

Supporting Information

Mechanism and Origins of Directing Group-Controlled *Endo*- Versus *Exo*- Selectivity of Iridium-Catalyzed Intramolecular Hydroalkenylation of 1,1- Disubstituted Alkenes

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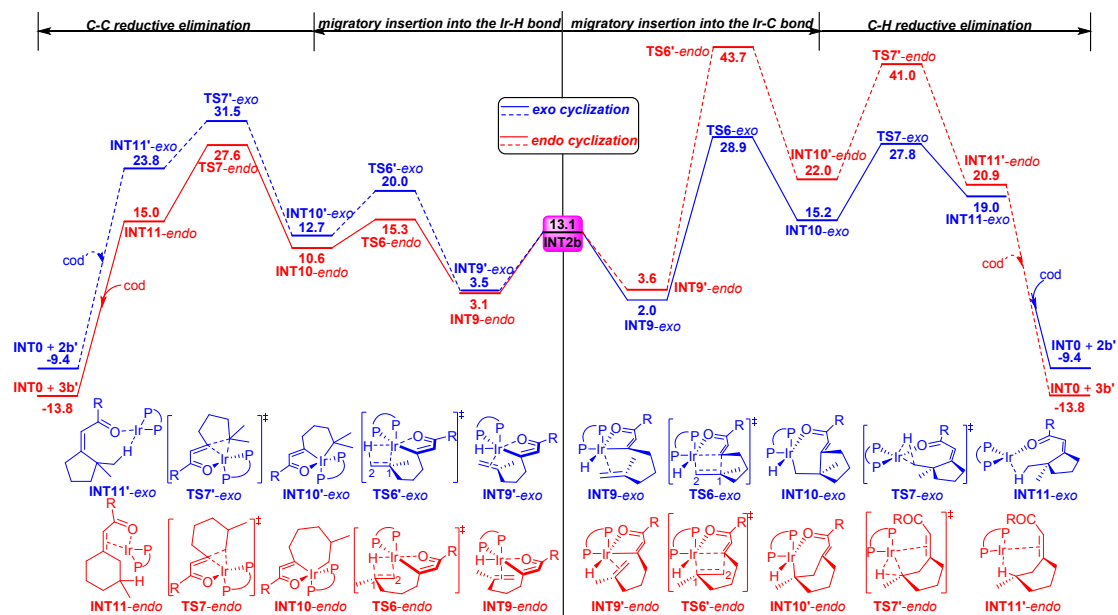
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1. Complete ref 14.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Mont-gomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Nor-mand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision A.02; Gaussian, Inc.: Wallingford, CT, 2009.

2. Results for reaction with INT2b.



3. Table of calculated energies and energy corrections

Stationary point	Single-point energy- B3LYP 6-311+G(d,p), SDD with DFT-D3(BJ) correction (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)	Optimization energy 6-31G(d) , lanl2dz (a.u.)	Solvation energy (1,4-Dioxane) (a.u.)
cod	-312.150608	0.149697	-312.024454	-0.005553
INT0	-4090.064384	0.355896	-4089.048344	-0.035120
1a'	-560.775661	0.237226	-560.554891	-0.008368
INT1a	-4338.673837	0.445520	-4337.569343	-0.034986
INT2a	-4338.686929	0.446168	-4337.570405	-0.033498
INT3-endo	-4338.708627	0.450775	-4337.577062	-0.031556
INT3-exo	-4338.708846	0.452163	-4337.575232	-0.031708
INT4-endo	-4338.697721	0.455409	-4337.577668	-0.032244
INT4-exo	-4338.695304	0.457409	-4337.570699	-0.032631
INT5-endo	-4338.711151	0.453863	-4337.601595	-0.034525
INT5-exo	-4338.682910	0.451549	-4337.568806	-0.035595
INT6-endo	-4338.709000	0.453760	-4337.576732	-0.031778
INT6-exo	-4338.711478	0.452149	-4337.578202	-0.031813
INT7-endo	-4338.687077	0.454733	-4337.561019	-0.033227
INT7-exo	-4338.695744	0.452912	-4337.575402	-0.032629
INT8-endo	-4338.670080	0.452195	-4337.548266	-0.040077
INT8-exo	-4338.684966	0.451339	-4337.570798	-0.035541
TS1a	-4338.658992	0.444923	-4337.540951	-0.035096
TS2-endo	-4338.684870	0.452249	-4337.552802	-0.032216
TS2-exo	-4338.680157	0.452164	-4337.546370	-0.032176
TS3-endo	-4338.661338	0.453281	-4337.542510	-0.035133
TS3-exo	-4338.654369	0.453455	-4337.526843	-0.034855
TS4-endo	-4338.637657	0.451066	-4337.505851	-0.032596
TS4-exo	-4338.670140	0.453144	-4337.541431	-0.032454
TS5-endo	-4338.643552	0.450962	-4337.514628	-0.035941
TS5-exo	-4338.665344	0.447997	-4337.545964	-0.033929
2a'	-560.799975	0.244947	-560.577379	-0.007068
3a'	-560.807410	0.247039	-560.585375	-0.007951
1b'	-466.068906	0.195557	-465.883822	-0.008292
INT1b	-4243.951574	0.402752	-4242.879604	-0.035611
INT2b	-4243.967639	0.402890	-4242.889962	-0.033126
INT9-endo	-4243.990020	0.408368	-4242.900436	-0.032135

INT9-<i>exo</i>	-4243.993109	0.409860	-4242.901708	-0.032300
INT10-<i>endo</i>	-4243.981086	0.412324	-4242.900960	-0.033175
INT10-<i>exo</i>	-4243.968988	0.407181	-4242.892348	-0.032800
INT11-<i>endo</i>	-4243.968014	0.412035	-4242.889895	-0.038915
INT11-<i>exo</i>	-4243.959999	0.407344	-4242.886313	-0.035893
TS1b	-4243.938819	0.401178	-4242.859708	-0.035970
TS6-<i>endo</i>	-4243.969420	0.408025	-4242.877590	-0.032943
TS6-<i>exo</i>	-4243.948997	0.409393	-4242.862417	-0.033104
TS7-<i>endo</i>	-4243.950611	0.411225	-4242.871782	-0.035407
TS7-<i>exo</i>	-4243.943370	0.403519	-4242.864468	-0.034596
2b'	-466.092863	0.202909	-465.907743	-0.006624
3b'	-466.100245	0.204475	-465.915654	-0.007923

4. Cartesian coordinates

cod			
C	0.52272600	1.16375200	6.70902400
H	0.84519300	0.58388900	5.84348300
C	1.06265600	0.66898200	8.03433000
H	0.29652600	0.69129100	8.81347500
H	1.33438400	-0.38818400	7.92171100
C	2.32417100	1.41860900	8.51529700
H	2.70617900	0.91910800	9.42056100
H	3.11529300	1.28366000	7.76256300
C	2.20961700	2.89771500	8.79289500
H	3.17940200	3.38680500	8.90111300
C	1.13358400	3.68326400	8.92698100
H	1.32897800	4.74065400	9.10881900
C	-0.33372400	3.32216200	8.82977500
H	-0.91311200	4.09555000	9.34966900
H	-0.55306800	2.39027200	9.35706500
C	-0.86671000	3.24473400	7.38248700
H	-0.73979400	4.23153600	6.91253700
H	-1.95689000	3.08627000	7.41807800
C	-0.26074000	2.21943400	6.45519000
H	-0.52093900	2.38560400	5.40826500

INT0

Ir	3.54512900	7.71826000	16.16200500
P	2.28138400	8.61989600	14.41093000
P	2.45998700	9.35319300	17.42635800
C	5.14630900	7.41367800	17.73150600
H	5.06247100	8.23714000	18.43873800
C	4.21724800	6.37479300	17.85837700
H	3.44479600	6.50288600	18.61397300
C	4.42910200	4.93909800	17.39364000
H	3.91966000	4.27166400	18.09604600
H	5.49189000	4.68910600	17.45723300
C	3.88774700	4.66258100	15.97233400
H	4.37643400	3.77092900	15.55174500
H	2.82090400	4.42844200	16.03091700
C	4.04113200	5.82520200	15.01828100
H	3.36951600	5.79373600	14.16297600
C	5.14296300	6.68109900	14.92541800
H	5.21320000	7.29143900	14.02725200
C	6.44435500	6.53062000	15.70346900
H	7.26754800	6.86709200	15.06498400
H	6.63035100	5.47138600	15.90171200
C	6.47682500	7.34565100	17.01605500
H	7.24215500	6.93737600	17.69304300
H	6.77867900	8.37333000	16.79446800
C	0.73625300	7.73058600	13.92757700
C	0.27069700	6.58158200	14.57919000
C	-0.91491900	5.94790100	14.21008500
C	-1.67861400	6.46327100	13.16552300
C	-1.25458200	7.61443800	12.49967800
C	-0.06915300	8.22541900	12.89028800
C	3.17449800	8.91213600	12.82485700
C	3.20411300	7.94563600	11.81065600
C	3.92484400	8.11681700	10.63266300
C	4.66969100	9.28121400	10.44783500
C	4.69377100	10.25127100	11.44890500
C	3.96239800	10.05158200	12.61665300
C	1.55842900	10.25186200	14.98031900
C	1.04891000	10.06292900	16.41775200
C	3.40034400	10.90216000	17.79008600
C	4.65139900	11.19184300	17.23012200
C	5.32144300	12.38708300	17.48799300
C	4.73956900	13.34164600	18.31847700
C	3.48533400	13.09810100	18.88042400
C	2.84010900	11.89921200	18.60343200
C	1.77221600	8.78644200	19.03888000
C	2.46338800	8.93430000	20.24809400
C	1.97638000	8.43849500	21.45394800
C	0.76667300	7.74506800	21.47248500
C	0.06735100	7.54440400	20.28289900
C	0.58026100	8.05175400	19.09267700
H	0.71939700	11.01180500	16.84949300
H	0.20859400	9.36825400	16.45436900
H	2.34079900	11.01056800	14.93698700
H	0.75395100	10.56106700	14.30853500
F	1.62626500	11.70880600	19.14774900
F	2.91525700	14.00791000	19.66525300
F	5.36828400	14.48147600	18.56615400

F	6.50904100	12.61924900	16.93263000
F	5.26150800	10.33520900	16.39640100
F	3.65393200	9.55923300	20.27702400
F	2.66515000	8.61333400	22.57850800
F	0.29279300	7.26249900	22.61264400
F	-1.07417600	6.86088500	20.28461900
F	-0.10808700	7.78566700	17.96693200
F	0.94400300	6.03884000	15.60473000
F	-1.31908100	4.85769800	14.85845400
F	-2.80820500	5.86867600	12.80993600
F	-1.98129400	8.11950900	11.50680300
F	0.30025700	9.33882500	12.23323800
F	2.53330600	6.78802400	11.95822600
F	3.91434800	7.17300400	9.69534000
F	5.36614200	9.45629400	9.33351700
F	5.42087800	11.35460900	11.29427900
F	4.05873100	11.00100600	13.56466200

1a'

C	-4.49612200	7.76589000	4.21935300
O	-4.29253200	7.35177400	3.07660900
N	-3.47347400	8.29100100	4.98511500
C	-2.11338700	8.22177600	4.47041900
H	-1.48053600	7.60826500	5.12691600
C	-3.61218800	8.83270400	6.32774300
H	-2.87679200	9.63384500	6.46139500
H	-3.43112500	8.07721400	7.10725700
C	-5.86132200	7.70578300	4.82443200
H	-6.01084000	7.94737800	5.87235900
C	-6.90290300	7.31086600	4.08063500
H	-6.70398600	7.06474900	3.03783100
C	-8.31831000	7.18910000	4.55939000
H	-8.65167000	6.14776200	4.42738200
H	-8.37783400	7.40467500	5.63448600
C	-9.28574400	8.11030900	3.78797900
H	-8.98504300	9.15593700	3.93155500
H	-9.19380900	7.90501800	2.71353700
C	-10.74959000	7.93301200	4.23809400
H	-11.04103800	6.88419200	4.07013000
H	-10.81272300	8.10510900	5.32016400
H	-1.67315400	9.22578500	4.40844300
C	-11.72915700	8.84541600	3.52839100
C	-12.37483000	9.81761200	4.18175900
H	-12.22489500	9.98990200	5.24510200
H	-13.07878000	10.47650400	3.67888300
C	-11.94673000	8.59920400	2.05415600
H	-12.27878200	7.56738400	1.87296000
H	-11.02164200	8.73469500	1.47882800
H	-12.70008900	9.27659600	1.64052500
H	-4.59837700	9.27103900	6.48333300
H	-2.14644200	7.77707200	3.47710800

INT1a

C	3.52174900	3.02362300	-4.52657600
C	4.83759200	3.03943900	-4.02123700
H	5.04980700	3.38933600	-3.01540500
Ir	4.30651400	0.92079200	-4.35772700
H	3.39717500	3.02800200	-5.61038900
C	5.93788400	2.82560500	-5.00264000
O	5.74066600	1.79815200	-5.73765300
N	7.03767100	3.56950000	-5.09291700
C	7.22171500	4.82035400	-4.35733900
H	8.02097100	4.71382500	-3.61562100
H	7.49827800	5.61316400	-5.05982700
C	8.11620400	3.18776200	-6.01086400
H	8.16022600	3.89015800	-6.85016400
H	7.92957200	2.18440700	-6.38996700
P	4.57928800	-1.33299600	-4.87971500
P	3.12095100	0.16922300	-2.62092700
C	6.36145600	-1.79921900	-4.88800600
C	7.15888500	-1.35461600	-5.95145200
C	8.52763600	-1.59296000	-6.00854700
C	9.14386600	-2.30023600	-4.97676700
C	8.38390400	-2.75358000	-3.89991800
C	7.01560200	-2.49611700	-3.86656100
C	3.95850400	-1.95698500	-6.48876800
C	4.03477100	-3.32260000	-6.79312800
C	3.57941000	-3.84370600	-7.99834700
C	3.02449400	-2.97934900	-8.94422900
C	2.93221800	-1.61469200	-8.67532700

C	3.39827500	-1.11802900	-7.45952200
C	3.66894100	-2.36462900	-3.61678400
C	3.60076300	-1.61148700	-2.28250800
C	1.27697800	-0.00857500	-2.72236700
C	0.53719300	-0.50932500	-1.64119700
C	-0.83328300	-0.72773000	-1.69644500
C	-1.51794800	-0.45110100	-2.88088300
C	-0.82071700	0.03564000	-3.98321100
C	0.55573600	0.24492500	-3.89597800
C	3.47055200	1.05750600	-1.03446900
C	2.57364600	1.88334200	-0.34546300
C	2.91676100	2.54468100	0.83183200
C	4.20036700	2.40330200	1.35426000
C	5.13077800	1.60879900	0.68617800
C	4.75952500	0.96127800	-0.48789500
H	2.88557700	-2.07633900	-1.59941600
H	4.57867700	-1.60573800	-1.80039300
H	2.66592600	-2.49784200	-4.03942100
H	4.11252100	-3.35360900	-3.50193600
F	2.58283000	-3.45919200	-10.09893600
F	3.66629900	-5.14730200	-8.25208400
F	4.56514700	-4.17270100	-5.89701600
F	2.40275900	-0.79185300	-9.57825400
F	3.29358700	0.19955100	-7.25617100
F	6.60459300	-0.66388100	-6.95837100
F	9.24741300	-1.14082600	-7.03531200
F	10.44976900	-2.53356800	-5.01663300
F	8.96428500	-3.42402000	-2.90692700
F	6.34024300	-2.94116500	-2.79263500
F	5.70648100	0.22998800	-1.10294800
F	6.36830100	1.48116800	1.16284300
F	4.54027400	3.03257700	2.47185800
F	2.02595400	3.31831900	1.44908600
F	1.33354400	2.09834700	-0.81343100
F	1.16123200	-0.79268300	-0.48390100
F	-1.48922300	-1.19782600	-0.63813400
F	-2.82621300	-0.65575400	-2.95608100
F	-1.46479300	0.29297500	-5.12110600
F	1.15760100	0.70041700	-5.00623700
H	6.29851300	5.11110200	-3.85652000
H	9.06993800	3.21472100	-5.47446200
C	2.34006800	3.55465000	-3.76053200
H	1.44515100	3.00094200	-4.06229100
H	2.47328900	3.40039500	-2.68461700
C	2.11216100	5.05808900	-4.03374600
H	2.99804800	5.62657900	-3.72104300
H	2.00064900	5.21813100	-5.11367000
C	0.87429400	5.59646200	-3.28714600
H	-0.00908300	5.03511400	-3.62785200
H	0.98620600	5.38648000	-2.21584800
C	0.64243000	7.08081000	-3.48928800
C	0.18791600	7.52101300	-4.86042400
H	0.92095800	7.26652000	-5.63776800
H	-0.75112600	7.02430600	-5.14074900
H	0.02355400	8.60152500	-4.89979800
C	0.82585800	7.94954300	-2.48932400
H	1.13594300	7.62646800	-1.49817800
H	0.66223700	9.01602300	-2.62038300

INT2a

C	3.65124500	3.06398700	-4.63451000
C	4.40171200	3.67596300	-5.59228800
H	4.31839300	4.73987800	-5.78988300
Ir	4.00096400	1.02773800	-4.54221000
H	5.09474000	1.35066200	-3.48707200
C	5.29636300	2.83432700	-6.36805500
O	5.28777700	1.57051800	-6.11880300
N	6.11459500	3.29745100	-7.32373600
C	6.15892200	4.70514700	-7.72591900
H	7.15845300	4.92195100	-8.10989700
H	5.42862200	4.91614100	-8.51636700
C	6.92336300	2.37631800	-8.12679700
H	6.54713000	2.34584200	-9.15636800
H	6.88067900	1.37969800	-7.69479600
P	4.76208800	-1.25810400	-4.60881300
P	2.63462200	0.28701300	-2.87837700
C	6.57707800	-1.39279800	-4.32616400
C	7.45757300	-1.15349000	-5.38897000
C	8.83889800	-1.14649100	-5.22771100

C	9.38280000	-1.37725600	-3.96465600
C	8.53793300	-1.60657800	-2.88009400
C	7.15898100	-1.60578800	-3.07283700
C	4.48840300	-2.30689200	-6.09242000
C	4.84947400	-3.65993100	-6.10210500
C	4.65958200	-4.47294400	-7.21408600
C	4.08715800	-3.92728400	-8.36478700
C	3.71270100	-2.58448100	-8.38994700
C	3.91632500	-1.79415300	-7.26116600
C	3.85701800	-2.21047900	-3.27301800
C	3.36324200	-1.27799200	-2.15925000
C	1.02715200	-0.27476500	-3.57472000
C	0.06640100	-0.96304500	-2.82255300
C	-1.13016200	-1.41030700	-3.36988300
C	-1.39448800	-1.17216800	-4.72058800
C	-0.46229000	-0.49527900	-5.50510000
C	0.72857500	-0.06887500	-4.92619100
C	2.29008600	1.31589500	-1.38682800
C	1.04592300	1.83033900	-0.99793000
C	0.89192900	2.62365800	0.13715900
C	2.00014200	2.93315800	0.92313200
C	3.25779500	2.45033400	0.56282400
C	3.38145700	1.66111000	-0.57517300
H	2.62131800	-1.77695700	-1.53044400
H	4.19598700	-0.96821500	-1.52531400
H	3.00678100	-2.66628500	-3.79271500
H	4.46450400	-3.02020900	-2.86670000
F	3.89575800	-4.68875800	-9.43357100
F	5.01335000	-5.75543900	-7.18674000
F	5.40158700	-4.20779300	-5.00703000
F	3.16452200	-2.06452400	-9.48679600
F	3.54363000	-0.50817200	-7.33376000
F	6.97617100	-0.91686700	-6.62178600
F	9.63705600	-0.91671100	-6.26954900
F	10.69879100	-1.37218800	-3.79492000
F	9.04701900	-1.82064800	-1.66899600
F	6.38976900	-1.81050100	-1.98711100
F	4.61549100	1.22762900	-0.89244400
F	4.32661300	2.74496100	1.29825300
F	1.86098100	3.68768400	2.00410300
F	-0.31000800	3.08951900	0.46670200
F	-0.06152400	1.59856600	-1.71857900
F	0.28281900	-1.18784300	-1.51712500
F	-2.01873500	-2.05608200	-2.62053700
F	-2.53213600	-1.59074700	-5.25620400
F	-0.70543500	-0.26836600	-6.79288600
F	1.60165500	0.56725000	-5.74213200
H	5.97517900	5.36193500	-6.87634400
H	7.95996300	2.72732000	-8.14239100
C	2.69984200	3.90563000	-3.82460700
H	2.91044900	3.75020200	-2.75825200
H	2.88587600	4.97037900	-4.02597400
C	1.20541000	3.60515500	-4.07251100
H	0.99332600	2.56633200	-3.80298000
H	0.61634000	4.22453000	-3.38523200
C	0.74084300	3.84906200	-5.51066300
H	0.89131400	4.90956100	-5.76774700
H	1.39105900	3.29598900	-6.20432300
C	-0.69953900	3.48109200	-5.81523800
C	-1.10342200	3.65922600	-7.25944900
H	-0.94421900	4.69464200	-7.58936600
H	-0.49896200	3.02244800	-7.92018600
H	-2.15645200	3.41098100	-7.41988700
C	-1.56440000	3.03484600	-4.89570600
H	-1.30154100	2.90887400	-3.84969700
H	-2.59142500	2.79873700	-5.16223600

INT3-endo

C	5.12029000	0.52263800	-6.83469600
C	3.74727100	2.67395400	-6.99052200
H	5.02891900	-0.54083400	-7.08152100
H	6.12953300	0.83107600	-7.14135300
C	4.97672800	0.71155700	-5.34904700
C	6.05442000	1.11634700	-4.62148300
H	7.01344000	1.29778400	-5.09768500
Ir	3.21829800	0.59547400	-4.28566800
H	2.28075100	0.10580000	-5.46710100
C	5.85949500	1.35468600	-3.19678500
O	4.68300600	1.21131000	-2.72048100

N	6.85129900	1.73188200	-2.36168900
C	8.26370300	1.81739700	-2.72514200
H	8.60053900	2.86076300	-2.72909600
H	8.86023600	1.26532300	-1.98986800
C	6.54105000	2.04731900	-0.96481700
H	7.17675600	2.87658200	-0.64127600
H	6.73217200	1.18376000	-0.31507400
P	3.59761100	-1.63286600	-3.78534400
P	1.32546700	0.43218200	-2.72798500
C	5.25540300	-1.88652700	-3.01720300
C	6.38768600	-2.11909000	-3.80589000
C	7.67087900	-2.18469900	-3.27018800
C	7.85371400	-1.98182900	-1.90362400
C	6.75064400	-1.72773400	-1.09130300
C	5.47902600	-1.68690700	-1.65278100
C	3.53134200	-2.99456000	-5.03963500
C	3.80876200	-4.30515800	-4.61640900
C	3.75407800	-5.40443200	-5.46518200
C	3.39914400	-5.21740400	-6.80081400
C	3.10398300	-3.93658400	-7.25811800
C	3.16940300	-2.85124100	-6.38440700
C	2.29382200	-2.26550100	-2.59761900
C	1.59383500	-1.17195000	-1.79496900
C	-0.37610200	0.38874500	-3.46236600
C	-1.02701900	1.59418000	-3.74440100
C	-2.29172700	1.65684800	-4.31893400
C	-2.95189600	0.47179000	-4.64241600
C	-2.33165200	-0.75058400	-4.39233100
C	-1.06487300	-0.77405700	-3.81337500
C	1.01839100	1.53098600	-1.25944600
C	-0.04376600	1.25006300	-0.38421800
C	-0.31143300	2.01012700	0.74909000
C	0.50704800	3.09821800	1.05081600
C	1.57602500	3.40501400	0.21424200
C	1.81728800	2.62766800	-0.91791500
H	0.65345200	-1.54217800	-1.38328400
H	2.22520200	-0.86489000	-0.95768300
H	1.57503700	-2.77942800	-3.23886000
H	2.73467600	-3.01249400	-1.93422400
F	3.33748800	-6.25301000	-7.62630400
F	4.03242800	-6.62299800	-5.00887200
F	4.14375600	-4.54122200	-3.33512100
F	2.75428900	-3.74524900	-8.52897100
F	2.86120600	-1.65824500	-6.90870800
F	6.26998800	-2.26366500	-5.13518200
F	8.72068100	-2.40347000	-4.06120400
F	9.07568700	-2.00169700	-1.38154000
F	6.91976700	-1.48129900	0.21013200
F	4.45459500	-1.41489900	-0.82636100
F	2.86353700	2.98811800	-1.67225500
F	2.36990600	4.43871100	0.49401400
F	0.27062700	3.83148500	2.13073600
F	-1.33250000	1.69944100	1.54491400
F	-0.85533300	0.20314900	-0.61756200
F	-0.40783600	2.76413100	-3.47829600
F	-2.86191000	2.83363800	-4.57076900
F	-4.15759600	0.50887600	-5.19591100
F	-2.94723700	-1.88964600	-4.70335100
F	-0.51867200	-1.98625900	-3.59987100
H	8.44901900	1.38136100	-3.70449400
H	5.49426900	2.33421400	-0.88041600
C	2.90642400	2.89776700	-4.59612000
H	3.87765500	3.26891600	-4.28352500
H	2.07065000	3.16102600	-3.96060400
C	4.07825600	1.31722600	-7.65117400
C	2.67178000	2.60421100	-5.92811400
C	1.26514100	2.49075800	-6.45691600
H	1.15680000	1.67936400	-7.18211000
H	0.53557600	2.36543300	-5.65980400
H	1.03161200	3.42632700	-6.98452500
H	4.47270500	1.48788600	-8.65821900
H	3.16296500	0.72947200	-7.76720200
H	3.36858600	3.36242900	-7.75767800
H	4.65836300	3.12174500	-6.58031200

INT3-exo

C	3.96673100	1.92094700	-7.35127900
C	5.03370000	0.97957600	-6.75318500
C	3.96167600	3.29137400	-6.65352400

H	4.86512000	-0.02851100	-7.14518200
H	6.03242000	1.29380200	-7.08848600
H	4.17009000	2.06852900	-8.41764100
H	2.97911000	1.45643300	-7.27551400
H	3.31096300	3.97659600	-7.21632100
H	4.96992300	3.71963600	-6.69818200
C	4.96787900	0.98050900	-5.25246000
C	6.06867800	1.27738700	-4.50751700
H	7.03505000	1.45802500	-4.97020600
Ir	3.20649500	0.79679500	-4.18990500
H	2.31031400	0.35176200	-5.41380600
C	5.86493000	1.48292700	-3.07751400
O	4.67188700	1.43418400	-2.62438800
N	6.87254500	1.76581200	-2.22129400
C	8.29068400	1.71679600	-2.56903100
H	8.71139900	2.72552800	-2.66203400
H	8.83358600	1.18885700	-1.77728000
C	6.57070900	2.13325200	-0.83627400
H	7.23485400	2.94801800	-0.53155600
H	6.72532500	1.28371000	-0.15925500
P	3.57395200	-1.43398300	-3.79357500
P	1.23710400	0.53043000	-2.79032700
C	5.15787400	-1.70201300	-2.88990900
C	6.36422200	-1.91451900	-3.56625200
C	7.58742800	-1.97289800	-2.90413600
C	7.62990400	-1.78633900	-1.52434900
C	6.44893300	-1.55973600	-0.82064100
C	5.24073700	-1.52008300	-1.50718800
C	3.64170000	-2.70880200	-5.13751100
C	3.98278400	-4.02720100	-4.79193000
C	4.02057400	-5.06849400	-5.71132000
C	3.69149500	-4.81494000	-7.04247100
C	3.32601700	-3.52762200	-7.42345400
C	3.29751200	-2.50127100	-6.47892600
C	2.18284600	-2.17558900	-2.77577300
C	1.35358100	-1.16234200	-1.98844700
C	-0.36602400	0.62501000	-3.71156300
C	-1.04837000	1.83910700	-3.85549700
C	-2.21819700	1.95957100	-4.60024900
C	-2.73668200	0.84026000	-5.24975600
C	-2.07290600	-0.38128800	-5.15071600
C	-0.90738000	-0.46646200	-4.39501700
C	0.85180200	1.53630300	-1.28282500
C	-0.23422100	1.20394300	-0.46026300
C	-0.54293200	1.90882900	0.69819000
C	0.25056400	2.99525900	1.06786100
C	1.33370700	3.36106400	0.27262700
C	1.61507200	2.63626200	-0.88334900
H	0.35856600	-1.55965100	-1.78165600
H	1.83374900	-0.95390300	-1.02982000
H	1.55552400	-2.68027200	-3.51187700
H	2.59448500	-2.94165800	-2.11426200
F	3.71692200	-5.79514900	-7.93477900
F	4.35960100	-6.29629200	-5.32588500
F	4.28741800	-4.33069800	-3.51714200
F	2.99259600	-3.27486100	-8.68782100
F	2.90826000	-1.30265800	-6.93292500
F	6.38224000	-2.05010200	-4.90047500
F	8.71579700	-2.16075600	-3.58850500
F	8.79624000	-1.78916100	-0.88598100
F	6.48771100	-1.33065700	0.49407900
F	4.13184000	-1.26798600	-0.78938400
F	2.65699300	3.04970500	-1.61928700
F	2.09502100	4.40090700	0.61367200
F	-0.02691800	3.67674200	2.17166300
F	-1.58222300	1.55328900	1.45001900
F	-1.02906800	0.16829300	-0.78110700
F	-0.57239600	2.95806600	-3.27645800
F	-2.83262600	3.13658500	-4.70114700
F	-3.84827500	0.94044800	-5.96791400
F	-2.54761100	-1.45574600	-5.77819400
F	-0.29186900	-1.66490500	-4.35354600
H	8.44918800	1.17471200	-3.49990400
H	5.53431900	2.45910400	-0.76605900
C	3.47528600	3.34183700	-5.21303900
C	2.23294800	2.87597400	-4.82793200
H	1.52335600	2.54206700	-5.57833700
H	1.81422300	3.25336100	-3.90311900
C	4.28158800	4.20701700	-4.28798700
H	5.33729300	3.91902600	-4.29626800

H	4.23419500	5.23702100	-4.67049300
H	3.90554300	4.19844300	-3.26527600

INT4-endo

C	6.74336700	-0.92977200	-4.49485600
C	5.45261200	-0.55764800	-5.26979800
C	6.59158600	-1.34652300	-3.02047700
C	4.71385300	0.55354200	-4.58323800
C	5.15423400	1.84325500	-4.68902000
H	5.96690600	2.10625000	-5.35807600
Ir	3.22195500	0.29750800	-3.30151900
C	4.56405800	2.78906900	-3.76833200
O	3.68477100	2.32584200	-2.94931700
P	1.43963700	0.88056000	-4.95123300
P	2.47333200	-1.84091000	-3.64918500
C	2.06229700	1.67851300	-6.49630600
C	2.41271500	3.03264800	-6.44476200
C	2.98829700	3.70333600	-7.51699300
C	3.23509900	3.01543300	-8.70388500
C	2.90671300	1.66403300	-8.79335000
C	2.33914700	1.01782800	-7.69687700
C	-0.02305700	1.92313700	-4.54251500
C	-1.08138500	2.08411500	-5.44728700
C	-2.19142300	2.87184500	-5.16396300
C	-2.26212500	3.53038000	-3.93473500
C	-1.22815800	3.39457300	-3.00994300
C	-0.12663400	2.59956600	-3.32140300
C	0.63115500	-0.74568500	-5.42526900
C	1.59701700	-1.93198500	-5.29065800
C	1.08993600	-2.10472700	-2.45250900
C	0.79651100	-1.13297200	-1.49662700
C	-0.21590400	-1.27419300	-0.55521000
C	-0.98088500	-2.44173500	-0.56381500
C	-0.72561000	-3.43914600	-1.50741000
C	0.29778800	-3.25778500	-2.43379800
C	3.46887400	-3.38195300	-3.46990400
C	4.02523100	-4.06964200	-4.55522300
C	4.80815200	-5.20985500	-4.39717700
C	5.05859900	-5.69948700	-3.11645800
C	4.52859200	-5.03865800	-2.00847800
C	3.75237900	-3.90025300	-2.19818900
H	1.06214200	-2.88188500	-5.38000300
H	2.35234900	-1.89775000	-6.07581500
H	-0.20503000	-0.85152800	-4.72479000
H	0.20928300	-0.70758200	-6.42915500
F	-3.31539900	4.28337300	-3.64739900
F	-3.17871300	2.99834200	-6.04787100
F	-1.04077500	1.46532800	-6.63954500
F	-1.29456800	4.02213900	-1.83727300
F	0.84192000	2.50507700	-2.40295400
F	2.21289900	3.73025600	-5.31063200
F	3.33250200	4.98946800	-7.39997500
F	3.78905400	3.63947200	-9.73590100
F	3.14284000	0.99253200	-9.91812600
F	2.07350500	-0.29376700	-7.84134700
F	3.27584700	-3.29381000	-1.09802000
F	4.76581300	-5.49341000	-0.78142300
F	5.80301700	-6.78338800	-2.95171200
F	5.31529500	-5.82735200	-5.46087400
F	3.83648400	-3.63368400	-5.81396300
F	1.51564200	0.02292700	-1.46455000
F	-0.46130100	-0.31526100	0.33251000
F	-1.95666700	-2.59908700	0.31846400
F	-1.45944100	-4.54719100	-1.51908900
F	0.51942800	-4.23497200	-3.32641000
C	6.14105800	-0.25300300	-2.01402100
H	4.82768700	-1.44474500	-5.39817100
H	5.74440400	-0.23251000	-6.27888900
H	7.22831700	-1.74706300	-5.04446200
H	7.43002600	-0.07498100	-4.54873400
H	5.92346200	-2.21442300	-2.94218000
C	4.62024200	-0.18324000	-1.77284200
H	6.48518700	0.71941000	-2.39049000
H	4.41858100	0.62542200	-1.05548100
H	4.30425400	-1.11950400	-1.29824200
H	7.57908400	-1.71026500	-2.70867400
C	6.83485700	-0.48232300	-0.65455600
H	7.92581400	-0.44157500	-0.75684800
H	6.53745200	0.27550400	0.07892000

H	6.57438700	-1.46524100	-0.24125100
N	4.89319900	4.08990500	-3.70493000
C	5.76882200	4.73070300	-4.68627200
H	6.20247300	5.62410500	-4.23129700
H	6.58854900	4.07111600	-4.97280700
H	5.20791400	5.03058900	-5.58015200
C	4.18320900	4.98826100	-2.79223500
H	4.90856100	5.59870400	-2.24579000
H	3.51724700	5.65015900	-3.35942800
H	3.59458600	4.40154300	-2.09066300

INT4-*exo*

C	6.69884600	-1.08447900	-3.72964100
C	5.78172700	-0.76690300	-4.94201300
C	5.95356200	-1.35799800	-2.41265400
C	4.92615000	0.39981900	-4.56930400
C	5.31755300	1.68038200	-4.84513000
H	6.15788800	1.87884800	-5.50163700
Ir	3.41738100	0.23765200	-3.29161900
C	4.67795200	2.70657900	-4.05174800
O	3.82707000	2.30180800	-3.17082300
P	1.54474200	0.87174000	-4.85964900
P	2.54131600	-1.89253600	-3.59195600
C	2.10461600	1.71354600	-6.40608900
C	2.33203100	3.09528000	-6.39693500
C	2.84091200	3.78097200	-7.49435800
C	3.14717600	3.08362700	-8.66097600
C	2.94536700	1.70549600	-8.70707500
C	2.44334200	1.04608100	-7.58785100
C	0.10120700	1.90737500	-4.35764500
C	-1.03816600	2.01566900	-5.16771000
C	-2.13934600	2.78645800	-4.81131800
C	-2.11674800	3.48870400	-3.60529000
C	-0.99775500	3.41422400	-2.77800900
C	0.09252200	2.63542100	-3.16141700
C	0.70753200	-0.72922900	-5.36529800
C	1.64202700	-1.93666700	-5.22694600
C	1.12001500	-2.05825600	-2.41584200
C	0.82415900	-1.03133200	-1.52069300
C	-0.23491400	-1.08324700	-0.62149700
C	-1.05275200	-2.21298100	-0.61118100
C	-0.80272300	-3.26128000	-1.49913300
C	0.26590400	-3.16732900	-2.38574500
C	3.38125300	-3.54352000	-3.49529400
C	3.99868100	-4.12238400	-4.61225300
C	4.65167800	-5.35046600	-4.56452600
C	4.70194800	-6.05487300	-3.36346500
C	4.10370700	-5.51473700	-2.22627200
C	3.46220200	-4.28246400	-2.30560600
H	1.07706200	-2.87075700	-5.30315700
H	2.39083500	-1.93294100	-6.01757600
H	-0.14530600	-0.82583600	-4.68496700
H	0.30742000	-0.67091300	-6.37703200
F	-3.15908000	4.22703500	-3.24849200
F	-3.20395300	2.85814300	-5.60745600
F	-1.09014400	1.36400400	-6.34208500
F	-0.97067300	4.08881500	-1.63006700
F	1.14838900	2.61827200	-2.34025400
F	2.07957000	3.81290700	-5.28752700
F	3.06672300	5.09615000	-7.41861400
F	3.63938800	3.72418500	-9.71387100
F	3.24200100	1.02325500	-9.81069900
F	2.30348600	-0.28880500	-7.68755300
F	2.91326500	-3.81782800	-1.17109300
F	4.14495600	-6.17417400	-1.07203600
F	5.31841700	-7.22625600	-3.30163700
F	5.22327800	-5.84755400	-5.65829400
F	4.00143800	-3.48887300	-5.80119300
F	1.57620000	0.10238800	-1.51544800
F	-0.47571800	-0.06825600	0.20409000
F	-2.07209100	-2.28621400	0.23204000
F	-1.58586300	-4.33519700	-1.49761300
F	0.47133100	-4.19404400	-3.22484900
C	5.01378800	-0.25972600	-1.87050400
N	4.93959400	4.02165800	-4.13519200
C	5.80053100	4.62215300	-5.15172100
H	6.43652000	3.87801700	-5.62685000
H	5.19239700	5.11846600	-5.91762600
H	6.44363800	5.37052700	-4.67856500

C	4.24305300	4.97851300	-3.27238400
H	4.97586600	5.55994300	-2.70280000
H	3.64992600	5.66299900	-3.88915800
H	3.58584000	4.44446900	-2.59050900
H	6.41020800	-0.51693100	-5.80772500
H	5.19197200	-1.64423700	-5.21488200
H	7.39367000	-0.24670800	-3.60024600
H	7.31200000	-1.95878300	-3.98124100
H	6.71548800	-1.55639300	-1.64144900
H	5.39448600	-2.29385700	-2.51610200
C	5.82076500	0.99324000	-1.48918800
H	5.18471700	1.76899100	-1.05319400
H	6.57055600	0.71816800	-0.73241100
H	6.36153500	1.43410900	-2.33005500
C	4.33953800	-0.76680400	-0.58315600
H	5.10773700	-0.95038400	0.18373200
H	3.64891600	-0.02795800	-0.16296500
H	3.80132400	-1.70940000	-0.71714300

INT5-endo

C	6.31947200	-1.06648800	-1.12776500
C	5.10778200	-1.19171700	-2.08173500
C	6.10031200	0.03538300	-0.08519300
C	4.81215900	0.14806700	-2.72491900
C	5.28657900	0.37135800	-4.03963000
H	5.85171200	-0.40552500	-4.54711900
Ir	3.08581200	0.36336000	-4.26182300
C	5.25259500	1.74261500	-4.62032400
O	4.08761000	2.26624700	-4.58174800
P	0.96439300	0.93714600	-4.99905500
P	2.32313200	-1.73645400	-4.32849700
C	1.03908500	1.83164000	-6.60980300
C	1.48831100	3.15899900	-6.61095900
C	1.64962400	3.89236100	-7.78139400
C	1.35716200	3.29730700	-9.00805100
C	0.91349400	1.97674500	-9.04692600
C	0.76551900	1.26511100	-7.85889700
C	-0.10501600	2.01992100	-3.96902400
C	-1.41546600	2.30627500	-4.37494700
C	-2.26685100	3.11684200	-3.63316600
C	-1.80573500	3.67022400	-2.43751000
C	-0.50779900	3.40825800	-2.00286300
C	0.32568700	2.59387600	-2.76718300
C	-0.05694300	-0.61453100	-5.19915300
C	0.86171600	-1.80423400	-5.49969300
C	1.55993100	-2.55347500	-2.84313000
C	1.34063100	-1.87183400	-1.64003100
C	0.69573600	-2.46341600	-0.55402000
C	0.23751700	-3.77418800	-0.65249600
C	0.42312200	-4.48351100	-1.84001900
C	1.06737100	-3.86509500	-2.90429300
C	3.53039900	-2.95983700	-5.01885900
C	3.92127700	-2.83124200	-6.36054300
C	4.83912100	-3.68581200	-6.96347800
C	5.41772900	-4.70934400	-6.21486000
C	5.07604900	-4.85539600	-4.87236500
C	4.15353600	-3.98487700	-4.29616500
H	0.33168600	-2.75413700	-5.39360100
H	1.24738000	-1.73996900	-6.51706100
H	-0.55515600	-0.74466500	-4.23101100
H	-0.83132700	-0.49799100	-5.95715000
F	-2.60460900	4.44416800	-1.71488600
F	-3.50601200	3.36399000	-4.05178000
F	-1.88458400	1.78732100	-5.52280800
F	-0.06714800	3.93771000	-0.86279700
F	1.56415000	2.38668900	-2.30643600
F	1.78725200	3.76346300	-5.45131900
F	2.08898200	5.15017600	-7.73332100
F	1.50841800	3.98326100	-10.13454200
F	0.63844100	1.39834400	-10.21429400
F	0.35379800	-0.01085800	-7.96314000
F	3.90245900	-4.15886000	-2.98856400
F	5.63861400	-5.81519300	-4.14024900
F	6.29937100	-5.52890500	-6.77364700
F	5.17291100	-3.52056100	-8.24272100
F	3.41978500	-1.84461700	-7.12526900
F	1.73009200	-0.59669400	-1.47666900
F	0.50987300	-1.77238400	0.57067200
F	-0.37914300	-4.34432100	0.37429100
F	-0.01802000	-5.73470900	-1.94780100

F	1.21479700	-4.57986300	-4.03379100
C	5.77828200	1.38747500	-0.74015400
H	4.23799000	-1.51249600	-1.49798400
H	5.30478600	-1.95612100	-2.83803700
H	6.49041100	-2.03364300	-0.64140500
H	7.22070400	-0.84620800	-1.71720200
H	5.27028400	-0.24817800	0.57878300
C	4.56589900	1.24767600	-1.70598900
H	6.65022000	1.68878600	-1.34246300
H	4.35628200	2.20654800	-2.18291900
H	3.68042400	0.98241500	-1.11719900
H	6.98858600	0.13154700	0.55105000
C	5.50777600	2.48401600	0.29605800
H	6.36972900	2.61390100	0.95987200
H	5.30515800	3.44827500	-0.18392300
H	4.64103600	2.23074500	0.91875300
N	6.29250900	2.35472100	-5.18393500
C	7.65225200	1.81797700	-5.14701200
H	8.33505100	2.59232800	-4.78269400
H	7.70813500	0.96261700	-4.47402400
H	7.97100000	1.51350000	-6.15020400
C	6.12027600	3.64399000	-5.86093400
H	6.64862300	4.42827900	-5.30847200
H	6.53649400	3.57973400	-6.87155200
H	5.06044900	3.88726000	-5.91002200

INT5-exo

C	8.18437600	-0.86134500	-3.81279000
C	7.33538600	-0.05647600	-4.80999900
C	7.16572900	-1.21660800	-2.72213800
C	6.32109600	0.68869500	-3.95452200
C	5.66955600	1.76796200	-4.42096800
H	5.92107600	2.12596600	-5.41898600
Ir	2.65942000	0.10334000	-3.56272200
C	4.61229400	2.55352500	-3.73502300
O	3.52065400	2.03769000	-3.34730900
P	1.08889600	0.73382200	-4.97148100
P	1.70250900	-1.91581900	-3.62187900
C	1.77433500	1.42260600	-6.54812500
C	2.22853500	2.74638600	-6.59963400
C	2.81639300	3.29548000	-7.73424900
C	2.97040200	2.51039800	-8.87572400
C	2.54049700	1.18492600	-8.86157300
C	1.96101200	0.66297800	-7.70786100
C	-0.13133100	2.03563800	-4.48478600
C	-1.18209100	2.36411500	-5.35217600
C	-2.14388200	3.31878100	-5.04176600
C	-2.06767200	3.98492200	-3.81810800
C	-1.03565700	3.68826700	-2.93060700
C	-0.08567500	2.72532600	-3.26810400
C	-0.03289500	-0.70805700	-5.37663500
C	0.71382800	-2.03273600	-5.19515000
C	0.46151500	-2.32735600	-2.30383000
C	0.25991400	-1.52479900	-1.17340200
C	-0.67582000	-1.84771600	-0.19174300
C	-1.43510600	-3.00891000	-0.31545300
C	-1.25183200	-3.84315700	-1.41847200
C	-0.31111800	-3.49518800	-2.38151700
C	2.81473600	-3.39217000	-3.51572300
C	3.13950000	-4.24809600	-4.57383600
C	4.00770100	-5.32757900	-4.41655500
C	4.58437700	-5.57740800	-3.17318800
C	4.29106200	-4.74184500	-2.09553500
C	3.41962600	-3.67521000	-2.28373200
H	0.02782900	-2.88111700	-5.18246600
H	1.42256400	-2.17646400	-6.00859400
H	-0.86319300	-0.62448300	-4.66592600
H	-0.44856500	-0.61699100	-6.38070900
F	-2.97563100	4.89919600	-3.50151400
F	-3.12590100	3.59663600	-5.89673200
F	-1.28371000	1.74275400	-6.54135000
F	-0.95663200	4.32654200	-1.76332800
F	0.88340600	2.49700800	-2.37291500
F	2.12197300	3.54228900	-5.51902900
F	3.23886200	4.56129600	-7.72851100
F	3.53212900	3.01993100	-9.96537800
F	2.68951800	0.42255100	-9.94267800
F	1.58456000	-0.62674100	-7.75104000
F	3.17179600	-2.88295300	-1.22211600
F	4.84327200	-4.96335200	-0.90330400

F	5.41487600	-6.60075600	-3.01587400
F	4.28671800	-6.11769800	-5.45123200
F	2.62627400	-4.06407500	-5.79923000
F	0.97096500	-0.40694300	-0.97591900
F	-0.84066400	-1.05338100	0.86534400
F	-2.32780100	-3.32373100	0.61454700
F	-1.96810800	-4.95920000	-1.54051900
F	-0.15138700	-4.33864700	-3.41876100
C	6.28478600	0.05649200	-2.54975400
N	4.79839900	3.87309000	-3.56040200
C	6.03808900	4.56798800	-3.90623200
H	6.83626900	3.85338500	-4.10093400
H	5.88936400	5.20101200	-4.78917000
H	6.33621700	5.20647100	-3.06840100
C	3.73364400	4.72225900	-3.01924100
H	4.09214200	5.22403600	-2.11437500
H	3.46109300	5.48225800	-3.75973000
H	2.86765300	4.11146600	-2.77866700
H	7.91229400	0.60798600	-5.46125500
H	6.78743700	-0.74861400	-5.46736700
H	8.98960000	-0.23985500	-3.40415800
H	8.65037800	-1.74112200	-4.26520300
H	7.62108000	-1.52524700	-1.77552000
H	6.53812400	-2.04984300	-3.06893700
C	6.94241300	1.02393400	-1.53414300
H	6.38563900	1.96483800	-1.46430800
H	6.96300300	0.56798400	-0.53769900
H	7.97303300	1.26297500	-1.81511500
C	4.88420400	-0.32871200	-2.02806600
H	4.94952200	-1.07683200	-1.23271300
H	4.33227200	0.52376200	-1.62429600
H	4.33190600	-0.85115100	-2.85709800

INT6-endo

C	4.93928900	0.95418200	-6.51419700
C	4.88800000	0.85321100	-5.01968900
C	6.01765200	1.03882800	-4.28285500
H	6.98385800	1.17728600	-4.75962300
Ir	3.14440000	0.77623100	-3.94014200
H	2.17986500	0.40096800	-5.14079600
C	5.85831300	1.16934600	-2.83980400
O	4.67689600	1.10746200	-2.35402400
N	6.89067200	1.37810000	-1.99546200
C	8.29881000	1.35794700	-2.38477400
H	8.71820900	2.37122000	-2.39354400
H	8.86108200	0.75802700	-1.66096300
C	6.62981700	1.62784700	-0.57540800
H	7.34091000	2.37522800	-0.21148200
H	6.75258100	0.70946800	0.01223700
P	3.35389100	-1.52666100	-3.58839400
P	1.21875500	0.61365100	-2.41687600
C	5.01263600	-1.96617200	-2.91320400
C	6.08718700	-2.26353500	-3.75859000
C	7.37061600	-2.50898500	-3.27807400
C	7.61712300	-2.42763500	-1.90894600
C	6.57603800	-2.10696000	-1.04032300
C	5.30113300	-1.88221900	-1.54823900
C	3.12616500	-2.77764400	-4.93301700
C	3.29759300	-4.13402500	-4.61019000
C	3.12664300	-5.16152100	-5.53003900
C	2.75744200	-4.84942600	-6.83801600
C	2.56592900	-3.51857200	-7.19687800
C	2.74698800	-2.50747000	-6.25337500
C	2.08455400	-2.15313900	-2.35136300
C	1.42214500	-1.04019200	-1.54100800
C	-0.45067300	0.58685300	-3.23473300
C	-1.38796900	1.62346600	-3.14842900
C	-2.60306900	1.59992900	-3.82847100
C	-2.91438800	0.51826800	-4.64984200
C	-1.99463400	-0.51884800	-4.79110000
C	-0.79230100	-0.46207300	-4.09400700
C	0.93114300	1.62677800	-0.88724300
C	-0.15567500	1.35546700	-0.04091200
C	-0.37395900	2.03356900	1.15195000
C	0.52612900	3.02268000	1.54966900
C	1.62533600	3.31268500	0.74746400
C	1.81520200	2.61678800	-0.44624100
H	0.45996500	-1.37060700	-1.14137500
H	2.05993100	-0.78115600	-0.69109000
H	1.34500000	-2.68910800	-2.94501200

H	2.55863000	-2.87613800	-1.68614200
F	2.58472000	-5.81438400	-7.73068100
F	3.30752000	-6.42929400	-5.16782500
F	3.64141200	-4.48635300	-3.35804800
F	2.20445000	-3.20840600	-8.44068300
F	2.53332800	-1.25881200	-6.68897700
F	5.91396400	-2.29764900	-5.08835200
F	8.36390600	-2.78560400	-4.12212200
F	8.84331100	-2.62533200	-1.43639600
F	6.81150600	-1.97349800	0.26750700
F	4.34360300	-1.54810400	-0.66575700
F	2.90698900	2.94037900	-1.15451600
F	2.50023600	4.24635400	1.12088100
F	0.33693500	3.67723100	2.68774600
F	-1.42629200	1.74179700	1.91313500
F	-1.04753400	0.40554100	-0.37455100
F	-1.12553700	2.72711700	-2.42668400
F	-3.45764900	2.61347500	-3.70640900
F	-4.06726900	0.48515700	-5.30606000
F	-2.26070300	-1.55149700	-5.58990900
F	0.07331900	-1.47859400	-4.29620000
H	8.43123000	0.90865200	-3.36719900
H	5.61370400	1.99891900	-0.45211500
C	2.45127300	2.78844900	-5.28967800
C	3.24457400	3.06652800	-4.18463400
C	2.96291900	2.63340400	-6.71108200
C	4.44505000	2.34581300	-6.97468100
C	0.96342400	3.03418400	-5.22257200
H	0.60949000	3.17238100	-4.19995500
H	0.74984700	3.96169000	-5.77162000
H	0.39023500	2.23751800	-5.70501000
H	5.96809200	0.81845200	-6.87490000
H	4.31782000	0.18343700	-6.97864800
H	2.79319600	3.48574600	-3.29446300
H	4.30798500	3.24589000	-4.29816500
H	5.07300000	3.12252900	-6.52063700
H	4.60143300	2.42133700	-8.05706900
H	2.34693800	1.87997000	-7.21815600
H	2.71085000	3.58683000	-7.20222000

INT6-*exo*

C	5.09513300	0.77659400	-6.70009400
C	3.54713200	2.80509800	-7.07718500
C	5.05740300	1.08124900	-5.22842300
C	6.20031300	1.42247400	-4.57225500
H	7.16424100	1.39189300	-5.07249900
Ir	3.31439300	1.26532800	-4.12504600
H	2.34001600	0.67132400	-5.21917000
C	6.05823700	1.95917200	-3.22449500
O	4.88091000	2.07201200	-2.74213700
N	7.10440500	2.37319000	-2.47476400
C	8.50968400	2.19819900	-2.83233300
H	8.97908400	3.16534300	-3.04861900
H	9.04247900	1.73717000	-1.99255200
C	6.86156100	3.02412000	-1.18517800
H	7.57847400	3.84126000	-1.06011900
H	6.98915400	2.31623000	-0.35662900
P	3.61618100	-0.89039700	-3.31786100
P	1.42844800	1.35856300	-2.59329600
C	5.22911000	-1.06723300	-2.44072000
C	6.38851900	-1.49813000	-3.09448900
C	7.63400800	-1.50937700	-2.47284500
C	7.75121400	-1.05080600	-1.16253300
C	6.62026100	-0.59875300	-0.48643100
C	5.38758800	-0.61256300	-1.12937400
C	3.54668200	-2.40568500	-4.38207300
C	3.87706300	-3.64724200	-3.81270100
C	3.81582300	-4.84458000	-4.51517500
C	3.38777400	-4.83687300	-5.84228600
C	3.02325800	-3.63251500	-6.43624700
C	3.09522900	-2.44545800	-5.70700300
C	2.25868600	-1.34310100	-2.10454000
C	1.52194000	-0.15527800	-1.48778100
C	-0.22973000	1.35990800	-3.41722000
C	-0.89677100	2.55268200	-3.72251200
C	-2.11724700	2.57989400	-4.39215800
C	-2.70557000	1.38286200	-4.79741700
C	-2.06027000	0.17589900	-4.53417000
C	-0.84274800	0.18522000	-3.86062200
C	1.19621600	2.65193800	-1.28428700

C	0.12890200	2.54809700	-0.37963800
C	-0.08469200	3.46452200	0.64389200
C	0.79305500	4.53877100	0.79126500
C	1.86432500	4.67785000	-0.08693000
C	2.05109400	3.74416100	-1.10485700
H	0.52381500	-0.45160000	-1.16056100
H	2.06384100	0.20503300	-0.61112200
H	1.56623700	-1.94672100	-2.69248300
H	2.67694400	-1.98789900	-1.32764500
F	3.31702700	-5.97008400	-6.52666100
F	4.15238700	-5.98932600	-3.92601700
F	4.26830900	-3.71757200	-2.52756900
F	2.59129700	-3.61171200	-7.69564400
F	2.68705600	-1.34175300	-6.34757400
F	6.33900800	-1.90253200	-4.37223400
F	8.71486100	-1.91742600	-3.13752600
F	8.94206900	-1.00941000	-0.57291400
F	6.73063800	-0.10997800	0.75132900
F	4.33332700	-0.13452400	-0.44548900
F	3.09494100	3.95018700	-1.92109300
F	2.70851900	5.70112100	0.04369900
F	0.60738400	5.42166200	1.76358500
F	-1.11218000	3.32037000	1.47755000
F	-0.74249600	1.52890600	-0.48323900
F	-0.35784100	3.73816100	-3.38274800
F	-2.71409100	3.74091700	-4.65379800
F	-3.86632400	1.39313600	-5.44034300
F	-2.60219500	-0.97503700	-4.92770100
F	-0.25039100	-1.00754100	-3.65307400
H	8.62164100	1.54842500	-3.69784900
H	5.84713600	3.41856300	-1.16250000
C	2.34169900	3.23969100	-4.90689200
C	4.82802400	2.06888700	-7.50672400
C	3.50921300	3.31817200	-5.65024700
C	4.58990100	4.27809600	-5.21791600
H	5.59515000	3.90982100	-5.43048600
H	4.45596800	5.20767000	-5.78896700
H	4.51524300	4.51744500	-4.15547500
H	6.07864500	0.38389900	-6.99198100
H	4.34409800	0.02932400	-6.96281100
H	5.69150700	2.73814200	-7.41246800
H	4.74492100	1.81749400	-8.57000100
H	3.43195400	3.69185600	-7.71942100
H	2.67287500	2.17064100	-7.25808000
H	2.21781200	3.90257300	-4.05932000
H	1.43350100	2.87747600	-5.37722100

INT7-endo

C	3.79745600	1.65015500	-6.91404500
C	4.40698400	1.81586900	-5.54297100
C	5.15164100	0.83048700	-4.90687600
H	5.42631300	-0.07111100	-5.43980300
Ir	3.05862800	0.67718300	-3.88938600
H	2.11435500	0.20524700	-5.05290600
C	5.78909900	1.14398800	-3.58403100
O	4.97302400	1.33745400	-2.64150200
N	7.11639300	1.21653900	-3.42915700
C	8.06903600	0.93991000	-4.50233100
H	8.83030200	1.72582300	-4.52198300
H	8.55965600	-0.02500400	-4.33042300
C	7.69663300	1.47843300	-2.10949100
H	8.34972900	2.35536500	-2.16445000
H	8.29059400	0.61446900	-1.79228100
P	3.41641400	-1.68020300	-3.34818000
P	1.11688200	0.46784800	-2.63237900
C	4.67331500	-2.00646100	-2.02416900
C	6.02628200	-1.95005900	-2.37155700
C	7.05340600	-2.07481900	-1.44569400
C	6.74207500	-2.27363200	-0.10176600
C	5.40596000	-2.34275800	0.28716100
C	4.40101300	-2.20385800	-0.66854000
C	3.84729300	-3.02668800	-4.55101600
C	3.95382700	-4.35848500	-4.12064700
C	4.24336700	-5.40893800	-4.98585300
C	4.43157800	-5.14546300	-6.34273800
C	4.32974400	-3.83776700	-6.81082400
C	4.03993700	-2.80839100	-5.91801800
C	1.76281300	-2.33864300	-2.77652000
C	0.91755900	-1.30732800	-2.03237800
C	-0.42297800	0.82850200	-3.59959800

C	-1.23392100	1.96053100	-3.44854700
C	-2.34228500	2.20284300	-4.25713800
C	-2.67726000	1.29935600	-5.26289400
C	-1.89426200	0.16170500	-5.44927100
C	-0.79566700	-0.05115800	-4.62389900
C	0.86573900	1.30790400	-1.00229200
C	-0.35087900	1.18783200	-0.31404900
C	-0.55972000	1.73327000	0.94622800
C	0.48412400	2.41029400	1.57859700
C	1.71645500	2.52521800	0.94195900
C	1.89524000	1.96795800	-0.32386900
H	-0.14154400	-1.57812500	-2.05648000
H	1.22150800	-1.27503600	-0.98483400
H	1.27251800	-2.63014300	-3.70811800
H	1.89220400	-3.23724100	-2.17140100
F	4.70556200	-6.13478300	-7.18225100
F	4.33520800	-6.65508800	-4.52785300
F	3.77190100	-4.66731200	-2.82514600
F	4.50804900	-3.57300900	-8.10418200
F	3.95883400	-1.57102800	-6.43616500
F	6.37616800	-1.74873000	-3.66217400
F	8.32911300	-1.96681900	-1.83401400
F	7.71037600	-2.38694500	0.79918600
F	5.09243700	-2.53332200	1.56656500
F	3.13280400	-2.26822200	-0.22356900
F	3.11636000	2.07414600	-0.86126300
F	2.72774300	3.14837600	1.54569400
F	0.30379400	2.93033000	2.78541100
F	-1.73762100	1.60419800	1.55269500
F	-1.37555600	0.52244400	-0.87508800
F	-0.97201000	2.88207200	-2.50827500
F	-3.07947400	3.29460800	-4.06809100
F	-3.73001500	1.52065000	-6.03895400
F	-2.19409400	-0.71219200	-6.40862800
F	-0.06710000	-1.16112900	-4.85657400
H	7.56618600	0.92159300	-5.46904500
H	6.89587700	1.66396600	-1.39578100
C	2.66434300	2.80454400	-4.49450000
C	4.10436400	3.14930900	-4.90518300
C	1.77092700	2.83286500	-5.75633900
C	2.53999300	2.54804500	-7.07544600
C	2.16762100	3.73696400	-3.39651100
H	2.79470000	3.68110600	-2.50417800
H	2.20194400	4.77585300	-3.76134600
H	1.13272600	3.53889200	-3.10761500
H	4.55284900	1.96707100	-7.64909300
H	3.58657100	0.59900400	-7.11489100
H	4.72790900	3.36165100	-4.03537200
H	4.19112000	3.98788600	-5.60964600
H	2.85759200	3.50434500	-7.50270400
H	1.87315400	2.09953900	-7.81834100
H	0.92932900	2.14510600	-5.64048800
H	1.32970600	3.83765800	-5.84416600

INT7-*exo*

C	4.19163400	1.28479400	-7.25784700
C	3.02053700	3.37744600	-7.09576900
C	4.51150000	1.90004900	-5.90168000
C	5.37442900	1.30686300	-5.00151400
H	5.81750300	0.35614500	-5.28053800
Ir	3.29471500	1.17162400	-3.86055200
H	2.24946600	0.59543400	-4.90112100
C	5.93203800	1.93782700	-3.75517300
O	5.12574500	2.07655100	-2.79522000
N	7.22603800	2.26482100	-3.66322700
C	8.18675400	2.05436800	-4.74384800
H	8.79761900	2.95419900	-4.86450800
H	8.84596600	1.21004700	-4.50943300
C	7.77967400	2.71424200	-2.38254100
H	8.42071700	3.58421900	-2.55108800
H	8.37550100	1.91086200	-1.93398400
P	3.63712400	-1.08185400	-2.99157400
P	1.42840900	1.22664900	-2.53026400
C	4.83440200	-1.16927800	-1.57457500
C	6.18170900	-0.92542600	-1.86010600
C	7.16737100	-0.85435000	-0.88517500
C	6.82039100	-1.04744900	0.45079400
C	5.49307600	-1.31227900	0.78005600
C	4.52824900	-1.37017400	-0.22514500
C	4.10376500	-2.60570700	-3.93240000

C	4.17764700	-3.85588900	-3.30023500
C	4.51257800	-5.02169900	-3.98128000
C	4.78307000	-4.96051300	-5.34885000
C	4.71489700	-3.73809500	-6.01384900
C	4.37721200	-2.58870900	-5.30309300
C	1.94967900	-1.57948000	-2.37171500
C	1.19898400	-0.43411100	-1.68989900
C	-0.10286700	1.57949700	-3.50265800
C	-0.56738400	2.88672300	-3.69173800
C	-1.69168400	3.17689400	-4.46027800
C	-2.38656300	2.14046200	-5.08097500
C	-1.94419700	0.82731700	-4.93012500
C	-0.81806900	0.57018700	-4.15452100
C	1.23035000	2.35555500	-1.07966100
C	0.04908600	2.30486700	-0.32427100
C	-0.17368700	3.11947900	0.77936600
C	0.81344700	4.02683500	1.16604200
C	2.00240200	4.10180700	0.44559200
C	2.19756400	3.27332700	-0.65890800
H	0.13581100	-0.66478100	-1.60157200
H	1.58647400	-0.28823100	-0.67848600
H	1.42835200	-1.88244400	-3.28417300
H	2.00612700	-2.44487100	-1.71097000
F	5.10235000	-6.06346500	-6.01258300
F	4.57109400	-6.18677800	-3.34089000
F	3.91581000	-3.96418100	-1.98677000
F	4.97027600	-3.66978000	-7.31995200
F	4.32391500	-1.43980000	-5.99723900
F	6.56847300	-0.74892300	-3.14311600
F	8.43312200	-0.58233500	-1.22156500
F	7.74681100	-0.97979000	1.39884100
F	5.14753600	-1.50736200	2.05078700
F	3.26984600	-1.62816000	0.17134300
F	3.36275200	3.38984400	-1.30209800
F	2.95323000	4.96027300	0.81227900
F	0.62109100	4.80914100	2.21971800
F	-1.31225500	3.03565000	1.46393100
F	-0.92642300	1.44303100	-0.66301900
F	0.07997000	3.92630400	-3.13936100
F	-2.09531800	4.43677800	-4.61022800
F	-3.45746200	2.40279300	-5.81937000
F	-2.59253900	-0.17160000	-5.52635200
F	-0.42352000	-0.71377300	-4.05913500
H	7.67072600	1.85816700	-5.68347200
H	6.96443600	2.98423300	-1.71344300
C	2.98924000	3.18374800	-4.51429700
C	3.76875400	2.49796900	-8.10783400
C	3.85314600	3.29219800	-5.78264300
C	4.88757500	4.43194600	-5.72870000
H	5.51740700	4.45559300	-6.62654900
H	4.36508400	5.39245800	-5.65955500
H	5.54201800	4.35154200	-4.85462500
H	5.04087900	0.72394900	-7.66071400
H	3.35855900	0.58163100	-7.16686300
H	4.65201300	3.01862000	-8.49736400
H	3.15494500	2.21060700	-8.96615100
H	2.89315400	4.41227400	-7.42772800
H	2.02002200	2.96124200	-6.92346000
H	3.35136400	3.82286100	-3.70457200
H	1.94675200	3.42493600	-4.72170200

INT8-endo

C	3.70639100	1.68991000	-6.38369600
C	4.32961200	1.78418600	-4.98798300
C	5.12359500	0.78383900	-4.45262200
H	5.32706300	-0.07674300	-5.08129800
Ir	2.90655400	0.47059900	-3.54054400
H	2.14414000	2.46064800	-3.79385300
C	6.04669800	1.03883700	-3.27611100
O	5.59657200	1.40537300	-2.18626400
N	7.38265300	0.85765200	-3.49232900
C	8.00701600	0.49327400	-4.76066300
H	8.83498200	1.18060100	-4.96738000
H	8.40610100	-0.52712100	-4.71627900
C	8.31563700	1.07519000	-2.38663300
H	8.98134900	1.91604100	-2.61417700
H	8.92628300	0.17788900	-2.23547900
P	3.35832700	-1.68435200	-3.21737800
P	0.95430200	0.07235200	-2.47102600
C	4.83383800	-1.93795100	-2.13272900

C	6.12196900	-2.12638000	-2.64494200
C	7.24122900	-2.24455900	-1.82950500
C	7.09940500	-2.16416000	-0.44616500
C	5.83404300	-1.96303200	0.10321000
C	4.73560800	-1.84351600	-0.74113300
C	3.69118400	-2.88927600	-4.58980200
C	3.91568700	-4.23960000	-4.28032300
C	4.12725300	-5.21097900	-5.25236700
C	4.12131000	-4.84264900	-6.59807400
C	3.90616700	-3.51177600	-6.94627100
C	3.69706100	-2.56261600	-5.94741600
C	1.90755700	-2.56312700	-2.40296800
C	0.96154600	-1.61127500	-1.67676100
C	-0.50242700	0.20759100	-3.59968800
C	-0.99290400	1.46919600	-3.95520300
C	-2.04562800	1.64538800	-4.84643600
C	-2.64327500	0.52620100	-5.42554200
C	-2.17324400	-0.74781500	-5.10968900
C	-1.11541700	-0.88771100	-4.21546600
C	0.47393500	1.13933800	-1.04769800
C	-0.75749700	0.95272100	-0.40604100
C	-1.14859900	1.70965900	0.69243000
C	-0.28503300	2.69003200	1.18484200
C	0.95380100	2.89469000	0.57983800
C	1.31950100	2.11849700	-0.51778800
H	-0.04906300	-2.01845300	-1.61508100
H	1.31360600	-1.42514300	-0.66046800
H	1.38783300	-3.04973200	-3.23150600
H	2.27654800	-3.34433000	-1.73595800
F	4.32150700	-5.75502400	-7.53897600
F	4.33490200	-6.47890300	-4.90689400
F	3.93780000	-4.63953600	-2.99628600
F	3.90332600	-3.14615200	-8.22727300
F	3.51296200	-1.29715800	-6.35310700
F	6.33296400	-2.16261000	-3.97652100
F	8.45387900	-2.38847600	-2.37260500
F	8.16363500	-2.26259200	0.34015500
F	5.68264000	-1.87383700	1.42212400
F	3.54226000	-1.61908800	-0.16341300
F	2.52861100	2.34682900	-1.05225300
F	1.78196900	3.82556400	1.04916800
F	-0.64239900	3.42157000	2.23163200
F	-2.32726700	1.50280200	1.27438700
F	-1.60111300	0.00346700	-0.84850300
F	-0.42559000	2.57701300	-3.43788800
F	-2.47251400	2.86897500	-5.15261200
F	-3.64705900	0.67365400	-6.28004200
F	-2.72961900	-1.82210500	-5.66469600
F	-0.68958400	-2.13992200	-3.96541600
H	7.30156600	0.56439300	-5.58734000
H	7.74796300	1.29886200	-1.48533700
C	2.61563900	3.37765600	-4.27185200
C	4.13703100	3.12890000	-4.31073800
C	2.02637300	3.48898100	-5.70534200
C	2.99890600	2.99077200	-6.79079000
C	2.23065900	4.55672600	-3.37624900
H	2.58276800	4.41843700	-2.35105900
H	2.68381900	5.47420300	-3.77206900
H	1.14543000	4.69815400	-3.36045800
H	4.49428300	1.44339600	-7.10764900
H	2.99544000	0.85986700	-6.41668400
H	4.56024200	3.13300700	-3.30609200
H	4.63570100	3.91601000	-4.89282500
H	3.74680200	3.76564400	-6.99601500
H	2.46331500	2.83307200	-7.73267300
H	1.08045500	2.93836500	-5.75554400
H	1.77700600	4.53819600	-5.90352900

INT8-*exo*

C	1.02672000	3.09016100	-6.36052200
C	2.78565200	4.41179200	-5.40827600
C	2.23323400	2.18153900	-6.18450500
C	2.19123700	0.87554300	-6.49817300
H	1.27026500	0.47424800	-6.92117500
Ir	2.99680700	0.16521400	-3.23809100
H	3.29421500	2.18955300	-3.66034300
C	3.26743600	-0.13746300	-6.31461100
O	3.69287500	-0.47391900	-5.16635700
N	3.76314700	-0.75823600	-7.39831800
C	3.36902700	-0.42992700	-8.76875000

H	4.26683600	-0.25064600	-9.36932600
H	2.81496400	-1.26431200	-9.21443600
C	4.73469400	-1.85035300	-7.27073300
H	5.57422400	-1.66144800	-7.94632000
H	4.26530300	-2.80192300	-7.54397300
P	2.28676100	-1.84017600	-2.69068300
P	2.30823300	0.80844900	-1.21602100
C	3.53997600	-3.07662600	-2.11576600
C	4.91371700	-2.81331600	-2.04659800
C	5.82439500	-3.76592300	-1.59044000
C	5.37453200	-5.02420700	-1.19747800
C	4.01372000	-5.32579800	-1.26101300
C	3.12857600	-4.35651100	-1.71754500
C	1.43198300	-2.72290900	-4.06905600
C	0.05879600	-2.60754700	-4.32141600
C	-0.55022700	-3.19292600	-5.42921500
C	0.22293000	-3.89927500	-6.34890600
C	1.59634200	-4.01348600	-6.14426100
C	2.17506900	-3.43604700	-5.01917100
C	1.14505500	-1.72695100	-1.22378200
C	1.73802200	-0.69380000	-0.25844700
C	0.92297700	2.04562000	-1.23228900
C	1.20837200	3.35783300	-1.62517000
C	0.23556700	4.34060100	-1.76010000
C	-1.09353200	4.02463900	-1.48130400
C	-1.42218800	2.73035800	-1.08311300
C	-0.42167000	1.76653800	-0.96991600
C	3.49296700	1.60114400	-0.04022700
C	3.10801200	1.89383600	1.27456500
C	3.97085500	2.47531100	2.19691600
C	5.27301000	2.78860900	1.80477100
C	5.69144800	2.51796200	0.50330800
C	4.80359800	1.93506000	-0.39860200
H	1.03404500	-0.43474400	0.53177800
H	2.64780300	-1.08079900	0.21600400
H	0.16980100	-1.39838400	-1.57795500
H	1.02800100	-2.70391300	-0.74934200
F	-0.34174400	-4.44367300	-7.42017800
F	-1.86133200	-3.06164000	-5.62124200
F	-0.73587100	-1.89731000	-3.50609400
F	2.35980900	-4.65084200	-7.03742900
F	3.50617000	-3.56283200	-4.89137900
F	5.42092800	-1.63248500	-2.41959600
F	7.12364300	-3.47622100	-1.53329700
F	6.23721200	-5.93430400	-0.76397600
F	3.57467000	-6.52725800	-0.89132800
F	1.82419800	-4.68535900	-1.77646500
F	5.26171900	1.70973200	-1.63959400
F	6.93245700	2.82065200	0.12503000
F	6.11083300	3.34456300	2.67042000
F	3.56550100	2.73245700	3.43875700
F	1.85825300	1.60910800	1.68259300
F	2.47943300	3.70543800	-1.91830400
F	0.56865500	5.56680100	-2.16557900
F	-2.03967800	4.94782400	-1.60348700
F	-2.68864400	2.41572500	-0.81899400
F	-0.81427300	0.53399000	-0.60149600
H	2.75154900	0.46646400	-8.78429700
H	5.09047200	-1.90414600	-6.24534300
C	4.09014900	2.46007800	-4.40255300
C	1.60820700	4.51319300	-6.38796100
C	3.42408600	3.01566400	-5.67705300
C	4.49629900	3.12938600	-6.78868100
H	4.08962000	3.59539900	-7.69210400
H	5.33445900	3.74434400	-6.44177400
H	4.89185500	2.14562200	-7.06445100
H	0.41943800	2.83110700	-7.23381600
H	0.37952300	2.97573500	-5.47729500
H	1.96121000	4.76212100	-7.39572100
H	0.87896600	5.27593700	-6.10091800
H	3.51835000	5.21768200	-5.51995100
H	2.41217400	4.45800600	-4.37753000
H	4.76283000	1.62480000	-4.60445200
H	4.67222700	3.23067200	-3.88704900
TS1a			
C	3.71081300	3.15579300	-4.52958800
C	4.46636400	3.70496100	-5.52077800
H	4.26413800	4.70950100	-5.87586200
Ir	4.02838400	1.02955300	-4.44715200

H	4.45676400	2.40527200	-3.60978900
C	5.48073400	2.86981400	-6.16184400
O	5.51744000	1.63304800	-5.84025000
N	6.34399900	3.35050800	-7.06819400
C	6.41092400	4.76100700	-7.45818600
H	7.44998800	5.00206300	-7.69659500
H	5.79605900	4.95590000	-8.34491300
C	7.25800400	2.45314200	-7.78022100
H	7.12107600	2.58023200	-8.85962000
H	7.05269300	1.42204000	-7.50467700
P	4.70764500	-1.19999500	-4.60980900
P	2.62698700	0.26161100	-2.84758700
C	6.53325400	-1.36067600	-4.45124000
C	7.36321000	-1.14685700	-5.55884400
C	8.75061300	-1.15511400	-5.46471200
C	9.35405600	-1.38108800	-4.22861200
C	8.56077700	-1.58781300	-3.10108500
C	7.17465400	-1.56686300	-3.22488600
C	4.30962300	-2.13945400	-6.13774400
C	4.55372200	-3.51543600	-6.22241200
C	4.25524200	-4.25606000	-7.36066100
C	3.69517500	-3.60837800	-8.46340000
C	3.44337200	-2.23771000	-8.41637400
C	3.75323000	-1.52140700	-7.26283900
C	3.87252200	-2.20103400	-3.26646800
C	3.39916700	-1.28636900	-2.12983500
C	0.97826000	-0.37124600	-3.39532900
C	0.10824800	-1.01798500	-2.50515500
C	-1.11062300	-1.55399700	-2.89889900
C	-1.49744500	-1.45396800	-4.23691900
C	-0.66294200	-0.82114900	-5.15404300
C	0.55537000	-0.29433900	-4.72810700
C	2.31478200	1.32935200	-1.37054000
C	1.08567300	1.90319200	-1.01710400
C	0.93744200	2.71851600	0.10298900
C	2.03914500	2.99454300	0.90993700
C	3.28327200	2.45745500	0.58283900
C	3.40198900	1.64689200	-0.54159300
H	2.68584900	-1.80149600	-1.48190100
H	4.24693100	-0.96344800	-1.52493100
H	3.01742100	-2.67702100	-3.75879200
H	4.52167300	-2.99503700	-2.89576700
F	3.40249900	-4.29839400	-9.55752700
F	4.49658500	-5.56406500	-7.40417300
F	5.09670000	-4.15750300	-5.17442400
F	2.91505500	-1.62042300	-9.47174800
F	3.51065200	-0.20305700	-7.27306700
F	6.83207300	-0.91223700	-6.77172600
F	9.49772400	-0.94192400	-6.54808100
F	10.67684400	-1.39225000	-4.12410800
F	9.12667500	-1.79725400	-1.91477800
F	6.45768000	-1.74426000	-2.10118900
F	4.62804200	1.17363100	-0.82528900
F	4.34821100	2.72414800	1.33563300
F	1.90727500	3.77151300	1.97662100
F	-0.25184900	3.23914900	0.39705900
F	-0.01418400	1.70936900	-1.76144400
F	0.43919200	-1.11732400	-1.20546400
F	-1.90563200	-2.15480400	-2.01662600
F	-2.65785300	-1.96158200	-4.63079700
F	-1.02339100	-0.72607100	-6.43228200
F	1.31439700	0.29152600	-5.66727400
H	6.09644400	5.41145700	-6.64290500
H	8.29426800	2.70222600	-7.52603700
C	2.61872800	3.96276700	-3.87096800
H	2.72760800	3.89283200	-2.78180000
H	2.75434800	5.02118300	-4.13091100
C	1.18256500	3.53491200	-4.24546900
H	1.01874600	2.50061000	-3.93286200
H	0.49260800	4.14897400	-3.65446400
C	0.84761200	3.66587900	-5.73240100
H	0.98328000	4.71277900	-6.04814500
H	1.57449900	3.08998900	-6.32369900
C	-0.54591200	3.22057800	-6.13520600
C	-0.83120800	3.30912800	-7.61525500
H	-0.70950200	4.33826100	-7.97965200
H	-0.13252600	2.68679200	-8.19121700
H	-1.84853900	2.98490200	-7.85166500
C	-1.46821200	2.78601900	-5.26789700
H	-1.29182400	2.72744000	-4.19803500

H	-2.45739500	2.48890500	-5.60625900
TS2-endo			
C	5.54406400	0.93330200	-6.58083100
C	3.36644000	2.05228600	-7.40421000
H	6.13328200	0.01540200	-6.71718600
H	6.21792600	1.76295700	-6.84095600
C	5.19549400	1.03383600	-5.11581100
C	6.16511800	1.37172700	-4.21541700
H	7.18838700	1.57145300	-4.51895700
Ir	3.35456600	0.80603700	-4.27811500
H	2.54049600	0.69894400	-5.77495000
C	5.76835300	1.41760000	-2.82720000
O	4.54346300	1.12718700	-2.53896300
N	6.61043400	1.72913900	-1.82362600
C	8.02742700	2.01402000	-2.05809600
H	8.41980700	2.54590400	-1.18923700
H	8.61140500	1.09512800	-2.19362100
C	6.17812600	1.63820800	-0.42746400
H	6.51555300	2.52610000	0.11492000
H	6.60267200	0.74692900	0.05064800
P	3.61522900	-1.55176200	-3.83329600
P	1.40629900	0.60794300	-2.77921500
C	5.30926500	-1.90683500	-3.18669400
C	6.36698300	-2.14331100	-4.07048200
C	7.68114800	-2.31364700	-3.64729700
C	7.97849300	-2.21779400	-2.28870600
C	6.95525600	-1.95568200	-1.38062700
C	5.64869300	-1.80317900	-1.83585300
C	3.36227600	-2.91652600	-5.05723200
C	3.73264800	-4.23313700	-4.74326100
C	3.53336800	-5.29981100	-5.61315500
C	2.91822200	-5.07297000	-6.84405300
C	2.50711900	-3.78579700	-7.18022000
C	2.72187600	-2.73732800	-6.28790300
C	2.39588400	-2.10813500	-2.51370100
C	1.74160700	-0.94599900	-1.76569500
C	-0.30383300	0.45867700	-3.48789700
C	-1.28785300	1.45504300	-3.41269200
C	-2.53425600	1.32362000	-4.02288700
C	-2.83090000	0.17776600	-4.75753500
C	-1.86851800	-0.82255100	-4.88222300
C	-0.63700000	-0.65992700	-4.25843100
C	1.16838300	1.77922000	-1.36223900
C	0.20831300	1.50929700	-0.37402600
C	0.02782700	2.30964400	0.74677600
C	0.82961400	3.43915200	0.91364400
C	1.78850900	3.74737900	-0.04592600
C	1.94431700	2.92752100	-1.16448000
H	0.82527200	-1.27284300	-1.26926600
H	2.42414100	-0.58022200	-0.99228700
H	1.64462700	-2.68932500	-3.04735900
H	2.89180700	-2.77976500	-1.81059700
F	2.71388400	-6.07998200	-7.68262500
F	3.91258600	-6.52900800	-5.27112200
F	4.29349100	-4.51116900	-3.55412600
F	1.89778800	-3.55949000	-8.34326500
F	2.26392700	-1.53219900	-6.66496000
F	6.13407700	-2.19742900	-5.39451200
F	8.65127800	-2.53980500	-4.53185000
F	9.23118900	-2.35180400	-1.86540100
F	7.23162900	-1.81671700	-0.08039400
F	4.71441000	-1.51943100	-0.90920200
F	2.87751700	3.30366000	-2.04529200
F	2.55919400	4.82528800	0.10107300
F	0.67534900	4.21406600	1.97936700
F	-0.90040400	2.00741100	1.65211900
F	-0.60456000	0.44421400	-0.49929900
F	-1.05929600	2.60964800	-2.76818000
F	-3.43507600	2.29733700	-3.91469900
F	-4.01278000	0.04650100	-5.34560100
F	-2.12214700	-1.91738300	-5.59749300
F	0.27168900	-1.64147100	-4.43932000
H	8.15660300	2.65556600	-2.93153400
H	5.09282400	1.58067100	-0.39003200
C	2.96090800	2.80344700	-4.95805000
H	3.87356800	3.38522700	-5.07034100
H	2.20380700	3.32281500	-4.37764400
C	4.37006000	0.90177600	-7.56621800
C	2.49255600	2.05504300	-6.12708500

C	0.99708200	2.12057400	-6.42644400
H	0.66556400	1.29025300	-7.05803500
H	0.39836000	2.13930600	-5.51482400
H	0.80982500	3.05352300	-6.97218200
H	4.77494700	0.94427000	-8.58390300
H	3.83769500	-0.05044500	-7.48498000
H	2.68882300	2.03102700	-8.26468500
H	3.89583400	3.01238300	-7.44614800

TS2-*exo*

C	4.79745800	2.70818900	-7.12474500
C	5.23786900	1.24806000	-6.75159000
C	4.14115700	3.52120200	-5.99181100
H	4.60785000	0.51890400	-7.26762000
H	6.26717500	1.08030300	-7.09194000
H	5.67955900	3.26898300	-7.44963200
H	4.13036100	2.67332300	-7.99378000
H	3.80069300	4.47149700	-6.42974600
H	4.89777600	3.79810200	-5.24774300
C	5.13269000	1.07468600	-5.26976200
C	6.21683700	1.28405300	-4.46880300
H	7.20371300	1.47136900	-4.88101200
Ir	3.35751000	0.92293000	-4.27947000
H	2.41478200	0.50193100	-5.58047900
C	5.94439000	1.39141100	-3.05268900
O	4.71657600	1.28705100	-2.67318300
N	6.87936100	1.62236800	-2.11224900
C	8.31570800	1.64855600	-2.38177500
H	8.69430500	2.67764600	-2.39487500
H	8.83647000	1.09756300	-1.59174800
C	6.48283900	1.87946300	-0.72495600
H	7.14398300	2.64369600	-0.30629800
H	6.56764800	0.96980800	-0.11781800
P	3.63229200	-1.42102900	-3.76625600
P	1.42134400	0.76198600	-2.76755300
C	5.26837700	-1.80101000	-3.00363000
C	6.38605700	-2.06761100	-3.80281800
C	7.66042700	-2.24861900	-3.27154800
C	7.85262200	-2.13002600	-1.89635400
C	6.76735800	-1.83540100	-1.07353700
C	5.50421700	-1.67455700	-1.63205100
C	3.48911700	-2.74448800	-5.04877200
C	3.62951200	-4.08673000	-4.66348100
C	3.52090900	-5.14606300	-5.55733800
C	3.25472300	-4.87926600	-6.90013500
C	3.10169700	-3.56121400	-7.32243400
C	3.21946400	-2.52044700	-6.40309200
C	2.31217700	-1.99761700	-2.55477300
C	1.61920400	-0.85107100	-1.81730200
C	-0.21841900	0.71228500	-3.64124900
C	-1.14487900	1.76402400	-3.64727300
C	-2.33081500	1.71694900	-4.37801400
C	-2.62099300	0.59847000	-5.15649900
C	-1.70990300	-0.45521000	-5.20580800
C	-0.53720500	-0.37452700	-4.46293500
C	1.09704100	1.84809100	-1.30156700
C	-0.01588800	1.61956800	-0.47708500
C	-0.27419300	2.36245200	0.66808900
C	0.61092900	3.37599400	1.03728200
C	1.73483200	3.62476600	0.25561700
C	1.96564000	2.86531000	-0.89135000
H	0.65186000	-1.17111800	-1.42125100
H	2.23531200	-0.54352300	-0.96718700
H	1.59500700	-2.55412200	-3.15765400
H	2.74896200	-2.69503100	-1.83892200
F	3.14302100	-5.87519700	-7.76839200
F	3.66519900	-6.40113900	-5.13895000
F	3.87958300	-4.39121300	-3.37793700
F	2.84060700	-3.29539900	-8.60118000
F	3.05463900	-1.28008800	-6.89185100
F	6.26129300	-2.13426900	-5.13730500
F	8.69502500	-2.49916300	-4.07303400
F	9.06787600	-2.26461800	-1.37512000
F	6.94813100	-1.66228000	0.23865100
F	4.50324300	-1.35213400	-0.79222700
F	3.07807100	3.15170800	-1.57946900
F	2.59586300	4.58061400	0.60507500
F	0.38470000	4.09229500	2.13050300
F	-1.34998500	2.11023600	1.41039500
F	-0.89454100	0.64974000	-0.78893600

F	-0.91315100	2.89074100	-2.95388100
F	-3.17936100	2.74109600	-4.33972200
F	-3.74487000	0.54449900	-5.85891300
F	-1.95329600	-1.52178200	-5.96555100
F	0.33191600	-1.40170300	-4.58523300
H	8.54492500	1.17032900	-3.33266700
H	5.45443900	2.23577600	-0.70012200
C	2.94592900	2.90282600	-5.25876400
C	2.16926200	1.89526900	-5.95711000
H	2.44124600	1.64888700	-6.98244400
H	1.09427000	1.88075200	-5.78754700
C	2.19845100	3.93477200	-4.43051100
H	2.83214600	4.33903200	-3.63812800
H	1.89971300	4.77662200	-5.07208800
H	1.28924400	3.53902500	-3.97067600

TS3-endo

C	7.03054500	-1.09380500	-4.50386000
C	5.57743900	-0.83805400	-4.94474900
C	7.12577900	-1.32415400	-2.99438800
C	4.94214300	0.34328700	-4.24801100
C	5.38876100	1.62542800	-4.56601100
H	6.21631600	1.77763300	-5.24906600
Ir	3.05121200	0.36875600	-3.50169600
C	4.66826900	2.70201800	-3.97069200
O	3.57947700	2.40193700	-3.32667000
P	1.33281100	0.89723200	-4.93310900
P	2.27945400	-1.77904000	-3.70820900
C	1.97301800	1.88815100	-6.34606700
C	2.09861700	3.27971500	-6.24436600
C	2.68579300	4.05025100	-7.24309500
C	3.16616600	3.43434100	-8.39724300
C	3.06589600	2.05021000	-8.53073300
C	2.48795100	1.30355500	-7.50826800
C	-0.14101100	1.84956700	-4.37701200
C	-1.25617900	2.00565600	-5.21013100
C	-2.38542400	2.71621300	-4.81974400
C	-2.41308800	3.30324200	-3.55327900
C	-1.31778500	3.17624500	-2.70003700
C	-0.19856400	2.45952600	-3.11849200
C	0.57505700	-0.68654900	-5.59389500
C	1.51355500	-1.88726900	-5.40292700
C	0.86246700	-2.15773800	-2.58003700
C	0.48488100	-1.29767400	-1.54404500
C	-0.56732500	-1.58660200	-0.67893000
C	-1.27600700	-2.77675100	-0.83731000
C	-0.92798100	-3.66447600	-1.85695700
C	0.12721400	-3.34515400	-2.70519400
C	3.33009400	-3.27437000	-3.44617500
C	3.72460800	-4.17413800	-4.44232900
C	4.51525000	-5.28764600	-4.16495200
C	4.93195500	-5.53050100	-2.85713100
C	4.55963300	-4.65457800	-1.83620600
C	3.77112800	-3.55246600	-2.14576000
H	0.97608800	-2.82746900	-5.54030900
H	2.33061800	-1.85063400	-6.12446300
H	-0.34429500	-0.82336100	-5.01480600
H	0.28656400	-0.58137000	-6.64022600
F	-3.48279600	3.98250400	-3.16236100
F	-3.42832900	2.83921500	-5.63769800
F	-1.24961900	1.46017600	-6.43913100
F	-1.34271900	3.74222200	-1.49538700
F	0.83503500	2.38488600	-2.27252800
F	1.66858200	3.92558800	-5.15048000
F	2.80380900	5.37037200	-7.08668600
F	3.72824000	4.15864500	-9.35674000
F	3.53285800	1.44728000	-9.62209700
F	2.44980200	-0.03095700	-7.67516700
F	3.43062700	-2.72535300	-1.13882000
F	4.95359100	-4.87561400	-0.58457300
F	5.68496800	-6.58676700	-2.58426300
F	4.87183800	-6.11612100	-5.14295300
F	3.36119100	-3.98796800	-5.71979400
F	1.13647500	-0.13707500	-1.34468400
F	-0.89768500	-0.73486300	0.28892300
F	-2.28165900	-3.06418500	-0.02302800
F	-1.60303100	-4.79998500	-2.01306000
F	0.43773700	-4.22738500	-3.67078400
C	6.56860900	-0.15535700	-2.16800500
H	4.99640200	-1.74390100	-4.75683700

H	5.53722800	-0.65476400	-6.02648100
H	7.42075600	-1.96139100	-5.04941000
H	7.65755200	-0.23852400	-4.78664000
H	6.59420800	-2.24858700	-2.72168500
C	5.03063400	0.03414100	-2.26362100
H	7.04037000	0.76980500	-2.52284300
H	4.77867700	0.93647300	-1.70281200
H	4.56089200	-0.83561500	-1.79934400
H	8.17535700	-1.48344000	-2.71787100
C	6.91678000	-0.32632300	-0.67694300
H	8.00406100	-0.36397800	-0.54427300
H	6.53379500	0.50492400	-0.07476600
H	6.49764100	-1.25609100	-0.27319100
N	5.04194200	3.99770800	-4.03103400
C	6.27400600	4.41346500	-4.69469700
H	6.60976500	5.35392100	-4.25057200
H	7.06005600	3.67083100	-4.54734300
H	6.12486800	4.57490400	-5.77071800
C	4.16104300	5.06543100	-3.55655500
H	4.70183700	5.70255000	-2.84904200
H	3.82415700	5.67956500	-4.40079200
H	3.29747500	4.62777400	-3.06177300

TS3-*exo*

C	6.78795300	-1.49947400	-3.95817400
C	5.70794200	-0.93021100	-4.89224500
C	6.19851000	-1.41261900	-2.54861100
C	5.06271500	0.25502000	-4.19697700
C	5.35576200	1.53175000	-4.70277100
H	6.05618900	1.66462100	-5.51941100
Ir	3.13456700	0.29202700	-3.40485600
C	4.68851200	2.61774400	-4.07482700
O	3.70675000	2.31657600	-3.27083300
P	1.47303800	0.86370600	-4.82076400
P	2.28081200	-1.83010900	-3.61136900
C	2.10359800	1.90234200	-6.20308100
C	2.06942800	3.30235700	-6.18367400
C	2.63702900	4.07284600	-7.19467200
C	3.26474900	3.44972700	-8.27164400
C	3.33317100	2.05792900	-8.31717700
C	2.77109000	1.31522700	-7.28447100
C	0.01780100	1.80189200	-4.19274900
C	-1.12107000	1.97531600	-4.98974500
C	-2.24290400	2.66855100	-4.55092900
C	-2.23827500	3.22405800	-3.27021000
C	-1.11790700	3.08324800	-2.45273800
C	-0.00643100	2.38429200	-2.91962300
C	0.69726800	-0.67533700	-5.56409100
C	1.57880000	-1.91046100	-5.33674400
C	0.78547300	-2.16729600	-2.56563000
C	0.40254000	-1.33367900	-1.50928900
C	-0.71839400	-1.58748800	-0.72257500
C	-1.49338300	-2.71760400	-0.97545200
C	-1.13894700	-3.58267800	-2.01119700
C	-0.01496600	-3.29946500	-2.78063200
C	3.23391800	-3.39225500	-3.33650300
C	3.79436300	-4.17204200	-4.35386800
C	4.49531800	-5.34771600	-4.09364600
C	4.65721800	-5.77641400	-2.77735900
C	4.12705100	-5.01827200	-1.73310700
C	3.43599500	-3.84791600	-2.02612700
H	1.00996900	-2.82883700	-5.49179000
H	2.42146400	-1.90919900	-6.02622900
H	-0.26865700	-0.79274000	-5.06346900
H	0.49632300	-0.52929300	-6.62675600
F	-3.29968600	3.88760800	-2.83283800
F	-3.30775500	2.80698200	-5.33742300
F	-1.14356600	1.46720300	-6.23491600
F	-1.11031100	3.62182600	-1.23541400
F	1.05217300	2.30667500	-2.10571300
F	1.50964700	3.96605100	-5.16171800
F	2.60303500	5.40445000	-7.11737500
F	3.81131100	4.17682400	-9.23778800
F	3.94805700	1.44934800	-9.32917200
F	2.89773000	-0.02149800	-7.35071100
F	2.96954700	-3.13007700	-0.98765900
F	4.29159300	-5.40732700	-0.47148400
F	5.32400400	-6.89231200	-2.51739000
F	5.00919100	-6.05738200	-5.09502800
F	3.69026200	-3.80074900	-5.64143100

F	1.11895500	-0.23947800	-1.20237800
F	-1.04737300	-0.75796400	0.26562800
F	-2.56332700	-2.97064400	-0.23469300
F	-1.87048200	-4.66664000	-2.25660500
F	0.29630400	-4.17200000	-3.75557500
C	5.54421800	-0.04120000	-2.33298200
N	5.00937800	3.92038200	-4.23700400
C	6.16398900	4.33210800	-5.02944000
H	6.97058200	3.60237200	-4.93921300
H	5.90957400	4.45934000	-6.09040100
H	6.52774300	5.28984900	-4.64810600
C	4.16276600	4.98972900	-3.70831300
H	4.74712400	5.63332400	-3.04175700
H	3.76986700	5.59944500	-4.53110600
H	3.33524600	4.55496700	-3.15265400
H	6.12506600	-0.62494100	-5.85861100
H	4.95713800	-1.69675800	-5.10740100
H	7.69826500	-0.89354700	-4.02954900
H	7.06570800	-2.52394600	-4.22696900
H	6.96347900	-1.56977300	-1.77643400
H	5.44860600	-2.19763600	-2.41478500
C	6.58808500	1.05989600	-2.10702500
H	6.12428800	2.04346300	-2.00168000
H	7.10775600	0.84452500	-1.16341900
H	7.33440100	1.11134700	-2.90191200
C	4.64770300	-0.06007600	-1.06743500
H	5.30903300	-0.25077400	-0.20773700
H	4.16143100	0.90210500	-0.87616500
H	3.89792100	-0.85464200	-1.05252000

TS4-endo

C	4.84506600	1.12412000	-6.48893100
C	4.84873000	1.33203600	-4.98721700
C	5.95284600	1.14194400	-4.18226100
H	6.92477400	0.90169300	-4.60298400
Ir	3.00119700	0.72236800	-3.89485300
H	2.03036800	0.28566600	-5.05447900
C	5.74531700	1.21678800	-2.74109600
O	4.54747100	1.13518200	-2.30210900
N	6.77089500	1.36822700	-1.86708800
C	8.17092600	1.47316600	-2.27345100
H	8.67884800	2.17367100	-1.60447600
H	8.68745800	0.50652600	-2.21155600
C	6.51307200	1.37432300	-0.42636500
H	7.06779000	2.19689100	0.03535800
H	6.83363500	0.43367600	0.03840400
P	3.33916300	-1.60813300	-3.58368400
P	1.16274300	0.53063300	-2.49524900
C	4.99140600	-2.01500500	-2.88092900
C	6.09772200	-2.07836000	-3.73645000
C	7.40139800	-2.21831700	-3.26941100
C	7.63175600	-2.26769300	-1.89736600
C	6.55656200	-2.19037600	-1.01352700
C	5.26454000	-2.05783400	-1.51016900
C	3.18398300	-2.86330400	-4.93250500
C	3.31430500	-4.22322900	-4.60941800
C	3.19611100	-5.23848300	-5.55197600
C	2.93035500	-4.90665900	-6.88030000
C	2.78989200	-3.56914100	-7.24109800
C	2.91694800	-2.57272300	-6.27468100
C	2.02283900	-2.23343300	-2.39804700
C	1.35807700	-1.11179300	-1.59482500
C	-0.50185100	0.54754500	-3.30765300
C	-1.42127400	1.60097000	-3.21364500
C	-2.63539900	1.59710900	-3.89842900
C	-2.96089100	0.52609900	-4.72726500
C	-2.06011800	-0.52819700	-4.87002600
C	-0.85929000	-0.49420600	-4.17114600
C	0.93827300	1.61808700	-1.01230300
C	-0.07104300	1.33320900	-0.07944900
C	-0.25399300	2.06665600	1.08622600
C	0.59578500	3.13957700	1.35657700
C	1.60406000	3.46164900	0.45314600
C	1.76125500	2.70808700	-0.70978100
H	0.39690200	-1.44049700	-1.19340900
H	1.99681000	-0.84726500	-0.74570400
H	1.28965900	-2.73702300	-3.02807200
H	2.44621500	-2.97885800	-1.72515800
F	2.81112500	-5.86042800	-7.79400800
F	3.33116900	-6.51331900	-5.19377600

F	3.56294100	-4.58968600	-3.33971600
F	2.53471200	-3.24209200	-8.50697600
F	2.77377600	-1.30997200	-6.70239900
F	5.92672500	-1.98196600	-5.06671900
F	8.42502500	-2.24846000	-4.12345700
F	8.87592000	-2.33633300	-1.43156200
F	6.77760700	-2.18366500	0.30314200
F	4.27239200	-1.93595900	-0.61009300
F	2.74208700	3.09881000	-1.53715200
F	2.41856900	4.48834100	0.69708700
F	0.43915600	3.85065600	2.46525400
F	-1.22882200	1.75406200	1.93681400
F	-0.92860100	0.32189200	-0.30666700
F	-1.15976600	2.68563300	-2.46777200
F	-3.47708100	2.62047300	-3.76934800
F	-4.11258500	0.51495900	-5.38581400
F	-2.34436100	-1.55264500	-5.67283300
F	-0.00995500	-1.52427300	-4.36863300
H	8.25497900	1.86162400	-3.28837300
H	5.44793200	1.51351700	-0.25324000
C	2.59153800	2.63526400	-5.05193200
C	3.97335500	2.82209200	-4.62945200
C	2.50215200	2.32541800	-6.55890800
C	3.86524000	2.05867100	-7.24500800
C	1.49574600	3.52684800	-4.51365100
H	1.61165800	3.72990100	-3.44914000
H	1.51671200	4.49106700	-5.04396900
H	0.50755300	3.09176500	-4.69211100
H	5.85481200	1.24662100	-6.90590000
H	4.56002000	0.08426100	-6.66753200
H	4.13336300	3.20480800	-3.62411400
H	4.60195800	3.36434400	-5.34515100
H	4.36406300	3.02211900	-7.41497300
H	3.68523500	1.64576900	-8.24265500
H	1.81171900	1.49549000	-6.73897800
H	2.04776800	3.19767500	-7.05273200

TS4-exo

C	5.16513600	0.86835300	-6.69630800
C	3.65495000	2.73439500	-7.10528100
C	5.05692800	1.51523400	-5.33510000
C	6.12236600	1.54701000	-4.48921500
H	7.06598800	1.09750900	-4.78870000
Ir	3.18236400	1.32761700	-3.92968300
H	2.14649000	0.81417500	-5.00617700
C	5.97835000	2.09608300	-3.12918600
O	4.81543200	2.16431300	-2.63302900
N	7.04475900	2.50918900	-2.41110100
C	8.42693200	2.46994600	-2.88950600
H	8.93896000	3.37989100	-2.56360000
H	8.96605300	1.60660100	-2.47934700
C	6.85180400	2.96062600	-1.02905600
H	7.47500900	3.84113300	-0.85071000
H	7.13981400	2.17565000	-0.31848600
P	3.56005500	-0.92732800	-3.25269000
P	1.39982000	1.31903600	-2.49683700
C	5.21103500	-1.13208200	-2.44957800
C	6.34087600	-1.37526000	-3.23820800
C	7.63578300	-1.32927000	-2.73093900
C	7.83297300	-1.01024400	-1.38995000
C	6.73305600	-0.75689700	-0.57327300
C	5.44979000	-0.82161500	-1.10832300
C	3.46150100	-2.43150000	-4.32861600
C	3.76911600	-3.69534900	-3.80298600
C	3.68299500	-4.86400100	-4.55171100
C	3.25824600	-4.79498000	-5.87859900
C	2.92466200	-3.56132100	-6.43179100
C	3.02319800	-2.40698800	-5.65661300
C	2.23189000	-1.37709400	-2.00706800
C	1.57494100	-0.15750000	-1.35803700
C	-0.23554200	1.25773400	-3.35515400
C	-0.74381600	2.43292800	-3.92086700
C	-1.93983500	2.46964500	-4.62977900
C	-2.67194800	1.29419500	-4.79465300
C	-2.19609700	0.10319900	-4.24988800
C	-0.99538100	0.10142700	-3.54434400
C	1.07035300	2.62828400	-1.22364700
C	-0.06277300	2.50957400	-0.40229600
C	-0.38373000	3.43923800	0.58053800
C	0.45233300	4.53772600	0.77938700

C	1.59379600	4.68305700	-0.00371000
C	1.89002900	3.73586600	-0.98318300
H	0.60954100	-0.41824000	-0.92111700
H	2.21297600	0.22808800	-0.55758500
H	1.49253200	-1.92984900	-2.59051400
H	2.62729500	-2.05519500	-1.24795200
F	3.16539800	-5.90025300	-6.60627100
F	3.99305200	-6.03913800	-4.00875000
F	4.15926600	-3.81427700	-2.52177500
F	2.50563500	-3.48497000	-7.69408100
F	2.66656200	-1.25664900	-6.24978700
F	6.20581700	-1.61926500	-4.55422100
F	8.68238200	-1.52672000	-3.53455500
F	9.06727000	-0.89784700	-0.90524100
F	6.91714500	-0.40190400	0.69996700
F	4.42899100	-0.53003800	-0.28268000
F	3.01245400	3.93523500	-1.68347300
F	2.40676100	5.72228400	0.18573500
F	0.16509700	5.43263100	1.71542000
F	-1.47160500	3.28066300	1.33102500
F	-0.89108000	1.45823200	-0.54068100
F	-0.06418300	3.58664700	-3.78883400
F	-2.38210100	3.61318300	-5.14928400
F	-3.81431700	1.30979800	-5.46990000
F	-2.88600300	-1.02566500	-4.40329100
F	-0.58684200	-1.07999500	-3.04389100
H	8.46541600	2.43683900	-3.97752700
H	5.80477500	3.21624000	-0.87763100
C	2.88444100	3.26476800	-4.73772700
C	4.78508500	1.92400700	-7.74668800
C	4.02337400	3.08300400	-5.65837600
C	5.08799400	4.17801600	-5.52980400
H	5.98447800	3.97475900	-6.12089900
H	4.63653600	5.11034200	-5.89337300
H	5.37418800	4.34033000	-4.48822400
H	6.16500000	0.45094100	-6.86422700
H	4.45155000	0.04020000	-6.74405900
H	5.64451300	2.56856800	-7.96496400
H	4.47480500	1.46945700	-8.69203100
H	3.45987300	3.66947600	-7.64479900
H	2.72669100	2.15267100	-7.10586900
H	3.02088400	4.04375500	-3.99056700
H	1.91509000	3.33325300	-5.22733700

TSS-endo

C	3.83168000	1.67525200	-6.75135100
C	4.37618000	1.78096900	-5.33295600
C	5.11803300	0.77297000	-4.73883500
H	5.33205800	-0.10740000	-5.33612100
Ir	2.93794200	0.62817800	-3.77316900
H	1.98848000	1.44173000	-4.78572100
C	5.97458700	1.03028800	-3.51932600
O	5.43052100	1.33070600	-2.44578000
N	7.32055000	0.92702900	-3.66169100
C	8.00364000	0.55273300	-4.89645600
H	8.89569200	1.17586900	-5.01474400
H	8.31589100	-0.49900200	-4.86929700
C	8.18138900	1.10507500	-2.49170300
H	8.93903400	1.86723400	-2.70271000
H	8.68636000	0.16315700	-2.24826000
P	3.35631600	-1.61294800	-3.28166600
P	1.00628200	0.30705100	-2.58724100
C	4.63185400	-1.82807100	-1.95452700
C	5.98568300	-2.02151300	-2.24285400
C	6.96116900	-2.07545800	-1.25416800
C	6.60062800	-1.90856300	0.08145700
C	5.26431400	-1.68497700	0.40724900
C	4.31537100	-1.63873300	-0.60847800
C	3.86332700	-2.88681000	-4.52750500
C	4.16408900	-4.19472500	-4.11597700
C	4.48946600	-5.20963700	-5.00919800
C	4.50716500	-4.93751200	-6.37730500
C	4.19444300	-3.65770300	-6.82756000
C	3.87344100	-2.66200300	-5.90657900
C	1.77331500	-2.43802500	-2.70284100
C	0.76646000	-1.48673100	-2.05872300
C	-0.50237300	0.68712700	-3.58962200
C	-1.36039400	1.77979500	-3.42474700
C	-2.44902700	2.00656200	-4.26498600
C	-2.70806500	1.12733800	-5.31445200

C	-1.86951200	0.03185400	-5.51821200
C	-0.79218900	-0.16622900	-4.66229000
C	0.77235800	1.14321300	-0.95968500
C	-0.42923900	1.00641100	-0.25128600
C	-0.61993000	1.54365400	1.01488900
C	0.42983200	2.23180600	1.62647500
C	1.64773200	2.36821300	0.96528000
C	1.80881500	1.81812500	-0.30589200
H	-0.25767300	-1.78796400	-2.29080600
H	0.87217900	-1.49310900	-0.97447900
H	1.35608100	-2.85070500	-3.62464900
H	2.01506300	-3.27579500	-2.04392700
F	4.81268500	-5.89393500	-7.24347900
F	4.77443200	-6.43172200	-4.56663000
F	4.13835000	-4.51455600	-2.81083000
F	4.19599800	-3.38655000	-8.13188300
F	3.56416000	-1.45736100	-6.41139700
F	6.40005100	-2.13137100	-3.52247800
F	8.24444400	-2.24801300	-1.58509300
F	7.52545700	-1.94707800	1.03293000
F	4.90297200	-1.50533100	1.67622000
F	3.04189400	-1.37620800	-0.24918100
F	3.01339000	1.95668100	-0.87583200
F	2.65838400	3.00899300	1.54995200
F	0.26756900	2.74689300	2.83787800
F	-1.78280900	1.39925200	1.64622800
F	-1.45036800	0.32824700	-0.80399500
F	-1.15601300	2.68032600	-2.44949000
F	-3.23714700	3.06082500	-4.06757500
F	-3.74129800	1.33490500	-6.12027000
F	-2.09794400	-0.81177700	-6.52309000
F	-0.00074700	-1.22940600	-4.89974000
H	7.36535700	0.71506000	-5.76494800
H	7.56870600	1.42349800	-1.65016200
C	2.54007800	2.93689200	-4.52595400
C	4.06250200	3.09327000	-4.64512600
C	1.89862900	3.19962900	-5.91037400
C	2.82980300	2.80501500	-7.08519100
C	1.90817300	3.73826900	-3.40603000
H	2.39691700	3.54757100	-2.45015800
H	2.02794000	4.80841200	-3.63607800
H	0.83683800	3.55153100	-3.30373300
H	4.68511100	1.75223200	-7.44036800
H	3.39719500	0.68807600	-6.91054400
H	4.53480600	3.16993500	-3.66566500
H	4.34783200	3.96721600	-5.24993900
H	3.39785100	3.69033400	-7.38846300
H	2.23885100	2.51709200	-7.95976200
H	0.92027700	2.71143700	-5.98991700
H	1.69962800	4.27950800	-5.96908800
TSS-<i>exo</i>			
C	0.80457700	2.82747000	-6.97729200
C	1.87627800	4.10761200	-5.25246500
C	2.04087300	2.06449300	-6.51554800
C	2.29352000	0.81895300	-6.95394100
H	1.61739300	0.39487900	-7.69533000
Ir	2.86933500	0.32780500	-3.44788400
H	2.07411700	1.62252100	-3.97621400
C	3.38385800	-0.08918300	-6.53383600
O	3.62018000	-0.37323400	-5.31914600
N	4.10969900	-0.70272800	-7.48817200
C	3.95120300	-0.43348100	-8.91779700
H	4.94235300	-0.35586200	-9.37477800
H	3.40574900	-1.24722600	-9.41143300
C	5.07969300	-1.74744400	-7.14492800
H	5.99947500	-1.57967300	-7.71205000
H	4.67801600	-2.73486500	-7.40060900
P	2.17023500	-1.78800600	-2.79896000
P	2.31174000	0.93881600	-1.36141900
C	3.35486700	-2.95529800	-1.99226900
C	4.70968000	-2.63777800	-1.85239800
C	5.61558700	-3.50544500	-1.24716100
C	5.16923600	-4.73480000	-0.76430900
C	3.82413400	-5.08752200	-0.88721800
C	2.94387700	-4.19843400	-1.49498300
C	1.44419000	-2.81534300	-4.14091200
C	0.07600400	-2.93340300	-4.40782600
C	-0.40752500	-3.63936800	-5.50814800
C	0.48724600	-4.24167600	-6.39096300

C	1.85803700	-4.13592400	-6.16006400
C	2.31103000	-3.43808100	-5.04703300
C	0.90854100	-1.50733500	-1.46211900
C	1.50597700	-0.50598700	-0.46393700
C	1.17477800	2.39024400	-1.19915200
C	1.67230600	3.69906600	-1.20026100
C	0.84583200	4.81702100	-1.13523400
C	-0.53645200	4.64430100	-1.07805700
C	-1.07169400	3.35755300	-1.09674100
C	-0.21713500	2.26020800	-1.16395300
C	3.68524900	1.37484200	-0.20582400
C	3.42368600	1.59868000	1.15199100
C	4.42175900	1.91458900	2.06644900
C	5.74071700	2.01741600	1.62204800
C	6.03997200	1.80656800	0.27747800
C	5.01754300	1.49381800	-0.61666500
H	0.75281300	-0.16072800	0.24507600
H	2.31129700	-0.97062800	0.11553900
H	0.01947000	-1.08941100	-1.93167200
H	0.63367500	-2.44371300	-0.97007900
F	0.03755400	-4.90405800	-7.45035900
F	-1.71843700	-3.73070000	-5.72252900
F	-0.83465200	-2.35651500	-3.60984800
F	2.73106200	-4.68582600	-7.00966800
F	3.64041800	-3.36255400	-4.86424800
F	5.18976800	-1.46770900	-2.30646800
F	6.89863200	-3.16705400	-1.12761400
F	6.02245900	-5.56892900	-0.18449400
F	3.39637400	-6.26005000	-0.42469000
F	1.65520600	-4.56619400	-1.60138800
F	5.36764800	1.32241600	-1.89906000
F	7.29737700	1.90891700	-0.14965500
F	6.70764100	2.31545400	2.48002700
F	4.12988200	2.11588500	3.34962900
F	2.16091100	1.51079300	1.60768900
F	2.99683400	3.92157000	-1.28694300
F	1.36888800	6.04169400	-1.13723200
F	-1.33887600	5.69974400	-1.01915200
F	-2.39068600	3.18079700	-1.05733700
F	-0.79097500	1.04403700	-1.20276400
H	3.42411000	0.50612500	-9.07528500
H	5.29221600	-1.71167800	-6.07982100
C	3.44219100	2.32251300	-4.29465100
C	1.01493900	4.27851300	-6.51074200
C	2.87440300	2.96314600	-5.58921200
C	4.06575700	3.53186300	-6.40618100
H	3.73130100	4.06966400	-7.29933600
H	4.64283200	4.22899900	-5.78799000
H	4.73592800	2.72794600	-6.72963200
H	0.62363600	2.72628100	-8.05262000
H	-0.07128000	2.39655700	-6.47042200
H	1.55152900	4.85631500	-7.27122100
H	0.07289000	4.79855900	-6.31577600
H	2.39696800	5.02075800	-4.94572700
H	1.23693300	3.79676200	-4.41310300
H	4.44763700	1.92283900	-4.46864300
H	3.51092400	3.08171800	-3.51530200
2a'			
C	-2.92925100	0.25990000	-0.92687300
C	-1.06584000	1.84369200	-1.42585700
C	-2.43605300	2.37176900	-1.94365000
C	-3.49206800	1.68389500	-1.06795900
H	-3.23305500	-0.33921300	-1.79858200
H	-3.28338600	-0.27547200	-0.03864300
H	-2.48650600	3.46584400	-1.91349900
H	-2.57628700	2.06761500	-2.99063000
H	-3.55423400	2.16901200	-0.08648700
H	-4.49576700	1.70277000	-1.50528100
C	-0.00478600	1.89037900	-2.53909800
H	0.08187600	2.91474200	-2.92321100
H	0.97468600	1.58208800	-2.16835500
H	-0.28569400	1.24248000	-3.37855500
C	-1.41093100	0.42355800	-0.94307400
C	-0.61256300	-0.60010500	-0.58458100
H	-1.11157800	-1.51698400	-0.27384400
C	0.87535200	-0.62141000	-0.50032700
O	1.54895800	0.37410000	-0.21715900
N	1.48150700	-1.84801700	-0.69501700
C	2.91168500	-1.97121600	-0.45994100

H	3.11431100	-2.83838600	0.18225100
H	3.45705500	-2.10808700	-1.40455600
H	3.26355700	-1.06147700	0.02413500
C	0.83619700	-3.02334200	-1.25529300
H	-0.13555800	-2.77010100	-1.67816200
H	1.45596500	-3.43018100	-2.06536300
H	0.70387600	-3.81544400	-0.50354800
C	-0.59914900	2.69974400	-0.22123900
H	0.31662100	2.28198900	0.20009800
H	-0.40735600	3.72805100	-0.55392900
H	-1.35985100	2.73946600	0.56730800
3a'			
C	-3.61536300	-2.75692400	-0.21845600
C	-2.08664500	-2.73400700	-0.43313100
C	-1.57711400	-1.26680400	-0.43141700
C	-3.50080000	-0.54282100	1.03523500
C	-4.05259600	-1.98636300	1.03751900
H	-0.49434500	-1.24100300	-0.55117500
H	-4.10310200	-2.30706100	-1.09596800
H	-3.97047600	-3.79456800	-0.16299000
H	-3.76815400	-0.02631800	1.96476000
H	-3.97779700	0.00901400	0.20967000
H	-3.69687600	-2.50215800	1.93830300
H	-5.14764900	-1.96081100	1.10349000
H	-2.03431900	-0.74837000	-1.28946300
C	-2.00323700	-0.54284900	0.82399900
C	-1.18175500	0.04048500	1.71788800
H	-1.63762900	0.53294900	2.57438200
C	0.30998100	0.02158800	1.67008300
O	0.94740500	-0.90953700	1.16978600
N	0.95967800	1.08458500	2.26883900
C	2.40713400	1.04041500	2.40137000
H	2.88542100	1.79252600	1.75810000
H	2.69886100	1.24277500	3.44064200
H	2.75050100	0.04976300	2.10699000
C	0.32757200	2.32082500	2.69681300
H	-0.68377700	2.40027300	2.29902800
H	0.28803300	2.40368600	3.79318200
H	0.90196100	3.17601000	2.31682700
H	-1.88248100	-3.14369300	-1.43228200
C	-1.32741200	-3.59812200	0.58571200
H	-1.66413800	-4.64121400	0.53865500
H	-0.25075000	-3.57103000	0.39037600
H	-1.46995500	-3.24229500	1.61181200
1b'			
C	-4.46478200	7.32913800	4.43432800
O	-3.60837100	7.68201600	5.23324400
C	-5.88783000	7.28534000	4.85333600
H	-6.04927400	7.58535900	5.88764800
C	-6.92130300	6.91748100	4.08046000
H	-6.73665900	6.62397100	3.04614400
C	-8.35763100	6.88958600	4.51507800
H	-8.74530100	5.86455600	4.40662100
H	-8.43086000	7.14406400	5.57988100
C	-9.24755600	7.83895200	3.68635900
H	-8.88631900	8.86866300	3.80065500
H	-9.14614100	7.58868900	2.62189300
C	-10.72946700	7.76849300	4.10697000
H	-11.07983700	6.73242500	3.97819600
H	-10.80499800	7.99355600	5.17822500
C	-11.63357200	8.70559200	3.33217600
C	-12.21105200	9.75975000	3.91873800
H	-12.05896400	9.98335800	4.97210500
H	-12.85848400	10.43803800	3.36814500
C	-11.85521800	8.38862100	1.87206200
H	-12.26719300	7.37739300	1.74772400
H	-10.91677800	8.41583600	1.30264500
H	-12.54789300	9.09717600	1.40788200
C	-4.09029200	6.93251400	3.01248500
H	-4.38800800	5.89885200	2.79962800
H	-4.59064700	7.57529700	2.27834200
H	-3.00914000	7.02724800	2.89661500
INT1b			
C	3.47751100	3.10705900	-5.07269500
C	4.76790300	3.27572100	-4.53337500
H	4.92712100	3.88689000	-3.65112700
Ir	4.30736800	1.07000500	-4.50770200

H	3.39907300	2.83151300	-6.12508100
C	5.93764100	2.88965500	-5.34413100
O	5.82579300	1.77782500	-5.91829500
P	4.72060100	-1.20536400	-4.67368200
P	2.99987200	0.48800800	-2.78694700
C	6.52706200	-1.55048900	-4.62557200
C	7.29254900	-1.33381800	-5.77991400
C	8.67079800	-1.52100600	-5.80500600
C	9.32829200	-1.92618700	-4.64348300
C	8.60144500	-2.13335700	-3.47180000
C	7.22325400	-1.93823700	-3.47527900
C	4.13516200	-2.09280100	-6.16864900
C	4.24352000	-3.48792100	-6.24354900
C	3.81673300	-4.21103000	-7.35114000
C	3.26139000	-3.52681400	-8.43404200
C	3.14157700	-2.13832500	-8.39648600
C	3.57892700	-1.43777700	-7.27427700
C	3.87956300	-2.09885500	-3.26263600
C	3.64307400	-1.12793400	-2.09954800
C	1.22994500	0.05062900	-3.12360600
C	0.41484200	-0.48583200	-2.11470800
C	-0.88970300	-0.90660300	-2.33775600
C	-1.42922800	-0.79785000	-3.62073800
C	-0.65732300	-0.26868200	-4.65123000
C	0.64974200	0.14682900	-4.39591100
C	2.98058400	1.64327000	-1.34788700
C	1.87194700	2.36208400	-0.88263000
C	1.95210100	3.24972600	0.18693600
C	3.17374100	3.45645800	0.82361100
C	4.30507300	2.77044900	0.38183700
C	4.19446900	1.88926300	-0.68880200
H	2.94277400	-1.54325800	-1.37150100
H	4.58135600	-0.90674600	-1.58787400
H	2.92641400	-2.44956800	-3.67380000
H	4.44521600	-2.97556400	-2.94741300
F	2.84622800	-4.19909400	-9.49834000
F	3.93212100	-5.53617200	-7.38357200
F	4.77904500	-4.16658000	-5.21442900
F	2.61521500	-1.48740700	-9.43122900
F	3.45459700	-0.10585700	-7.29906000
F	6.69789600	-0.92119900	-6.90839700
F	9.35953600	-1.30678100	-6.92375500
F	10.64268800	-2.10442600	-4.65057300
F	9.22298100	-2.50885100	-2.35632500
F	6.57616900	-2.12862400	-2.31172300
F	5.31743500	1.27098600	-1.09682700
F	5.48211600	2.96860700	0.97232100
F	3.26410700	4.30774100	1.83520100
F	0.86881800	3.91381300	0.58352100
F	0.67384800	2.25817500	-1.48202000
F	0.89051000	-0.59174600	-0.86116400
F	-1.62170100	-1.40470800	-1.34473800
F	-2.67168800	-1.19619800	-3.85497400
F	-1.16342500	-0.16276400	-5.87892300
F	1.32633600	0.64403000	-5.44252100
C	2.24441800	3.79232500	-4.51060300
H	1.76536600	4.31327100	-5.35143600
H	1.51446300	3.03418200	-4.20139900
C	2.48920200	4.79416900	-3.37332200
H	3.02282100	4.30579900	-2.54912200
H	3.14336300	5.59733600	-3.73626500
C	1.18685500	5.39614900	-2.83400000
H	0.65702400	5.91110800	-3.65039000
H	0.51392400	4.58106800	-2.52886300
C	1.32375400	6.35700000	-1.66761400
C	0.01203100	6.83242300	-1.09092500
H	-0.61165500	7.30517500	-1.86129600
H	-0.56544600	5.99009400	-0.68741600
H	0.16359000	7.55630100	-0.28541900
C	2.49836200	6.76190900	-1.17079300
H	3.45338700	6.44010700	-1.57605900
H	2.54564100	7.45708000	-0.33719300
C	7.18281300	3.70752300	-5.43282100
H	6.94734000	4.72362500	-5.77058100
H	7.62977600	3.79896400	-4.43390100
H	7.89995900	3.24127700	-6.11088100
INT2b			
C	3.59528300	3.05752500	-4.68857600
C	4.32674500	3.65851600	-5.68066000

H	4.27185300	4.72477600	-5.89187800
Ir	3.95475900	1.02198300	-4.59162300
H	5.09256900	1.37211900	-3.59131300
C	5.18016400	2.81901700	-6.46788800
O	5.21644200	1.57690300	-6.20792700
P	4.74869800	-1.26189800	-4.64266100
P	2.63713900	0.28763100	-2.88116500
C	6.56140200	-1.37670800	-4.34912800
C	7.43793500	-1.10838300	-5.40932500
C	8.82015700	-1.10776400	-5.25111700
C	9.36631900	-1.37087100	-3.99520200
C	8.52460800	-1.62791900	-2.91406300
C	7.14544000	-1.62321900	-3.10260400
C	4.48666000	-2.30970800	-6.12629400
C	4.85433600	-3.66119400	-6.13370000
C	4.67985700	-4.47290100	-7.24905300
C	4.11752300	-3.92756300	-8.40511600
C	3.73725400	-2.58618600	-8.43267100
C	3.92545100	-1.79722600	-7.30058400
C	3.84641300	-2.20905700	-3.30271600
C	3.37609100	-1.27757900	-2.17767300
C	1.02869500	-0.27161900	-3.57147600
C	0.06071100	-0.94584900	-2.81644700
C	-1.13997400	-1.38193400	-3.36468600
C	-1.39836600	-1.14885800	-4.71772100
C	-0.45573200	-0.48978300	-5.50612900
C	0.73761300	-0.07608100	-4.92521800
C	2.31648300	1.32288800	-1.39255000
C	1.07835100	1.83494500	-0.98142800
C	0.94501100	2.62811600	0.15626500
C	2.06795800	2.93941500	0.92097700
C	3.32012800	2.45931900	0.53721000
C	3.42336500	1.67041100	-0.60290700
H	2.64176100	-1.77412900	-1.53764100
H	4.22019100	-0.97285000	-1.55639600
H	2.98545900	-2.65205000	-3.81602100
H	4.44858300	-3.02776900	-2.90697600
F	3.94033400	-4.68813100	-9.47627600
F	5.03829800	-5.75364800	-7.21980500
F	5.39706400	-4.20735600	-5.03329300
F	3.19768300	-2.06738600	-9.53352500
F	3.54722200	-0.51248500	-7.37390700
F	6.94945100	-0.83662500	-6.62799700
F	9.61629500	-0.85207700	-6.28695100
F	10.68211600	-1.37079600	-3.82814000
F	9.03710900	-1.87368100	-1.71044000
F	6.37967500	-1.86055100	-2.02061500
F	4.65033500	1.23784200	-0.94711800
F	4.40155300	2.75629000	1.25180500
F	1.94776500	3.69343700	2.00367900
F	-0.25060300	3.09213700	0.50842100
F	-0.04085400	1.60025300	-1.68223900
F	0.27610600	-1.16789200	-1.51120900
F	-2.03709500	-2.01314800	-2.61452100
F	-2.53910700	-1.55682100	-5.25295300
F	-0.69142000	-0.27052600	-6.79588500
F	1.62952600	0.53797400	-5.74411900
C	2.67165400	3.90722000	-3.86179800
H	2.90885800	3.75531700	-2.80026100
H	2.85299300	4.96950400	-4.07650900
C	1.17043400	3.60203100	-4.07043400
H	0.96465100	2.56880700	-3.77595800
H	0.59936300	4.23509100	-3.38086500
C	0.67466300	3.82208300	-5.50238900
H	0.82498900	4.87647600	-5.78225700
H	1.30579400	3.25297300	-6.20116300
C	-0.77387700	3.45602500	-5.76777800
C	-1.21457500	3.63135600	-7.20152500
H	-1.06448400	4.66621500	-7.53698800
H	-0.62719900	2.99397800	-7.87689500
H	-2.27130900	3.38264200	-7.33423200
C	-1.61464500	3.01345400	-4.82441100
H	-1.32540100	2.89101900	-3.78494600
H	-2.64873900	2.77879500	-5.06326300
C	6.02763700	3.33721800	-7.58827500
H	5.40084000	3.84884500	-8.32862000
H	6.73708400	4.08134800	-7.20521300
H	6.57400300	2.52360400	-8.06791700

INT9-endo

C	5.10929300	0.52834100	-6.92407200
C	3.67980800	2.63874400	-7.13309700
H	5.04051700	-0.54365200	-7.13897800
H	6.11041400	0.85015800	-7.24134800
C	4.96478200	0.75416300	-5.44585500
C	6.04331300	1.20023400	-4.72519500
H	7.01845400	1.36511700	-5.18143400
Ir	3.23362000	0.63263800	-4.35689700
H	2.28995500	0.09412800	-5.51035000
C	5.85628800	1.47493900	-3.32778800
O	4.71045600	1.32126500	-2.81907600
P	3.64046000	-1.59383600	-3.81667000
P	1.36243800	0.48290800	-2.74628300
C	5.29732900	-1.86373400	-3.05129700
C	6.42280000	-2.05626700	-3.86110900
C	7.70056200	-2.23094300	-3.33828100
C	7.88422300	-2.20278900	-1.95622800
C	6.78957600	-1.99404500	-1.11825100
C	5.52397500	-1.82407800	-1.67262300
C	3.57279000	-2.97253900	-5.05403900
C	3.85089900	-4.27769400	-4.61265300
C	3.79625000	-5.38861700	-5.44666700
C	3.43897500	-5.22118600	-6.78418500
C	3.14068100	-3.94713900	-7.25845800
C	3.20599200	-2.85026400	-6.39965000
C	2.33037200	-2.20417500	-2.62935000
C	1.68162600	-1.10042100	-1.80062200
C	-0.36083900	0.41055800	-3.42653300
C	-1.00663200	1.60981400	-3.74599100
C	-2.29127400	1.66320600	-4.27499100
C	-2.97973400	0.47329400	-4.51013100
C	-2.36858000	-0.74387800	-4.21616500
C	-1.08112800	-0.75818100	-3.68384600
C	1.09023000	1.61012100	-1.29641400
C	0.07662200	1.32432900	-0.36674600
C	-0.16091600	2.10952000	0.75584600
C	0.63652900	3.23043400	0.98690200
C	1.65415600	3.54641800	0.09134100
C	1.86719800	2.74216200	-1.02764200
H	0.76667200	-1.46328900	-1.33027200
H	2.36161400	-0.78208100	-1.00594200
H	1.58697100	-2.67698400	-3.27488200
H	2.74858400	-2.98046400	-1.98603500
F	3.37716000	-6.26796500	-7.59471300
F	4.07536300	-6.59993600	-4.97314200
F	4.18318800	-4.49930600	-3.32836000
F	2.78764200	-3.77328200	-8.53065200
F	2.89239100	-1.66507700	-6.93945000
F	6.29451800	-2.07681300	-5.19811300
F	8.74082000	-2.41342800	-4.14930800
F	9.09622100	-2.36421100	-1.44110200
F	6.95584900	-1.95467000	0.20193800
F	4.50671600	-1.61750700	-0.81815100
F	2.85848300	3.11046400	-1.84645400
F	2.42241500	4.61424900	0.30109700
F	0.42639200	3.98828000	2.05470200
F	-1.13468700	1.79364700	1.60677000
F	-0.71597000	0.25071700	-0.53625600
F	-0.36293900	2.78202300	-3.55944500
F	-2.85418000	2.83406700	-4.56606400
F	-4.20457500	0.50055000	-5.01935500
F	-3.01306300	-1.88713200	-4.43943100
F	-0.55067800	-1.96680000	-3.41878000
C	2.86123400	2.91016900	-4.73696400
H	3.82410300	3.32746000	-4.45701900
H	2.02772600	3.17694100	-4.10076200
C	4.04536800	1.27472000	-7.75921900
C	2.61813900	2.56733500	-6.05753400
C	1.21093200	2.39512800	-6.56749200
H	1.12703400	1.57759800	-7.28898500
H	0.49565400	2.24289300	-5.76251900
H	0.93483600	3.31903200	-7.09529500
H	4.43705000	1.43010800	-8.76961400
H	3.14594700	0.66082100	-7.86092300
H	3.27119700	3.29194200	-7.91564600
H	4.58093400	3.12720000	-6.74753400
C	6.98124500	1.96097600	-2.45625900
H	7.84936300	1.29669200	-2.53681000
H	7.31105400	2.95194400	-2.79298600
H	6.65898900	2.02807000	-1.41567700

INT9-*exo*

C	5.16896900	0.78534700	-6.66933800
C	3.58379600	2.76429600	-7.12606600
C	5.07776600	1.12040000	-5.21001600
C	6.19864500	1.50871300	-4.52090900
H	7.19390300	1.47984400	-4.96308600
Ir	3.32330900	1.27301900	-4.13750000
H	2.38133300	0.64445500	-5.23864000
C	6.01691300	2.04195800	-3.20063400
O	4.85083900	2.11369800	-2.71771700
P	3.63723400	-0.88011900	-3.31381100
P	1.42746900	1.37181000	-2.60292400
C	5.24791900	-1.09128300	-2.44134100
C	6.39997500	-1.48478600	-3.13171000
C	7.63543000	-1.62007500	-2.50487200
C	7.74815700	-1.34190600	-1.14311700
C	6.62666700	-0.92309300	-0.42820800
C	5.40548000	-0.79863200	-1.08383600
C	3.56378400	-2.39328200	-4.38361900
C	3.86791100	-3.63772300	-3.80445100
C	3.80963800	-4.83625000	-4.50585000
C	3.41217800	-4.82757100	-5.84229900
C	3.07412800	-3.62057600	-6.44663600
C	3.14226900	-2.43272500	-5.71865000
C	2.26918700	-1.32169300	-2.11280800
C	1.56000100	-0.12585000	-1.48183800
C	-0.24426600	1.35689700	-3.39874500
C	-0.89945000	2.54938700	-3.73198900
C	-2.13509600	2.57401400	-4.37285800
C	-2.75330900	1.37340700	-4.71910600
C	-2.12220600	0.16578600	-4.42618600
C	-0.88837400	0.17771000	-3.78257200
C	1.21126200	2.68687400	-1.31568600
C	0.18758500	2.56917700	-0.36311900
C	-0.00940400	3.50039800	0.65027300
C	0.83615200	4.60698400	0.73303800
C	1.85722500	4.76605600	-0.20038400
C	2.02897900	3.81631700	-1.20583500
H	0.57673500	-0.41830800	-1.11006100
H	2.13838100	0.24573100	-0.63258800
H	1.56536900	-1.89869400	-2.71415100
H	2.66668900	-1.98744200	-1.34353800
F	3.34477400	-5.96111500	-6.52561600
F	4.11927500	-5.98258300	-3.90608100
F	4.22613000	-3.71150200	-2.51002800
F	2.67194900	-3.59749300	-7.71559200
F	2.76269500	-1.32692500	-6.37417000
F	6.34237100	-1.74893500	-4.44652000
F	8.70468700	-2.00257400	-3.20049200
F	8.92003000	-1.46313900	-0.53278700
F	6.72637600	-0.63974500	0.86896600
F	4.35877400	-0.37362500	-0.35385000
F	3.01312300	4.04684600	-2.08604600
F	2.66340500	5.82448600	-0.13596700
F	0.66442900	5.50459400	1.69382200
F	-0.99267200	3.34153600	1.53286300
F	-0.65757000	1.52391500	-0.41054600
F	-0.33380800	3.73703600	-3.44764500
F	-2.71805200	3.73501500	-4.66270500
F	-3.92866300	1.38070800	-5.33405900
F	-2.69303800	-0.98889900	-4.76272000
F	-0.31441200	-1.01755900	-3.54281900
C	2.31260500	3.19460200	-4.99228900
C	4.89805500	2.06087600	-7.50494700
C	3.49287600	3.30729700	-5.71319100
C	4.52614500	4.31773000	-5.28067200
H	5.55012100	3.97918200	-5.44978900
H	4.37958000	5.22123400	-5.88923800
H	4.40855900	4.59483400	-4.23150600
H	6.17013400	0.41167900	-6.92152600
H	4.44070900	0.02020200	-6.94314000
H	5.74040600	2.75337000	-7.39296000
H	4.85738400	1.78904400	-8.56538600
H	3.45773000	3.63326000	-7.79009000
H	2.73562500	2.09770500	-7.31506100
H	2.14400600	3.87037900	-4.16401400
H	1.42993900	2.78925300	-5.47596400
C	7.17200800	2.55959000	-2.38700600
H	6.86263300	2.74413600	-1.35645900

H	8.01517000	1.86085400	-2.40885300
H	7.53153300	3.50333400	-2.81742400
INT10-endo			
C	6.73979500	-0.90221400	-4.49474100
C	5.44079000	-0.54715700	-5.26933100
C	6.59436400	-1.32681600	-3.02184800
C	4.70112400	0.55561900	-4.57775100
C	5.15195900	1.85729700	-4.67064500
H	5.96912100	2.14064500	-5.32951400
Ir	3.21628800	0.30874200	-3.30709200
C	4.58367700	2.78019500	-3.75079600
O	3.69466900	2.33926400	-2.95077400
P	1.41088900	0.88606800	-4.92160800
P	2.47608800	-1.84143500	-3.66552400
C	2.01230300	1.73388800	-6.44430800
C	2.31887200	3.09705600	-6.36296800
C	2.86424000	3.81292200	-7.42201200
C	3.12273200	3.15930300	-8.62632300
C	2.84268000	1.79848800	-8.74390400
C	2.30436600	1.10797500	-7.66011000
C	-0.05665400	1.89315900	-4.45680700
C	-1.14679200	2.03579200	-5.32670900
C	-2.26175900	2.80085200	-5.00428300
C	-2.30445400	3.45471500	-3.77102500
C	-1.23790900	3.33779700	-2.88096800
C	-0.13183400	2.56574200	-3.23120600
C	0.62766200	-0.74087000	-5.43063600
C	1.60712200	-1.91710400	-5.31120100
C	1.09446100	-2.11306800	-2.47195200
C	0.80150000	-1.14935900	-1.50762400
C	-0.20926300	-1.29924300	-0.56595900
C	-0.97265400	-2.46810700	-0.58334200
C	-0.71785800	-3.45755700	-1.53572200
C	0.30392000	-3.26754900	-2.46217200
C	3.47925200	-3.37602400	-3.49451400
C	4.03103000	-4.06086300	-4.58432500
C	4.81252400	-5.20281300	-4.43230700
C	5.06592200	-5.69698700	-3.15367600
C	4.54047000	-5.03898900	-2.04152800
C	3.76560000	-3.89872000	-2.22494100
H	1.08430800	-2.87193000	-5.41696700
H	2.36479200	-1.86106600	-6.09313300
H	-0.21457800	-0.87086500	-4.74206300
H	0.21666600	-0.68678400	-6.43817400
F	-3.36218700	4.18496400	-3.44658900
F	-3.27963300	2.91005300	-5.85463900
F	-1.13192900	1.42142500	-6.52187500
F	-1.27819900	3.96068000	-1.70570400
F	0.87097200	2.49106000	-2.34955600
F	2.11071200	3.75795000	-5.20889700
F	3.15718900	5.10497800	-7.27698700
F	3.64461000	3.82379000	-9.64875900
F	3.09528600	1.16119800	-9.88466900
F	2.08446300	-0.20970400	-7.82891400
F	3.29219000	-3.29492600	-1.12216400
F	4.78050300	-5.49814600	-0.81717000
F	5.80870500	-6.78214200	-2.99481900
F	5.31524800	-5.81736200	-5.49921100
F	3.83800100	-3.62001900	-5.84049800
F	1.51948000	0.00767400	-1.46844800
F	-0.45465500	-0.34827100	0.32938500
F	-1.94650000	-2.63392500	0.29859200
F	-1.45034800	-4.56577300	-1.55567200
F	0.52614600	-4.23602100	-3.36369200
C	6.13671800	-0.24329700	-2.00752400
H	4.82605000	-1.44143400	-5.39309500
H	5.72740900	-0.21691900	-6.27802700
H	7.23198100	-1.71138200	-5.04927000
H	7.41504600	-0.03886800	-4.54837000
H	5.93570500	-2.20226300	-2.94623600
C	4.61505000	-0.17919300	-1.77169700
H	6.48093900	0.73313100	-2.37352100
H	4.40579500	0.62144600	-1.04802600
H	4.29680000	-1.12077000	-1.31052100
H	7.58637800	-1.68165300	-2.71465700
C	6.82469500	-0.48351000	-0.64702000
H	7.91578100	-0.43933500	-0.74468100
H	6.52286600	0.26728300	0.09167200
H	6.56448100	-1.47064500	-0.24388300

C	4.96814600	4.22631800	-3.66521000
H	4.68871600	4.63731800	-2.69289600
H	6.04037800	4.36149200	-3.83602600
H	4.43384800	4.78703500	-4.44304100

INT10-*exo*

C	0.99205300	2.64701500	-7.16477900
C	1.39098000	3.64698000	-4.98148800
C	2.20718700	2.00777900	-6.50331100
C	2.70349900	0.83825600	-6.98242900
H	2.30496300	0.48286800	-7.93348800
Ir	3.00838700	0.46913500	-3.46474900
H	1.57202200	0.62718800	-4.04099500
C	3.74730200	-0.00821300	-6.44507500
O	3.97823900	-0.17887000	-5.22170300
P	2.24734400	-1.75256400	-2.78782400
P	2.30721800	1.10998600	-1.42558000
C	3.29927000	-2.99910600	-1.92664700
C	4.67796400	-2.81112300	-1.78125700
C	5.49415400	-3.75208900	-1.15780300
C	4.92982500	-4.92627900	-0.66149200
C	3.55797300	-5.15202100	-0.79130100
C	2.76955300	-4.19320900	-1.41830700
C	1.47965300	-2.75945100	-4.12769800
C	0.12209100	-3.06358000	-4.27447900
C	-0.36754900	-3.75091700	-5.38473200
C	0.50715800	-4.15562500	-6.39153600
C	1.86866300	-3.87866800	-6.27196000
C	2.32926200	-3.20582300	-5.14737400
C	0.91792100	-1.35078200	-1.53858500
C	1.45379100	-0.31140400	-0.54097600
C	1.23453800	2.59439600	-1.24438400
C	1.75303600	3.88615300	-1.09547100
C	0.93658500	5.01093200	-1.01451000
C	-0.44744100	4.86427100	-1.10155400
C	-0.99920100	3.59553400	-1.27673600
C	-0.15640400	2.49121200	-1.35177900
C	3.76890300	1.43162500	-0.35995100
C	3.64666800	1.77536100	0.99002600
C	4.75292000	2.00481500	1.80079200
C	6.03346000	1.88287400	1.25636200
C	6.19446300	1.53110200	-0.08422600
C	5.06488300	1.30986500	-0.86583400
H	0.65365200	0.05466500	0.10573500
H	2.21867300	-0.75509800	0.10553100
H	0.07334500	-0.93753600	-2.09128000
H	0.57036800	-2.24493900	-1.01716600
F	0.04705400	-4.79778500	-7.45794600
F	-1.66804200	-4.01651900	-5.48664500
F	-0.77468700	-2.69741600	-3.34708100
F	2.72151100	-4.23740900	-7.23549700
F	3.65033300	-2.97409600	-5.05728300
F	5.26682800	-1.69900900	-2.24775200
F	6.80215800	-3.53445000	-1.03363600
F	5.69551600	-5.82883200	-0.06348000
F	3.01783200	-6.27214800	-0.31733500
F	1.45457100	-4.44305500	-1.53342900
F	5.27087300	0.96321300	-2.15862600
F	7.41257500	1.40542500	-0.60291000
F	7.09809100	2.09377700	2.01695100
F	4.60049700	2.33226600	3.08032400
F	2.42352400	1.89110700	1.53087400
F	3.07983400	4.08625500	-1.04329100
F	1.47246100	6.21980800	-0.86565100
F	-1.23543800	5.92835200	-1.03035600
F	-2.31750500	3.44518900	-1.37843900
F	-0.72892700	1.28913300	-1.55252600
C	3.49962600	2.37683200	-4.20318200
C	0.60158900	3.85895100	-6.28639600
C	2.70509600	2.93684400	-5.40213700
C	3.63246400	3.96977900	-6.12467700
H	3.14012900	4.47764000	-6.95984300
H	3.94427800	4.73288500	-5.40291600
H	4.52981600	3.47684100	-6.51141900
H	1.20070500	2.92401900	-8.20535100
H	0.18656500	1.90314300	-7.20707000
H	0.89261600	4.79774000	-6.76682500
H	-0.47779500	3.91162500	-6.11888000
H	1.59414000	4.58096600	-4.44633700
H	0.83300600	2.98919300	-4.30238900

H	4.55390000	2.25314600	-4.49133600
H	3.49166500	3.15407200	-3.43072100
C	4.56570800	-0.84060300	-7.40033400
H	5.56481800	-1.00024400	-6.98749000
H	4.09630100	-1.82817500	-7.50562200
H	4.63285500	-0.38394800	-8.39056600

INT11-endo

C	6.81496700	-0.81279300	-5.04488900
C	5.27601000	-0.66192300	-5.03477600
C	7.33886800	-1.18418600	-3.65282200
C	4.83142200	0.35339700	-3.99075500
C	5.10843700	1.75961600	-4.31243000
H	5.85844700	2.02307900	-5.05250900
Ir	2.80891200	0.38231700	-3.25224800
C	4.41220800	2.71406100	-3.61598100
O	3.36673900	2.32079100	-2.90379000
P	1.39883400	0.87424100	-4.91444300
P	2.10043400	-1.80346000	-3.51937800
C	2.18100900	1.81939700	-6.27412400
C	2.28905200	3.21594600	-6.22235800
C	2.93749100	3.94829300	-7.21227300
C	3.51420100	3.28390600	-8.29387900
C	3.44568400	1.89239500	-8.36792900
C	2.79361900	1.18799500	-7.36235100
C	-0.07461300	1.87255500	-4.46289800
C	-1.02108700	2.20741400	-5.44018500
C	-2.14767300	2.96897300	-5.15522700
C	-2.35240200	3.41449900	-3.84727200
C	-1.43650000	3.09197500	-2.84673700
C	-0.31434100	2.32833400	-3.16219100
C	0.63840700	-0.69589500	-5.59698100
C	1.49273800	-1.92765300	-5.27471300
C	0.65525200	-2.23576400	-2.45621300
C	0.31870000	-1.46470300	-1.33716900
C	-0.74613300	-1.79000500	-0.50109500
C	-1.50522700	-2.92819000	-0.77219400
C	-1.19008400	-3.73351800	-1.86837400
C	-0.11872700	-3.38282700	-2.68293300
C	3.21828500	-3.23391600	-3.20150200
C	3.58164100	-4.22285100	-4.12299300
C	4.43434100	-5.27175700	-3.78203600
C	4.94670400	-5.35461500	-2.48786600
C	4.60381600	-4.38771000	-1.54089800
C	3.74591000	-3.35904900	-1.90955000
H	0.93397100	-2.84706300	-5.45012700
H	2.38374400	-1.94437300	-5.90371300
H	-0.34046100	-0.76760200	-5.11040600
H	0.46349400	-0.60788100	-6.67105600
F	-3.42410300	4.13742200	-3.55686000
F	-3.02418000	3.26917200	-6.10944500
F	-0.84257900	1.78533500	-6.70418600
F	-1.63794500	3.50609200	-1.59909200
F	0.52904300	2.03577200	-2.16396700
F	1.77406500	3.90091000	-5.19216300
F	3.01759600	5.27298500	-7.11960600
F	4.13665900	3.96948400	-9.24158000
F	4.00667600	1.24673700	-9.38715100
F	2.77986800	-0.15539300	-7.46187400
F	3.42793500	-2.43785500	-0.98025100
F	5.09674500	-4.45042200	-0.30670200
F	5.76165800	-6.34605300	-2.15796700
F	4.75883700	-6.19096300	-4.68688300
F	3.12607400	-4.19403400	-5.38347500
F	1.03345400	-0.37120600	-1.01928900
F	-1.03746500	-1.02676300	0.54841600
F	-2.52308000	-3.24860500	0.01309900
F	-1.90649400	-4.82462600	-2.12320400
F	0.17405100	-4.19675300	-3.71157700
C	6.89003900	-0.19083400	-2.57160100
H	4.84555300	-1.64378100	-4.80398300
H	4.91358700	-0.37553100	-6.02717700
H	7.09593100	-1.57682600	-5.77899100
H	7.27760200	0.12461000	-5.37904100
H	6.98643200	-2.19192300	-3.38343700
C	5.32973500	-0.05206500	-2.55837700
H	7.28666400	0.80266600	-2.82224100
H	5.07810500	0.70619500	-1.80705500
H	4.93173900	-1.01526900	-2.22414900
H	8.43460000	-1.23504800	-3.66633700

C	7.39075600	-0.58710500	-1.17850700
H	8.48490600	-0.64520300	-1.16602500
H	7.08613100	0.14161500	-0.41902800
H	7.00249400	-1.56891600	-0.87900700
C	4.71571400	4.18314800	-3.58597300
H	4.90454100	4.49741700	-2.55259800
H	5.59464600	4.42436300	-4.18921300
H	3.85818600	4.76203500	-3.94504200

INT11-exo

C	1.41604700	3.28004800	-6.96339300
C	2.84644200	4.43961600	-5.42136300
C	2.41741100	2.27568800	-6.40954900
C	2.33281400	0.96793300	-6.75038600
H	1.60913200	0.71720300	-7.52647100
Ir	2.89540400	0.20905100	-3.20545800
H	2.96163300	2.17773400	-3.68275400
C	3.13377200	-0.18557800	-6.34149800
O	3.47183400	-0.45964200	-5.16881500
P	2.26600300	-1.83576800	-2.65555400
P	2.27042800	0.80607500	-1.14582500
C	3.60888700	-3.04771100	-2.27221600
C	4.97339300	-2.74539000	-2.36872500
C	5.95941200	-3.67906900	-2.05142600
C	5.59616200	-4.95709700	-1.63375000
C	4.24659000	-5.29742000	-1.53356900
C	3.28550100	-4.34695100	-1.85525700
C	1.26322100	-2.68493400	-3.95370800
C	-0.12217500	-2.50092500	-4.06923800
C	-0.87574000	-3.09218500	-5.07975400
C	-0.24347900	-3.87991400	-6.03988800
C	1.13721800	-4.05792800	-5.98040300
C	1.86395800	-3.46296600	-4.95346100
C	1.27623800	-1.80571500	-1.07614600
C	1.87164400	-0.73088500	-0.16097500
C	0.79836800	1.93449100	-1.10941000
C	0.96046400	3.25059100	-1.55570500
C	-0.08928300	4.15532300	-1.65268300
C	-1.37077300	3.75201400	-1.27899700
C	-1.57632300	2.45084300	-0.82444500
C	-0.50139700	1.56691700	-0.74884100
C	3.44320100	1.68446000	-0.02146400
C	3.05067300	2.03108200	1.27867200
C	3.89853000	2.67766700	2.17108200
C	5.19522400	2.99748000	1.76620100
C	5.62377700	2.66560600	0.48236200
C	4.75116100	2.01784500	-0.38988700
H	1.21634300	-0.51409900	0.68277900
H	2.84073500	-1.05323400	0.23806100
H	0.24647500	-1.56078400	-1.32803200
H	1.28751900	-2.78970600	-0.60269000
F	-0.94813500	-4.43901900	-7.01528300
F	-2.19075700	-2.89295000	-5.13924900
F	-0.78863600	-1.71432600	-3.20819600
F	1.76181600	-4.77876100	-6.91134800
F	3.19603400	-3.64060400	-4.97917800
F	5.39929000	-1.54279100	-2.77305200
F	7.24691000	-3.35177500	-2.14971400
F	6.52977100	-5.84900200	-1.33028400
F	3.89040300	-6.51767100	-1.13835200
F	1.99347200	-4.71324700	-1.76016000
F	5.22428800	1.72423500	-1.61119500
F	6.86119000	2.96770300	0.09285100
F	6.01875700	3.61380300	2.60346600
F	3.48487900	2.98673600	3.39771800
F	1.81056000	1.73133300	1.70342700
F	2.18336900	3.67954400	-1.93516500
F	0.12512900	5.39063400	-2.10664400
F	-2.38837200	4.59992800	-1.36295100
F	-2.79560700	2.05382000	-0.46751100
F	-0.77415600	0.32396600	-0.31412000
C	3.89766300	2.43591100	-4.25278400
C	2.01176600	4.67105800	-6.68791600
C	3.48497300	3.03305600	-5.60918200
C	4.75616700	3.14257100	-6.49582700
H	4.54373900	3.61800900	-7.45784700
H	5.51484200	3.74421200	-5.98263700
H	5.18182000	2.15337400	-6.69608100
H	1.16872600	3.09462200	-8.01373700
H	0.48032700	3.15742500	-6.39695400

H	2.64880100	4.98966700	-7.52019000
H	1.24360700	5.43793800	-6.55721000
H	3.60939600	5.20678100	-5.25359300
H	2.19488500	4.43283000	-4.53724500
H	4.60091800	1.60570900	-4.35843900
H	4.38791000	3.18633100	-3.62724700
C	3.55911000	-1.15021500	-7.42039000
H	4.45426800	-0.75323000	-7.91834000
H	3.80286800	-2.12340500	-6.99031500
H	2.78947700	-1.25274000	-8.19179400

TS1b

C	3.69917300	3.16023100	-4.53038400
C	4.46915500	3.70121600	-5.52659700
H	4.31496500	4.71752500	-5.88054300
Ir	4.03104500	1.03754900	-4.42909400
H	4.43834000	2.43425100	-3.60490100
C	5.48234200	2.87367600	-6.13770000
O	5.54436800	1.66060200	-5.79694800
P	4.71149600	-1.19961400	-4.60628400
P	2.63053600	0.26346300	-2.82295800
C	6.53449100	-1.35635500	-4.45252300
C	7.35742700	-1.12480400	-5.56333300
C	8.74583100	-1.15436300	-5.47736400
C	9.35313300	-1.40919000	-4.24846500
C	8.56561900	-1.62733000	-3.11849300
C	7.17962200	-1.59087400	-3.23282600
C	4.29826600	-2.11163300	-6.14277600
C	4.51309600	-3.49153500	-6.24211200
C	4.20606900	-4.21034500	-7.39203400
C	3.66856800	-3.53584900	-8.49023500
C	3.44676600	-2.16013300	-8.42823800
C	3.76463900	-1.46654800	-7.26365800
C	3.87370100	-2.19704400	-3.26303100
C	3.41444400	-1.28372800	-2.11850700
C	0.98908700	-0.36988100	-3.38104500
C	0.11537100	-1.01779800	-2.49527400
C	-1.10171200	-1.55238300	-2.89651800
C	-1.48132500	-1.44994000	-4.23674300
C	-0.64186000	-0.81644900	-5.14947700
C	0.57408800	-0.29131400	-4.71599300
C	2.32051800	1.33329900	-1.35088900
C	1.09046100	1.90693900	-0.99953800
C	0.94159200	2.72167900	0.12079500
C	2.04315400	2.99728300	0.92865100
C	3.28821500	2.46088800	0.60255900
C	3.40797200	1.65088400	-0.52202900
H	2.70806900	-1.79979100	-1.46344700
H	4.26911400	-0.96233200	-1.52236500
H	3.01201900	-2.66338200	-3.75301800
H	4.51756500	-2.99811300	-2.89860600
F	3.36781500	-4.20512600	-9.59417900
F	4.41757600	-5.52238900	-7.45069000
F	5.03351400	-4.15685400	-5.19762500
F	2.93937500	-1.51849900	-9.47839900
F	3.55300900	-0.14188300	-7.25573300
F	6.81732700	-0.85681100	-6.76080100
F	9.49041300	-0.93266700	-6.55893300
F	10.67559900	-1.43766500	-4.15233600
F	9.13717800	-1.86385600	-1.94015000
F	6.46583500	-1.78374600	-2.10903700
F	4.63346200	1.17759300	-0.80755600
F	4.35201400	2.72789500	1.35571000
F	1.91032700	3.77344100	1.99490800
F	-0.24739500	3.24208900	0.41408100
F	-0.00730300	1.71246900	-1.74631800
F	0.44239100	-1.11934600	-1.19526000
F	-1.90110000	-2.15428600	-2.01993500
F	-2.63932400	-1.95616400	-4.63710600
F	-0.99508900	-0.72000200	-6.42899100
F	1.34164500	0.29513000	-5.64910600
C	2.60773100	3.97020100	-3.88117200
H	2.71253900	3.90637000	-2.79112200
H	2.74016700	5.02599800	-4.15117800
C	1.17332300	3.53127800	-4.25754200
H	1.01259100	2.49966600	-3.93439900
H	0.48092000	4.14926400	-3.67394000
C	0.84336600	3.64784600	-5.74688100
H	0.97707700	4.69196000	-6.07146900
H	1.57326400	3.06877800	-6.33153100

C	-0.54800900	3.19457500	-6.14862700
C	-0.83126900	3.27215100	-7.62957400
H	-0.71520100	4.29968600	-7.99992000
H	-0.12800700	2.65073200	-8.20083400
H	-1.84631300	2.94051100	-7.86531800
C	-1.46979700	2.76327300	-5.27903800
H	-1.29540200	2.71424500	-4.20829700
H	-2.45781200	2.46123800	-5.61630500
C	6.45054400	3.40423700	-7.14794500
H	5.90800600	3.83822300	-7.99691500
H	7.04922300	4.21146900	-6.70747400
H	7.10889100	2.60949400	-7.50199000

TS6-endo

C	5.56715200	0.98067500	-6.55635000
C	3.38347700	2.05454700	-7.41368100
H	6.19018300	0.08338800	-6.68601800
H	6.22332900	1.83139500	-6.79433200
C	5.19705300	1.05500400	-5.09979500
C	6.16397800	1.38140500	-4.16971600
H	7.19575000	1.59554200	-4.44111200
Ir	3.36325200	0.81383600	-4.28312000
H	2.57170000	0.65976300	-5.77247200
C	5.75197500	1.42181300	-2.81250500
O	4.52779400	1.17412700	-2.53653200
P	3.62397200	-1.53873200	-3.83242600
P	1.41171100	0.61838000	-2.77515300
C	5.32412700	-1.90293800	-3.21377700
C	6.36645400	-2.15184800	-4.11270000
C	7.68029700	-2.35638400	-3.70502400
C	7.99340000	-2.28723000	-2.34783600
C	6.98834600	-2.00587600	-1.42465700
C	5.68109800	-1.81598900	-1.86592500
C	3.34953200	-2.89459700	-5.06051300
C	3.69115100	-4.21569000	-4.73088100
C	3.48222800	-5.28655600	-5.59316000
C	2.88666700	-5.05913000	-6.83359900
C	2.50428600	-3.76731700	-7.18571000
C	2.72774100	-2.71443600	-6.30071300
C	2.41802800	-2.08894100	-2.49884600
C	1.76635400	-0.92424600	-1.75312600
C	-0.29858200	0.45461000	-3.47703100
C	-1.29339700	1.44030500	-3.39748700
C	-2.54042800	1.29461600	-4.00373700
C	-2.82697700	0.14563700	-4.73761000
C	-1.85404500	-0.84419700	-4.86592200
C	-0.62247000	-0.66763000	-4.24660300
C	1.18482500	1.80537200	-1.37270000
C	0.23680900	1.53931100	-0.37166000
C	0.06476300	2.34903500	0.74333300
C	0.86249000	3.48448300	0.89032000
C	1.80863400	3.78944000	-0.08302700
C	1.95644100	2.95967400	-1.19493200
H	0.85660700	-1.25190500	-1.24522000
H	2.45437900	-0.54862000	-0.98899700
H	1.66526500	-2.67838400	-3.02112600
H	2.92540300	-2.75158200	-1.79573500
F	2.67339900	-6.06892800	-7.66575300
F	3.83354500	-6.51886900	-5.23496200
F	4.23153100	-4.49236700	-3.53223600
F	1.91386500	-3.53978400	-8.35794900
F	2.29758700	-1.50522700	-6.69783300
F	6.11679100	-2.18146700	-5.43543600
F	8.63473400	-2.59680300	-4.60206900
F	9.24417100	-2.46588800	-1.94089400
F	7.27830000	-1.89638700	-0.12849500
F	4.76250200	-1.51196800	-0.93017100
F	2.87634600	3.33298000	-2.09132800
F	2.57327000	4.87333900	0.04371400
F	0.71499800	4.26871900	1.94948100
F	-0.85207500	2.05095000	1.66116900
F	-0.57188000	0.46904500	-0.48046300
F	-1.07718100	2.59598600	-2.75186600
F	-3.45160900	2.25766800	-3.89178700
F	-4.00903600	0.00131800	-5.32133200
F	-2.09758500	-1.94135300	-5.58076500
F	0.29741600	-1.63846800	-4.43131400
C	2.92575400	2.80867700	-4.98172200
H	3.82676600	3.41031200	-5.07837600
H	2.15190600	3.30213500	-4.40176100

C	4.41051100	0.92217400	-7.56007200
C	2.49228000	2.05044800	-6.15075700
C	1.00025200	2.05392800	-6.46521600
H	0.70869500	1.20446700	-7.09073400
H	0.39045700	2.06081500	-5.56075000
H	0.78469900	2.97266500	-7.02487500
H	4.83006400	0.97339900	-8.57118300
H	3.89709200	-0.04060200	-7.48535300
H	2.71819400	2.01935600	-8.28312500
H	3.89798200	3.02290900	-7.45191800
C	6.66215100	1.76047300	-1.66763300
H	7.71465500	1.63798700	-1.93421700
H	6.50343000	2.80859100	-1.38212600
H	6.42346200	1.14477600	-0.79554400

TS6-exo

C	5.23618100	0.93429900	-6.72056500
C	3.60045200	2.67244800	-7.16950600
C	5.05972000	1.59075800	-5.37221600
C	6.10742000	1.66674300	-4.49629500
H	7.09688000	1.31409800	-4.78667300
Ir	3.17896100	1.35412500	-3.93782700
H	2.14825100	0.78432200	-4.98987900
C	5.93801600	2.19545700	-3.15213500
O	4.78710200	2.25697100	-2.66206900
P	3.60587900	-0.88753800	-3.24596600
P	1.40433700	1.34098000	-2.49281400
C	5.23780500	-1.12625600	-2.41093700
C	6.38087000	-1.36195000	-3.18370500
C	7.65027800	-1.49402900	-2.62801600
C	7.80800600	-1.37432400	-1.24755000
C	6.69604500	-1.11539900	-0.44657700
C	5.44007400	-0.98915400	-1.03484100
C	3.53078600	-2.38181700	-4.33939900
C	3.81182200	-3.65119300	-3.81030100
C	3.74204000	-4.81604800	-4.56687500
C	3.36081500	-4.73886100	-5.90639100
C	3.05323200	-3.50034900	-6.46381000
C	3.13403100	-2.35031100	-5.68044600
C	2.25073300	-1.34921500	-2.03742900
C	1.60589100	-0.13762900	-1.36326100
C	-0.24184300	1.27259700	-3.32804500
C	-0.75691700	2.44485800	-3.89498000
C	-1.96839600	2.48056900	-4.57704100
C	-2.71062300	1.30745200	-4.71184600
C	-2.22944800	0.11983300	-4.16422700
C	-1.01294400	0.11849100	-3.48614600
C	1.09354300	2.65902000	-1.22763500
C	0.00121700	2.51751600	-0.35595900
C	-0.30620900	3.45205600	0.62618000
C	0.49859000	4.58268300	0.76722500
C	1.59358000	4.75740000	-0.07438900
C	1.87721500	3.80429400	-1.05190200
H	0.65097900	-0.40616300	-0.90945600
H	2.25881900	0.24250500	-0.57165800
H	1.51174300	-1.86902300	-2.65134500
H	2.61774500	-2.05749300	-1.29259700
F	3.28414400	-5.83983200	-6.64152900
F	4.02576600	-5.99491500	-4.01873700
F	4.15708400	-3.78128600	-2.51745300
F	2.67510000	-3.41479800	-7.73814600
F	2.80287300	-1.19594100	-6.28167900
F	6.27687500	-1.46343500	-4.52220800
F	8.70732100	-1.71892900	-3.40797500
F	9.01134500	-1.49329100	-0.70000300
F	6.83816600	-0.98585600	0.87052500
F	4.40668400	-0.72254600	-0.21590100
F	2.94549900	4.03809700	-1.82030300
F	2.37070800	5.83158200	0.05435900
F	0.22279100	5.48323400	1.70055000
F	-1.35360600	3.27067800	1.42697200
F	-0.80179100	1.44185000	-0.44898900
F	-0.06913100	3.59628400	-3.78987000
F	-2.41592200	3.62052000	-5.09896000
F	-3.86754200	1.32215900	-5.36078400
F	-2.92909300	-1.00614100	-4.28841200
F	-0.60196400	-1.05919500	-2.98022500
C	2.80290100	3.24263500	-4.82446600
C	4.77817600	1.92674700	-7.80078400
C	3.95949800	3.06629400	-5.73007700

C	4.97250000	4.21770200	-5.63184100
H	5.88671700	4.03523000	-6.20174500
H	4.48368600	5.11280700	-6.03706100
H	5.23418600	4.43121000	-4.59298600
H	6.26715800	0.59307100	-6.86802500
H	4.59222700	0.04952600	-6.74817500
H	5.58910300	2.62185500	-8.04613000
H	4.49457600	1.42193100	-8.72861400
H	3.33916800	3.58333200	-7.72155400
H	2.71319400	2.03045900	-7.15070000
H	2.89804100	4.05914300	-4.11232700
H	1.83725600	3.25186200	-5.32533500
C	7.12177500	2.66114900	-2.35235900
H	6.81477500	2.94140600	-1.34337100
H	7.88496200	1.87514500	-2.30447200
H	7.59131000	3.52440600	-2.84080000

TS7-endo

C	6.97318500	-1.02073500	-4.59038900
C	5.50209100	-0.78031000	-4.98303200
C	7.11812600	-1.29923200	-3.09296300
C	4.86658300	0.36623300	-4.23722700
C	5.33114700	1.68125000	-4.48311600
H	6.21485000	1.87497200	-5.08306400
Ir	3.03227800	0.35844200	-3.44919900
C	4.60636500	2.70323500	-3.87526700
O	3.52446500	2.37956200	-3.23461600
P	1.34245700	0.88964700	-4.92769000
P	2.28416400	-1.81206300	-3.69285500
C	2.01356900	1.84130900	-6.35019100
C	2.17736900	3.23027800	-6.25946700
C	2.76151800	3.98038000	-7.27570200
C	3.20691800	3.34407800	-8.43301300
C	3.07396400	1.96119400	-8.55298700
C	2.49550500	1.23567400	-7.51606200
C	-0.12108100	1.87121300	-4.40575100
C	-1.20350500	2.06051100	-5.27533900
C	-2.32192500	2.80570300	-4.92121900
C	-2.37354200	3.39186700	-3.65467500
C	-1.31326900	3.22795500	-2.76428500
C	-0.20357200	2.47669100	-3.14631000
C	0.57338000	-0.69852000	-5.56216300
C	1.50624300	-1.90501400	-5.38169100
C	0.87923100	-2.17093200	-2.55055100
C	0.53049300	-1.28820900	-1.52503100
C	-0.50723500	-1.54601000	-0.63457100
C	-1.23244600	-2.73104700	-0.76128200
C	-0.91530500	-3.64039300	-1.77261300
C	0.12796700	-3.35002400	-2.64623100
C	3.33830500	-3.30464300	-3.44955800
C	3.73424400	-4.19003400	-4.45848400
C	4.52911800	-5.30424300	-4.19684700
C	4.94940600	-5.56207600	-2.89288000
C	4.57691300	-4.70002800	-1.85990100
C	3.78389300	-3.59691000	-2.15338000
H	0.96164900	-2.84197800	-5.51582300
H	2.31624300	-1.87382000	-6.11121900
H	-0.33634800	-0.82470800	-4.96528400
H	0.26645400	-0.59797200	-6.60373700
F	-3.43412500	4.10270800	-3.29862300
F	-3.33306900	2.96070100	-5.77229200
F	-1.17325200	1.51272200	-6.50289500
F	-1.36304700	3.78781700	-1.55838600
F	0.79280400	2.35845800	-2.26289600
F	1.79056100	3.89093100	-5.15864000
F	2.91035600	5.29599100	-7.13167800
F	3.76582000	4.04670000	-9.40875400
F	3.50741600	1.33911900	-9.64704600
F	2.42186200	-0.09929800	-7.67389300
F	3.44280800	-2.78311600	-1.13608400
F	4.97463700	-4.93534000	-0.61264700
F	5.70589900	-6.61885200	-2.63512000
F	4.88604500	-6.11862300	-5.18582600
F	3.36740800	-3.98833200	-5.73257900
F	1.20433700	-0.12954300	-1.36711000
F	-0.81009900	-0.67413800	0.32304000
F	-2.22641600	-2.99182700	0.07483900
F	-1.60890900	-4.76772900	-1.89719900
F	0.41054400	-4.24715000	-3.60537600
C	6.57522100	-0.16617800	-2.20846000

H	4.94351700	-1.70365300	-4.81141200
H	5.43145800	-0.55879400	-6.05682000
H	7.35930100	-1.86271100	-5.17690400
H	7.57793000	-0.14710600	-4.86401400
H	6.60803800	-2.23970600	-2.83430100
C	5.03153100	-0.01187600	-2.22433400
H	7.01155500	0.77915300	-2.55477400
H	4.78292300	0.86607500	-1.62494500
H	4.59838600	-0.90616800	-1.77438800
H	8.17841100	-1.45313300	-2.85796700
C	6.99652200	-0.37181600	-0.74031100
H	8.08934900	-0.38606300	-0.65910200
H	6.62318500	0.43225900	-0.09684200
H	6.61865100	-1.32295300	-0.34562500
C	4.97413000	4.15799800	-3.89615400
H	5.08676200	4.52514900	-2.86958900
H	5.90453200	4.33352600	-4.44102000
H	4.16842100	4.74074000	-4.35600900

TS7-exo

C	1.19747100	3.09153300	-7.27262800
C	1.88908300	4.09810000	-5.18339100
C	2.23558500	2.20114000	-6.59737300
C	2.43303700	0.93739700	-7.04540600
H	1.92267700	0.66874400	-7.97022700
Ir	2.83975800	0.32621000	-3.44238700
H	2.09184300	1.65198200	-3.97291600
C	3.28521900	-0.12876800	-6.54152700
O	3.50976600	-0.38094100	-5.33508900
P	2.14717200	-1.80486500	-2.79710300
P	2.28770900	0.92829800	-1.34463700
C	3.38130400	-2.94838700	-2.03736700
C	4.73589600	-2.60914200	-1.95639700
C	5.68189700	-3.46384400	-1.39596100
C	5.27662700	-4.70132400	-0.89766500
C	3.93283900	-5.07501000	-0.96051600
C	3.01198300	-4.19898400	-1.52522100
C	1.38783100	-2.85001900	-4.10638400
C	0.01336600	-3.04917600	-4.27895700
C	-0.50101300	-3.80187900	-5.33306700
C	0.36632900	-4.37581400	-6.26067700
C	1.74196100	-4.19201100	-6.12424700
C	2.22706700	-3.44337300	-5.05832800
C	0.92104900	-1.53931100	-1.42513900
C	1.52839000	-0.53312300	-0.43912900
C	1.11626900	2.35189200	-1.18855900
C	1.58346500	3.67141100	-1.22274200
C	0.73330100	4.77154300	-1.16698600
C	-0.64362700	4.56905800	-1.08230800
C	-1.14942200	3.27044700	-1.06467200
C	-0.27154900	2.19108500	-1.12532500
C	3.65614400	1.40317600	-0.20017500
C	3.38939800	1.64914600	1.15315300
C	4.38183600	1.99661100	2.06223600
C	5.70031000	2.10742800	1.61784600
C	6.00492100	1.87196900	0.27850200
C	4.98813700	1.52768000	-0.61050200
H	0.78926800	-0.20356300	0.29203300
H	2.35788100	-0.98610600	0.11522200
H	0.01371800	-1.13354500	-1.86971200
H	0.67092100	-2.48041800	-0.92916600
F	-0.11426300	-5.08676000	-7.27301100
F	-1.81581800	-3.96875900	-5.45690900
F	-0.87472900	-2.51369100	-3.42820100
F	2.58444900	-4.71885200	-7.01357400
F	3.55960200	-3.28865700	-4.96707600
F	5.17506800	-1.42889300	-2.42448800
F	6.96280200	-3.10497100	-1.33184300
F	6.16738000	-5.52301200	-0.35899400
F	3.54495500	-6.25439800	-0.48143400
F	1.72567600	-4.58597800	-1.57366300
F	5.34328100	1.32850300	-1.88752700
F	7.26145200	1.97986600	-0.14865500
F	6.66140000	2.43528900	2.47078300
F	4.08515400	2.21942800	3.34033700
F	2.12776600	1.55083500	1.60918500
F	2.90196500	3.92145000	-1.33270300
F	1.22878300	6.00708400	-1.20444400
F	-1.46868400	5.60686400	-1.03133300
F	-2.46270100	3.06506700	-0.99775500

F	-0.81851000	0.96227100	-1.12818900
C	3.47511600	2.30744600	-4.25233700
C	1.22159300	4.44075000	-6.52442800
C	2.95099000	3.01567500	-5.52221200
C	4.17787600	3.68613500	-6.21154100
H	3.89486400	4.27155900	-7.09133000
H	4.67007400	4.36009200	-5.50143300
H	4.90348100	2.93038200	-6.52883500
H	1.38105700	3.18834100	-8.34889900
H	0.21779100	2.60513500	-7.17386400
H	1.81354700	5.18041800	-7.07256400
H	0.22083300	4.86305200	-6.40060200
H	2.33894900	4.96278800	-4.68433700
H	1.14463500	3.67066100	-4.49585800
H	4.46833000	1.88040000	-4.43353600
H	3.56819000	3.04361900	-3.45410300
C	3.92831300	-1.04454900	-7.55423500
H	4.86586200	-0.58679300	-7.89846100
H	4.16302600	-2.01055200	-7.10360300
H	3.29554100	-1.17726700	-8.43667600
2b'			
C	-2.83950800	0.12476000	-1.28974200
C	-1.09241700	1.89306400	-1.42445700
C	-2.53048700	2.47189300	-1.60283700
C	-3.38492500	1.30314000	-2.11108000
C	-0.29217400	2.07203000	-2.73743900
H	-0.15902300	3.14178400	-2.94161300
H	0.69267700	1.60950900	-2.65259300
H	-0.81719600	1.62974100	-3.59228000
C	-1.34731400	0.39692000	-1.16676700
C	-0.49162300	-0.61459100	-0.89490800
H	-0.93891400	-1.60069400	-0.76346800
C	0.97987900	-0.60552100	-0.74042500
O	1.70257300	0.36665600	-0.93312300
C	-0.36585100	2.59749300	-0.26296400
H	0.65642000	2.23177400	-0.15693200
H	-0.33251300	3.67773300	-0.45386900
H	-0.89772300	2.44276200	0.68363600
H	-2.53716800	3.34155600	-2.26880500
H	-2.91618800	2.80595300	-0.62979100
H	-3.21184600	1.13186900	-3.18095700
H	-4.45979800	1.45943800	-1.97325900
H	-3.05577700	-0.86380500	-1.70893600
H	-3.28703000	0.14863300	-0.28345100
C	1.58885800	-1.93901600	-0.32178100
H	1.16863700	-2.27352600	0.63539900
H	1.35828200	-2.71726900	-1.06071600
H	2.67143800	-1.83427600	-0.22931800
3b'			
C	-3.63807300	-2.79404600	-0.13661300
C	-2.11908600	-2.79891200	-0.41010900
C	-1.59139100	-1.34176700	-0.51977400
C	-3.45980300	-0.50626000	0.96345200
C	-4.01972000	-1.94138400	1.08327300
H	-0.51305000	-1.32732500	-0.67298700
H	-4.15572700	-2.39580500	-1.02170200
H	-3.99822200	-3.82263400	-0.00235600
H	-3.68811000	0.07581700	1.86363400
H	-3.96383400	-0.00872800	0.11969200
H	-3.63309900	-2.40112400	2.00166300
H	-5.11074300	-1.90016100	1.19067000
H	-2.06502000	-0.87442500	-1.39791000
C	-1.97256000	-0.52449300	0.69106400
C	-1.11528100	0.12528300	1.50980200
H	-1.54062000	0.67812400	2.34747000
C	0.36347600	0.19789300	1.40978400
O	1.03742400	-0.37734800	0.56275100
H	-1.95541700	-3.27224500	-1.38801300
C	-1.32948800	-3.60831500	0.63073600
H	-1.68783000	-4.64400600	0.67480200
H	-0.26359300	-3.62778600	0.37818600
H	-1.41553100	-3.18040400	1.63591900
C	1.03727500	1.06445900	2.46725500
H	0.66448600	2.09562400	2.41658400
H	0.80920100	0.69186900	3.47429000
H	2.11777000	1.05831000	2.31187700