0.65443700
C	-1.91831500	-2.80707800	-0.30804900
C	-3.10545200	-3.60756800	-0.12395500
C	-4.05626200	-2.79414400	0.41193400
C	-3.48749300	-1.46817800	0.49097800
C	-4.19214300	-0.29676600	0.79157800
C	-3.68406600	0.98915400	0.56405900
C	-4.47791400	2.19440700	0.52177800
C	-3.67215300	3.18969900	0.05760200
C	-2.35993700	2.62031400	-0.13055000
C	-1.20447900	3.34995000	-0.43344600
C	0.08886600	2.83378400	-0.30000900
C	1.29651300	3.61456700	-0.18994700
C	2.28582000	2.76795800	0.21480800
C	1.71640200	1.44881100	0.26039500
C	2.44341000	0.26167900	0.45636800
H	3.74289200	-2.29482300	0.27908100
H	2.08194700	-4.21793000	-0.62586200
H	-3.17729000	-4.66451800	-0.33482600
H	-5.06157500	-3.05812100	0.70292700
H	-5.52554400	2.25448100	0.77715000
H	-3.92619700	4.22617000	-0.10900500
H	1.36539600	4.67655600	-0.36691300
H	3.32394000	2.98588100	0.41849000
Mn	-0.89073000	0.00313900	-0.03664200
Cl	-0.66832800	-0.08782900	2.33245300
O	-1.19005900	0.06262200	-1.71847200
C	-5.60141600	-0.40226100	1.26128100
C	-6.63018100	-0.86766000	0.43619900
C	-5.94930800	0.00196100	2.55513400
C	-7.94822000	-0.95010700	0.87877700
C	-7.26226500	-0.06459400	3.01686000
C	-8.26348800	-0.54472700	2.17454100
C	-0.58496400	-4.72712300	-1.11576100
C	-0.92797400	-5.05828200	-2.42950800
C	-0.19091800	-5.76575900	-0.26803200
C	-0.87755900	-6.37129100	-2.89190600
C	-0.12979100	-7.08631300	-0.70901800

C	-0.47694200	-7.38704200	-2.02532000
C	-1.37269100	4.77932200	-0.81626500
C	-1.90024500	5.11092300	-2.06885200
C	-1.04030000	5.83120500	0.04149300
C	-2.07991200	6.43588600	-2.46051400
C	-1.20453700	7.16308200	-0.33152500
C	-1.72820000	7.46392000	-1.58760300
F	-6.36005800	-1.25045500	-0.81955500
F	-8.91085100	-1.40315000	0.06833500
F	-9.52403100	-0.61530000	2.60765900
F	-7.56692200	0.32527100	4.25868300
F	-5.01000500	0.47182300	3.38202400
F	0.14432900	-5.50028100	0.99908600
F	0.25192000	-8.06390800	0.11893400
F	-0.42354100	-8.64901000	-2.45707100
F	-1.20718100	-6.66257800	-4.15457100
F	-1.31396800	-4.09789900	-3.28065200
F	-0.54243200	5.57093100	1.25880600
F	-2.25259300	4.14365500	-2.92080100
F	-2.58481300	6.72746800	-3.66338500
F	-1.89380000	8.73713700	-1.95358900
F	-0.87284000	8.15076500	0.50782900
C	3.76475000	0.35639800	0.95613900
C	4.80550900	0.39757100	1.57598500
C	5.94742700	0.38119300	2.46753500
H	6.83147500	0.77107600	1.94691600
C	5.75665600	1.11108200	3.83881900
H	5.48670200	2.16797400	3.77172800
C	6.25859200	-0.99548900	3.13199300
H	6.40752700	-1.83057500	2.44523400
C	7.48517100	-0.61217500	3.99156700
H	7.63297400	-1.30891300	4.82170600
H	8.39950200	-0.62327700	3.38945100
C	7.14287600	0.84055900	4.47369000
H	7.11450200	0.92826100	5.56380900
H	7.88094500	1.56151300	4.10823300
C	4.72127200	0.23465400	4.59139000
H	4.87195700	0.34047300	5.66875200
C	5.05990100	-1.19802700	4.08606000
H	5.32126500	-1.90144900	4.88291600
C	3.21300200	0.44599100	4.25925800
H	3.06625500	1.25307500	3.53179100
H	2.63637600	0.69741700	5.15574600
C	3.77611700	-1.71233900	3.42467000

O	3.68191600	-2.75023600	2.78154400
N	2.77759600	-0.83043200	3.70843300
H	1.86100800	-0.93211000	3.28309400
C	6.89077500	0.80539300	-1.22575400
C	5.91231400	1.70342900	-1.64211900
C	4.70485500	1.24048400	-2.18555400
C	4.47099000	-0.14738200	-2.33875600
C	5.47904800	-1.04189800	-1.92890900
C	6.66087200	-0.57885500	-1.37808200
H	6.07028100	2.77342500	-1.52581500
C	3.19709900	-0.57312300	-2.84352100
H	5.30068300	-2.10870700	-2.03076300
H	7.42057900	-1.28293900	-1.05027900
C	2.19655300	0.30135500	-3.15170900
C	2.42298300	1.75028500	-2.99317800
H	3.02720200	-1.64107400	-2.93635600
C	8.20202600	1.30054200	-0.65783200
H	8.05443000	2.27696800	-0.18124200
H	8.53997100	0.61453400	0.12894100
O	1.57964100	2.61878900	-3.20805200
C	0.82743000	-0.09328300	-3.58241900
H	0.13047900	0.13525800	-2.72070200
C	9.29676800	1.41510500	-1.73421100
H	10.23900600	1.76639900	-1.30153100
H	9.47805800	0.44515200	-2.20805600
H	8.99613900	2.11688700	-2.51866000
N	3.69933900	2.10748400	-2.56071800
H	3.82032500	3.10278100	-2.42299900
C	0.61130600	-1.54767300	-3.97957300
H	0.85764000	-2.23100200	-3.16223200
H	-0.43815000	-1.71689000	-4.22928800
H	1.22245400	-1.81951400	-4.84821900
H	0.47032000	0.60340400	-4.34885400

**<sup>5</sup>TS5-S**

N	0.23486100	1.63800700	0.01194500
N	-2.55565000	1.15755500	0.18341400
N	-2.09425500	-1.61746700	-0.00652700
N	0.69483100	-1.14813200	-0.18761700
C	1.57291500	1.66302700	0.26236200
C	2.04650300	3.02001900	0.25408400
C	0.97232400	3.80932800	-0.04625100
C	-0.16904900	2.93463200	-0.15498300
C	-1.50534100	3.34829200	-0.25550900

C	-2.60084200	2.51766500	-0.02088900
C	-3.95218200	2.98463600	0.17883700
C	-4.69838000	1.90714400	0.53935500
C	-3.82749300	0.75494000	0.49445000
C	-4.24232500	-0.57712300	0.60971100
C	-3.42936900	-1.67114200	0.29444000
C	-3.90967100	-3.02140800	0.10653900
C	-2.86381800	-3.75791800	-0.35064400
C	-1.71411000	-2.88511800	-0.39199400
C	-0.40987000	-3.29392900	-0.66400700
C	0.72009500	-2.48137900	-0.47729300
C	2.07141400	-2.97564300	-0.36496300
C	2.84100800	-1.93495800	0.05932300
C	1.97397500	-0.78645800	0.13623700
C	2.39505200	0.52516200	0.41281000
H	3.07404600	3.30833000	0.41999100
H	0.94718300	4.88402400	-0.14784200
H	-4.26965900	4.01364000	0.09502000
H	-5.74778800	1.88527700	0.79045500
H	-4.92717000	-3.34428300	0.26918500
H	-2.85826400	-4.80338200	-0.61964300
H	2.37070900	-3.99994500	-0.52769900
H	3.88612000	-1.93009700	0.32370300
Mn	-0.94875000	0.00074300	-0.03582200
Cl	-0.63446600	-0.12535000	2.33821800
O	-1.14421100	0.10004800	-1.74961400
C	-5.65712600	-0.85862600	0.98037400
C	-6.72435600	-0.54582300	0.13250100
C	-5.96300600	-1.48346200	2.19458200
C	-8.04466700	-0.82209300	0.47931400
C	-7.27565800	-1.77560200	2.55932100
C	-8.31889600	-1.44092300	1.69776500
C	-1.77776800	4.78117100	-0.56116800
C	-2.23965700	5.15258500	-1.82748400
C	-1.59590600	5.79463500	0.38293500
C	-2.50972600	6.48083700	-2.14906300
C	-1.85567000	7.13030200	0.08326100
C	-2.31642000	7.47145300	-1.18743600
C	-0.17196200	-4.71383200	-1.04755900
C	0.24518100	-5.04392800	-2.34138200
C	-0.32018900	-5.75632600	-0.12748700
C	0.50691200	-6.36343700	-2.70718700
C	-0.06886200	-7.08143600	-0.47450900
C	0.34891800	-7.38249000	-1.76993600

F	-6.49004600	0.03792000	-1.05072200
F	-9.04578000	-0.50812800	-0.35008500
F	-9.58024600	-1.71362600	2.03849300
F	-7.54081200	-2.37006600	3.72676900
F	-4.98119300	-1.82020700	3.03672700
F	-1.15447300	5.49178000	1.61038000
F	-1.67137200	8.08272000	1.00364300
F	-2.56961900	8.74787800	-1.48429400
F	-2.94753300	6.81126000	-3.36808200
F	-2.42940600	4.21903100	-2.76890200
F	-0.71409600	-5.49076800	1.12420500
F	0.39406200	-4.08843800	-3.25883400
F	0.90126100	-6.65860400	-3.95061800
F	0.59449700	-8.64932300	-2.11339500
F	-0.21807000	-8.06152900	0.42339300
C	3.70888600	0.72450300	0.89367700
C	4.74721500	0.86702000	1.50398300
C	5.89846300	0.97046900	2.37536900
H	6.73114500	1.43262200	1.82906300
C	6.34993700	-0.35670400	3.05950000
H	6.56634600	-1.18835800	2.38649800
C	5.66034000	1.70700600	3.73608400
H	5.29062000	2.73200700	3.65306000
C	7.07552600	1.58103500	4.35194000
H	7.05463800	1.68478600	5.44077300
H	7.73565900	2.36274500	3.96310300
C	7.54846700	0.15925500	3.88810000
H	7.77796500	-0.50419000	4.72682100
H	8.44818300	0.22519900	3.26774900
C	5.19097500	-0.65229300	4.03812700
H	5.53036300	-1.31110100	4.84354900
C	4.72357900	0.75149500	4.52084100
H	4.87777700	0.89382600	5.59346500
C	3.95384100	-1.30075800	3.40601700
N	2.88010400	-0.50995900	3.67999500
H	1.96971600	-0.70762800	3.27418100
C	6.86981100	0.84272700	-1.29503100
C	6.04509300	-0.17009300	-1.77613900
C	4.76330500	0.12408700	-2.26270600
C	4.28686200	1.46023400	-2.27531400
C	5.14507800	2.47623000	-1.80490800
C	6.40719000	2.17691600	-1.32468200
H	6.38365300	-1.20340400	-1.75598400
C	2.94288900	1.70076100	-2.70081200

H	4.78601700	3.50180000	-1.80808000
H	7.05030900	2.97010700	-0.95355400
C	2.09559200	0.69605500	-3.09732500
C	2.58872400	-0.69930400	-3.10556000
H	2.58229000	2.72407800	-2.67276900
C	8.25687100	0.52568400	-0.78351900
H	8.27075100	-0.48452200	-0.35795700
H	8.51073000	1.21264800	0.03328500
O	1.91606900	-1.67617500	-3.41773100
C	0.68581500	0.88362100	-3.46749200
H	0.01807100	0.45285800	-2.58477900
H	0.40130800	0.17721400	-4.25404000
C	0.18191500	2.29724900	-3.71314400
H	0.67372600	2.75607100	-4.58002200
H	0.34981400	2.94292900	-2.84598300
H	-0.89497400	2.28415200	-3.89322400
C	9.32397900	0.63418200	-1.88799000
H	9.10947300	-0.06396300	-2.70329700
H	10.32020000	0.40737600	-1.49514200
H	9.34409400	1.64345700	-2.31144500
N	3.91780500	-0.86389600	-2.71625400
H	4.20947600	-1.83212900	-2.66823100
C	3.19754800	0.81058000	4.20708600
H	2.61101500	1.01864700	5.10818400
H	2.96302100	1.58903400	3.47135800
O	3.95444300	-2.35833400	2.78809100

**<sup>5</sup>TS5-R**

N	0.60074000	-1.30637700	-0.20962700
N	-2.22608200	-1.53443700	-0.02848400
N	-2.43256900	1.27903200	0.14935000
N	0.38059500	1.51379100	-0.01256700
C	1.90765500	-1.05078500	0.09679000
C	2.68098100	-2.26037500	-0.00059400
C	1.82279300	-3.24028500	-0.40397400
C	0.51234100	-2.64183500	-0.48949800
C	-0.68444900	-3.36193600	-0.64150800
C	-1.95013200	-2.84050400	-0.37181500
C	-3.16333900	-3.61944800	-0.28627800
C	-4.14191900	-2.79014200	0.15886800
C	-3.55927400	-1.47375000	0.28385100
C	-4.27314100	-0.30347400	0.56367300
C	-3.74076900	0.98316700	0.42636000
C	-4.52202200	2.19793700	0.41238300

C	-3.67965900	3.20918200	0.07188400
C	-2.36298500	2.63562400	-0.07267800
C	-1.19737400	3.37283400	-0.28661300
C	0.09491600	2.84166400	-0.17334600
C	1.30570200	3.61359700	-0.03362200
C	2.29879000	2.73567100	0.28518700
C	1.71325400	1.42184900	0.25844500
C	2.43630200	0.22023100	0.39071500
H	3.72851200	-2.33813900	0.24085900
H	2.03989200	-4.28693100	-0.55576500
H	-3.24481000	-4.67151800	-0.51307500
H	-5.17271700	-3.03684000	0.36162300
H	-5.58313600	2.25437300	0.60425400
H	-3.91311600	4.25746500	-0.04149400
H	1.37722400	4.68457000	-0.14202600
H	3.34320900	2.93265200	0.47652100
Mn	-0.93969100	-0.01361300	-0.06121200
Cl	-0.64540600	-0.17345000	2.31458500
O	-1.12777100	0.10077200	-1.77300600
C	-5.71357700	-0.41159100	0.92756500
C	-6.68198800	-0.83551900	0.01223200
C	-6.15191400	-0.05438900	2.20746500
C	-8.02947900	-0.92130400	0.35391600
C	-7.49549100	-0.12572500	2.56949000
C	-8.43576900	-0.56288000	1.63815700
C	-0.56473200	-4.81017900	-0.97361400
C	-0.13171800	-5.22831900	-2.23536000
C	-0.83407400	-5.80520200	-0.02741000
C	0.01981200	-6.57554900	-2.55406600
C	-0.69645300	-7.15917800	-0.32493100
C	-0.26589000	-7.54390500	-1.59352200
C	-1.34446400	4.82673400	-0.57671400
C	-1.83247300	5.24979600	-1.81755300
C	-1.02176500	5.81243800	0.35960500
C	-1.98510700	6.60082700	-2.12188600
C	-1.16032700	7.16880300	0.07482600
C	-1.64550900	7.56181000	-1.17124600
F	-6.32195200	-1.17572400	-1.23287100
F	-8.93331100	-1.33392700	-0.54130500
F	-9.72507700	-0.63737700	1.97521700
F	-7.88741800	0.21891900	3.80011900
F	-5.27191000	0.37441300	3.11786500
F	-1.23755500	-5.46635600	1.20222300
F	-0.96482900	-8.08836000	0.59756700

F	-0.12766900	-8.83809400	-1.88832800
F	0.43265500	-6.94374600	-3.77154600
F	0.15390000	-4.32242200	-3.18190400
F	-0.55861800	5.46195900	1.56753900
F	-2.17261600	4.34790100	-2.74281600
F	-2.45268300	6.98101100	-3.31511300
F	-1.78579000	8.85922300	-1.45340100
F	-0.83947500	8.09231900	0.98816600
C	3.76229100	0.29876100	0.87334500
C	4.80479200	0.33365600	1.49237900
C	5.94578500	0.31815200	2.38311200
H	6.83312500	0.68950200	1.85370600
C	5.76022800	1.07781100	3.73963500
H	5.50122800	2.13575500	3.65024500
C	6.24182100	-1.04826000	3.07540300
H	6.38291600	-1.89875100	2.40612900
C	7.47131500	-0.65968000	3.92839800
H	7.61124100	-1.34130400	4.77225100
H	8.38620900	-0.69160500	3.32785400
C	7.14288200	0.80561000	4.38139200
H	7.11362800	0.91488300	5.46947800
H	7.88864300	1.51192500	4.00315800
C	4.71467000	0.22667800	4.50734500
H	4.86547800	0.35294300	5.58246000
C	5.03982800	-1.21894300	4.03134300
H	5.29318100	-1.90883200	4.84243300
N	2.76247400	-0.83586300	3.63828800
H	1.83956400	-0.93944200	3.22505500
C	6.92846100	0.82075600	-1.31117900
C	5.96917800	1.75924100	-1.68085800
C	4.72791700	1.34787500	-2.18824500
C	4.43692300	-0.03082300	-2.34715500
C	5.42625300	-0.96749800	-1.97958800
C	6.64245100	-0.55363000	-1.46938000
H	6.17132800	2.82114500	-1.56000300
C	3.14016600	-0.40397900	-2.81726900
H	5.20352900	-2.02538100	-2.08480800
H	7.38760400	-1.28794000	-1.17660700
C	2.16149800	0.51255000	-3.11385300
C	2.44756900	1.95287300	-2.93745500
H	2.92555800	-1.46384500	-2.91113300
C	8.27666000	1.25883900	-0.78517300
H	8.19178800	2.25167200	-0.32807800
H	8.59708200	0.57291400	0.00912600



O	1.63868800	2.85748500	-3.12466500
C	0.80275500	0.16458600	-3.55124800
H	0.07655000	0.26328100	-2.62099600
H	0.39618900	0.95209700	-4.19313600
C	0.55916000	-1.24006400	-4.08140700
H	1.16115700	-1.44486500	-4.97539200
H	0.79069200	-2.00196100	-3.33331800
H	-0.49553100	-1.35914900	-4.33971600
C	9.34952300	1.29134400	-1.88910300
H	9.06797500	1.99162600	-2.68185200
H	10.31890000	1.60061000	-1.48552600
H	9.46803300	0.30329600	-2.34501300
N	3.74523200	2.25453500	-2.52380600
H	3.90733400	3.24337300	-2.38045400
C	3.75143900	-1.73440000	3.37843300
C	3.20841100	0.44487800	4.16959900
H	2.63283900	0.71561000	5.06105100
H	3.06821500	1.24231800	3.42996100
O	3.65041900	-2.78604500	2.75865600

**<sup>3</sup>TS6-S**

N	-0.17724300	2.47508400	0.41258300
N	-2.62181500	1.00086100	0.34466600
N	-1.15709500	-1.40900200	0.71724100
N	1.27437200	0.07994200	0.78938400
C	1.01370400	3.04696300	0.79821600
C	0.88702300	4.48101300	0.75281700
C	-0.36162000	4.76016700	0.28882100
C	-1.03786900	3.50229900	0.10461500
C	-2.39169600	3.38279600	-0.22078200
C	-3.12707200	2.20363200	-0.07942400
C	-4.55944900	2.09901500	-0.22126200
C	-4.90453700	0.84107500	0.16526000
C	-3.68300400	0.15398000	0.49957800
C	-3.61447200	-1.20954800	0.84174900
C	-2.40958900	-1.92884500	0.91180100
C	-2.32592900	-3.36026900	1.05945000
C	-1.01458600	-3.69221700	0.90427300
C	-0.28175500	-2.46487800	0.70854800
C	1.11255000	-2.37716100	0.62870400
C	1.82348700	-1.17784300	0.69883600
C	3.25883600	-1.07748100	0.80625100
C	3.55315000	0.23247900	1.01064100
C	2.30668400	0.95921500	0.98739300

H	1.65964200	5.18288900	1.02680000
H	-0.80624400	5.73049200	0.12491800
H	-5.21084000	2.89410100	-0.55215800
H	-5.88584500	0.39274800	0.20810500
H	-3.15542000	-4.02810500	1.24375000
H	-0.57574100	-4.67733300	0.95628100
H	3.94774100	-1.90428400	0.72588200
H	4.52905300	0.67990600	1.11833100
Mn	-0.65984600	0.53589500	0.52882600
Cl	-0.89805600	0.74881800	2.83929300
O	-0.58692700	0.25022300	-1.17314700
C	-3.11276000	4.62188400	-0.62887000
C	-2.90081300	5.20329900	-1.88194200
C	-4.01072900	5.26300600	0.23117300
C	-3.54983100	6.37234100	-2.27220900
C	-4.67642800	6.42979900	-0.13823900
C	-4.44162300	6.98628900	-1.39466200
C	1.87048900	-3.65689800	0.54348100
C	1.79502000	-4.45517600	-0.59989300
C	2.65842500	-4.13310500	1.59511500
C	2.46927200	-5.66344900	-0.71929000
C	3.35292900	-5.33783300	1.50113300
C	3.25454900	-6.10573700	0.34289000
F	-4.24931100	4.75459000	1.44525000
F	-5.52969800	7.02167500	0.70331400
F	-5.07183800	8.10505300	-1.75781600
F	-3.32860100	6.90287000	-3.47935200
F	-2.05679800	4.63233400	-2.75485100
F	2.76481700	-3.42404600	2.72686300
F	1.09150600	-4.01883800	-1.67101700
F	2.38297300	-6.37994100	-1.83767000
F	3.92243900	-7.25447900	0.24613900
F	4.10571200	-5.76447600	2.52072600
C	6.05591900	-2.62777200	-1.90046800
C	6.02958300	-1.26732600	-1.94300700
C	4.82914600	-0.52179200	-2.20001900
C	4.81895600	-3.38864500	-2.14712600
H	6.94594300	-0.70886500	-1.75985800
C	3.56384300	1.54811900	-2.37095300
H	2.84367600	-3.15176000	-2.58176700
C	2.36961600	0.82558600	-2.59486800
C	2.42077500	-0.57212900	-2.62266600
H	3.54387900	2.62876300	-2.33976700
C	7.29612800	-3.43610100	-1.63005200

H	7.05828700	-4.19464800	-0.87547000
H	8.07095100	-2.78335600	-1.21249200
C	1.04674400	1.49365200	-2.77169900
H	0.35962500	1.07919700	-1.91080700
C	7.82346800	-4.14650800	-2.89069000
H	8.71735300	-4.73299900	-2.65602900
H	8.08427400	-3.42097900	-3.66826700
H	7.06094400	-4.82234200	-3.28456700
C	0.99002000	3.01096400	-2.77028900
H	1.51989600	3.41984700	-3.63997600
H	1.44461900	3.43442300	-1.87300900
H	-0.04485100	3.35334000	-2.81506700
H	0.51315500	1.06865400	-3.63038200
C	2.19486800	2.35094000	1.07265600
C	3.42233400	3.11738900	1.42073600
C	4.04327500	2.93709900	2.66430200
C	4.02992600	4.01682400	0.53814300
C	5.21164700	3.61200500	3.01177200
C	5.19420300	4.70690700	0.86386000
C	5.78839600	4.50170600	2.10740300
F	3.49349200	4.24825400	-0.67427500
F	5.74600600	5.55647400	-0.00961700
F	6.90601100	5.15505300	2.43014500
F	5.77895100	3.41592800	4.20519300
F	3.51961900	2.08943100	3.55430200
C	3.63086800	-1.24247300	-2.42901500
H	1.50322700	-1.14150800	-2.74452800
C	4.76457200	0.88398500	-2.18642000
H	5.67795600	1.44772300	-2.01448500
N	3.69238600	-2.62318900	-2.41925600
O	4.74625100	-4.61925800	-2.11443700
C	-5.89895800	-2.50411100	1.07465900
C	-7.19230300	-3.16769100	1.12974100
H	-7.80163200	-2.65662100	1.88705200
C	-7.99172400	-3.26643800	-0.21169700
H	-8.16296200	-2.31680300	-0.72497200
C	-7.22262200	-4.70769000	1.37561900
H	-6.68063900	-5.06209900	2.25358800
C	-8.74919700	-4.94974000	1.39239300
H	-8.99667900	-5.99345500	1.17863900
H	-9.16821800	-4.70942300	2.37426300
C	-9.27822200	-3.96399800	0.29353800
H	-9.80525600	-4.47761500	-0.51616700
H	-9.97086400	-3.23178000	0.71933300

C	-7.19331000	-4.30172500	-1.04187100
H	-7.85450400	-4.78919400	-1.76258900
C	-6.67660100	-5.28557800	0.05026700
H	-7.00482600	-6.32054600	-0.08487200
C	-5.91923100	-3.78211800	-1.77323800
H	-5.78687700	-2.70336100	-1.63200800
H	-5.96558000	-3.98040100	-2.84982600
C	-5.15555000	-5.25561500	-0.05639700
O	-4.37312900	-5.79675000	0.71462900
N	-4.82531400	-4.52277800	-1.15806200
H	-3.85563700	-4.28134000	-1.31171800
C	-4.84036600	-1.91480800	1.00237500

**<sup>3</sup>TS6-R**

N	-0.38910700	2.25712000	-0.44179200
N	-2.59452200	0.44538100	-0.43079900
N	-0.78972200	-1.72472100	-0.77321300
N	1.40006500	0.10125600	-0.79815100
C	0.71262100	2.99908400	-0.80328300
C	0.37885200	4.39950600	-0.74503800
C	-0.90214100	4.48976600	-0.29450200
C	-1.39225700	3.14500800	-0.13448900
C	-2.71952300	2.82706200	0.16575200
C	-3.27628200	1.55859600	-0.00904700
C	-4.68407100	1.25290300	0.08331800
C	-4.84466800	-0.03164700	-0.33542800
C	-3.52561100	-0.53716000	-0.63146000
C	-3.25050900	-1.87437500	-0.96431800
C	-1.95126600	-2.41531000	-0.98393900
C	-1.66074400	-3.81952200	-1.10996300
C	-0.31800300	-3.96448500	-0.93823100
C	0.22804100	-2.64365700	-0.74337000
C	1.59392900	-2.35472600	-0.64670400
C	2.12441200	-1.06467700	-0.70526100
C	3.53089400	-0.75722200	-0.79514800
C	3.63484200	0.58290100	-0.99115200
C	2.29643600	1.12115700	-0.98099000
H	1.04528400	5.20891200	-1.00057200
H	-1.48465800	5.38309700	-0.12496000
H	-5.45294100	1.94118100	0.40120100
H	-5.76779600	-0.58877400	-0.41143300
H	-2.40461200	-4.58107400	-1.29019400
H	0.26196000	-4.87463900	-0.97198400
H	4.33168000	-1.47558200	-0.70930300

H	4.53707100	1.16710900	-1.08510000
Mn	-0.58557300	0.27263800	-0.57288100
Cl	-0.80347800	0.45623900	-2.88830500
O	-0.50595100	-0.00645200	1.13006500
C	-3.61866400	3.94255400	0.57776300
C	-3.54320800	4.49623900	1.85816300
C	-4.55692400	4.48861900	-0.30405900
C	-4.36237500	5.55059100	2.25475900
C	-5.39073100	5.54015900	0.07036100
C	-5.28960100	6.07282800	1.35476800
C	2.53000300	-3.51032700	-0.55564800
C	2.56244400	-4.31465000	0.58561400
C	3.39088600	-3.86105300	-1.59963400
C	3.40768000	-5.40980300	0.70998900
C	4.25608700	-4.94924100	-1.50006400
C	4.26118600	-5.72690200	-0.34416700
F	-4.66891400	3.99925500	-1.54348600
F	-6.27787000	6.04535800	-0.79185400
F	-6.08113500	7.08200400	1.72305400
F	-4.26909700	6.05834100	3.48820400
F	-2.66861000	4.00795000	2.75163600
F	3.40230200	-3.14119200	-2.72940300
F	1.79025000	-3.99253400	1.64937000
F	3.41603400	-6.13609000	1.82554600
F	5.09076300	-6.76466800	-0.24253900
F	5.07379000	-5.25659100	-2.51267300
C	-5.24817900	-3.56010500	-1.30322800
C	-6.30332300	-4.55229500	-1.43769800
H	-6.22642200	-4.99514300	-2.43969900
C	-6.34526200	-5.68587500	-0.36034800
H	-5.41778000	-6.25139200	-0.23990500
C	-7.77235200	-4.10400400	-1.16622100
H	-8.11942400	-3.23740800	-1.73082000
C	-8.51818200	-5.42748400	-1.45164600
H	-9.49926400	-5.45230300	-0.96876400
H	-8.67986100	-5.55641900	-2.52617700
C	-7.53903700	-6.51649900	-0.89090700
H	-7.99139000	-7.12566700	-0.10258800
H	-7.21160500	-7.19851100	-1.68136000
C	-6.81550700	-4.95743000	0.92314600
H	-7.31345300	-5.66514700	1.59050400
C	-7.79276000	-3.88077900	0.36296500
H	-8.81314900	-3.95366400	0.75119200
C	-5.73274500	-4.16693700	1.71733900

H	-4.74018000	-4.28159600	1.26700500
H	-5.67385300	-4.50270400	2.75861300
C	-7.21719400	-2.53720000	0.79894200
O	-7.62338200	-1.43645400	0.44824200
N	-6.17654800	-2.78047700	1.64600900
H	-5.58643700	-2.00987800	1.92864500
C	6.48394000	-1.87722500	1.94010800
C	6.25461100	-0.53608400	1.98772500
C	4.95391800	0.02085100	2.23415600
C	5.37194300	-2.81511200	2.17056500
H	7.07930500	0.15367300	1.81669300
C	3.39191300	1.87750300	2.39652200
H	3.37967600	-2.87742900	2.58700200
C	2.31618300	0.98381500	2.60295000
C	2.57537800	-0.39064600	2.62840000
H	3.21113900	2.94307600	2.36872700
C	7.83356300	-2.49015300	1.68014600
H	7.71900600	-3.27274700	0.92133600
H	8.50611500	-1.72736100	1.27198500
C	0.90627400	1.44667900	2.76178400
H	0.30131700	0.94147900	1.88655100
C	8.44898900	-3.11859900	2.94433400
H	9.42256800	-3.56439200	2.71740000
H	8.59119700	-2.36511500	3.72603000
H	7.79208600	-3.90199500	3.32924900
C	0.62567800	2.93894600	2.76878500
H	1.07667700	3.41371400	3.64943000
H	1.02609500	3.43287500	1.88169300
H	-0.44891200	3.12486200	2.79976900
H	0.42793000	0.94003200	3.60860700
C	1.98512500	2.48345000	-1.06338300
C	3.09348300	3.42154800	-1.39039800
C	3.75220700	3.33921500	-2.62485000
C	3.55124700	4.39547100	-0.49641800
C	4.81533400	4.17793000	-2.95281900
C	4.60781700	5.24855100	-0.80271400
C	5.24369100	5.13756300	-2.03755300
C	-4.34025700	-2.76499800	-1.17554800
F	2.96895200	4.54181600	0.70811300
F	5.01756100	6.16505600	0.08117800
F	6.25935000	5.94755000	-2.34156600
F	5.42254000	4.07170600	-4.13799700
F	3.37027200	2.42868300	-3.52489200
C	3.87424500	-0.87156000	2.44732400

H	1.75189400	-1.09130500	2.73764700
C	4.68039900	1.40129000	2.22456500
H	5.50107200	2.09609300	2.06530500
N	4.14150600	-2.22762900	2.43419500
O	5.48351700	-4.04290400	2.13167200

**<sup>5</sup>TS6-S**

N	0.14592500	2.47028700	-0.39233600
N	2.61536000	1.00729300	-0.37388200
N	1.17415600	-1.40097200	-0.71199300
N	-1.28100900	0.04671500	-0.77771200
C	-1.05621900	3.02694700	-0.75351900
C	-0.94775500	4.46410300	-0.71876400
C	0.30986400	4.75822200	-0.28883400
C	0.99672400	3.50354400	-0.11239100
C	2.36426700	3.39534400	0.18242900
C	3.10908800	2.22800500	0.03369400
C	4.54456400	2.14304000	0.16571200
C	4.90425800	0.88644800	-0.20694700
C	3.68835200	0.17922800	-0.52328900
C	3.63180700	-1.19082400	-0.84231100
C	2.43296000	-1.91936100	-0.89127400
C	2.36103500	-3.35224000	-1.01671200
C	1.05199900	-3.69387600	-0.86649500
C	0.30379600	-2.47446300	-0.69648500
C	-1.08725000	-2.40444600	-0.63119300
C	-1.81747300	-1.21093400	-0.70185300
C	-3.25406000	-1.13176400	-0.80673700
C	-3.56473500	0.17891300	-0.98311100
C	-2.32440000	0.91811100	-0.95304300
H	-1.73308400	5.15676300	-0.97950900
H	0.75029300	5.73328300	-0.14314700
H	5.18740500	2.94990200	0.48426800
H	5.89101000	0.45035800	-0.25067100
H	3.19705700	-4.01574800	-1.18670600
H	0.62487100	-4.68456900	-0.90660200
H	-3.93216000	-1.96839200	-0.73799500
H	-4.54655500	0.61636000	-1.07642600
Mn	0.67358000	0.51009700	-0.54914300
Cl	0.80836500	0.83819400	-2.85561600
O	0.59299400	0.26832900	1.18760100
C	3.07871900	4.64452400	0.57197100
C	2.87516100	5.23367000	1.82289600
C	3.95738700	5.28929900	-0.30507600

C	3.51511000	6.41348600	2.19519300
C	4.61308000	6.46730100	0.04618900
C	4.38775800	7.03109700	1.30106600
C	-1.83216800	-3.69286700	-0.55886500
C	-1.76596600	-4.49496600	0.58215400
C	-2.60209300	-4.17032300	-1.62336900
C	-2.43302100	-5.70860300	0.68718700
C	-3.28753300	-5.38106800	-1.54447100
C	-3.19906100	-6.15287700	-0.38791600
F	4.18664400	4.77397500	-1.51800500
F	5.44796000	7.06260600	-0.81122100
F	5.00891100	8.16029900	1.64699900
F	3.30328600	6.95111200	3.40079800
F	2.04931500	4.65966900	2.71038700
F	-2.69821400	-3.45653500	-2.75295300
F	-1.07879600	-4.05855100	1.66358400
F	-2.35859900	-6.42850800	1.80415600
F	-3.85924500	-7.30737500	-0.30513600
F	-4.02213600	-5.80977800	-2.57628700
C	-6.02042800	-2.63149000	1.85707800
C	-6.00171200	-1.27109000	1.92224500
C	-4.80802800	-0.52467500	2.19942100
C	-4.78063500	-3.38948600	2.09932700
H	-6.92006200	-0.71473600	1.74275400
C	-3.55860400	1.54974200	2.42036100
H	-2.80880600	-3.14972900	2.54690000
C	-2.35838200	0.83082600	2.63570600
C	-2.40203700	-0.56935800	2.63606800
H	-3.54490900	2.63066700	2.41545700
C	-7.25455200	-3.44145700	1.56630300
H	-7.00781800	-4.18796700	0.80263200
H	-8.02976100	-2.78645700	1.15307900
C	-1.04211200	1.50003300	2.81811500
H	-0.35443700	1.08500300	1.95120400
C	-7.78692900	-4.17279700	2.81301800
H	-8.67630700	-4.75994800	2.56345900
H	-8.05657900	-3.45999200	3.59926300
H	-7.02376500	-4.85065500	3.20210000
C	-0.98840000	3.01780900	2.82409400
H	-1.50649300	3.42844800	3.70039500
H	-1.45212500	3.44332400	1.93216500
H	0.04721200	3.36025900	2.85565400
H	-0.50749500	1.06998500	3.67400700
C	-2.23148300	2.31304400	-1.01767400



C	-3.47002200	3.06642900	-1.35681000
C	-4.09877600	2.87643000	-2.59544100
C	-4.07708000	3.96699400	-0.47470900
C	-5.27536700	3.54000300	-2.93672100
C	-5.25036400	4.64460500	-0.79428700
C	-5.85304600	4.42838600	-2.03176900
F	-3.53204500	4.21321100	0.73037100
F	-5.80184600	5.49411400	0.07940000
F	-6.97881400	5.07044000	-2.34844500
F	-5.84958200	3.33421900	-4.12515900
F	-3.57449800	2.03175500	-3.48768500
C	-3.60584500	-1.24245300	2.42414900
H	-1.48016200	-1.13352900	2.74890300
C	-4.75270700	0.88297800	2.21469300
H	-5.66948700	1.44362200	2.05071800
N	-3.65968200	-2.62317800	2.38875000
O	-4.70284400	-4.61932500	2.04864100
C	5.92636600	-2.46912700	-1.05794400
C	7.22454000	-3.12340200	-1.10533200
H	7.82589300	-2.62335000	-1.87626100
C	8.03159500	-3.18769100	0.23378200
H	8.19798900	-2.22617100	0.72604700
C	7.26536900	-4.66800300	-1.31887500
H	6.72172000	-5.04486500	-2.18640100
C	8.79365500	-4.89884400	-1.33840400
H	9.05007700	-5.93579600	-1.10341100
H	9.20585300	-4.67676300	-2.32742100
C	9.32078400	-3.88563600	-0.26389400
H	9.85642000	-4.37756100	0.55356800
H	10.00507900	-3.15718700	-0.70918600
C	7.24576200	-4.21154700	1.08973500
H	7.91483200	-4.67907000	1.81634200
C	6.73015200	-5.22155000	0.02115900
H	7.06600900	-6.25125900	0.17621900
C	5.97219600	-3.68633500	1.81784200
H	5.83142900	-2.61150000	1.65616500
H	6.02567200	-3.86285600	2.89784000
C	5.20943900	-5.19945800	0.13533900
O	4.42662400	-5.76121900	-0.62052200
N	4.88017800	-4.44645600	1.22341600
H	3.90964300	-4.21047600	1.37998400
C	4.86246800	-1.88806100	-0.99374800

N	-0.37748200	2.25544600	-0.42428200
N	-2.59516900	0.43559500	-0.45251100
N	-0.80190700	-1.72453200	-0.76386600
N	1.40501100	0.07901900	-0.78443800
C	0.73143000	2.99058500	-0.76577600
C	0.40597800	4.39483700	-0.71821800
C	-0.88487400	4.49055900	-0.29714900
C	-1.37586900	3.14409100	-0.14150000
C	-2.71490200	2.82612500	0.13532900
C	-3.27429000	1.56431700	-0.04292500
C	-4.68463000	1.26652300	0.04674900
C	-4.85244800	-0.01994000	-0.35898500
C	-3.53439600	-0.53655800	-0.64435400
C	-3.26262400	-1.87989000	-0.95839500
C	-1.96522400	-2.42189600	-0.96054200
C	-1.67722600	-3.82754300	-1.06479200
C	-0.33480600	-3.97356400	-0.89612300
C	0.21881300	-2.65410400	-0.72614200
C	1.58255000	-2.37401200	-0.64217600
C	2.12478800	-1.08367000	-0.70368900
C	3.53339600	-0.78790500	-0.79416600
C	3.64372400	0.55536800	-0.96805500
C	2.30604700	1.09775400	-0.95033200
H	1.07996700	5.20119100	-0.96318800
H	-1.46923800	5.38560400	-0.14428100
H	-5.45040900	1.96154900	0.35694800
H	-5.77865800	-0.57229900	-0.43233000
H	-2.42307400	-4.59000800	-1.23248700
H	0.24072900	-4.88679500	-0.91747700
H	4.33012900	-1.51185000	-0.71889000
H	4.54902100	1.13622300	-1.05197600
Mn	-0.60238900	0.24265500	-0.58987700
Cl	-0.73802300	0.54839700	-2.90045200
O	-0.52145000	0.01776200	1.14814300
C	-3.61405900	3.94698500	0.53314700
C	-3.53836400	4.51525000	1.80728100
C	-4.54773600	4.48704700	-0.35722400
C	-4.35447200	5.57701200	2.19001000
C	-5.37792900	5.54619000	0.00348600
C	-5.27757800	6.09281200	1.28203800
C	2.51424000	-3.53403200	-0.55920000
C	2.56047200	-4.33540000	0.58343300
C	3.36028300	-3.88822600	-1.61414500
C	3.40566900	-5.43166300	0.69857400

C	4.22398800	-4.97828400	-1.52441600
C	4.24332600	-5.75321500	-0.36675000
F	-4.65884300	3.98479900	-1.59156900
F	-6.26088100	6.04526200	-0.86653500
F	-6.06597700	7.10908000	1.63716700
F	-4.26206400	6.09823700	3.41780000
F	-2.66710500	4.03406200	2.70712800
F	3.35730700	-3.17015000	-2.74496700
F	1.80210000	-4.01027400	1.65591100
F	3.42916700	-6.15481300	1.81591000
F	5.07220700	-6.79250000	-0.27412800
F	5.02675700	-5.28992500	-2.54749500
C	6.47485100	-1.86058100	1.89451500
C	6.24582200	-0.51920000	1.95556500
C	4.94931800	0.03458400	2.22220200
C	5.36543900	-2.80028200	2.13093400
H	7.06849900	0.17190000	1.78037100
C	3.39235400	1.89108400	2.42534600
H	3.37814600	-2.86680300	2.56887500
C	2.31578200	0.99594800	2.63471600
C	2.57587800	-0.38057200	2.64252800
H	3.21154300	2.95676100	2.41568900
C	7.82129600	-2.47077200	1.61431100
H	7.69796800	-3.24890900	0.85230800
H	8.48846200	-1.70504600	1.20289300
C	0.91061300	1.45457800	2.80226600
H	0.30307600	0.94525600	1.92460800
C	8.45226500	-3.10671400	2.86727100
H	9.42335100	-3.55017100	2.62566600
H	8.60328600	-2.35804500	3.65190000
H	7.80056900	-3.89305400	3.25498900
C	0.62487100	2.94632600	2.81354900
H	1.06446400	3.42620200	3.69753600
H	1.02753400	3.44333400	1.92894000
H	-0.45128100	3.12625900	2.83463800
H	0.43752400	0.94293900	3.64939800
C	2.00312700	2.46399800	-1.01686300
C	3.11747400	3.39664400	-1.34114400
C	3.78071000	3.30698200	-2.57307600
C	3.57258900	4.37585200	-0.45141200
C	4.84721400	4.14135600	-2.90092900
C	4.63358100	5.22351200	-0.75755000
C	5.27477900	5.10420600	-1.98877500
F	2.98427800	4.53374400	0.74821600

F	5.04148400	6.14391800	0.12305400
F	6.29404000	5.90960200	-2.29253500
F	5.45839400	4.02773200	-4.08332300
F	3.39939000	2.39501400	-3.47163200
C	3.87091200	-0.85972100	2.44172300
H	1.75195800	-1.08059900	2.75244200
C	4.67686000	1.41672700	2.23163100
H	5.49697000	2.11212600	2.07183900
N	4.13819800	-2.21568900	2.41251700
O	5.47805700	-4.02772900	2.08185900
C	-5.26387800	-3.56476100	-1.27412900
C	-6.32198800	-4.55529600	-1.39442300
H	-6.24249300	-5.01635400	-2.38799200
C	-6.37161700	-5.66941300	-0.29701500
H	-5.44642900	-6.23562900	-0.16304600
C	-7.79055500	-4.09743100	-1.13652700
H	-8.13262100	-3.23988500	-1.71774200
C	-8.53944300	-5.42344100	-1.40145100
H	-9.52246800	-5.43652400	-0.92212200
H	-8.69731700	-5.57093300	-2.47415500
C	-7.56604600	-6.50540600	-0.81756600
H	-8.02341100	-7.09890500	-0.02026500
H	-7.23777800	-7.20248100	-1.59440600
C	-6.84439600	-4.91670000	0.97140300
H	-7.34716800	-5.61093900	1.64919100
C	-7.81598000	-3.84707100	0.38838900
H	-8.83806500	-3.90974000	0.77387200
C	-5.76219300	-4.11569300	1.75575000
H	-4.76801500	-4.24222800	1.31214600
H	-5.70896200	-4.43250900	2.80322000
C	-7.23765400	-2.49773200	0.80254300
O	-7.63927500	-1.40224200	0.43073100
N	-6.20047100	-2.72922100	1.65696100
H	-5.60994100	-1.95564900	1.93053200
C	-4.35325700	-2.77054500	-1.15820100

**<sup>3</sup>TS7-S**

N	-0.66047800	2.23401500	0.30512000
N	1.28023000	0.18700100	0.17253600
N	-0.75982200	-1.71848300	-0.17065100
N	-2.71920600	0.30103900	0.02592900
C	-1.72058100	3.04464800	0.60673600
C	-1.27075500	4.41631400	0.65118800
C	0.05251700	4.41604900	0.32914100
C	0.43974900	3.04052800	0.14154000

C	1.75235200	2.59641600	-0.01670100
C	2.13553600	1.25658200	0.09418400
C	3.48999500	0.80145500	0.29634800
C	3.42498100	-0.53822000	0.54077000
C	2.04092500	-0.91707900	0.43432200
C	1.56285800	-2.23723000	0.48070100
C	0.25538800	-2.59647500	0.11398200
C	-0.19270000	-3.93998000	-0.12544900
C	-1.46693400	-3.85626000	-0.60508000
C	-1.83816400	-2.46523500	-0.58567200
C	-3.13164800	-1.97750500	-0.79836400
C	-3.54390600	-0.69248500	-0.43007700
C	-4.91508200	-0.24553600	-0.34986200
C	-4.89732300	0.99728200	0.20052200
C	-3.51086400	1.36038600	0.38834500
H	-1.89988100	5.26619100	0.87066200
H	0.72303200	5.26025700	0.25905600
H	4.36651100	1.43126200	0.25635900
H	4.23368300	-1.22839900	0.72730900
H	0.39441600	-4.82128300	0.07753900
H	-2.12686800	-4.66808700	-0.87213300
H	-5.77768100	-0.82461300	-0.64217600
H	-5.74233700	1.62831500	0.42991400
Mn	-0.71499600	0.24383200	0.03105700
Cl	-0.78908100	-0.03413000	2.38913400
O	-0.69044500	0.56199500	-1.66123300
C	2.84078300	3.59659600	-0.21587100
C	3.25570000	3.94582000	-1.49957600
C	3.54303200	4.15332000	0.85534800
C	4.34413700	4.77638200	-1.73521100
C	4.62659900	5.00522400	0.65158100
C	5.02823400	5.31395700	-0.64768100
C	-4.12669800	-2.92269500	-1.37483600
C	-4.01773500	-3.32769500	-2.70912200
C	-5.17356200	-3.46561000	-0.62415300
C	-4.90994600	-4.22950100	-3.28211100
C	-6.08400100	-4.36419300	-1.17689700
C	-5.94840400	-4.74815000	-2.50997000
F	3.19080000	3.85112800	2.11135400
F	5.28606300	5.52446200	1.69219600
F	6.07028400	6.12175100	-0.84712400
F	4.72769400	5.05730800	-2.97977000
F	2.61659100	3.42179400	-2.57233100
F	-5.32355700	-3.12054400	0.66012800

F	-3.02790400	-2.84339100	-3.47830200
F	-4.78126100	-4.59575400	-4.56146200
F	-6.81293300	-5.61051700	-3.04781200
F	-7.07808300	-4.86523600	-0.43762300
C	3.06394700	-4.05456000	1.61037400
C	3.67455100	-4.96145400	2.56412400
H	4.53507500	-5.46873500	2.10891300
C	4.08307300	-4.33042700	3.93834600
H	4.78339200	-3.49360700	3.87802600
C	2.70588100	-5.99693300	3.21766100
H	2.15159400	-6.63287100	2.52522300
C	3.68908800	-6.73401500	4.15675500
H	3.16721700	-7.22823000	4.98125000
H	4.24286600	-7.50509800	3.61195900
C	4.64373600	-5.58915800	4.64488400
H	4.64635300	-5.47612400	5.73299000
H	5.67632800	-5.77743100	4.33464700
C	2.73050800	-3.98462100	4.61536600
H	2.85272800	-4.01642500	5.70100600
C	1.79301300	-5.11263800	4.09473900
H	1.33382800	-5.71019000	4.88870300
N	0.77005600	-3.06129900	3.62208700
H	0.15178200	-2.38680900	3.18045800
C	6.17600700	-0.23788400	-2.09335200
C	5.50709100	-1.41552500	-2.23190300
C	4.11911200	-1.47768400	-2.60396100
C	5.47373800	1.03281600	-2.35060100
H	6.01142000	-2.35568800	-2.02509700
C	2.00679100	-2.64560100	-2.87659700
H	3.69918600	1.78753000	-2.98729900
C	1.34593300	-1.42751000	-3.15310300
C	2.08462600	-0.24287000	-3.17314000
H	1.42900700	-3.56367200	-2.83844100
C	7.60838000	-0.09542500	-1.64979000
H	8.14684000	0.46951400	-2.42221700
H	7.62189000	0.56934500	-0.77619100
C	-0.13254900	-1.37388400	-3.32068500
H	-0.60539900	-2.33370200	-3.10191100
H	-0.49364200	-0.63853500	-2.47784200
C	-0.67500500	-0.75937800	-4.60698300
H	-1.76702700	-0.72445900	-4.57455300
H	-0.30136800	0.25755600	-4.75624500
H	-0.37531600	-1.36099800	-5.47357700
C	8.33961000	-1.40052500	-1.33808100

H	9.36694000	-1.19569600	-1.02400600
H	7.84870200	-1.95350500	-0.52936000
H	8.38472000	-2.05687400	-2.21403000
C	2.43593100	-3.25075000	0.95346700
C	-3.05655700	2.63922000	0.72371900
C	-4.05181100	3.67377600	1.12301600
C	-4.07476700	4.17024700	2.43089700
C	-4.96981100	4.21164600	0.21590600
C	-4.98008300	5.15274000	2.82703100
C	-5.88883100	5.18864800	0.59092200
C	-5.89090900	5.66079900	1.90240500
F	-4.98255000	3.78522800	-1.05494100
F	-6.75837100	5.68177900	-0.29764300
F	-6.76434000	6.59992800	2.27180700
F	-4.98256700	5.60828000	4.08359200
F	-3.20787800	3.70480700	3.33560300
C	3.45215200	-0.26179000	-2.89324700
C	3.36797400	-2.66887400	-2.62251700
H	3.86513900	-3.60638300	-2.38958500
H	1.57949300	0.70802900	-3.31141800
N	4.17722700	0.91025500	-2.82221600
O	5.96920800	2.14748000	-2.16169000
C	0.65851800	-4.39169600	3.35639500
C	2.03309700	-2.64899900	4.21719000
H	1.86026200	-2.01007700	5.08961300
H	2.63228900	-2.07518400	3.49942000
O	-0.20267900	-4.93779800	2.67776700

**<sup>3</sup>TS7-R**

N	0.86324200	2.12072100	0.23294100
N	-1.16123800	0.14927800	0.09622600
N	0.80168300	-1.84792900	-0.12501200
N	2.83446200	0.08771700	0.08402900
C	1.94016000	2.89169600	0.58744500
C	1.52749700	4.27556500	0.65110800
C	0.22212900	4.32411200	0.27090900
C	-0.20148100	2.96426300	0.04166900
C	-1.52388000	2.57020100	-0.16518600
C	-1.96721900	1.25022500	-0.03891000
C	-3.34525300	0.86254600	0.15042300
C	-3.34677800	-0.46381000	0.45507500
C	-1.97867000	-0.91051000	0.38579300
C	-1.55806300	-2.24440000	0.48549700
C	-0.25723000	-2.66945700	0.15398400

C	0.13202800	-4.03440800	-0.05219800
C	1.42545300	-4.02015800	-0.49583100
C	1.85601700	-2.64759900	-0.49986200
C	3.17196600	-2.21527700	-0.70436800
C	3.62755600	-0.93872000	-0.36293500
C	5.00980800	-0.52623000	-0.31216000
C	5.03095100	0.73093700	0.20770700
C	3.65751100	1.12827400	0.41581200
H	2.16376400	5.10121800	0.93124400
H	-0.41868800	5.19034300	0.19424000
H	-4.19045800	1.53154900	0.08975300
H	-4.18276800	-1.09387400	0.70934800
H	-0.51999500	-4.88189000	0.10119900
H	2.04965600	-4.86451600	-0.74937600
H	5.85276200	-1.13122200	-0.61021300
H	5.89128200	1.35662900	0.39341500
Mn	0.83037600	0.12361200	0.02037100
Cl	0.80349100	-0.07796600	2.38906800
O	0.88117700	0.38170800	-1.68088100
C	-2.56515000	3.60827300	-0.41528200
C	-2.97389800	3.90028400	-1.71513100
C	-3.23430300	4.25598800	0.62576900
C	-4.03038000	4.75829200	-1.99360300
C	-4.28377700	5.13857200	0.37768000
C	-4.68425500	5.38490400	-0.93533600
C	4.13799700	-3.20907600	-1.24683200
C	4.02922300	-3.64550700	-2.57143100
C	5.16146300	-3.76342900	-0.47238900
C	4.89936100	-4.58839900	-3.11180100
C	6.04926300	-4.70325600	-0.99224700
C	5.91460400	-5.11766400	-2.31630900
F	-2.88043200	4.01756300	1.89389100
F	-4.91172600	5.74695700	1.38857300
F	-5.69367000	6.22238900	-1.17630300
F	-4.40875700	4.98463500	-3.25083100
F	-2.35663500	3.29790900	-2.75973700
F	5.30867900	-3.39165400	0.80521800
F	3.06359600	-3.15103300	-3.36356800
F	4.77161600	-4.98391800	-4.38229700
F	6.75697000	-6.02004400	-2.82254400
F	7.01963900	-5.21587700	-0.22941200
C	-3.17029700	-3.95301200	1.63380400
C	-3.91986300	-4.73868300	2.59619700
H	-4.45142800	-5.55265600	2.08620200



C	-4.89456100	-3.93576000	3.51409800
H	-5.63752900	-3.32358200	2.99991200
C	-3.09506900	-5.30389300	3.80202900
H	-2.24827900	-5.93938800	3.53094700
C	-4.22535800	-6.03156800	4.57104300
H	-3.96811200	-6.18161400	5.62371400
H	-4.41255800	-7.01901600	4.13766700
C	-5.46186500	-5.08577000	4.37854500
H	-5.86365300	-4.71827600	5.32714900
H	-6.27523200	-5.59983000	3.85673500
C	-3.93707800	-3.11089600	4.40156900
H	-4.44005200	-2.80903000	5.32569100
C	-2.71255200	-4.04504400	4.62396000
H	-2.58944000	-4.32366800	5.67362400
C	-3.37106200	-1.84081400	3.75644200
N	-2.01284900	-1.91324900	3.81643800
H	-1.43192800	-1.20186000	3.38241800
C	-6.05385600	-0.17894200	-2.19750700
C	-5.42201000	-1.38177700	-2.28078200
C	-4.03560700	-1.50387100	-2.64368500
C	-5.31261700	1.05597300	-2.51421100
H	-5.95484100	-2.29487100	-2.02951200
C	-1.95939800	-2.74806000	-2.84517200
H	-3.51145700	1.72599700	-3.16787600
C	-1.25558600	-1.56361200	-3.16044300
C	-1.95663400	-0.35857900	-3.24028400
H	-1.41206200	-3.68196400	-2.76479000
C	-7.47869300	0.02841100	-1.75648700
H	-8.00489700	0.56914800	-2.55437000
H	-7.46586200	0.73612800	-0.91749900
C	0.22607700	-1.56541600	-3.30416200
H	0.65933300	-2.53739300	-3.05795600
H	0.60419400	-0.82876300	-2.47245400
C	0.81175000	-1.00051800	-4.59458200
H	1.90372300	-1.00667600	-4.54485000
H	0.48137700	0.02692200	-4.77095200
H	0.50231100	-1.60810700	-5.45346300
C	-8.24524300	-1.23674200	-1.37339700
H	-9.26404800	-0.98539500	-1.06546300
H	-7.76507500	-1.75898200	-0.53841500
H	-8.31521100	-1.93672500	-2.21335900
C	-2.47655500	-3.21113700	0.97002300
C	3.25235000	2.43126500	0.73525900
C	4.31105400	3.39531800	1.14484500

C	4.96663300	3.25098700	2.37281400
C	4.71665800	4.45046300	0.32147000
C	5.97505500	4.12500200	2.77379600
C	5.71690500	5.34064500	0.70448100
C	6.34852300	5.17428000	1.93586600
F	4.13757200	4.62662800	-0.87463400
F	6.08157400	6.34258400	-0.10292000
F	7.31146700	6.01875500	2.31118200
F	6.58312700	3.96616400	3.95344100
F	4.63237400	2.25017300	3.19335700
C	-3.32788600	-0.32316100	-2.97948200
C	-3.32294800	-2.71784100	-2.60559100
H	-3.85222800	-3.62821300	-2.33836800
H	-1.42129600	0.57014200	-3.41207300
N	-4.01759000	0.87138400	-2.97134000
O	-5.77424600	2.19286000	-2.38565300
C	-1.47284300	-3.21999600	4.16329800
H	-0.72949500	-3.13233200	4.96280200
H	-0.97758700	-3.67847500	3.29862300
O	-4.04142500	-0.92357800	3.29956600

**<sup>5</sup>TS7-s**

N	-0.67913100	2.21252000	0.32419200
N	1.28181600	0.18766200	0.20366900
N	-0.75329100	-1.74189800	-0.17143300
N	-2.73278500	0.28335300	0.09348300
C	-1.74524900	3.03276700	0.59760200
C	-1.29930700	4.40529100	0.61489500
C	0.02798800	4.40406700	0.31347900
C	0.42717700	3.02918500	0.16560400
C	1.74158000	2.59598700	0.03997600
C	2.13400100	1.25471900	0.15237400
C	3.49190600	0.80481800	0.33880400
C	3.43442900	-0.54321100	0.53310100
C	2.05001100	-0.92359800	0.41863500
C	1.58623900	-2.24811000	0.41266800
C	0.27261000	-2.61417400	0.05568700
C	-0.16551800	-3.95994000	-0.19851400
C	-1.45837400	-3.87773600	-0.62436900
C	-1.83438200	-2.48649200	-0.56361900
C	-3.13916500	-2.00369200	-0.72388100
C	-3.55516700	-0.72597900	-0.33697300
C	-4.93035900	-0.29132000	-0.24256100
C	-4.91776200	0.96210900	0.28138300

C	-3.53130700	1.33912000	0.44087900
H	-1.93364700	5.25759500	0.80829700
H	0.69482700	5.25027700	0.23465700
H	4.36461900	1.44048800	0.31444500
H	4.24718200	-1.23587100	0.69005600
H	0.43585900	-4.83969200	-0.03446600
H	-2.12294400	-4.68959600	-0.87941200
H	-5.79142400	-0.88302700	-0.51289900
H	-5.76494100	1.59077000	0.50909000
Mn	-0.72862700	0.25174100	0.08527200
Cl	-0.77518000	-0.16386100	2.42586000
O	-0.73863900	0.51399300	-1.64375800
C	2.82277700	3.60589400	-0.14845600
C	3.19468300	4.01677700	-1.42714700
C	3.55543900	4.11725600	0.92501600
C	4.26711900	4.86952800	-1.65682800
C	4.62540500	4.98746100	0.72756900
C	4.98123100	5.36226000	-0.56757000
C	-4.13941900	-2.94723600	-1.29485300
C	-4.04723600	-3.33385900	-2.63606900
C	-5.17145100	-3.50584600	-0.53568600
C	-4.94327900	-4.23287500	-3.20742000
C	-6.08465300	-4.40267100	-1.08666200
C	-5.96690300	-4.76794000	-2.42665100
F	3.24608300	3.75284300	2.17588500
F	5.31399600	5.46301600	1.77017800
F	6.01022800	6.18791200	-0.76180700
F	4.61096600	5.20949600	-2.89839700
F	2.53279100	3.52909300	-2.50287400
F	-5.30421000	-3.17812000	0.75506000
F	-3.07154700	-2.83386300	-3.41237900
F	-4.83202300	-4.58166900	-4.49328500
F	-6.83448700	-5.62830800	-2.96294600
F	-7.06455000	-4.91957200	-0.33929100
C	3.12289000	-4.08325300	1.46029600
C	3.76175700	-5.00574700	2.37942100
H	4.61883000	-5.49093800	1.89448400
C	4.19120500	-4.40128500	3.75941400
H	4.87954400	-3.55423700	3.70403900
C	2.81999100	-6.06872400	3.02823300
H	2.25883400	-6.69519000	2.33273200
C	3.83277600	-6.81470800	3.92808700
H	3.33512400	-7.33561200	4.75108400
H	4.38489200	-7.56485200	3.35317500

C	4.78260700	-5.66898300	4.42379400
H	4.80632100	-5.58168800	5.51399400
H	5.81088100	-5.83600200	4.08807000
C	2.84898000	-4.08917500	4.47209400
H	2.99487400	-4.14370100	5.55388600
C	1.91540900	-5.21752100	3.94559700
H	1.48179900	-5.83973800	4.73493300
N	0.85738700	-3.16975900	3.53794000
H	0.21753800	-2.49268600	3.13157200
C	6.14931700	-0.08883600	-2.10845000
C	5.50510600	-1.28044100	-2.24799300
C	4.11780800	-1.37036600	-2.61112600
C	5.41629900	1.16753700	-2.35263800
H	6.03109200	-2.21045900	-2.04981100
C	2.03406300	-2.58610500	-2.88321600
H	3.61906300	1.88873600	-2.96740100
C	1.34199000	-1.38223800	-3.16520000
C	2.05535000	-0.17916800	-3.17811100
H	1.47686300	-3.51671100	-2.84664100
C	7.58148500	0.08249500	-1.67601400
H	8.10118800	0.66210600	-2.45044800
H	7.58767800	0.74427600	-0.80002900
C	-0.12965800	-1.36469300	-3.33121000
H	-0.58035400	-2.34082300	-3.13950000
H	-0.49293400	-0.63781100	-2.45062600
C	-0.70628700	-0.70979500	-4.58280500
H	-1.79778000	-0.69672300	-4.52546200
H	-0.35862400	0.32061000	-4.69710000
H	-0.41555100	-1.26879700	-5.48093200
C	8.34307200	-1.20775700	-1.37544600
H	9.36807300	-0.98174000	-1.06856300
H	7.87074000	-1.77425200	-0.56505300
H	8.39566400	-1.85947000	-2.25439900
C	2.47544300	-3.26806900	0.83641900
C	-3.07803200	2.62893000	0.73580500
C	-4.07343100	3.67093200	1.11390400
C	-4.08275900	4.21038200	2.40488500
C	-5.00799900	4.17143100	0.20217300
C	-4.99053900	5.19821900	2.78111500
C	-5.92965500	5.15330400	0.55771300
C	-5.91799500	5.66834400	1.85287800
F	-5.03427000	3.70387400	-1.05357000
F	-6.81491200	5.61027500	-0.33448400
F	-6.79382000	6.61243600	2.20317400

F	-4.97957400	5.69495300	4.02189300
F	-3.19929500	3.78206100	3.31227000
C	3.41979300	-0.16681000	-2.89268900
C	3.39481100	-2.57950200	-2.63346300
H	3.91401000	-3.50563900	-2.40360400
H	1.52722400	0.75930800	-3.31422100
N	4.11777800	1.02086600	-2.81226500
O	5.89181400	2.29027100	-2.16295600
C	0.75511300	-4.49585900	3.24891800
C	2.12565300	-2.75446300	4.11906300
H	1.96095900	-2.13890200	5.00967000
H	2.70322100	-2.15469300	3.40457700
O	-0.11461600	-5.04002100	2.57987200

**<sup>5</sup>TS7-R**

N	0.88440500	2.10280900	0.26439600
N	-1.16632700	0.16195100	0.12355100
N	0.78311100	-1.86452700	-0.13764300
N	2.84139800	0.06919300	0.13358000
C	1.97183400	2.87664200	0.59189000
C	1.57022800	4.26397200	0.63893200
C	0.25984300	4.31904700	0.28060600
C	-0.18282700	2.96250200	0.08191900
C	-1.50793000	2.58512000	-0.09838700
C	-1.96572300	1.26434500	0.02188700
C	-3.34701500	0.88765000	0.20252000
C	-3.35969500	-0.44949100	0.45695700
C	-1.99311400	-0.90312700	0.37129200
C	-1.58995200	-2.24338500	0.41633700
C	-0.28620200	-2.67858100	0.08769900
C	0.08812300	-4.04618000	-0.14087800
C	1.39497200	-4.03567300	-0.54159200
C	1.83453100	-2.66387200	-0.50159800
C	3.16030200	-2.23849400	-0.66308400
C	3.62556000	-0.97209500	-0.29968800
C	5.01379000	-0.57727100	-0.24024900
C	5.04816500	0.68496100	0.26392400
C	3.67716400	1.09989200	0.45592200
H	2.21663500	5.08829800	0.89876600
H	-0.37349900	5.19048500	0.20164700
H	-4.18583300	1.56619400	0.16450600
H	-4.20069500	-1.08205400	0.68710600
H	-0.57733500	-4.88920600	-0.02586000
H	2.01936800	-4.88042800	-0.79333300

H	5.85112900	-1.19535300	-0.52671800
H	5.91470800	1.30251900	0.44763200
Mn	0.84011100	0.13723100	0.06682600
Cl	0.78253600	-0.20654400	2.42319100
O	0.91728000	0.34656400	-1.66542400
C	-2.53976000	3.63661100	-0.33151600
C	-2.92523400	3.97461400	-1.62730300
C	-3.21981500	4.25528600	0.72002800
C	-3.96819800	4.85294500	-1.89321500
C	-4.25708500	5.15573800	0.48500800
C	-4.63311600	5.45053300	-0.82518300
C	4.12415100	-3.23072000	-1.21322800
C	4.02184000	-3.64057300	-2.54702000
C	5.13544000	-3.80897800	-0.44078700
C	4.88834900	-4.58073900	-3.09785900
C	6.01873600	-4.74720100	-0.97108700
C	5.89166200	-5.13471200	-2.30399200
F	-2.88904800	3.97086800	1.98477900
F	-4.89575200	5.73596000	1.50562800
F	-5.63090800	6.30515500	-1.05407600
F	-4.32563900	5.12312700	-3.14798400
F	-2.30118900	3.39657700	-2.68142000
F	5.27518100	-3.46253800	0.84478900
F	3.06725400	-3.12236900	-3.33660300
F	4.76813700	-4.95103900	-4.37671800
F	6.73001000	-6.03524300	-2.82035900
F	6.97769100	-5.28364000	-0.21003800
C	-3.22554400	-3.97869100	1.48713200
C	-3.98476900	-4.79405600	2.41614600
H	-4.52820300	-5.57781200	1.87240400
C	-4.94602400	-4.01713900	3.36988000
H	-5.68078800	-3.37268400	2.88410600
C	-3.16602800	-5.42257200	3.59476900
H	-2.32904200	-6.05784500	3.29439600
C	-4.30585300	-6.16635300	4.33367600
H	-4.04904700	-6.36605000	5.37815100
H	-4.50843100	-7.13102900	3.85798100
C	-5.52850900	-5.19485200	4.18559200
H	-5.92246200	-4.86253800	5.15030000
H	-6.35070600	-5.67387900	3.64462800
C	-3.97468400	-3.24498200	4.28898700
H	-4.47158100	-2.97447300	5.22600800
C	-2.76414000	-4.20601500	4.46941500
H	-2.64462300	-4.53158800	5.50588700

C	-3.38978800	-1.95757400	3.69641200
N	-2.03331800	-2.05248300	3.75137800
H	-1.43995200	-1.33102900	3.35099400
C	-6.05379700	-0.02738200	-2.18106400
C	-5.44248100	-1.24095700	-2.26966400
C	-4.05968000	-1.38427900	-2.63214600
C	-5.28907900	1.19623300	-2.48846600
H	-5.99103000	-2.14607600	-2.02384500
C	-2.01027300	-2.66689000	-2.84872100
H	-3.47459800	1.84044200	-3.13372200
C	-1.28211500	-1.49414400	-3.17234700
C	-1.96316200	-0.27401500	-3.24026500
H	-1.47939700	-3.61057900	-2.77521900
C	-7.47533400	0.20180300	-1.74197200
H	-7.99071500	0.75453400	-2.53876000
H	-7.45195500	0.90637200	-0.90052800
C	0.18986200	-1.52703400	-3.32357900
H	0.60474100	-2.51515900	-3.11248300
H	0.57658400	-0.80223700	-2.45305200
C	0.80132900	-0.91366000	-4.58016800
H	1.89198500	-0.93998100	-4.51208300
H	0.49494300	0.12749800	-4.71290600
H	0.49794600	-1.47461000	-5.47277400
C	-8.26357600	-1.05178800	-1.36497100
H	-9.27835400	-0.78417000	-1.05768100
H	-7.79372900	-1.58499300	-0.53110400
H	-8.34428000	-1.74719200	-2.20772800
C	-2.52288000	-3.21652400	0.85590500
C	3.28031500	2.41145200	0.75000600
C	4.34501300	3.37620800	1.14147500
C	5.00306100	3.24794300	2.36991000
C	4.75554100	4.41455500	0.29936200
C	6.01866600	4.12144800	2.75336800
C	5.76303100	5.30399700	0.66461500
C	6.39711400	5.15380500	1.89682300
F	4.17317300	4.57520400	-0.89724800
F	6.13204100	6.28983000	-0.16035200
F	7.36691500	5.99769500	2.25525500
F	6.62878600	3.97830200	3.93390100
F	4.66390300	2.26351400	3.20812100
C	-3.32860700	-0.21319500	-2.96523600
C	-3.37047900	-2.61296100	-2.60424600
H	-3.91569000	-3.51386600	-2.33753400
H	-1.41105700	0.64421000	-3.41406200

N	-3.99618800	0.99325600	-2.94427900
O	-5.73279400	2.33899200	-2.35358900
C	-1.51266400	-3.38025900	4.04323600
H	-0.76807100	-3.33689300	4.84514100
H	-1.02357500	-3.80925200	3.16003100
O	-4.04783400	-1.01285900	3.27853000

**<sup>3</sup>TS8-S**

N	-1.00031600	-1.84074900	0.37010800
N	-2.71074600	0.39021300	0.24290000
N	-0.47472600	2.06962300	0.63803500
N	1.19180700	-0.20512500	0.83511600
C	-0.14956800	-2.81051600	0.83404200
C	-0.70715400	-4.10327400	0.53176600
C	-1.87067700	-3.89529300	-0.14537100
C	-2.07908100	-2.47017800	-0.20147000
C	-3.26908600	-1.84730600	-0.59626400
C	-3.58357600	-0.51518500	-0.29301200
C	-4.89288000	0.08963400	-0.38303200
C	-4.79167800	1.33973100	0.14448700
C	-3.40187100	1.54765900	0.48476700
C	-2.82535100	2.78133700	0.81400100
C	-1.44455300	3.02032700	0.79834100
C	-0.82591300	4.32531100	0.76513300
C	0.50086700	4.13523300	0.51672300
C	0.72123100	2.70987300	0.46279200
C	1.97399100	2.08724800	0.40063200
C	2.18192100	0.73079100	0.68944100
C	3.44570800	0.13591100	1.05864900
C	3.18001700	-1.12210100	1.50646500
C	1.76962400	-1.35642600	1.30967800
C	1.11768500	-2.59170800	1.39263700
H	-0.23524600	-5.04649800	0.76165000
H	-2.55301000	-4.63698700	-0.53330600
H	-5.77977100	-0.39354200	-0.76321500
H	-5.57717400	2.07118600	0.25809200
H	-1.35117800	5.26210200	0.87948900
H	1.27324900	4.88465400	0.42245700
H	4.40555800	0.62497900	1.01717400
H	3.88753400	-1.84466700	1.88104400
Mn	-0.74995600	0.10196700	0.49082500
Cl	-1.12028700	0.04283200	2.79948300
O	-0.51352500	0.36611900	-1.18926800
C	-3.71467200	3.94949200	1.06717300



C	-4.47968600	4.53851300	0.05576300
C	-3.78048700	4.52536700	2.34083600
C	-5.29558900	5.64094000	0.29777700
C	-4.58440000	5.63268000	2.60455200
C	-5.34532000	6.18955500	1.57819800
C	-4.26773500	-2.68728300	-1.31180400
C	-3.99189900	-3.14659200	-2.60466400
C	-5.48228500	-3.07698800	-0.74005700
C	-4.88549000	-3.94884100	-3.30895800
C	-6.39573800	-3.87374600	-1.42717500
C	-6.09348200	-4.31214800	-2.71528600
C	3.14308900	2.92393000	0.01762200
C	3.24175000	3.38409100	-1.29952200
C	4.19637900	3.23386900	0.88256200
C	4.35278000	4.08571800	-1.75300000
C	5.32408100	3.92492300	0.44658900
C	5.40104900	4.34716000	-0.87777500
F	-4.44024600	4.04205400	-1.18893500
F	-6.01947200	6.18112300	-0.68867000
F	-6.12036100	7.24873000	1.82027400
F	-4.63166100	6.16189200	3.83087800
F	-3.05602200	4.01527600	3.34115900
F	-5.79567900	-2.68067800	0.50038400
F	-7.55147300	-4.22793800	-0.85682300
F	-6.95989400	-5.07858400	-3.38014700
F	-4.59608000	-4.36852100	-4.54438400
F	-2.83537100	-2.81523100	-3.20012300
F	4.15754300	2.83218700	2.16055600
F	2.27585200	3.09715200	-2.18372000
F	4.45848900	4.42935400	-3.04339500
F	6.51062600	4.94552000	-1.32455800
F	6.34830700	4.15024400	1.27638100
C	6.37841400	0.43355400	-2.06110700
C	5.66038600	-0.69395000	-1.67205700
C	4.33291200	-0.87902400	-2.09181400
C	3.69352300	0.08938700	-2.90266200
C	4.43952000	1.21726000	-3.30155400
C	5.75070600	1.38738000	-2.89251700
H	6.12501700	-1.44344800	-1.03564600
C	2.31216300	-0.10873200	-3.23558100
H	3.95724100	1.97584400	-3.90982200
H	6.29752000	2.27518000	-3.19757700
C	1.60666800	-1.20295900	-2.82323100
C	2.27251100	-2.23480000	-2.00751700

H	1.81739400	0.66687500	-3.81248000
C	7.79589900	0.65540400	-1.58021400
H	8.18191100	-0.27093600	-1.14049500
H	8.43786200	0.88253900	-2.44072500
O	1.72036100	-3.24959900	-1.58034700
C	0.14552900	-1.38568000	-3.01890500
H	-0.12031700	-2.44400300	-2.95493600
H	-0.31168100	-0.92258200	-2.07523000
C	-0.51148200	-0.67080500	-4.19107200
H	-1.57600400	-0.91397000	-4.22078700
H	-0.42141200	0.41569700	-4.09774700
H	-0.06153100	-0.97444700	-5.14346200
C	7.91267100	1.79713100	-0.55435000
H	8.94177900	1.89090700	-0.19378500
H	7.62729300	2.75739400	-0.99111000
H	7.26742400	1.61732500	0.31179500
N	3.61099600	-1.99134700	-1.71980200
H	4.03377300	-2.67705800	-1.10909700
C	1.77385000	-3.75386500	2.05263800
C	2.96799200	-4.34960400	1.63437600
C	1.14847100	-4.32963800	3.17099300
C	3.52263700	-5.44696200	2.28855200
C	1.67937300	-5.43177300	3.83636500
C	2.87418500	-5.99383200	3.39246300
F	3.65290400	-3.87297100	0.57921600
F	0.00046700	-3.82134700	3.62762700
F	1.05332300	-5.94958300	4.89683000
F	3.39637300	-7.04743700	4.02244600
F	4.67084100	-5.97963600	1.85523100

**<sup>3</sup>TS8-R**

N	1.00031500	-1.84075000	0.37010900
N	2.71074600	0.39021100	0.24290000
N	0.47472700	2.06962200	0.63803900
N	-1.19180700	-0.20512500	0.83512100
C	0.14956700	-2.81051700	0.83404300
C	0.70715200	-4.10327500	0.53176600
C	1.87067500	-3.89529500	-0.14537100
C	2.07907900	-2.47017900	-0.20147000
C	3.26908400	-1.84730800	-0.59626500
C	3.58357500	-0.51518700	-0.29301300
C	4.89287900	0.08963100	-0.38303200
C	4.79167800	1.33972800	0.14448700
C	3.40187100	1.54765700	0.48476700

C	2.82535300	2.78133500	0.81400200
C	1.44455400	3.02032600	0.79834400
C	0.82591500	4.32531000	0.76513600
C	-0.50086600	4.13523200	0.51672600
C	-0.72123000	2.70987300	0.46279600
C	-1.97399000	2.08724800	0.40063700
C	-2.18192000	0.73079100	0.68944600
C	-3.44570800	0.13591200	1.05865400
C	-3.18001700	-1.12210100	1.50646900
C	-1.76962500	-1.35642700	1.30968200
C	-1.11768500	-2.59170900	1.39263900
H	0.23524400	-5.04649900	0.76165200
H	2.55300700	-4.63698800	-0.53330700
H	5.77976900	-0.39354500	-0.76321700
H	5.57717500	2.07118200	0.25809200
H	1.35118000	5.26210100	0.87949200
H	-1.27324700	4.88465400	0.42246100
H	-4.40555700	0.62498000	1.01718000
H	-3.88753400	-1.84466700	1.88104800
Mn	0.74995600	0.10196600	0.49082800
Cl	1.12029000	0.04282900	2.79948500
O	0.51352200	0.36612100	-1.18926400
C	3.71467400	3.94948900	1.06717500
C	4.47968800	4.53851000	0.05576400
C	3.78049000	4.52536400	2.34083700
C	5.29559200	5.64093600	0.29777700
C	4.58440400	5.63267700	2.60455300
C	5.34532400	6.18955200	1.57819900
C	4.26773200	-2.68728500	-1.31180600
C	3.99189800	-3.14659000	-2.60466700
C	5.48228100	-3.07699300	-0.74005800
C	4.88548800	-3.94883900	-3.30896200
C	6.39573400	-3.87375100	-1.42717600
C	6.09347900	-4.31214900	-2.71528900
C	-3.14308700	2.92393000	0.01762500
C	-3.24174800	3.38408900	-1.29952000
C	-4.19637700	3.23387100	0.88256500
C	-4.35277700	4.08571700	-1.75299800
C	-5.32407900	3.92492500	0.44659100
C	-5.40104600	4.34716100	-0.87777400
F	4.44024700	4.04205100	-1.18893400
F	6.01947400	6.18111900	-0.68867000
F	6.12036600	7.24872600	1.82027400
F	4.63166500	6.16188900	3.83087900

F	3.05602500	4.01527400	3.34116000
F	5.79567300	-2.68068600	0.50038400
F	7.55146700	-4.22794600	-0.85682300
F	6.95989100	-5.07858600	-3.38015000
F	4.59608000	-4.36851500	-4.54438900
F	2.83537100	-2.81522600	-3.20012700
F	-4.15754200	2.83218900	2.16055900
F	-2.27584900	3.09714900	-2.18371700
F	-4.45848500	4.42935300	-3.04339300
F	-6.51062200	4.94552200	-1.32455700
F	-6.34830400	4.15024900	1.27638200
C	-6.37841300	0.43356000	-2.06111000
C	-5.66038500	-0.69394400	-1.67206000
C	-4.33291100	-0.87901900	-2.09181700
C	-3.69352300	0.08939200	-2.90266700
C	-4.43952000	1.21726500	-3.30155900
C	-5.75070600	1.38738500	-2.89252000
H	-6.12501600	-1.44344200	-1.03564900
C	-2.31216300	-0.10872700	-3.23558700
H	-3.95724100	1.97584800	-3.90982700
H	-6.29752000	2.27518500	-3.19758100
C	-1.60666800	-1.20295300	-2.82323600
C	-2.27251000	-2.23479400	-2.00752100
H	-1.81739400	0.66687900	-3.81248700
C	-7.79589800	0.65540800	-1.58021800
H	-8.18191100	-0.27093300	-1.14050200
H	-8.43786100	0.88254700	-2.44072800
O	-1.72035900	-3.24959300	-1.58035200
C	-0.14552800	-1.38567300	-3.01890900
H	0.12031800	-2.44399600	-2.95494700
H	0.31168000	-0.92258100	-2.07523100
C	0.51148300	-0.67078800	-4.19107000
H	1.57600200	-0.91396500	-4.22079800
H	0.42142600	0.41571300	-4.09772800
H	0.06152100	-0.97441000	-5.14346200
C	-7.91267100	1.79713200	-0.55434900
H	-8.94177900	1.89090900	-0.19378700
H	-7.62728900	2.75739600	-0.99110600
H	-7.26742500	1.61732100	0.31179600
N	-3.61099500	-1.99134000	-1.71980500
H	-4.03377100	-2.67705100	-1.10909900
C	-1.77385100	-3.75386600	2.05263900
C	-2.96799300	-4.34960400	1.63437400
C	-1.14847500	-4.32964000	3.17099300

C	-3.52264000	-5.44696300	2.28854800
C	-1.67937800	-5.43177500	3.83636500
C	-2.87419000	-5.99383300	3.39246000
F	-3.65290400	-3.87297000	0.57921400
F	-0.00047100	-3.82134900	3.62763000
F	-1.05333000	-5.94958600	4.89683000
F	-3.39637900	-7.04743900	4.02244200
F	-4.67084400	-5.97963500	1.85522600

**<sup>5</sup>TS8-S**

C	2.03700000	0.50673000	0.82716500
C	3.26506800	-0.21110900	1.06741800
C	2.92164800	-1.47985500	1.41684000
C	1.48297100	-1.57159900	1.33441600
N	0.97560200	-0.34544900	0.98989100
H	4.25777300	0.20233900	0.98340400
H	3.57925100	-2.30707100	1.63173700
C	-2.50954400	-2.42594500	0.06806100
C	-2.49357000	-3.84489200	0.32714300
C	-1.32538300	-4.11784000	0.96842100
C	-0.58447800	-2.88208400	1.04571300
N	-1.34808300	-1.86777400	0.52077800
H	-3.29537100	-4.52796000	0.08937900
H	-0.98509400	-5.07191000	1.33962200
C	-1.42781900	3.06457200	0.70854000
C	-0.71059000	4.31514200	0.76334900
C	0.61340600	4.02253000	0.64885400
C	0.72754800	2.58667400	0.58249800
N	-0.53062900	2.03251200	0.62509700
H	-1.17001700	5.28915200	0.84331900
H	1.44522100	4.71104700	0.64761200
C	-3.45177400	1.75246000	0.23464900
C	-4.82128500	1.63936000	-0.20819100
C	-5.00336500	0.35847900	-0.62425000
C	-3.77406000	-0.35159900	-0.36298900
N	-2.84217700	0.52683600	0.13957200
H	-5.53828500	2.44573300	-0.22571200
H	-5.90029200	-0.07848800	-1.03561900
C	1.93425800	1.88350000	0.57645900
C	-3.61243600	-1.73410200	-0.45348100
C	0.75330100	-2.76395400	1.43864100
C	-2.81581800	2.94610900	0.58477600
Mn	-0.94001600	0.09684400	0.56722500
Cl	-1.41665700	0.08620800	2.84243300

O	-0.56601400	0.11979200	-1.16585300
C	-3.62806500	4.18720700	0.72117500
C	-4.23657600	4.80280900	-0.37678000
C	-3.78018100	4.80228400	1.96868500
C	-4.98394400	5.97059700	-0.24475900
C	-4.51661200	5.97508700	2.12354400
C	-5.12159200	6.55844900	1.01159000
C	-4.69573600	-2.55355700	-1.06336600
C	-4.46728400	-3.23504000	-2.26408400
C	-5.95014400	-2.71055100	-0.46601700
C	-5.44470800	-4.03014700	-2.85703300
C	-6.94582300	-3.49558400	-1.04338000
C	-6.68941600	-4.15836500	-2.24250600
C	1.49254200	-3.98637500	1.85208800
C	1.65847900	-5.08321000	0.99603800
C	2.10649400	-4.05819300	3.10865300
C	2.40482200	-6.19731800	1.37013900
C	2.85882200	-5.16195500	3.50090600
C	3.00735800	-6.23587400	2.62557000
C	3.16538800	2.66978200	0.29518000
C	3.31030400	3.28888400	-0.95175300
C	4.20093900	2.84985400	1.21791400
C	4.43259700	4.04020700	-1.27915700
C	5.34347800	3.58485700	0.90624200
C	5.45167000	4.18897900	-0.34405400
F	4.11651700	2.30413700	2.43777800
F	6.32828400	3.72356300	1.79919900
F	6.54950000	4.88535500	-0.65927300
F	-3.20430700	4.26729200	3.04976700
F	-6.22092500	-2.09620700	0.69272800
F	-8.13747600	-3.62516600	-0.45172200
F	-7.63501800	-4.91534100	-2.80203000
F	1.99029400	-3.03740800	3.96741100
F	3.43365800	-5.19969700	4.70836300
F	3.72383100	-7.30177700	2.99103700
F	2.54743000	-7.22967800	0.53215400
F	1.08766800	-5.09872700	-0.21230800
F	2.35905200	3.14159100	-1.88677700
F	4.55677300	4.58028500	-2.49805700
F	-3.27869700	-3.13392700	-2.87584600
F	-5.19986600	-4.66609900	-4.00681100
F	-4.11158700	4.26574200	-1.59868100
F	-5.55884600	6.53459300	-1.31243900
F	-5.83147200	7.68013100	1.14896500

F	-4.64797700	6.54141800	3.32689100
C	6.78899000	0.96485600	-2.67487100
C	6.40291400	-0.26373200	-2.14405300
C	5.05719500	-0.65619000	-2.15920500
C	4.06217000	0.19035000	-2.71017900
C	4.47314400	1.42437400	-3.25537000
C	5.80405700	1.80509000	-3.23654700
H	7.14819500	-0.92755300	-1.71136800
C	2.69856800	-0.24927500	-2.66787600
H	3.72153000	2.09028300	-3.66582500
H	6.09188600	2.77184700	-3.63777000
C	2.32248200	-1.45648500	-2.14204200
C	3.34881200	-2.33714500	-1.55080100
H	1.93143200	0.42218000	-3.04609000
C	8.23092400	1.41117400	-2.59202200
H	8.88989100	0.53902400	-2.67507500
H	8.46270800	2.06318500	-3.44188800
O	3.13239800	-3.41683900	-1.00098900
C	0.90444800	-1.90454200	-2.08843900
H	0.81749800	-2.81293900	-1.49009800
C	8.53475200	2.15602000	-1.27818100
H	9.59260600	2.43175100	-1.22347200
H	7.94383700	3.07129400	-1.19667100
H	8.30220600	1.52745300	-0.41204000
N	4.65461800	-1.86496200	-1.63376600
H	5.34151300	-2.48383500	-1.22080300
C	0.18344000	-2.04034300	-3.43065400
H	0.22834800	-1.10978000	-4.00475600
H	0.63663100	-2.83551800	-4.03410100
H	-0.86904900	-2.28592700	-3.26600200
H	0.31454900	-1.08077300	-1.53093100

**<sup>5</sup>TS8-R**

C	-2.03700000	0.50673000	0.82716500
C	-3.26506800	-0.21110900	1.06741800
C	-2.92164800	-1.47985500	1.41684000
C	-1.48297100	-1.57159900	1.33441600
N	-0.97560200	-0.34544900	0.98989100
H	-4.25777300	0.20233900	0.98340400
H	-3.57925100	-2.30707100	1.63173700
C	2.50954400	-2.42594500	0.06806100
C	2.49357000	-3.84489200	0.32714300
C	1.32538300	-4.11784000	0.96842100
C	0.58447800	-2.88208400	1.04571300

N	1.34808300	-1.86777400	0.52077800
H	3.29537100	-4.52796000	0.08937900
H	0.98509400	-5.07191000	1.33962200
C	1.42781900	3.06457200	0.70854000
C	0.71058900	4.31514200	0.76334900
C	-0.61340600	4.02253000	0.64885400
C	-0.72754800	2.58667400	0.58249800
N	0.53062900	2.03251200	0.62509700
H	1.17001700	5.28915200	0.84331900
H	-1.44522100	4.71104700	0.64761200
C	3.45177400	1.75246000	0.23464900
C	4.82128500	1.63936100	-0.20819100
C	5.00336500	0.35847900	-0.62425000
C	3.77406000	-0.35159900	-0.36298900
N	2.84217700	0.52683600	0.13957200
H	5.53828400	2.44573400	-0.22571200
H	5.90029200	-0.07848800	-1.03561900
C	-1.93425800	1.88350000	0.57645900
C	3.61243600	-1.73410200	-0.45348100
C	-0.75330100	-2.76395400	1.43864100
C	2.81581800	2.94610900	0.58477600
Mn	0.94001600	0.09684400	0.56722500
Cl	1.41665700	0.08620800	2.84243300
O	0.56601400	0.11979200	-1.16585300
C	3.62806500	4.18720700	0.72117500
C	4.23657600	4.80281000	-0.37678000
C	3.78018100	4.80228400	1.96868500
C	4.98394400	5.97059700	-0.24475900
C	4.51661200	5.97508700	2.12354400
C	5.12159200	6.55844900	1.01159000
C	4.69573600	-2.55355700	-1.06336600
C	4.46728400	-3.23504000	-2.26408400
C	5.95014500	-2.71055100	-0.46601700
C	5.44470900	-4.03014700	-2.85703300
C	6.94582300	-3.49558400	-1.04338000
C	6.68941700	-4.15836500	-2.24250600
C	-1.49254200	-3.98637500	1.85208800
C	-1.65847900	-5.08321000	0.99603800
C	-2.10649400	-4.05819300	3.10865300
C	-2.40482200	-6.19731800	1.37013900
C	-2.85882200	-5.16195500	3.50090600
C	-3.00735800	-6.23587400	2.62557000
C	-3.16538800	2.66978200	0.29518000
C	-3.31030400	3.28888400	-0.95175300



C	-4.20093900	2.84985400	1.21791400
C	-4.43259700	4.04020600	-1.27915700
C	-5.34347800	3.58485700	0.90624300
C	-5.45167000	4.18897900	-0.34405400
F	-4.11651700	2.30413700	2.43777800
F	-6.32828400	3.72356300	1.79919900
F	-6.54950000	4.88535500	-0.65927300
F	3.20430600	4.26729200	3.04976700
F	6.22092500	-2.09620700	0.69272800
F	8.13747600	-3.62516600	-0.45172200
F	7.63501800	-4.91534100	-2.80203000
F	-1.99029400	-3.03740900	3.96741100
F	-3.43365700	-5.19969700	4.70836300
F	-3.72383100	-7.30177700	2.99103700
F	-2.54743000	-7.22967800	0.53215300
F	-1.08766700	-5.09872700	-0.21230800
F	-2.35905200	3.14159100	-1.88677700
F	-4.55677300	4.58028400	-2.49805700
F	3.27869700	-3.13392700	-2.87584600
F	5.19986700	-4.66609800	-4.00681100
F	4.11158700	4.26574200	-1.59868100
F	5.55884600	6.53459300	-1.31243900
F	5.83147200	7.68013200	1.14896500
F	4.64797600	6.54141800	3.32689100
C	-6.78899000	0.96485600	-2.67487200
C	-6.40291400	-0.26373200	-2.14405300
C	-5.05719500	-0.65618900	-2.15920500
C	-4.06217000	0.19034900	-2.71017900
C	-4.47314400	1.42437400	-3.25537100
C	-5.80405700	1.80509000	-3.23654700
H	-7.14819400	-0.92755300	-1.71136800
C	-2.69856800	-0.24927500	-2.66787600
H	-3.72153000	2.09028300	-3.66582500
H	-6.09188600	2.77184700	-3.63777000
C	-2.32248200	-1.45648500	-2.14204200
C	-3.34881200	-2.33714500	-1.55080100
H	-1.93143200	0.42218000	-3.04609000
C	-8.23092400	1.41117400	-2.59202200
H	-8.88989100	0.53902400	-2.67507500
H	-8.46270800	2.06318500	-3.44188900
O	-3.13239800	-3.41683900	-1.00098900
C	-0.90444800	-1.90454200	-2.08843900
H	-0.81749800	-2.81293900	-1.49009800
C	-8.53475200	2.15602000	-1.27818100

H	-9.59260600	2.43175100	-1.22347200
H	-7.94383700	3.07129400	-1.19667100
H	-8.30220600	1.52745300	-0.41204000
N	-4.65461800	-1.86496200	-1.63376600
H	-5.34151300	-2.48383400	-1.22080300
C	-0.18344000	-2.04034300	-3.43065400
H	-0.22834800	-1.10978000	-4.00475600
H	-0.63663100	-2.83551800	-4.03410100
H	0.86904900	-2.28592700	-3.26600200
H	-0.31454900	-1.08077300	-1.53093100

**<sup>3</sup>TS9-S**

N	0.13203300	1.97918100	-0.67924300
N	-0.95681300	-0.62164700	-1.03007000
N	1.56437100	-1.74408400	-0.39685900
N	2.67814900	0.84948200	-0.14848100
C	0.86346400	3.13697400	-0.75425900
C	-0.03933600	4.25860300	-0.86610800
C	-1.30357100	3.76434000	-0.79421800
C	-1.19309700	2.32695100	-0.70905000
C	-2.27660000	1.44982800	-0.82289400
C	-2.13252300	0.08138100	-1.08523100
C	-3.18442400	-0.78867600	-1.55947900
C	-2.61852600	-2.00227200	-1.80483000
C	-1.22862300	-1.90634200	-1.42900300
C	-0.34689500	-2.98558400	-1.34069600
C	0.93949200	-2.89740400	-0.80168000
C	1.77508500	-4.02602300	-0.48103900
C	2.88700800	-3.54006800	0.13788000
C	2.76405700	-2.10461600	0.16628800
C	3.77193700	-1.22871900	0.58414000
C	3.73616400	0.15172400	0.37372300
C	4.84377800	1.05454800	0.58387900
C	4.44756300	2.27885700	0.14677100
C	3.07368000	2.15254400	-0.28294100
H	0.26088500	5.28999800	-0.97023200
H	-2.23395900	4.30958600	-0.84796400
H	-4.20800700	-0.49341700	-1.73157400
H	-3.09699200	-2.88923800	-2.19299400
H	1.52871100	-5.05669900	-0.68862900
H	3.73513200	-4.09579100	0.50915600
H	5.80212600	0.77809300	0.99663000
H	5.01266800	3.19889500	0.14966900
Mn	0.85012700	0.10935300	-0.52946000

C1	1.37734800	0.17579800	-2.79900500
O	0.47322200	0.18430300	1.14337000
C	-3.64290600	2.02643900	-0.68408700
C	-4.04429600	2.55129800	0.55064200
C	-4.56710300	2.08467600	-1.73153400
C	-5.30612300	3.10620700	0.73649000
C	-5.84816100	2.60144900	-1.55813700
C	-6.21462000	3.11705000	-0.31811500
C	4.98805700	-1.82598300	1.20419200
C	4.93902600	-2.37784000	2.48774600
C	6.21037600	-1.88277400	0.52726200
C	6.05487200	-2.96220800	3.08171700
C	7.34268000	-2.45479000	1.10345000
C	7.26167800	-2.99815100	2.38476900
F	-4.23422600	1.61794100	-2.94452100
F	-6.71456000	2.61975300	-2.57278100
F	-7.44246300	3.60609500	-0.13127500
F	-5.66260500	3.59628400	1.92955300
F	-3.20733000	2.51974900	1.59580500
F	6.31370200	-1.37428900	-0.70631100
F	3.79171100	-2.35354100	3.18188900
F	5.97790900	-3.48083800	4.31108600
F	8.33871900	-3.55155300	2.94419500
F	8.49916900	-2.49339400	0.43537200
C	-6.35701900	0.63557900	2.43436200
C	-5.37398100	0.66674800	3.37673000
C	-4.13162600	-0.04039500	3.22931500
C	-6.14156600	-0.11559500	1.18563000
H	-5.51748300	1.26194100	4.27622200
C	-1.88146400	-0.64729100	3.92782900
H	-4.84081300	-1.39588400	0.29273400
C	-1.71379700	-1.44495700	2.77301000
C	-2.77078000	-1.54985700	1.86878900
H	-1.06920400	-0.55185100	4.63955600
C	-7.67052600	1.35828000	2.57015600
H	-7.61476300	2.05050600	3.41677100
H	-7.84290800	1.95904900	1.67202900
C	-0.40546800	-2.07800200	2.41412500
H	-0.56534300	-2.89712100	1.70489700
H	0.12743800	-1.27858200	1.80981800
C	0.52975300	-2.50102600	3.54300400
H	1.43352600	-2.95609600	3.13202500
H	0.84467300	-1.64901500	4.15240400
H	0.04444900	-3.22917100	4.20296800

C	-8.85368200	0.38979400	2.74613600
H	-9.79402700	0.94304100	2.83479800
H	-8.92609900	-0.27335700	1.88054800
H	-8.73062500	-0.22214300	3.64584300
C	2.25242000	3.23140300	-0.62841500
C	2.89624400	4.56729700	-0.77036700
C	3.75769000	4.83140900	-1.84099400
C	2.69579100	5.59081000	0.16112000
C	4.38760000	6.06558900	-1.98812800
C	3.30888500	6.83443100	0.03042300
C	4.15927000	7.06986400	-1.04881400
F	1.89188400	5.38806700	1.21424300
F	3.09599800	7.79592900	0.93475300
F	4.75518300	8.25611300	-1.18149200
F	5.20424200	6.29288700	-3.02090600
F	3.99836600	3.88328100	-2.75175700
C	-3.95712100	-0.84214000	2.07668900
C	-3.06911300	0.02790000	4.15245600
H	-3.18967400	0.64054600	5.04180600
H	-2.66243600	-2.16173800	0.98050200
N	-4.98155200	-0.87705600	1.14986400
O	-6.89727600	-0.08942400	0.21075200
C	-0.84412100	-4.33664100	-1.72230000
C	-1.77612100	-5.01454900	-0.93187600
C	-0.37853900	-4.98569300	-2.86948200
C	-2.24675600	-6.28065500	-1.26744800
C	-0.83022300	-6.25586100	-3.22444400
C	-1.76879900	-6.90181300	-2.42111100
F	-2.23779600	-4.44368500	0.19527500
F	0.52546700	-4.38891600	-3.65149100
F	-3.13894900	-6.90454300	-0.49256300
F	-2.20804100	-8.11636900	-2.75339000
F	-0.37312100	-6.85568000	-4.32669200

**<sup>3</sup>TS9-R**

N	-0.13203300	1.97918100	-0.67924300
N	0.95681300	-0.62164700	-1.03007000
N	-1.56437100	-1.74408400	-0.39685900
N	-2.67814900	0.84948200	-0.14848100
C	-0.86346400	3.13697400	-0.75425900
C	0.03933600	4.25860300	-0.86610800
C	1.30357100	3.76434000	-0.79421800
C	1.19309700	2.32695100	-0.70905000
C	2.27660000	1.44982800	-0.82289400

C	2.13252300	0.08138100	-1.08523100
C	3.18442400	-0.78867600	-1.55947900
C	2.61852600	-2.00227200	-1.80483000
C	1.22862300	-1.90634200	-1.42900300
C	0.34689500	-2.98558400	-1.34069600
C	-0.93949200	-2.89740400	-0.80168000
C	-1.77508500	-4.02602300	-0.48103900
C	-2.88700800	-3.54006800	0.13788000
C	-2.76405700	-2.10461600	0.16628800
C	-3.77193700	-1.22871900	0.58414000
C	-3.73616400	0.15172400	0.37372300
C	-4.84377800	1.05454800	0.58387900
C	-4.44756300	2.27885700	0.14677100
C	-3.07368000	2.15254400	-0.28294100
H	-0.26088500	5.28999800	-0.97023200
H	2.23395900	4.30958600	-0.84796400
H	4.20800700	-0.49341700	-1.73157400
H	3.09699200	-2.88923800	-2.19299400
H	-1.52871100	-5.05669900	-0.68862900
H	-3.73513200	-4.09579100	0.50915600
H	-5.80212600	0.77809300	0.99663000
H	-5.01266800	3.19889500	0.14966900
Mn	-0.85012700	0.10935300	-0.52946000
Cl	-1.37734800	0.17579800	-2.79900500
O	-0.47322200	0.18430300	1.14337000
C	3.64290600	2.02643900	-0.68408700
C	4.04429600	2.55129800	0.55064200
C	4.56710300	2.08467600	-1.73153400
C	5.30612300	3.10620700	0.73649000
C	5.84816100	2.60144900	-1.55813700
C	6.21462000	3.11705000	-0.31811500
C	-4.98805700	-1.82598300	1.20419200
C	-4.93902600	-2.37784000	2.48774600
C	-6.21037600	-1.88277400	0.52726200
C	-6.05487200	-2.96220800	3.08171700
C	-7.34268000	-2.45479000	1.10345000
C	-7.26167800	-2.99815100	2.38476900
F	4.23422600	1.61794100	-2.94452100
F	6.71456000	2.61975300	-2.57278100
F	7.44246300	3.60609500	-0.13127500
F	5.66260500	3.59628400	1.92955300
F	3.20733000	2.51974900	1.59580500
F	-6.31370200	-1.37428900	-0.70631100
F	-3.79171100	-2.35354100	3.18188900

F	-5.97790900	-3.48083800	4.31108600
F	-8.33871900	-3.55155300	2.94419500
F	-8.49916900	-2.49339400	0.43537200
C	6.35701900	0.63557900	2.43436200
C	5.37398100	0.66674800	3.37673000
C	4.13162600	-0.04039500	3.22931500
C	6.14156600	-0.11559500	1.18563000
H	5.51748300	1.26194100	4.27622200
C	1.88146400	-0.64729100	3.92782900
H	4.84081300	-1.39588400	0.29273400
C	1.71379700	-1.44495700	2.77300900
C	2.77078000	-1.54985700	1.86878900
H	1.06920400	-0.55185100	4.63955600
C	7.67052600	1.35828000	2.57015600
H	7.61476300	2.05050600	3.41677100
H	7.84290800	1.95904900	1.67202900
C	0.40546800	-2.07800200	2.41412500
H	0.56534300	-2.89712100	1.70489700
H	-0.12743800	-1.27858200	1.80981800
C	-0.52975300	-2.50102600	3.54300400
H	-1.43352600	-2.95609600	3.13202500
H	-0.84467300	-1.64901500	4.15240400
H	-0.04444900	-3.22917100	4.20296800
C	8.85368200	0.38979400	2.74613600
H	9.79402700	0.94304100	2.83479800
H	8.92609900	-0.27335700	1.88054800
H	8.73062500	-0.22214300	3.64584300
C	-2.25242000	3.23140300	-0.62841500
C	-2.89624400	4.56729700	-0.77036700
C	-3.75769000	4.83140900	-1.84099400
C	-2.69579100	5.59081000	0.16112000
C	-4.38760000	6.06558900	-1.98812800
C	-3.30888500	6.83443100	0.03042300
C	-4.15927000	7.06986400	-1.04881400
F	-1.89188400	5.38806700	1.21424300
F	-3.09599800	7.79592900	0.93475300
F	-4.75518300	8.25611300	-1.18149300
F	-5.20424200	6.29288700	-3.02090600
F	-3.99836600	3.88328100	-2.75175700
C	3.95712100	-0.84214000	2.07668900
C	3.06911300	0.02790000	4.15245600
H	3.18967400	0.64054600	5.04180600
H	2.66243600	-2.16173800	0.98050200
N	4.98155200	-0.87705600	1.14986400

O	6.89727600	-0.08942400	0.21075200
C	0.84412100	-4.33664100	-1.72230000
C	1.77612100	-5.01454900	-0.93187600
C	0.37853900	-4.98569300	-2.86948200
C	2.24675600	-6.28065500	-1.26744800
C	0.83022300	-6.25586100	-3.22444400
C	1.76879900	-6.90181300	-2.42111100
F	2.23779600	-4.44368500	0.19527500
F	-0.52546700	-4.38891600	-3.65149100
F	3.13894900	-6.90454300	-0.49256400
F	2.20804100	-8.11636900	-2.75339000
F	0.37312100	-6.85568000	-4.32669200

**<sup>5</sup>TS9-S**

N	-0.47100200	-1.88173600	0.43565300
N	-2.79909800	-0.23427400	0.26620400
N	-1.10020300	2.05631800	0.22260200
N	1.16718800	0.41287100	0.56078300
C	0.66419700	-2.50219500	0.89799500
C	0.44870500	-3.92510500	0.93580200
C	-0.80915900	-4.15142700	0.46299400
C	-1.39679500	-2.86248900	0.19577900
C	-2.75677000	-2.66802900	-0.08785300
C	-3.40634900	-1.43453200	0.00653800
C	-4.83760300	-1.23648300	-0.07285600
C	-5.07129100	0.07771500	0.17467700
C	-3.78071000	0.71162300	0.33705200
C	-3.56993500	2.09478600	0.39192400
C	-2.31708100	2.69953300	0.26595300
C	-2.11176800	4.11092900	0.06130900
C	-0.77893300	4.30269200	-0.13721000
C	-0.13844900	3.02084500	-0.00368200
C	1.24036500	2.81185700	0.01269900
C	1.83413800	1.58504000	0.33628200
C	3.24186500	1.40123500	0.61096200
C	3.39952400	0.12397200	1.04528900
C	2.09752700	-0.50089500	0.98965300
H	1.16723700	-4.65693500	1.27137800
H	-1.31645000	-5.09917200	0.36127700
H	-5.56500300	-2.00899400	-0.26951700
H	-6.02392100	0.58341200	0.21284200
H	-2.89582100	4.85312500	0.04477600
H	-0.26884900	5.23328900	-0.33495800
H	4.00357700	2.15784700	0.50216600

H	4.32050000	-0.37211500	1.31455300
Mn	-0.81422000	0.10780100	0.36727000
Cl	-1.00432800	0.10539900	2.68833700
O	-0.78016800	0.14820000	-1.39015600
C	-3.55656600	-3.87734600	-0.42846000
C	-3.32196900	-4.56992700	-1.62093900
C	-4.53872000	-4.39100000	0.42492400
C	-4.03593300	-5.71453000	-1.96461400
C	-5.27108300	-5.53118000	0.10087700
C	-5.01627600	-6.19534800	-1.09792200
C	2.15352000	3.96766600	-0.21318600
C	2.99922200	4.00413000	-1.32517100
C	2.26308400	5.02061000	0.70152300
C	3.93043500	5.01913600	-1.51919500
C	3.17098500	6.06230800	0.51843500
C	4.01253200	6.05764500	-0.59354400
F	-4.79797600	-3.78299900	1.58878800
F	-6.20577600	-5.99691100	0.93441900
F	-5.70931200	-7.28984000	-1.41551700
F	-3.79001800	-6.35032700	-3.11412900
F	-2.38063500	-4.13449800	-2.47435700
F	1.48783600	5.04228300	1.79177600
F	2.94022300	3.02508300	-2.23919300
F	4.73901700	4.99791800	-2.58586600
F	4.89307200	7.04388600	-0.76973400
F	3.25135200	7.05568600	1.40839900
C	5.87074600	0.32910400	-1.73247900
C	4.94064300	0.79162300	-2.61557200
C	3.72578500	0.08297000	-2.89975500
C	5.65580300	-0.96186700	-1.05686600
H	5.08361700	1.76283900	-3.08409900
C	1.49420500	-0.07634100	-3.84512900
H	4.38029200	-2.54238100	-0.99301900
C	1.25643600	-1.28032400	-3.13435400
C	2.29040700	-1.82860100	-2.37335400
H	0.70140700	0.35820800	-4.44245000
C	7.12318500	1.07891100	-1.36951200
H	7.04737900	2.10974700	-1.73421600
H	7.19803400	1.11719500	-0.27607400
C	-0.11142600	-1.84851500	-3.01460600
H	-0.09473000	-2.85845300	-2.59356700
H	-0.55577500	-1.17968300	-2.18161900
C	-1.06097300	-1.74728100	-4.20391900
H	-2.02168900	-2.19916400	-3.94782000



H	-1.24710500	-0.70812200	-4.48857800
H	-0.65804700	-2.27389900	-5.07706500
C	8.39546200	0.41103800	-1.92318000
H	9.28625600	0.97512200	-1.62928900
H	8.48420100	-0.60426700	-1.52956600
H	8.36656500	0.36177200	-3.01657000
C	1.86510800	-1.85740800	1.22524600
C	2.97613600	-2.63434000	1.84329700
C	3.41958000	-2.31219100	3.13379200
C	3.65939000	-3.66084300	1.19008200
C	4.49284800	-2.97085200	3.73002900
C	4.73905100	-4.32929600	1.75481000
C	5.15452400	-3.98410600	3.03881100
F	3.30986100	-4.00950100	-0.07342900
F	5.37330800	-5.28749200	1.07513200
F	6.18222200	-4.61822400	3.60204700
F	4.88858500	-2.63973600	4.96117700
F	2.81809400	-1.33851400	3.82180700
C	3.51040200	-1.15828000	-2.25145900
C	2.70121300	0.58234600	-3.73172500
H	2.85847200	1.52762200	-4.24097200
H	2.12467300	-2.74160500	-1.81111400
N	4.51756600	-1.64954500	-1.44641600
O	6.39278300	-1.42892900	-0.18317600
C	-4.75558300	2.99279000	0.49106900
C	-4.99041100	3.73795100	1.65155100
C	-5.65654000	3.14867000	-0.56659300
C	-6.08231400	4.59649100	1.76335500
C	-6.75860800	3.99529100	-0.47507300
C	-6.96931200	4.72237900	0.69548000
F	-4.15061600	3.64066900	2.68692100
F	-6.28513700	5.29615100	2.88354000
F	-8.01949700	5.53969800	0.79263800
F	-7.60647700	4.12167000	-1.50135900
F	-5.47219300	2.46887200	-1.70694400

**<sup>5</sup>TS9-R**

N	0.47100200	-1.88173600	0.43565300
N	2.79909800	-0.23427400	0.26620400
N	1.10020300	2.05631800	0.22260200
N	-1.16718800	0.41287100	0.56078300
C	-0.66419700	-2.50219500	0.89799500
C	-0.44870500	-3.92510500	0.93580200
C	0.80915900	-4.15142700	0.46299400

C	1.39679500	-2.86248900	0.19577900
C	2.75677000	-2.66802900	-0.08785300
C	3.40634900	-1.43453200	0.00653800
C	4.83760300	-1.23648300	-0.07285600
C	5.07129100	0.07771500	0.17467700
C	3.78071000	0.71162300	0.33705200
C	3.56993500	2.09478600	0.39192400
C	2.31708100	2.69953300	0.26595300
C	2.11176800	4.11092900	0.06130900
C	0.77893300	4.30269200	-0.13721000
C	0.13844900	3.02084500	-0.00368200
C	-1.24036500	2.81185700	0.01269900
C	-1.83413800	1.58504000	0.33628200
C	-3.24186500	1.40123500	0.61096200
C	-3.39952400	0.12397200	1.04528900
C	-2.09752700	-0.50089500	0.98965300
H	-1.16723700	-4.65693500	1.27137800
H	1.31645000	-5.09917200	0.36127700
H	5.56500300	-2.00899400	-0.26951700
H	6.02392000	0.58341200	0.21284200
H	2.89582100	4.85312500	0.04477600
H	0.26884900	5.23328900	-0.33495800
H	-4.00357700	2.15784700	0.50216600
H	-4.32050000	-0.37211500	1.31455300
Mn	0.81422000	0.10780100	0.36727000
Cl	1.00432800	0.10539900	2.68833700
O	0.78016800	0.14820000	-1.39015600
C	3.55656600	-3.87734600	-0.42846000
C	3.32196900	-4.56992700	-1.62093900
C	4.53872000	-4.39100000	0.42492400
C	4.03593300	-5.71453000	-1.96461400
C	5.27108300	-5.53118000	0.10087700
C	5.01627600	-6.19534800	-1.09792200
C	-2.15352000	3.96766600	-0.21318600
C	-2.99922200	4.00413000	-1.32517100
C	-2.26308400	5.02061000	0.70152300
C	-3.93043500	5.01913600	-1.51919500
C	-3.17098500	6.06230800	0.51843500
C	-4.01253200	6.05764500	-0.59354400
F	4.79797600	-3.78299900	1.58878800
F	6.20577600	-5.99691100	0.93441900
F	5.70931100	-7.28984000	-1.41551700
F	3.79001800	-6.35032700	-3.11412900
F	2.38063500	-4.13449800	-2.47435700

F	-1.48783600	5.04228200	1.79177600
F	-2.94022300	3.02508300	-2.23919300
F	-4.73901700	4.99791800	-2.58586600
F	-4.89307100	7.04388600	-0.76973400
F	-3.25135100	7.05568600	1.40839900
C	-5.87074600	0.32910400	-1.73247900
C	-4.94064300	0.79162300	-2.61557200
C	-3.72578500	0.08297000	-2.89975500
C	-5.65580300	-0.96186700	-1.05686600
H	-5.08361600	1.76283900	-3.08409900
C	-1.49420500	-0.07634100	-3.84512900
H	-4.38029200	-2.54238100	-0.99301900
C	-1.25643600	-1.28032400	-3.13435400
C	-2.29040700	-1.82860100	-2.37335400
H	-0.70140700	0.35820800	-4.44245000
C	-7.12318500	1.07891200	-1.36951200
H	-7.04737900	2.10974800	-1.73421600
H	-7.19803400	1.11719600	-0.27607400
C	0.11142600	-1.84851500	-3.01460600
H	0.09473000	-2.85845300	-2.59356700
H	0.55577500	-1.17968300	-2.18161900
C	1.06097300	-1.74728100	-4.20391900
H	2.02168900	-2.19916400	-3.94782000
H	1.24710500	-0.70812200	-4.48857800
H	0.65804700	-2.27389900	-5.07706500
C	-8.39546200	0.41103900	-1.92318000
H	-9.28625600	0.97512300	-1.62928900
H	-8.48420100	-0.60426600	-1.52956600
H	-8.36656500	0.36177300	-3.01657000
C	-1.86510800	-1.85740800	1.22524600
C	-2.97613600	-2.63434000	1.84329700
C	-3.41958000	-2.31219100	3.13379200
C	-3.65939000	-3.66084300	1.19008200
C	-4.49284800	-2.97085200	3.73002900
C	-4.73905100	-4.32929600	1.75481000
C	-5.15452400	-3.98410600	3.03881100
F	-3.30986100	-4.00950100	-0.07342900
F	-5.37330800	-5.28749200	1.07513200
F	-6.18222100	-4.61822400	3.60204700
F	-4.88858500	-2.63973600	4.96117700
F	-2.81809400	-1.33851400	3.82180700
C	-3.51040200	-1.15828000	-2.25145900
C	-2.70121300	0.58234600	-3.73172500
H	-2.85847200	1.52762200	-4.24097200

H	-2.12467300	-2.74160500	-1.81111400
N	-4.51756600	-1.64954500	-1.44641600
O	-6.39278300	-1.42892900	-0.18317600
C	4.75558300	2.99279000	0.49106900
C	4.99041100	3.73795100	1.65155100
C	5.65654000	3.14867000	-0.56659300
C	6.08231400	4.59649100	1.76335500
C	6.75860800	3.99529100	-0.47507300
C	6.96931200	4.72237800	0.69548000
F	4.15061600	3.64066900	2.68692100
F	6.28513700	5.29615200	2.88354000
F	8.01949700	5.53969700	0.79263800
F	7.60647700	4.12166900	-1.50135900
F	5.47219300	2.46887200	-1.70694400