

Supporting Information

A DFT Study on Rhodium(III)-Catalyzed Synthesis of Indanones from N- methoxybenzamides via C-H activation Reaction

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1. Free energy profile of the entire reaction

Because the energy barrier of intramolecular hydrogen transfer is too high and the 5a product cannot be obtained in dichloroethane, we believe that the correct route for this reaction is the catalytic cyclization step, Claisen condensation reaction and retro-Claisen condensation reaction.

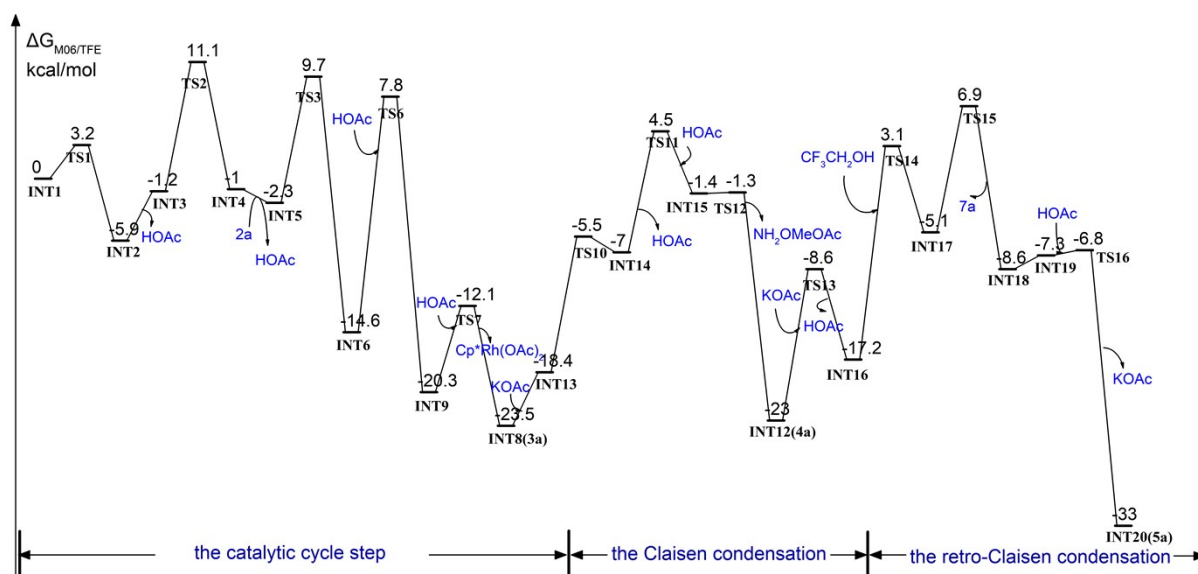
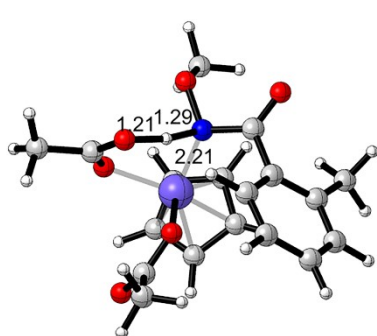
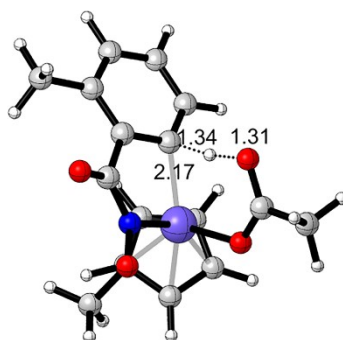


Figure S1. Calculated free energy profile for the entire reaction. The energy values are calculated using M06 method in 2,2,2-trifluoroethanol.

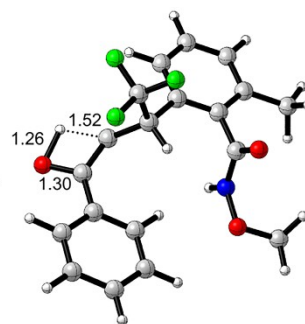
2. 3D Optimized Structures:



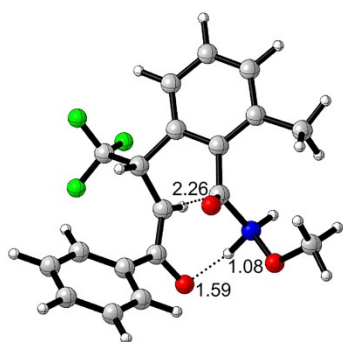
TS1



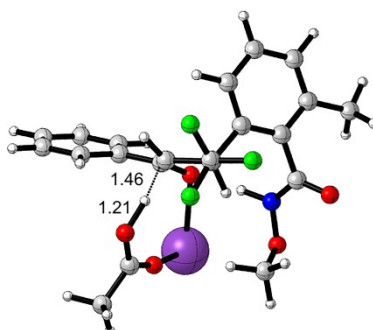
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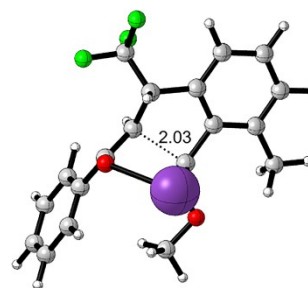
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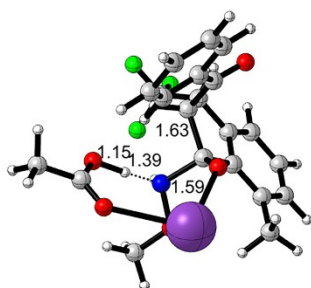
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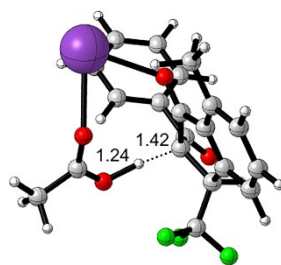
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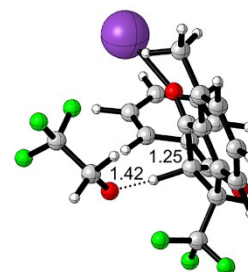
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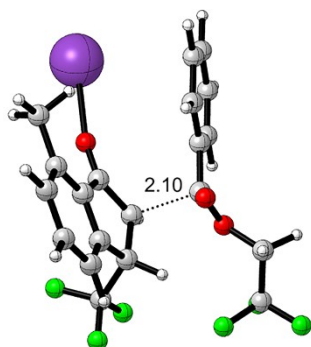
TS12



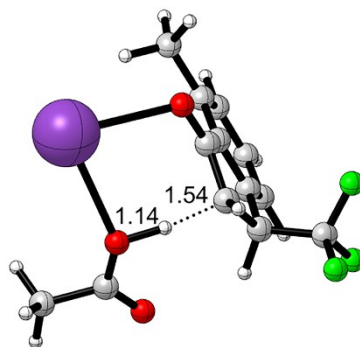
TS13



TS14



TS15



TS16

3. Calculated absolute energies, and free energies of all structures at the M06-D3/ma-TZVP-SDD-SMD(2,2,2-trifluoroethanol) //B3LYP-D3/6-31G+(d)-SDD-PCM(2,2,2-trifluoroethanol) level of theory

Geometry	E _(elec-B3LYP-D3) ¹	G _(corr-B3LYP-D3) ²	H _(corr-B3LYP-D3) ³	E _(solv-M06) ⁴
2a	-760.064660	0.107925	0.161270	-759.905437
INT1	-1315.959711	0.316130	0.406648	-1315.557912
TS1	-1315.950704	0.314602	0.401348	-1315.551339
INT2	-1315.965408	0.316228	0.405712	-1315.567412
INT3	-1086.826775	0.257545	0.336159	-1086.471554
TS2	-1086.810362	0.255563	0.330408	-1086.449943
INT4	-1086.832272	0.258906	0.336262	-1086.472558
INT5	-1617.794392	0.339401	0.431273	-1617.32296
TS3	-1617.770918	0.341072	0.430233	-1617.305487
INT6	-1617.809246	0.341750	0.432681	-1617.34501
TS4	-1846.929826	0.395875	0.496827	-1846.418047
INT7	-1846.939881	0.400592	0.502270	-1846.424942
TS5	-2076.004762	0.449452	0.566639	-2075.472085
INT8(3a)	-1314.871254	0.282740	0.365336	-1314.531412
Cp[*]Rh(OAc)₂	-761.172984	0.140294	0.203929	-760.968557
HOAc	-229.103276	0.034005	0.067016	-229.063683
KOAc	-828.506628	0.016593	0.056946	-828.452774
TS6	-1846.893465	0.394111	0.495727	-1846.391229
INT9	-1846.947047	0.400483	0.502389	-1846.442372
TS7	-2076.058881	0.452395	0.566793	-2075.510909
TS8	-1314.769489	0.275699	0.358452	-1314.429091
INT10	-1314.846829	0.284895	0.364977	-1314.511486
TS9	-1314.802679	0.288394	0.363479	-1314.456198
INT11	-1314.867891	0.281300	0.365465	-1314.517605

INT12(4a)	-1143.828275	0.218782	0.289154	-1143.520992
INT13	-2143.402943	0.324796	0.391953	-2143.001367
TS10	-2143.380235	0.318996	0.418707	-2142.974913
INT14	-2143.380490	0.324176	0.423279	-2142.982541
TS11	-1914.235273	0.268773	0.326423	-1913.866437
INT15	-2143.374510	0.325682	0.423755	-2142.975052
TS12	-2143.373549	0.322483	0.419610	-2142.972714
NH2OMe	-171.032782	0.042714	0.073791	-170.988252
TS13	-1972.330723	0.254031	0.342323	-1971.969439
INT16	-1743.222008	0.203475	0.278362	-1742.902916
CF ₃ CH ₂ OH	-452.797332	0.027122	0.063839	-452.794271
TS14	-2196.013898	0.248270	0.338997	-2195.682420
INT17	-2196.018795	0.248411	0.343965	-2195.695711
TS15	-2196.004757	0.251741	0.342486	-2195.679946
7a	-797.219021	0.107517	0.161448	-797.080330
INT18	-1398.786267	0.119432	0.180470	-1398.599428
INT19	-1627.910815	0.172379	0.248541	-1627.679995
TS16	-1627.910006	0.170174	0.244767	-1627.676951
INT20(5a)	-1028.074477	0.178579	0.247783	-799.250232

¹The electronic energy calculated by B3LYP-D3(BJ) in 2,2,2-trifluoroethanol solvent.

²The thermal correction to Gibbs free energy calculated by B3LYP-D3(BJ) in 2,2,2-trifluoroethanol solvent.

³The thermal correction to enthalpy calculated by B3LYP-D3(BJ) in 2,2,2-trifluoroethanol solvent.

⁴The electronic energy calculated by M06 in 2,2,2-trifluoroethanol solvent.

**4. Calculated absolute energies, and free energies of all structures
at the M06-D3/ma-TZVP- SDD-SMD(1,2-dichloroethane)**

**//B3LYP-D3/6-31G+(d)-SDD-PCM(1,2-dichloroethane) level of
theory**

Geometry	E _(elec-B3LYP-D3) ¹	G _(corr-B3LYP-D3) ²	H _(corr-B3LYP-D3) ³	E _(solv-M06) ⁴
2a	-760.063770	0.107935	0.161299	-759.909513
INT1	-1315.957089	0.317117	0.406740	-1315.552452
TS1	-1315.947980	0.314851	0.401386	-1315.547301
INT2	-1315.962295	0.316368	0.405750	-1315.562506
INT3	-1086.822690	0.258256	0.336173	-1086.4646
TS2	-1086.807517	0.255525	0.330435	-1086.448718
INT4	-1086.829992	0.259034	0.336289	-1086.472691
INT5	-1617.791151	0.339423	0.431329	-1617.324278
TS3	-1617.767614	0.341343	0.430291	-1617.305701
INT6	-1617.805576	0.341489	0.432654	-1617.344761
TS4	-1846.926993	0.396019	0.496904	-1846.418068
INT8	-1846.937471	0.400989	0.502392	-1846.425283
INT9	-2076.000493	0.453171	0.570973	-2075.45845
TS5	-2075.999582	0.450694	0.567300	-2075.454728
INT8(3a)	-1314.873832	0.282647	0.365526	-1314.534576
Cp*Rh(OAc)₂	-761.170955	0.144422	0.202991	-760.961856
HOAc	-229.102560	0.034088	0.067044	-229.065121
KOAc	-828.502833	0.018350	0.056009	-828.445443
TS6	-1846.888837	0.393941	0.495713	-1846.436416
INT9	-1846.943703	0.400780	0.502429	-1846.436416
TS7	-2076.055129	0.452109	0.566837	-2075.505866
TS8	-1314.767254	0.275501	0.358491	-1314.433594
INT10	-1314.847490	0.281748	0.364759	-1314.513004

TS9	-1314.800085	0.288508	0.363451	-1314.457307
INT11	-1314.866140	0.281533	0.365529	-1314.522329
INT12(4a)	-1143.827151	0.219058	0.289189	-1143.52729
NH₂OMe	-171.032200	0.042586	0.073808	-170.988029
INT13	-2143.397213	0.324714	0.425087	-2142.996562
TS10	-2143.375862	0.318820	0.418794	-2142.976100
INT14	-2143.380491	0.324180	0.423280	-2142.983830
TS11	-1914.235273	0.268773	0.352761	-1913.876010
INT15	-2143.371156	0.325755	0.423813	-2142.972888
TS12	-2143.369923	0.323975	0.419846	-2142.971090

¹The electronic energy calculated by B3LYP-D3(BJ) in 1,2-dichloroethane solvent.

²The thermal correction to Gibbs free energy calculated by B3LYP-D3(BJ) in 1,2-dichloroethane solvent.

³The thermal correction to enthalpy calculated by B3LYP-D3(BJ) in 1,2-dichloroethane solvent.

⁴The electronic energy calculated by M06 in 1,2-dichloroethane solvent.

5. Cartesian coordinates of the structures (optimization in 2,2,2-trifluoroethanol)

1a				C	-3.77673100	-1.37208600	0.13973000
O	-3.04993100	-0.82126000	0.05531600	H	-4.76760700	0.20419700	1.23805000
C	-0.87477800	0.05323100	0.48715200	H	-2.55405800	-2.73871500	-1.00116900
C	0.58211100	-0.16137100	0.18817800	H	-4.59958100	-2.07343300	0.24840400
C	1.11231800	-1.45895800	0.26068600	C	0.86510400	1.01978100	-0.41253100
C	1.41287500	0.93913100	-0.11962500	H	1.49794600	1.71707200	-0.95502500
C	2.47287900	-1.68535700	0.03838900	INT1			
H	0.46348500	-2.29285000	0.51695100	Rh	1.07975700	-0.40492700	-0.46356500
C	2.77182300	0.68596800	-0.35273700	C	1.23241300	-0.78010400	-2.62392800
C	3.30302600	-0.60591700	-0.27246400	H	0.94468500	-0.00927500	-3.32508100
H	2.87582600	-2.69176100	0.10783700	C	2.52037800	-0.91369100	-2.03207200
H	3.42588100	1.51753000	-0.60424300	H	3.37671100	-0.28375400	-2.23253200
H	4.36261900	-0.76546100	-0.45423500	C	2.47113300	-2.00944300	-1.09162700
O	-1.28864600	0.86683300	1.31642200	H	3.29369000	-2.36800600	-0.48776900
C	-3.84368900	0.09220200	-0.73122800	C	1.14561900	-2.52487900	-1.10533700
H	-4.87083200	-0.06493100	-0.39446600	H	0.76801600	-3.32731800	-0.48553600
H	-3.53497000	1.12449900	-0.54004800	C	0.36174200	-1.75774800	-2.03519200
H	-3.75474900	-0.14375500	-1.79758900	H	-0.68115900	-1.91205800	-2.27504300
C	0.87494100	2.34887600	-0.21269000	O	-0.08291200	1.29065200	-0.64588000
H	-0.04287800	2.39280300	-0.81011200	O	1.20017000	2.29588000	-2.21698800
H	0.62508300	2.74046600	0.77929500	C	0.23782700	2.27400600	-1.43564500
H	1.61310800	3.01483200	-0.67028500	C	-0.70655100	3.46159400	-1.29766200
N	-1.70727700	-0.71089300	-0.27918700	H	-0.47346700	3.99060400	-0.36553100
H	-1.37204700	-1.46651700	-0.86667000	H	-0.58089200	4.14881300	-2.13769600
2a				H	-1.74474700	3.12474800	-1.23048800
C	-0.56355600	1.44195700	-0.28453100	O	0.53292600	-1.18429700	2.57463500
O	-0.80151700	2.65113600	-0.28445600	C	-1.37598200	-1.19765500	1.17060900
C	1.38837700	-0.04647600	0.20094600	C	-2.43550600	-0.27532600	0.69523100
H	0.79791300	-0.74168500	0.78964400	C	-2.45725400	1.05794800	1.14656700
C	2.84917600	-0.37335700	0.15849000	C	-3.45768100	-0.75381100	-0.16550200
F	3.38815600	-0.38427400	1.40849900	C	-3.48244200	1.92253400	0.77306700
F	3.05397600	-1.61636000	-0.35876500	H	-1.67717400	1.43148700	1.80025800
F	3.58073600	0.49007600	-0.58206300	C	-4.45729400	0.14838300	-0.55406600
C	-1.65039000	0.43480000	-0.13199000	C	-4.48197600	1.46629800	-0.08931900
C	-2.82142400	0.81383200	0.55043700	H	-3.49017000	2.94455400	1.13983600
C	-1.56007400	-0.85440300	-0.68776200	H	-5.23735100	-0.19325200	-1.22984000
C	-3.87322600	-0.08870700	0.69533700	H	-5.28040000	2.13360500	-0.40306300
H	-2.88690100	1.81284500	0.97027900	O	-1.52064000	-2.39618700	1.34105800
C	-2.62472200	-1.74949300	-0.55799000	C	1.40642000	-2.29379100	2.33137100
H	-0.67659700	-1.14943200	-1.24439400	H	1.73018400	-2.59209400	3.33131100

H	0.87497500	-3.11853400	1.85254300	H	-4.86689900	0.27448100	-1.41975400
H	2.27267900	-1.98207900	1.74177300	H	-4.76167900	2.59056600	-0.55516400
C	-3.51738300	-2.17421800	-0.67723500	O	-1.88296300	-2.17147600	1.88887000
H	-2.53697900	-2.54799400	-0.98491300	C	0.95740600	-3.06046200	1.65206200
H	-3.87296700	-2.85480700	0.10426500	H	1.36297600	-3.62860400	2.49322900
H	-4.20023800	-2.24273700	-1.52954300	H	0.04644200	-3.54286900	1.29053000
O	2.40131000	0.75717800	0.67597100	H	1.71004400	-3.00064900	0.85981900
C	2.08532800	1.63910100	1.57101800	C	-3.43000500	-1.88717900	-0.68010600
O	0.95404800	1.80338900	2.07427000	H	-2.48234600	-2.43202900	-0.69638800
C	3.24267400	2.53458800	1.98647100	H	-4.10480200	-2.45846200	-0.03117700
H	4.18653300	1.98256300	1.98662500	H	-3.85194800	-1.89449700	-1.69063300
H	3.33128200	3.35023600	1.25799000	O	2.50054200	0.34471600	0.64360400
H	3.05553900	2.96715600	2.97235200	C	2.30657100	0.98095200	1.72335400
N	-0.06817000	-0.61396400	1.41381100	O	1.18835000	1.01854300	2.34969000
H	-0.03861600	0.40198200	1.63881900	C	3.45297000	1.76779100	2.30428800
TS1				H	4.40164000	1.45281100	1.86608800
Rh	0.92056100	-0.39367800	-0.58184900	H	3.29314200	2.82864200	2.07583000
C	0.78823200	-0.30162100	-2.77221900	H	3.47579800	1.65746900	3.39178700
H	0.55838600	0.63641100	-3.25751800	N	-0.04049600	-0.87458300	1.34460600
C	2.08981600	-0.73984000	-2.40901200	H	0.43077200	0.21573600	1.85184000
H	3.01256500	-0.20856100	-2.59968800	INT2			
C	1.95951500	-2.00112900	-1.71196600	Rh	-0.63928600	0.13200800	0.78123700
H	2.77288500	-2.59337600	-1.31444800	C	-0.04228000	1.51788000	2.42874300
C	0.57701100	-2.31444300	-1.64256600	H	-0.17287300	2.58681100	2.34940100
H	0.14755200	-3.18520200	-1.16527400	C	-0.97753300	0.59334000	2.93669200
C	-0.16591500	-1.24801000	-2.26372700	H	-1.95822100	0.83125500	3.32886800
H	-1.23936500	-1.19396100	-2.37885300	C	-0.43940700	-0.74289600	2.76860100
O	0.14044600	1.49824500	-0.30414600	H	-0.92041200	-1.66632600	3.06308800
O	1.49825200	2.51912800	-1.80453500	C	0.85346000	-0.61263100	2.18455400
C	0.61555200	2.53489200	-0.93431200	H	1.50855300	-1.42914300	1.91865900
C	-0.03781300	3.83372100	-0.47876800	C	1.08750600	0.77482200	1.90818100
H	0.20786900	4.01310700	0.57429000	H	1.96643100	1.19501800	1.44015100
H	0.31451100	4.67216800	-1.08362800	O	-0.92812900	1.50619000	-0.80487500
H	-1.12667900	3.74980100	-0.54768100	O	0.15405000	3.29728300	0.03216600
O	0.68760600	-1.76439400	2.19692600	C	-0.53328800	2.75874700	-0.83674900
C	-1.42448000	-1.14938100	1.38689100	C	-0.97656600	3.49193300	-2.09293900
C	-2.31314800	-0.10369800	0.78835800	H	-2.05414500	3.37366200	-2.24908700
C	-2.24202600	1.21306900	1.26387600	H	-0.72676000	4.55232200	-2.02227800
C	-3.27954200	-0.46964100	-0.17382000	H	-0.46940000	3.05788900	-2.96275000
C	-3.13387500	2.18181900	0.80338900	O	-1.18561700	-2.05277400	-1.19666700
H	-1.48777600	1.48123900	1.99575000	C	1.03723700	-1.47449700	-1.36074300
C	-4.13434400	0.53074800	-0.65760100	C	2.18001600	-0.56912700	-0.97848800
C	-4.07474500	1.84057500	-0.17133400	C	2.18831100	0.75948500	-1.42108400
H	-3.07978700	3.19628800	1.18799300	C	3.26732900	-1.08175600	-0.24234800

C	3.25939000	1.60398100	-1.12335300	H	-4.25062900	1.43470900	2.74584200
H	1.33847600	1.12923700	-1.98413600	O	-1.36245800	2.03461800	-1.21406400
C	4.32501000	-0.21365100	0.06807300	C	0.74461800	1.93796900	-0.22135400
C	4.32835200	1.11627300	-0.36511000	C	1.64853800	0.97497400	0.51181400
H	3.24891100	2.63577200	-1.46360300	C	1.06426400	0.20193900	1.54404900
H	5.15900300	-0.58794600	0.65802500	C	2.99623400	0.78845000	0.14687500
H	5.16126200	1.76640000	-0.10980700	C	1.82503000	-0.77592000	2.21516800
O	1.22984300	-2.38889600	-2.19219100	H	0.08073500	0.49390700	1.92753700
C	-1.28338900	-3.22192800	-0.37635000	C	3.72593500	-0.18947700	0.83707500
H	-2.11331500	-3.80314100	-0.78808300	C	3.15461300	-0.97020700	1.85499100
H	-0.35688500	-3.80533100	-0.42336200	H	1.37187300	-1.35608300	3.01385900
H	-1.50439200	-2.94465500	0.66182500	H	4.76426900	-0.35984100	0.56174000
C	3.32339600	-2.52870300	0.19616500	H	3.75750900	-1.72025400	2.35921400
H	2.33002200	-2.94310800	0.39783500	O	0.99776100	3.15190400	-0.34109400
H	3.76619200	-3.15273600	-0.59012200	C	-1.45354200	1.84327800	-2.62977300
H	3.93629900	-2.64299600	1.09673600	H	-1.66655300	0.79279400	-2.86437800
O	-2.72188200	-0.40051500	0.44999000	H	-2.28565700	2.47056000	-2.95947000
C	-3.40602900	-0.32484000	-0.58869300	H	-0.52515600	2.15327600	-3.12425700
O	-3.07398700	0.38899600	-1.63708600	C	3.62633700	1.57877400	-0.97533100
C	-4.69262200	-1.08281500	-0.71975800	H	3.02337100	1.51380400	-1.88913100
H	-5.04045700	-1.41200300	0.26027500	H	3.69601200	2.64064000	-0.71750000
H	-5.45161500	-0.47257300	-1.21611500	H	4.63089500	1.20739100	-1.19974600
H	-4.50415600	-1.96379600	-1.34548800	TS2			
N	-0.13759600	-1.21563600	-0.74832200	Rh	-0.90537500	-0.47824600	-0.09782300
H	-2.19908800	0.88050400	-1.46051600	N	0.00395800	1.15143700	-0.95563300
INT3				C	-0.49954600	-2.41918400	-1.04377600
Rh	-0.52472600	-0.72762300	-0.16747700	H	0.50595000	-2.78851200	-1.19528400
N	-0.32238900	1.26403700	-0.68624100	C	-1.33620800	-2.67284400	0.10870300
C	1.02214400	-2.06704900	-0.99056100	H	-1.06511000	-3.25299400	0.98008900
H	2.07893100	-1.89013300	-0.84023000	C	-2.56572700	-2.00361800	-0.10215100
C	0.16295000	-2.85889000	-0.12047600	H	-3.38532500	-1.95291900	0.60388700
H	0.47680900	-3.36149500	0.78486400	C	-2.52851600	-1.35087100	-1.38685600
C	-1.14423700	-2.81667200	-0.64017400	H	-3.32845600	-0.77646200	-1.83450900
H	-2.02393600	-3.26224900	-0.19419100	C	-1.25549000	-1.63658800	-1.96945400
C	-1.13501700	-1.97027300	-1.81493300	H	-0.89648200	-1.27657700	-2.92481800
H	-1.98748900	-1.74812100	-2.44331100	O	-1.93400300	0.89706500	1.14025300
C	0.23180500	-1.56826900	-2.05304500	O	-0.15483600	1.24661800	2.45718100
H	0.57335900	-0.92706300	-2.85497200	C	-1.36784600	1.46289000	2.12377800
O	-2.33702800	-0.26129800	0.72172200	C	-2.16297300	2.44976200	2.94334600
O	-1.74404200	1.35380100	2.19434400	H	-1.71552100	3.44378200	2.83348700
C	-2.58823900	0.67533900	1.58837200	H	-3.20340800	2.47925300	2.61598400
C	-4.07932200	0.90184000	1.80744400	H	-2.10813400	2.17612400	4.00166900
H	-4.46534000	1.51149200	0.98100400	O	-0.74315100	2.21842800	-1.46791500
H	-4.62615600	-0.04560000	1.80518600	C	1.32388700	1.39656600	-0.77594400

C	1.94705500	0.27365500	0.00829900	C	1.21388000	-1.39777300	-1.82951000
C	1.05404600	-0.44843200	0.84201000	H	1.33664700	-1.46700000	0.83764800
C	3.31220800	-0.05732500	-0.06722300	C	3.52772300	-0.68700700	-1.66017900
C	1.54649900	-1.51915500	1.61414200	C	2.55498300	-1.52866700	-2.20702200
H	0.32588000	0.36532900	1.61827500	H	0.46717500	-2.06456100	-2.25202700
C	3.75751600	-1.13937200	0.71358100	H	4.56555100	-0.80096000	-1.96470400
C	2.89713600	-1.85958200	1.54999900	H	2.84272500	-2.28957300	-2.92914500
H	0.87763200	-2.05872300	2.27964600	O	2.06038900	2.20715600	1.31950100
H	4.80671400	-1.42224800	0.66419200	C	-0.89446400	3.33497600	1.31799300
H	3.28585600	-2.68111800	2.14659100	H	-1.55302300	3.26139300	0.44460900
O	1.94639300	2.40273800	-1.17036000	H	-1.40719200	3.86517200	2.12540200
C	-1.12284300	1.96822300	-2.82473300	H	0.02792600	3.85953900	1.04746600
H	-1.77573800	1.08905200	-2.88674400	C	4.29938300	1.16522900	-0.14270500
H	-1.67206200	2.85732900	-3.14565700	H	4.10524500	2.22687400	-0.32477300
H	-0.23836600	1.82159600	-3.45597900	H	4.37281500	1.05161600	0.94344000
C	4.29286400	0.67427200	-0.95511700	H	5.26350000	0.90068200	-0.59030100
H	3.90508800	0.78765500	-1.97222300	INT5			
H	4.48289400	1.68609600	-0.58220100	Rh	-0.14846300	0.63402000	0.55876900
H	5.24514100	0.13517400	-0.99984200	N	-1.48495800	1.27890400	-0.84334300
INT4				C	-0.39267000	1.16775100	2.77109000
Rh	-1.06024900	-0.08402200	-0.27139500	H	-1.15620700	0.70027200	3.37636600
N	0.01318900	1.22545100	0.86464700	C	0.94185700	0.70786300	2.60048500
C	-1.88109000	-0.15865000	-2.32203000	H	1.39174600	-0.14331100	3.09330100
H	-1.23048800	-0.40470700	-3.15059800	C	1.60225200	1.63278800	1.72308200
C	-2.64299900	-1.07015100	-1.55350100	H	2.63945600	1.58480000	1.42295900
H	-2.71320500	-2.13907200	-1.70796100	C	0.67809500	2.64193600	1.33814300
C	-3.38594300	-0.30149300	-0.56582600	H	0.88709100	3.47483600	0.68098100
H	-4.04944300	-0.72030700	0.18074800	C	-0.57105300	2.34226000	1.96992600
C	-3.05467300	1.04962200	-0.70607800	H	-1.48877300	2.90760100	1.87587500
H	-3.42432000	1.86373900	-0.09691200	O	-1.08747300	2.13630700	-1.86932900
C	-2.04671800	1.15307700	-1.74867800	C	-2.72658100	0.73615200	-0.95494300
H	-1.61514500	2.07017100	-2.12889000	C	-2.91928700	-0.30153300	0.10433000
O	-0.95058300	-1.50058800	1.40716600	C	-1.79491600	-0.58304800	0.89076500
O	1.23613000	-2.02335200	1.64729900	C	-4.12567700	-1.01611300	0.29699500
C	-0.03849800	-2.07708000	2.01004500	C	-1.82877400	-1.57299100	1.87140300
C	-0.28289500	-2.90881500	3.23309100	C	-4.14647100	-2.00078600	1.29537200
H	0.22724900	-2.44945600	4.08707900	C	-3.01767500	-2.28057800	2.07172500
H	-1.35228200	-2.97518100	3.43381100	H	-0.95115700	-1.80513100	2.46776100
H	0.14050200	-3.90840000	3.09254100	H	-5.06302000	-2.56133300	1.46380000
O	-0.59914000	2.03056900	1.83675100	H	-3.06237900	-3.05434600	2.83475300
C	1.34771100	1.39244000	0.69812200	O	-3.56379400	1.06150900	-1.81539600
C	1.84225600	0.42014000	-0.33836100	C	2.53232300	0.59687700	-1.10387200
C	0.84726800	-0.41484900	-0.90005800	O	2.76099000	1.61584500	-1.75784900
C	3.20078700	0.29776200	-0.71412100	C	0.61387300	-1.10637500	-0.54802600

H	1.22538800	-1.71928000	0.10209200	C	-0.89626700	-1.60920600	1.90574900
C	-0.25764100	-1.99540400	-1.39864400	C	-3.22867900	-2.23934700	2.01647400
F	0.55372300	-2.71169900	-2.24446300	C	-1.92834700	-2.31398300	2.52342100
F	-0.94623700	-2.91630000	-0.68756100	H	0.11856400	-1.68518100	2.28426500
F	-1.13613600	-1.34137000	-2.18861200	H	-4.02179200	-2.80063800	2.50410200
C	3.67401000	-0.13674800	-0.46082400	H	-1.71839000	-2.92921300	3.39423800
C	4.92560300	-0.02242100	-1.09599400	O	-3.67804600	0.12676800	-1.66827900
C	3.58300500	-0.90211300	0.71533900	C	2.34209100	0.45316400	-1.27291900
C	6.04871200	-0.66850500	-0.58035300	O	2.67363600	1.27829600	-2.13067000
H	5.00210900	0.56883200	-2.00268900	C	0.36044000	-1.06586300	-0.49733800
C	4.71165300	-1.53292700	1.24200500	H	1.04084000	-1.58510000	0.16768500
H	2.65056000	-0.98154200	1.25827900	C	-0.26517800	-2.12144100	-1.40493100
C	5.94551100	-1.42526000	0.59251800	F	0.74778200	-2.66392200	-2.14301600
H	7.00340700	-0.58031000	-1.09128600	F	-0.84019900	-3.14765400	-0.74222700
H	4.62441200	-2.10519600	2.16118100	F	-1.16828400	-1.64045400	-2.28254300
H	6.82058100	-1.92471400	0.99910200	C	3.41414000	-0.20468700	-0.44776700
C	1.12185300	0.07581900	-1.13084700	C	4.67262300	-0.35832300	-1.05883800
H	0.61131300	0.46185800	-2.00819700	C	3.24827700	-0.66067800	0.87099300
C	-5.36994200	-0.76373600	-0.52363000	C	5.72795600	-0.96469200	-0.37712200
H	-5.68667600	0.28220700	-0.46176800	H	4.80815400	-0.00535400	-2.07607100
H	-5.19427000	-0.96742200	-1.58485000	C	4.30865400	-1.25198900	1.56083300
H	-6.18970100	-1.40078200	-0.17466100	H	2.30648900	-0.52496500	1.38637500
C	-1.46919000	3.49107800	-1.58915300	C	5.54991200	-1.41246800	0.93704600
H	-1.01947700	3.83312500	-0.65063000	H	6.68877700	-1.08619700	-0.86969000
H	-1.08252700	4.08260200	-2.42308300	H	4.16271700	-1.58270000	2.58531500
H	-2.55950400	3.57513900	-1.53554400	H	6.37253300	-1.87967000	1.47147100
TS3				C	0.89672900	0.09138300	-1.19389900
Rh	-0.15183300	1.02739900	0.39738000	H	0.40149400	0.36403500	-2.12244300
N	-1.71816000	1.11419600	-0.92829500	C	-4.97926300	-1.38363700	0.42011300
C	-0.51555200	1.93686700	2.48241200	H	-5.32602100	-0.34871000	0.33864100
H	-1.26591300	1.55117200	3.15979700	H	-5.08271400	-1.82162000	-0.57737200
C	0.85028800	1.49993700	2.39706100	H	-5.63605900	-1.92153400	1.11139400
H	1.31960500	0.76629100	3.03911500	C	-2.14912300	3.18383500	-1.91889900
C	1.49221800	2.24703400	1.36596300	H	-1.52666600	3.73407200	-1.20386800
H	2.52894200	2.15708400	1.07005300	H	-2.09227200	3.66389000	-2.89935800
C	0.52301600	3.11671100	0.77360800	H	-3.18749200	3.15851100	-1.56956500
H	0.70423700	3.82877700	-0.02020900	INT6			
C	-0.71707300	2.92237000	1.48565500	Rh	0.61986700	-1.05484600	-0.10706000
H	-1.65289700	3.42244000	1.27312500	N	2.05724900	-0.04959900	-1.20845000
O	-1.64810800	1.85678500	-2.11229900	C	1.30706200	-2.84910600	1.18071700
C	-2.72165800	0.20309700	-0.87657400	H	2.05104500	-2.76670400	1.96241400
C	-2.50478300	-0.72699400	0.28332900	C	-0.11693400	-2.61090300	1.34198200
C	-1.18650500	-0.81365400	0.78963300	H	-0.60956200	-2.36326500	2.27376600
C	-3.54659800	-1.44981100	0.89750000	C	-0.74605700	-2.80242100	0.08960800

H	-1.80520500	-2.72796500	-0.11363300	H	2.95794100	-1.10572800	-4.13141600
C	0.28787700	-3.04790400	-0.88445800	H	3.78618500	-1.42290800	-2.56906500
H	0.13057900	-3.25684200	-1.93463200	TS4			
C	1.54875300	-3.14098700	-0.17040200	Rh	-0.02559100	-1.51124800	-0.02285600
H	2.51601900	-3.32241400	-0.62025700	N	1.94860200	-0.93703600	-0.74204000
O	2.25098100	-0.00782100	-2.59302500	C	-1.75712300	-2.80208900	-0.55592900
C	2.45453600	1.01639800	-0.50892700	H	-2.67252700	-2.40956600	-0.97267100
C	1.80514800	0.88541300	0.86821400	C	-0.59612900	-3.19122500	-1.30069100
C	0.42775900	1.19672400	1.08860800	H	-0.49462900	-3.18768100	-2.37740500
C	2.65712500	0.57302500	1.97346900	C	0.36103600	-3.73177600	-0.35415200
C	-0.04616500	1.23362000	2.42328500	H	1.34991500	-4.09008500	-0.60426400
C	2.13393300	0.60090300	3.25906800	C	-0.16013800	-3.58283800	0.94012500
C	0.79044400	0.94592900	3.48712600	H	0.34709200	-3.82472400	1.86525600
H	-1.08307800	1.49866200	2.60806600	C	-1.46900800	-2.96348800	0.82588900
H	2.77580800	0.35782700	4.10182700	H	-2.12741100	-2.71025300	1.64652400
H	0.40619700	0.98211600	4.50257500	O	2.31663400	-1.93478100	-1.69842300
O	3.21556600	1.94691900	-0.81270500	C	2.13206600	0.35858400	-1.24774600
C	-2.00019800	-0.21795200	-1.37972300	C	2.07509400	1.41041200	-0.16805900
O	-2.17658200	-0.68219800	-2.51423600	C	0.87568900	1.95145200	0.31457000
C	-0.59475300	1.51436900	-0.01546200	C	3.32078500	1.79178900	0.38541000
H	-1.55682300	1.61589900	0.49053400	C	0.92942600	2.86567000	1.37881600
C	-0.43091000	2.87788200	-0.67830700	C	3.33599300	2.71884800	1.43155700
F	-1.55075400	3.18393600	-1.39264000	C	2.14565900	3.24811000	1.93571200
F	-0.26435700	3.86875300	0.23811300	H	0.00426400	3.28075300	1.76833600
F	0.60712900	2.96065900	-1.54013400	H	4.28782600	3.01408500	1.86569300
C	-3.14733400	-0.25013300	-0.40474300	H	2.16781300	3.95338600	2.76196200
C	-4.44834200	-0.15140200	-0.92817300	O	2.42402800	0.61100500	-2.40938700
C	-2.98569500	-0.38966200	0.98428400	C	-2.24421700	0.05352400	-1.19500200
C	-5.55892000	-0.17722800	-0.08321100	O	-2.62629200	-0.32961900	-2.30892500
H	-4.57552900	-0.04713500	-2.00125200	C	-0.49951800	1.66813700	-0.28228100
C	-4.09660800	-0.43420700	1.82921300	H	-1.22557100	1.83775700	0.51532400
H	-1.99469100	-0.49447400	1.40985500	C	-0.80841700	2.78794600	-1.29860700
C	-5.38624900	-0.32161400	1.29866400	F	-2.07971400	2.70740000	-1.77734500
H	-6.55786600	-0.08737700	-0.50133400	F	-0.69424700	4.03037500	-0.75687100
H	-3.95290100	-0.55765800	2.89915600	F	0.01595500	2.75762000	-2.37586900
H	-6.25061300	-0.34842800	1.95666800	C	-3.26722500	0.24313000	-0.10410100
C	-0.67257000	0.36478600	-1.03436700	C	-4.59999400	0.46853400	-0.48855800
H	-0.17299500	0.59936400	-1.97331900	C	-2.95651500	0.18926800	1.26672900
C	4.10134700	0.21656600	1.72518400	C	-5.59922700	0.64333800	0.47005400
H	4.18333800	-0.57798100	0.97356500	H	-4.83867100	0.51139400	-1.54661700
H	4.65616200	1.07899300	1.33943200	C	-3.95837600	0.35147800	2.22630200
H	4.58453400	-0.12583800	2.64461800	H	-1.94022200	-0.00216100	1.59327400
C	2.82162600	-1.23473600	-3.05512400	C	-5.28095900	0.58253100	1.83208800
H	2.13957800	-2.07238000	-2.86817300	H	-6.62361400	0.82634900	0.15675500

H	-3.70464800	0.29545200	3.28158600	O	2.33185400	0.50877100	-2.37352800
H	-6.05781900	0.71405500	2.58068900	C	-2.23370200	-0.08963900	-1.20708500
C	-0.78680900	0.29895700	-0.94725900	O	-2.62409900	-0.55526000	-2.28673800
H	-0.30682100	0.25448000	-1.92731900	C	-0.52235300	1.61441600	-0.41224100
C	4.61451700	1.18777600	-0.11109100	H	-1.27869100	1.81563700	0.34824400
H	4.65117700	0.11181900	0.09948700	C	-0.82096800	2.66146600	-1.50622600
H	4.73101600	1.31330300	-1.19253200	F	-2.07442700	2.52079500	-2.01663100
H	5.47402600	1.65052300	0.38218900	F	-0.75076200	3.93819100	-1.04183700
C	3.73201000	-2.16272100	-1.67574800	F	0.03746800	2.58359900	-2.55396000
H	4.06115700	-2.47241600	-0.67587300	C	-3.25434600	0.16943400	-0.12850500
H	3.89905200	-2.97607900	-2.38641900	C	-4.58756400	0.36814400	-0.52715400
H	4.28281100	-1.27259500	-1.99723100	C	-2.94237200	0.20304400	1.24253800
O	2.61660100	-1.06030600	1.67602300	C	-5.58737700	0.60218300	0.41815300
H	2.38971200	-1.08266300	0.51661200	H	-4.82682700	0.34270200	-1.58563600
C	1.59086800	-0.62608100	2.32766700	C	-3.94637100	0.42318000	2.18878900
O	0.43405000	-0.53307100	1.82977200	H	-1.92541900	0.03465700	1.57967800
C	1.81863200	-0.17538000	3.74376700	C	-5.26941000	0.62733300	1.78147300
H	2.34137900	0.78757200	3.71524000	H	-6.61189000	0.76369600	0.09344300
H	0.86989000	-0.05409500	4.26870700	H	-3.69315600	0.43293400	3.24580900
H	2.45937500	-0.89087800	4.26699500	H	-6.04670000	0.80478800	2.52018300
INT7				C	-0.77462500	0.20094500	-1.00093500
Rh	0.05200200	-1.55292700	-0.00929700	H	-0.31021600	0.12037100	-1.98694600
N	2.11808400	-0.94261600	-0.58511100	C	4.60028700	1.31974300	0.02928400
C	-1.25443800	-3.00760300	-1.05951100	H	4.69797000	0.28422900	0.37778900
H	-1.86117500	-2.70721900	-1.90144800	H	4.74200300	1.32013700	-1.05674800
C	0.08027500	-3.47648300	-1.12084200	H	5.42004300	1.89020300	0.47464300
H	0.67111100	-3.59703600	-2.01830800	C	4.07554300	-1.97903400	-1.42402600
C	0.52781900	-3.77094400	0.22803800	H	4.48722800	-2.08400200	-0.41370900
H	1.50829900	-4.13357600	0.50571100	H	4.33634200	-2.85444300	-2.02193900
C	-0.51888100	-3.43050800	1.10534900	H	4.45397700	-1.07281700	-1.90508800
H	-0.47707200	-3.46576500	2.18680100	O	2.38659800	-0.92216500	2.14349500
C	-1.62242600	-2.90675900	0.32927700	H	2.47696300	-0.98422200	0.40059500
H	-2.57992500	-2.58829400	0.71815200	C	1.28229600	-0.43957200	2.48871900
O	2.63518300	-1.98699600	-1.38873100	O	0.21248700	-0.44028400	1.76484600
C	2.18051700	0.35615200	-1.17941600	C	1.14477400	0.25642100	3.82963000
C	2.06020500	1.45416200	-0.16211700	H	1.47635700	1.29413500	3.70866200
C	0.81742800	1.97695300	0.22500000	H	0.10703300	0.26304800	4.17140200
C	3.26425900	1.90447500	0.42614100	H	1.78852000	-0.22401100	4.57127800
C	0.79309400	2.95446000	1.23138400	TS5			
C	3.19830200	2.89720400	1.40808000	C	-1.77573700	-0.57072400	-1.96812300
C	1.96833900	3.41478100	1.81734000	H	-2.14157100	0.22248400	-1.33357700
H	-0.16234900	3.35851300	1.55295700	Rh	-0.75171700	-2.23707000	-1.14539000
H	4.11793900	3.25433500	1.86400800	C	-0.46112200	-0.64179400	-2.57975800
H	1.92642300	4.17247400	2.59488000	H	0.35907700	0.06146400	-2.45578900

C	-0.37485300	-1.87239700	-3.27876500	H	-4.93134100	2.51675600	1.44697400
H	0.49421700	-2.25221900	-3.79954500	H	-4.12950400	0.96077500	1.70380700
C	-1.62729500	-2.56843800	-3.10574900	H	-3.51762800	2.41046900	2.50599200
H	-1.84658200	-3.56667800	-3.46490100	C	1.41921100	-2.06866800	0.94840300
C	-2.50140500	-1.75456600	-2.32289700	O	1.08844600	-2.51692500	-0.18290400
H	-3.50122100	-2.00850800	-1.99951900	C	2.29220800	-2.88766800	1.85220900
O	-1.05241400	-0.12195100	3.23909100	H	1.90865500	-2.83764200	2.87560400
C	-1.05903800	1.74409500	1.74664800	H	2.34323100	-3.92254000	1.51185900
C	-1.66141900	2.19195000	0.43177200	H	3.29676200	-2.44896500	1.84942900
C	-0.86830000	2.48492100	-0.69675800	O	1.07553400	-0.90811100	1.39415700
C	-3.07301000	2.31225200	0.37634100	H	0.94410900	-0.10867300	0.66157200
C	-1.51536300	2.86936600	-1.88267700	N	-1.40093100	0.46922500	2.03511000
C	-3.67353600	2.70691600	-0.82619600	H	-1.97716800	-0.11626900	1.42633000
C	-2.90211000	2.97624900	-1.95592700	C	-2.62418900	-2.48617100	1.15013100
H	-0.91706800	3.07974200	-2.76488700	O	-1.50474900	-2.90351300	0.62403400
H	-4.75554900	2.80090700	-0.87306500	C	-3.15442300	-3.37491300	2.25696200
H	-3.37774100	3.26811300	-2.88826500	H	-3.21979800	-4.41223500	1.91362500
O	-0.39159500	2.47078800	2.48786700	H	-2.45459300	-3.35024200	3.10013100
C	2.45567900	0.70020900	-0.81305800	H	-4.13357300	-3.02561200	2.58967000
O	2.38457200	0.58368200	-2.07338100	O	-3.19356200	-1.43169100	0.82217800
C	1.46091800	1.35451900	-0.02548600	INT8(3a)			
C	0.66044300	2.41648500	-0.76759600	C	-2.22258000	-0.00977800	-1.48532200
H	1.73418800	1.62423600	0.99189500	H	-1.94239400	0.76605000	-0.79027100
H	0.89502300	2.26554100	-1.82679300	Rh	-2.09419100	-2.04324300	-0.92280800
C	1.26251700	3.80426800	-0.49719400	C	-1.34557600	-0.68477000	-2.42387600
F	2.59196200	3.83377900	-0.79861400	H	-0.27933600	-0.51640300	-2.52551400
F	0.68827400	4.78039000	-1.26421500	C	-2.10642400	-1.67519700	-3.09237100
F	1.15152600	4.22181400	0.78633700	H	-1.74023400	-2.38384900	-3.82340900
C	3.61318300	0.01489000	-0.12157000	C	-3.46389800	-1.60144900	-2.58820600
C	4.21655400	-1.08808800	-0.74925400	H	-4.26999600	-2.27006300	-2.86483200
C	4.12749500	0.44775400	1.11227400	C	-3.54445700	-0.55732000	-1.63301900
C	5.29167800	-1.75275900	-0.15566400	H	-4.41616300	-0.27222200	-1.06036700
H	3.82196700	-1.42093300	-1.70402000	O	0.27400800	0.83462700	3.47495700
C	5.21061900	-0.20775500	1.70468500	C	0.19475000	2.40235700	1.69528900
H	3.69200100	1.30739700	1.61181200	C	-0.56602100	2.77386000	0.43870000
C	5.79397000	-1.31356700	1.07540100	C	-0.01048200	2.61735100	-0.84960300
H	5.73554600	-2.61360500	-0.64944400	C	-1.85317600	3.33780600	0.60641600
H	5.59888500	0.14547500	2.65654700	C	-0.75854500	3.04432500	-1.95812000
H	6.63210600	-1.82716400	1.53935600	C	-2.56370800	3.75285900	-0.52707900
C	-2.08756700	0.08700100	4.22266100	C	-2.02150300	3.61133600	-1.80400300
H	-1.73413900	-0.42596500	5.12007600	H	-0.34956800	2.91214300	-2.95582000
H	-2.21672700	1.15522400	4.42431000	H	-3.55215300	4.18798400	-0.40389400
H	-3.03228200	-0.35381600	3.88489000	H	-2.58475500	3.92893300	-2.67700900
C	-3.95698000	2.03563400	1.57631600	O	1.15257400	3.06205100	2.11276300

C	2.43569600	-0.34119200	-0.97775800	H	-3.53183500	-0.97607200	3.85272700
O	2.08401100	-0.58698600	-2.13238300	O	-2.66417400	-0.11636400	1.57101300
C	1.81086000	0.82960200	-0.22737500	TS6			
C	1.33138600	1.95319600	-1.16603400	N	-1.57193600	-1.04457600	0.70649600
H	2.47085700	1.22153100	0.54662500	C	-0.17999600	-0.82419600	-2.57191300
H	1.22383400	1.50417500	-2.15843400	H	-0.62830300	0.08456900	-2.95253300
C	2.44723600	2.97896700	-1.36620400	Rh	0.15642500	-1.20543300	-0.42365200
F	3.60089700	2.36315600	-1.75709400	C	1.23945300	-1.07799900	-2.39925700
F	2.14378100	3.87898400	-2.33962200	H	2.03841100	-0.37330700	-2.59149500
F	2.74847100	3.69184200	-0.25816600	C	1.39423300	-2.37568400	-1.87224000
C	3.41049600	-1.22464200	-0.27547400	H	2.32936800	-2.83649300	-1.58170100
C	3.99833200	-2.27870900	-0.99926000	C	0.07867400	-2.95716700	-1.70627900
C	3.74238700	-1.05910000	1.08066100	H	-0.13685900	-3.95204000	-1.34030800
C	4.90277600	-3.14260500	-0.38519700	C	-0.87791000	-2.00412900	-2.18875400
H	3.73329100	-2.40893300	-2.04351000	H	-1.95092900	-2.13373500	-2.19100500
C	4.64517300	-1.92792400	1.69672000	O	-1.67712600	-1.85993900	1.84698700
H	3.28452300	-0.27508400	1.67225600	C	-2.64686500	-0.25627200	0.51004500
C	5.22865800	-2.96852800	0.96612500	C	-2.51925000	0.71942700	-0.63636700
H	5.35126600	-3.95207300	-0.95452200	C	-1.63148500	1.81723100	-0.61756700
H	4.88747500	-1.79565600	2.74739800	C	-3.38695000	0.51571700	-1.73437000
H	5.93118800	-3.64343600	1.44777200	C	-1.62396400	2.69343000	-1.71545200
C	-0.40623600	1.36242600	4.63222700	C	-3.32975500	1.39668700	-2.82085900
H	0.10318600	0.91746800	5.49006800	C	-2.45697100	2.48532700	-2.81333600
H	-0.31901300	2.45346200	4.66418400	H	-0.94226000	3.54008700	-1.71544900
H	-1.46078100	1.06484200	4.62434200	H	-3.97702700	1.22701500	-3.67785800
C	-2.48034000	3.49708300	1.97557400	H	-2.42421000	3.16777200	-3.65821700
H	-3.33344800	4.18049100	1.92849900	O	-3.70373500	-0.29586500	1.16913900
H	-2.83916700	2.53331600	2.35486800	C	1.98443500	1.86153500	0.40951300
H	-1.76970100	3.89406500	2.70827500	O	2.07119800	2.98527400	0.90815300
C	0.38121900	-2.78535700	0.55276100	C	0.66432100	1.15643200	0.25736600
O	-0.40904000	-3.08285000	-0.44810500	C	-0.56411500	2.08948300	0.44394000
C	1.32871300	-3.91174400	0.93374500	H	0.66798200	0.88986300	-0.80700800
H	0.83025200	-4.54634200	1.67749200	H	-0.19836300	3.10355200	0.24576000
H	1.57944300	-4.53321700	0.07050200	C	-1.08596600	2.26342400	1.87357200
H	2.23790200	-3.50204000	1.37785500	F	-0.12755600	2.78013300	2.68717600
O	0.38102800	-1.70695200	1.15455200	F	-2.11927700	3.15979800	1.88220500
H	0.96325600	0.37355500	0.29630900	F	-1.53856400	1.15575700	2.49447000
N	-0.30773600	1.31318600	2.31101600	C	3.21728700	1.22392400	-0.16885100
H	-1.10016800	0.75775600	1.96610900	C	4.07829100	2.04943100	-0.91369900
C	-2.74951900	-1.32246400	1.87265700	C	3.54893600	-0.12799800	0.00223600
O	-2.61466300	-2.30768400	1.04103100	C	5.23018400	1.52507500	-1.50190400
C	-2.97891800	-1.74814200	3.31215900	H	3.82849400	3.09927500	-1.03576300
H	-3.50308100	-2.70542200	3.37073500	C	4.71512700	-0.64772600	-0.56756200
H	-1.99802700	-1.86737300	3.78934200	H	2.91932100	-0.77910200	0.59264400

C	5.55200300	0.17284000	-1.32978400	O	-2.72639400	-0.42087200	2.13973100
H	5.87749400	2.16942900	-2.09075300	C	0.96075600	2.12752400	-0.79598000
H	4.96586800	-1.69403900	-0.41452600	O	0.49411800	2.13183100	-1.93492800
H	6.45177500	-0.23550600	-1.78216800	C	0.04135700	2.08398900	0.41400000
C	-2.12103800	-3.17483000	1.49865800	C	-1.42831500	2.36660400	0.04170400
H	-2.20545500	-3.71547200	2.44518300	H	0.16146000	1.11521700	0.90922400
H	-3.09525100	-3.13502700	0.99820800	H	-1.41264700	3.20812800	-0.65693300
H	-1.38604200	-3.67272900	0.85438000	C	-2.14408300	2.95855600	1.25989600
C	-4.37723200	-0.62895800	-1.76364200	F	-1.69177900	4.22862800	1.49651700
H	-4.66552500	-0.86424000	-2.79320000	F	-3.48519500	3.06004600	1.07976300
H	-3.98317300	-1.53818300	-1.29852800	F	-1.94576000	2.27634100	2.41047500
H	-5.28472300	-0.36732400	-1.20727600	C	2.43787900	2.16908100	-0.57957000
C	1.13449900	-1.48641300	2.37241900	C	3.27791000	2.25506300	-1.70613100
O	1.03507000	-2.09739000	1.26617800	C	3.01547700	2.12650600	0.70078100
C	1.46364300	-2.27688900	3.60695500	C	4.66289300	2.29118400	-1.55714200
H	0.52092200	-2.49249600	4.12460700	H	2.82976400	2.29706500	-2.69422900
H	1.94263700	-3.22178100	3.34397300	C	4.40282800	2.16804000	0.85041200
H	2.09773300	-1.69356200	4.27869100	H	2.39409400	2.03630800	1.58334700
O	0.96260500	-0.22502600	2.49309100	C	5.22874300	2.24814600	-0.27559500
H	0.76948400	0.27215700	1.41296000	H	5.30138100	2.35610300	-2.43391600
INT9				H	4.83816200	2.12920200	1.84508600
N	-0.78189500	-1.17631900	1.15269400	H	6.30866500	2.27742700	-0.15684000
C	-0.12215700	-0.97690900	-2.25448200	C	-0.92043800	-2.89450200	2.73991100
H	-0.75819800	-0.11320300	-2.37486400	H	-0.55395800	-3.14172600	3.74056300
Rh	0.63762600	-1.68570600	-0.32455200	H	-2.01588200	-2.89801400	2.72987800
C	1.31015600	-0.96855800	-2.29688100	H	-0.52626500	-3.61477800	2.01397300
H	1.92667200	-0.08504900	-2.39129100	C	-3.64800300	-2.28712000	-0.33943500
C	1.78423200	-2.29868900	-2.09676800	H	-4.09798800	-2.92474800	-1.10693300
H	2.81859500	-2.61143000	-2.04684900	H	-2.76963600	-2.80126000	0.06472500
C	0.63096700	-3.14480100	-1.94501400	H	-4.36515800	-2.19311100	0.48492600
H	0.64826700	-4.20710900	-1.73576200	C	2.23316900	-1.73274100	1.65579700
C	-0.53998800	-2.33782900	-2.05083100	O	1.72612700	-2.81036000	1.19724000
H	-1.55704700	-2.69174600	-1.98436200	C	3.05610800	-1.72673300	2.90815900
O	-0.41764600	-1.58347500	2.46111300	H	2.37727500	-1.59258500	3.75901300
C	-1.97917600	-0.54454400	1.14989900	H	3.57936500	-2.67850100	3.03005000
C	-2.46627000	-0.03591200	-0.18580000	H	3.76786500	-0.89756800	2.89643900
C	-2.23075600	1.26923800	-0.66503000	O	1.98625600	-0.65083800	1.02632800
C	-3.30424500	-0.92363200	-0.90110100	H	0.37967400	2.83773000	1.13322300
C	-2.80060800	1.63882000	-1.89559000	TS7			
C	-3.84195900	-0.52128400	-2.12768700	Rh	-2.19551800	-1.26182500	-0.07853300
C	-3.58543300	0.75490400	-2.63144900	N	-1.17997500	0.18566500	-1.46036800
H	-2.60950900	2.63327600	-2.28855300	C	-4.09934900	-0.71068400	0.84361200
H	-4.46663500	-1.21194100	-2.68898800	H	-4.23205400	0.18363400	1.43257200
H	-3.99955700	1.06148400	-3.58806200	C	-4.31921300	-0.85650800	-0.56287300

H	-4.63389000	-0.07326700	-1.23956000	H	-2.95047000	0.86158200	-3.32822800
C	-4.00469500	-2.19731500	-0.93987300	H	-2.29094000	-0.28906200	-4.52341300
H	-4.06965600	-2.62497400	-1.93085300	O	0.89085800	-1.14016900	-1.14318700
C	-3.62529000	-2.89969600	0.25872900	H	-0.08101000	-0.38583200	-1.17983700
H	-3.28524700	-3.92649300	0.30605200	C	0.50754900	-2.33813900	-0.91935700
C	-3.69396500	-1.99780700	1.35231100	O	-0.69169800	-2.65996700	-0.66611500
H	-3.42934200	-2.20979800	2.37733700	C	1.55557500	-3.42017300	-0.94368900
O	-1.20910600	-0.20316600	-2.83702300	H	2.16067200	-3.33391200	-0.03346400
C	-1.17579300	1.59420500	-1.33861700	H	1.09463100	-4.40877100	-0.97750100
C	-0.93920400	2.14508400	0.04348900	H	2.22557400	-3.27648900	-1.79510800
C	0.37137700	2.31095500	0.52834400	C	2.47741100	0.91100200	0.35748100
C	-2.04890400	2.60693400	0.77882800	H	3.09120900	1.35985300	1.14727100
C	0.55021900	2.84376500	1.81183500	H	1.80015700	0.20909700	0.85187300
C	-1.83307000	3.13661400	2.05601500	C	-0.89860600	-0.51272300	2.53631200
C	-0.54495700	3.23661500	2.57983600	O	-1.99880900	-0.38055000	3.08914400
H	1.55076400	2.96264600	2.21326200	C	0.39805300	-0.43204800	3.33559600
H	-2.68499900	3.47351700	2.64145900	H	0.87297500	0.53714900	3.15577700
H	-0.39034900	3.63609900	3.57832000	H	0.18879900	-0.52616700	4.40366800
O	-1.33339700	2.34430700	-2.29415500	H	1.09487700	-1.21428800	3.01984300
C	3.37277000	0.10201000	-0.57378100	O	-0.69772400	-0.72907600	1.26748200
O	3.48917400	0.37972000	-1.76129800	CpRh(OAc) ₂			
C	1.59453800	1.97331800	-0.32571000	Rh	0.42151300	0.20995400	-0.06127000
H	1.28956300	1.58726900	-1.30182400	C	1.95548100	-0.87802300	1.01157100
C	2.35042500	3.26879600	-0.65488900	H	1.74861800	-1.44616300	1.90726000
F	3.31444700	3.10928800	-1.58903600	C	1.89858700	-1.37415700	-0.33017100
F	1.50708600	4.22298600	-1.13444100	H	1.58796400	-2.36958800	-0.61453800
F	2.96912900	3.80865200	0.43455200	C	2.19115600	-0.29723600	-1.21844500
C	4.09386200	-1.07382600	0.01216500	H	2.19312100	-0.34418400	-2.29962700
C	4.87402100	-1.87204100	-0.84271700	C	2.48653300	0.87285100	-0.41716300
C	3.99058900	-1.42699100	1.36901100	H	2.73218000	1.85638600	-0.79618400
C	5.52844700	-3.00266100	-0.35697800	C	2.34807400	0.51132800	0.94675500
H	4.94647600	-1.59902300	-1.89063000	H	2.45412100	1.17793000	1.79331600
C	4.64623300	-2.56034600	1.85659300	C	-1.33986200	2.03000100	0.09899100
H	3.40068600	-0.82976700	2.05551300	O	-0.77247300	1.76508700	-1.01243800
C	5.41292100	-3.35193800	0.99494700	O	-0.91788100	1.41643600	1.13763100
H	6.12313700	-3.61543800	-1.02898200	C	-2.48490000	2.99649900	0.18033700
H	4.55565900	-2.82520400	2.90636100	H	-3.42104500	2.44476100	0.03081600
H	5.91861400	-4.23597800	1.37414700	H	-2.51783400	3.46926900	1.16504100
C	-3.43893000	2.62360400	0.18813800	H	-2.40246600	3.75339700	-0.60359200
H	-4.20285800	2.60861900	0.97153900	O	-1.28891500	-0.90308900	-0.41983700
H	-3.58735700	3.53754000	-0.40081800	C	-1.44816600	-2.10919900	0.04970100
H	-3.61767900	1.78338600	-0.48419800	O	-0.62946100	-2.72928900	0.74374100
C	-2.49435700	-0.12183700	-3.46269300	C	-2.78993600	-2.71990800	-0.33862200
H	-3.15611300	-0.90960600	-3.09487300	H	-3.60495200	-2.11364400	0.07240500

H	-2.90074800	-2.72092100	-1.42842800	F	-0.21878300	-3.35825500	0.96939500
H	-2.86901200	-3.74124700	0.04016700	C	0.73127600	-1.47153200	-1.09233200
HOAc				H	1.51660100	-2.63635700	-1.68554200
C	1.39625800	-0.11911200	0.00000400	H	0.23774000	-1.34213500	-2.05885200
H	1.67718400	-0.70266500	-0.88323900	C	2.14190700	-1.19725600	-1.18703300
H	1.67719200	-0.70249200	0.88336100	O	2.67427900	-2.16872100	-1.87667300
H	1.92615600	0.83389500	-0.00009700	C	2.97770600	-0.13080200	-0.65058600
C	-0.08883500	0.12134100	-0.00001700	C	4.35165400	-0.35899400	-0.43474200
O	-0.63590800	1.21077300	0.00000500	C	2.42875000	1.13524000	-0.36693100
O	-0.78708300	-1.03781700	-0.00000100	C	5.16007700	0.66463000	0.05664400
H	-1.74114500	-0.82576500	0.00002700	H	4.76517000	-1.34121800	-0.64036000
KOAc				C	3.24079700	2.15604600	0.12178200
C	-2.61375900	-0.00063800	0.00340700	H	1.37964800	1.32811700	-0.55638000
H	-2.95535400	-0.03020900	1.04673200	C	4.60499100	1.92046400	0.33703000
H	-3.01360200	-0.88458700	-0.50304100	H	6.21755500	0.48581100	0.22809900
H	-3.01707300	0.90707000	-0.45574800	H	2.81052000	3.13093300	0.33037400
C	-1.08062000	0.00088400	-0.01353600	H	5.23606000	2.71563700	0.72464700
O	-0.49085800	-1.12452500	-0.00551300	C	-4.45095600	1.59674200	-0.16034900
O	-0.49096200	1.12622300	-0.00548900	H	-5.48984600	1.50528700	-0.49011400
K	2.05299300	-0.00038600	0.00320300	H	-4.45329200	1.87624700	0.89972600
TS8				H	-3.99411700	2.42803100	-0.71132600
C	-3.63629100	-2.01090900	-1.12711200	INT10			
C	-4.33666800	-0.82004700	-0.91572700	C	3.53742500	-2.06805300	1.04471800
C	-3.69678800	0.30490500	-0.38217500	C	4.19969700	-0.85444100	0.85217800
C	-2.32849700	0.20114500	-0.05719100	C	3.51857200	0.26735600	0.36268900
C	-1.61489100	-0.99484200	-0.25090200	C	2.14640200	0.13645800	0.05752600
C	-2.28377100	-2.09889100	-0.79890500	C	1.47130900	-1.08770800	0.22790600
H	-4.14662500	-2.87222400	-1.54957100	C	2.18245500	-2.18361000	0.73535700
H	-5.39095500	-0.75965900	-1.17391200	H	4.07886300	-2.92788300	1.42956200
H	-1.74278400	-3.02382400	-0.96840700	H	5.25919600	-0.77433000	1.08188800
C	-1.63108100	1.41005600	0.51759100	H	1.68115200	-3.13486200	0.88079300
O	-1.62617400	1.69880200	1.71500500	C	1.40426100	1.33136500	-0.49084700
N	-1.00212600	2.14564800	-0.43675300	O	1.05741200	1.44139400	-1.66855600
H	-1.05041200	1.92964200	-1.42752600	N	1.16918100	2.27905300	0.45330000
O	-0.25167700	3.26247800	-0.11233600	H	1.36682800	2.14012200	1.43891000
C	-1.07719000	4.44948600	-0.08108900	O	0.42130200	3.40742400	0.16560900
H	-0.39362600	5.25947300	0.18139100	C	1.28126400	4.51048300	-0.19833900
H	-1.51958900	4.63058200	-1.06690400	H	0.60149900	5.34088600	-0.40020400
H	-1.85744500	4.34744400	0.67882700	H	1.95135800	4.76126700	0.63122300
C	-0.13532600	-1.09196800	0.10153000	H	1.85726800	4.26329000	-1.09525600
H	0.19333500	-0.14179200	0.53420600	C	-0.01209900	-1.23278300	-0.11751300
C	0.09638700	-2.07140300	1.25818200	H	-0.38628300	-0.29552800	-0.53023700
F	-0.62356700	-1.73204800	2.36087000	C	-0.21119300	-2.22073000	-1.27665300
F	1.40601700	-2.06885600	1.63360300	F	0.58991300	-1.93953600	-2.33610300

F	-1.48991000	-2.18225000	-1.73425900	F	0.20809900	-3.83281200	-0.41461000
F	0.03680500	-3.51373700	-0.93260000	F	-1.19672100	-3.12653900	1.08371700
C	-0.85262500	-1.65328000	1.06721600	F	0.92959600	-3.15797100	1.53499800
H	-2.39207400	-2.46107800	2.78618500	C	-0.26805000	-0.44635700	1.02979600
H	-0.46587800	-2.48560600	1.65161300	H	-0.05854000	1.74877300	1.81741900
C	-2.05431400	-1.14416000	1.40024300	H	0.36505800	-0.44000500	1.91708500
O	-2.81073500	-1.65926600	2.42667000	C	-1.46889800	0.27154500	1.17806400
C	-2.75558200	-0.01314800	0.74127200	O	-1.51163400	1.15965700	2.10855800
C	-4.06336900	-0.19090500	0.25883100	C	-2.58471400	0.25151300	0.18547900
C	-2.13953500	1.23914100	0.60158600	C	-3.09244400	-0.92990800	-0.37992600
C	-4.72763700	0.85963600	-0.37809700	C	-3.15548700	1.48303500	-0.18558700
H	-4.54958900	-1.15543900	0.37366900	C	-4.14349100	-0.87993300	-1.30110000
C	-2.80291600	2.28950100	-0.03850100	H	-2.69712800	-1.89160500	-0.07722100
H	-1.14463400	1.39596400	1.00319800	C	-4.19327100	1.53366000	-1.11638400
C	-4.09741800	2.10105700	-0.53280500	H	-2.76405600	2.39452600	0.25387700
H	-5.73511000	0.70902300	-0.75692300	C	-4.69111800	0.35048100	-1.67738600
H	-2.30133500	3.24681000	-0.14490100	H	-4.53557400	-1.80313100	-1.71965600
H	-4.61497800	2.91602600	-1.03197800	H	-4.61514700	2.49307700	-1.40450300
C	4.25578200	1.57393400	0.15599700	H	-5.50380300	0.38812100	-2.39819600
H	3.99463600	2.31125900	0.92434600	C	3.58321900	2.18631300	-0.67073200
H	5.33747700	1.41655500	0.20051900	H	3.53669700	2.63417400	0.32822100
H	4.01936600	2.02276600	-0.81519600	H	4.60927700	2.31459100	-1.02625600
TS9				H	2.93053200	2.76328600	-1.33184300
C	3.86023500	-1.58708400	-1.06957200	INT11			
C	4.17088800	-0.23013200	-1.00788600	C	-2.36245300	-1.07346400	-2.79443500
C	3.20431700	0.72514200	-0.65977100	C	-2.61920500	-2.07921800	-1.85100000
C	1.91097300	0.26976300	-0.32722100	C	-1.99450500	-2.08719400	-0.59866200
C	1.59427400	-1.10238100	-0.38329000	C	-1.09980700	-1.02741000	-0.33997400
C	2.56993000	-2.02532300	-0.76730400	C	-0.84653400	-0.01508700	-1.27913100
H	4.62272500	-2.30733800	-1.35287600	C	-1.46996700	-0.02991000	-2.52367800
H	5.17698000	0.10355800	-1.24824900	H	-2.86671300	-1.10741300	-3.75634900
H	2.34220500	-3.08268200	-0.82169800	H	-3.32149400	-2.87125600	-2.09744500
C	0.74291900	1.21574200	-0.11797400	H	-1.27721800	0.74027000	-3.26258000
O	0.09363500	1.67617900	-1.04555500	C	-0.31894500	-0.78534500	0.88036200
N	0.73297800	2.12383600	1.18758500	O	-0.23712700	-1.48015700	1.88377200
H	1.62734600	2.11302900	1.69455200	N	-2.60235700	0.48810000	2.75669700
O	0.26695400	3.44787100	1.01458700	H	-3.08904000	0.75081600	3.61801900
C	1.12850300	4.31129900	0.24976600	O	-3.54922500	-0.34375100	2.04797500
H	0.62053200	5.27598000	0.29544500	C	-4.08024900	0.38864100	0.94616600
H	2.11637000	4.39443600	0.71311800	H	-4.74664300	-0.30599200	0.42643000
H	1.19689800	3.97356400	-0.78498100	H	-4.65263600	1.26153000	1.28886800
C	0.15592500	-1.46289200	0.00998400	H	-3.28342400	0.71441000	0.26853600
H	-0.48901100	-1.42441500	-0.87612800	C	0.17286800	0.98493000	-0.75397900
C	0.03085300	-2.88924200	0.55289800	H	1.10199600	0.92047100	-1.33043100

C	-0.26922500	2.43498300	-0.87453300	C	-1.39270300	0.26753600	0.87742900
F	-0.40937700	2.81432600	-2.17028700	O	-1.13804500	0.40565500	2.07056800
F	0.64428300	3.27019100	-0.31510100	C	-2.77327300	-0.02817300	0.40566100
F	-1.45410300	2.67674700	-0.26017500	C	-3.08595700	-0.26541800	-0.94522600
C	0.39182300	0.57888500	0.72647800	C	-3.80400200	-0.07124700	1.36574600
H	-1.88173100	-0.17973700	3.03651400	C	-4.40133000	-0.54060500	-1.32545800
H	-0.16650200	1.25221700	1.38617600	H	-2.31204800	-0.26222300	-1.70323700
C	1.83013800	0.58750900	1.24846400	C	-5.11559600	-0.34085300	0.98344400
O	2.07844200	1.22477300	2.26738100	H	-3.55903900	0.11085100	2.40708800
C	2.89948600	-0.16996000	0.53363500	C	-5.41716000	-0.57664200	-0.36508500
C	2.62336700	-1.15737900	-0.42925500	H	-4.63098100	-0.72735000	-2.37060900
C	4.24011800	0.11237900	0.85752300	H	-5.90319000	-0.36842300	1.73126900
C	3.66425600	-1.85091800	-1.04943700	H	-6.44037300	-0.78754400	-0.66426400
H	1.60337600	-1.41258300	-0.69651000	C	2.11222500	-3.56118500	-0.66394200
C	5.27873900	-0.57172100	0.22933400	H	1.81855000	-3.47429400	-1.71625600
H	4.45080600	0.87516000	1.60023100	H	2.91642500	-4.29871600	-0.58422300
C	4.99262800	-1.55698000	-0.72493100	H	1.23355300	-3.93736900	-0.12820100
H	3.43674400	-2.61789200	-1.78405600	INT13			
H	6.30976600	-0.34009800	0.48145700	C	-2.69185300	-3.39494000	0.52385300
H	5.80213900	-2.09290400	-1.21289600	C	-3.59136300	-3.03555900	-0.48145200
C	-2.28317300	-3.15133400	0.42458100	C	-3.61488100	-1.73334800	-0.99382300
H	-2.71165700	-2.69624100	1.32492500	C	-2.70318900	-0.78728800	-0.47481300
H	-2.98606700	-3.89138500	0.03023300	C	-1.78032200	-1.14199800	0.53094900
H	-1.36530000	-3.66280100	0.73387400	C	-1.79361400	-2.45452800	1.02483300
INT12(4a)				H	-2.68778700	-4.40882300	0.91455300
C	4.25304900	-0.79247700	0.89903300	H	-4.28168300	-3.77533100	-0.87890300
C	3.84457000	-2.03114500	0.38118800	H	-1.10296800	-2.74710400	1.80874200
C	2.55068200	-2.22912900	-0.11490800	C	-2.76678000	0.61294000	-1.04214700
C	1.68499600	-1.11515000	-0.06542500	O	-3.74908600	1.34969200	-0.91593800
C	2.09267800	0.12470800	0.44620100	N	-1.65160800	0.93501000	-1.74316400
C	3.38227200	0.30189400	0.93961000	H	-0.80149300	0.37013700	-1.65506800
H	5.26553900	-0.68459600	1.27852300	O	-1.46190700	2.20521200	-2.28052700
H	4.54856300	-2.85928000	0.36933100	C	-1.24190000	3.20080200	-1.24543200
H	3.70586300	1.25544100	1.34378800	H	-1.06459400	4.13001100	-1.79201100
C	0.28035200	-1.04622700	-0.49204900	H	-2.13277400	3.29659000	-0.61923900
O	-0.39222400	-1.92038500	-1.01663300	H	-0.36185500	2.93743100	-0.65116800
C	0.97009800	1.14623800	0.39011300	C	-0.78973700	-0.13620200	1.12052000
H	0.76639700	1.55188400	1.38552800	H	-0.79528400	0.79156600	0.54741700
C	1.30419700	2.33878400	-0.49143400	C	-1.23886400	0.29945600	2.51383400
F	2.37704300	3.02776900	-0.02766100	F	-2.51700100	0.75868100	2.50780600
F	0.26758200	3.21631500	-0.54930700	F	-0.46595100	1.30726600	2.99607000
F	1.58700100	1.98334100	-1.77251100	F	-1.18622700	-0.70126000	3.43296800
C	-0.25456100	0.37557500	-0.15128700	C	0.66535300	-0.63514700	1.17686500
H	-0.63496300	0.81372200	-1.07656500	H	1.29705900	0.12071100	1.66140600

H	0.74936000	-1.54413800	1.78123400	H	0.12417800	-2.98821700	-0.20877400
C	1.27690100	-0.89186000	-0.18467500	C	0.88295500	0.12317000	1.16898500
O	0.67687000	-0.62594800	-1.23215500	H	0.92073400	-0.89086600	0.76685000
C	2.63786900	-1.49319900	-0.24479400	C	1.27251400	-0.07694800	2.63123600
C	3.46261400	-1.59549300	0.89003500	F	2.55659100	-0.51344600	2.75799800
C	3.11154700	-1.96464900	-1.48389800	F	0.49169800	-1.00532100	3.24080100
C	4.73877000	-2.15142800	0.78312800	F	1.17609700	1.05674500	3.38028500
H	3.12834200	-1.22278200	1.85175600	C	-0.55280900	0.63990800	1.06234500
C	4.38261000	-2.52658000	-1.58677300	H	-1.43860600	-0.43025300	1.51885400
H	2.46900100	-1.89240500	-2.35578500	H	-0.80349900	1.42276100	1.77836900
C	5.20023400	-2.61832400	-0.45259900	C	-1.09143800	0.82338200	-0.24493200
H	5.37309400	-2.21675400	1.66251800	O	-0.58341100	0.32472400	-1.29536000
H	4.73701300	-2.89387900	-2.54588500	C	-2.38905000	1.56537100	-0.40394400
H	6.19302700	-3.05300700	-0.53227700	C	-3.29654000	1.74429900	0.65536800
C	-4.59146000	-1.36768200	-2.08981000	C	-2.71601200	2.08354600	-1.66934700
H	-5.35987300	-0.68045200	-1.72021100	C	-4.49877200	2.42686400	0.45205500
H	-4.08994800	-0.86532600	-2.92572400	H	-3.08164200	1.32839200	1.63421400
H	-5.08725600	-2.26157300	-2.47992500	C	-3.91202800	2.77584700	-1.87015400
C	2.01070300	2.55075500	1.09517000	H	-2.01778400	1.94336000	-2.48871900
C	1.30076900	3.85400700	1.48730700	C	-4.80944000	2.94774800	-0.80947700
H	1.79130000	4.33715700	2.33739500	H	-5.19531800	2.54672500	1.27780500
H	1.25331800	4.54723500	0.64095200	H	-4.14448900	3.18011200	-2.85211800
H	0.26982300	3.61536900	1.77887900	H	-5.74350100	3.48141700	-0.96489400
O	2.73371400	1.98126000	1.95792100	C	4.76941500	0.74424800	-2.12378900
O	1.77969100	2.10483400	-0.07543600	H	5.48088200	0.04747100	-1.66788600
K	1.99228200	1.73312100	-2.62561500	H	4.24264500	0.19105500	-2.91088400
TS10				H	5.33421800	1.55274800	-2.59780000
C	2.95484900	3.17922700	0.18862200	C	-2.61428900	-2.12698300	1.13380000
C	3.85223200	2.64849000	-0.74264400	C	-3.65648800	-3.08651300	1.67829800
C	3.80780500	1.29490000	-1.09375300	H	-4.56765500	-2.53006800	1.92747800
C	2.83798300	0.47058200	-0.47924700	H	-3.89318100	-3.85781400	0.94224700
C	1.93157600	0.99409000	0.46478300	H	-3.29491600	-3.55115700	2.60172800
C	2.00022100	2.35789700	0.78359800	O	-2.19439700	-1.24507400	1.99500500
H	2.99874500	4.23435800	0.44555200	O	-2.21838100	-2.19759800	-0.04289700
H	4.58880500	3.29557300	-1.21274100	K	-1.86224900	-1.74112200	-2.63418900
H	1.29903600	2.77404800	1.49968300	INT14			
C	2.79033700	-0.98380800	-0.89009400	C	3.25828300	3.05876900	-0.05744300
O	3.71223300	-1.78198800	-0.69080800	C	4.10051500	2.38086800	-0.94423400
N	1.63740500	-1.27947500	-1.54094100	C	3.94118400	1.01205700	-1.18328200
H	0.81949700	-0.64488800	-1.47177500	C	2.91145500	0.32322400	-0.50211000
O	1.31920900	-2.59433100	-1.89078100	C	2.06055500	0.99613500	0.39729400
C	0.99801000	-3.39727800	-0.72669200	C	2.24291500	2.37155300	0.60228300
H	0.76483200	-4.38658200	-1.12715500	H	3.39144100	4.12421100	0.11165100
H	1.86021600	-3.45641800	-0.05699000	H	4.88406400	2.92423900	-1.46691500

H	1.57775300	2.90145600	1.27666000	TS11			
C	2.74367900	-1.15262100	-0.78906100	C	-4.52369300	0.74369000	-0.32767200
O	3.60355100	-2.00051700	-0.52669300	C	-3.93508900	1.99085800	-0.56162800
N	1.56284200	-1.40820300	-1.40576600	C	-2.54258700	2.15168700	-0.54691300
H	0.77571000	-0.71543700	-1.37270100	C	-1.74522400	1.01288200	-0.30260200
O	1.14207500	-2.72649200	-1.62873600	C	-2.33113600	-0.23812700	-0.08170100
C	0.80433300	-3.40029000	-0.39263700	C	-3.72524200	-0.37484800	-0.08095400
H	0.48200100	-4.39917700	-0.69626000	H	-5.60634500	0.64501000	-0.33543500
H	1.68124400	-3.46957600	0.25625500	H	-4.56698700	2.85617600	-0.75112300
H	-0.01770800	-2.88271100	0.11380200	H	-4.18835900	-1.33737500	0.10612900
C	0.93561500	0.27932500	1.15847000	C	-0.22754300	1.13748600	-0.13640200
H	0.91218300	-0.76892000	0.85254900	O	0.18532500	1.62066700	0.96260600
C	1.27031000	0.18528500	2.64289700	N	0.50924400	1.50501800	-1.35314500
F	2.50419600	-0.34640000	2.85587100	H	-0.12262000	1.56153400	-2.15068600
F	0.38873400	-0.61603100	3.30160400	O	1.11441200	2.79528500	-1.26384200
F	1.24972800	1.38429500	3.28656800	C	2.53496100	2.64354900	-1.23588500
C	-0.43695200	0.89385000	0.95415200	H	2.93446400	3.66029900	-1.16000100
H	-1.67645900	-0.52613700	1.53230500	H	2.85023900	2.04849300	-0.37289300
H	-0.77722800	1.60745400	1.69789000	H	2.89804600	2.16671900	-2.15509800
C	-1.04453500	0.86647700	-0.28992300	C	-1.32797000	-1.35673800	0.19029800
O	-0.58037400	0.22770800	-1.31853000	H	-1.30123200	-1.58497900	1.26301100
C	-2.34663600	1.59563500	-0.49880300	C	-1.68664400	-2.67426300	-0.48312300
C	-3.24643600	1.87556900	0.54572700	F	-2.84258300	-3.22435900	-0.00636200
C	-2.69194800	1.99870800	-1.80074000	F	-0.72510600	-3.61798300	-0.28929600
C	-4.44624700	2.54750300	0.29692700	F	-1.84666500	-2.55695700	-1.83052400
H	-3.02392000	1.55046700	1.55758900	C	0.03878400	-0.88779200	-0.25241800
C	-3.88781800	2.67722200	-2.05106600	H	0.21641600	-0.97887100	-1.31894700
H	-2.00301500	1.78339400	-2.61165800	C	1.15325100	-1.06621000	0.62338200
C	-4.77246600	2.95365300	-1.00248900	C	2.54176400	-0.87607800	0.08515800
H	-5.13090700	2.74588200	1.11794400	C	2.88209700	-1.10739400	-1.25818000
H	-4.12851500	2.99133800	-3.06398700	C	3.54387400	-0.42980100	0.96509600
H	-5.70600200	3.47627200	-1.19502500	C	4.18733600	-0.89507400	-1.70980700
C	4.84554200	0.30041000	-2.16531900	H	2.13305700	-1.46439000	-1.95725000
H	5.49234300	-0.42107500	-1.65503400	C	4.84463800	-0.20217400	0.51375800
H	4.26790000	-0.26210900	-2.90901000	H	3.28204700	-0.25200000	2.00340400
H	5.47874500	1.01620000	-2.69864000	C	5.17148100	-0.43556200	-0.82807700
C	-2.82608700	-2.06463000	1.19729300	H	4.43445900	-1.08487100	-2.75126500
C	-3.81994900	-2.96287900	1.88750900	H	5.60290300	0.15814900	1.20460700
H	-4.63430500	-2.36240700	2.30678900	H	6.18455000	-0.26250600	-1.18241100
H	-4.22023900	-3.69256500	1.18235200	C	-1.93099600	3.51154300	-0.79858500
H	-3.33203500	-3.48011800	2.72093500	H	-2.68121100	4.30190900	-0.69110700
O	-2.31879700	-1.14271600	2.01236200	H	-1.10260900	3.71095100	-0.11363100
O	-2.50825600	-2.17006800	0.01627000	H	-1.51918400	3.58103200	-1.81380200
K	-1.83128000	-1.78938500	-2.56229400	O	1.00889600	-1.21112100	1.86854700

K	-0.01497700	0.77941200	3.45280000	O	2.51117700	-2.57003200	0.77018300
INT15				O	3.86576600	-1.54299300	-0.71109600
C	-4.39677400	0.01846900	-1.55110700	C	3.68507900	-2.10946300	0.36637600
C	-3.64529100	-0.64892800	-2.52880400	C	4.78243800	-2.33967500	1.37643400
C	-2.28601400	-0.93992500	-2.34254800	H	5.75849800	-2.14980600	0.92693200
C	-1.69386400	-0.53792900	-1.13163700	H	4.63321100	-1.65294200	2.21837000
C	-2.44727900	0.11140800	-0.15480700	H	4.73739000	-3.35933900	1.77087100
C	-3.79972600	0.40876600	-0.35047900	O	2.02592400	0.57412800	1.34328800
H	-5.44592700	0.23755100	-1.73309100	O	0.63886900	-0.07370200	-1.61435900
H	-4.12599300	-0.94457600	-3.45947700	K	3.03639300	0.71570200	-1.98759300
H	-4.37286100	0.93151100	0.40961100	TS12			
C	-0.20371900	-0.65215700	-0.75880900	C	-4.77784900	-0.09169800	-1.31309500
N	0.23485400	-2.10801700	-0.63600000	C	-4.02615900	-1.01948500	-2.04576800
H	0.34229800	-2.42928000	-1.60053400	C	-2.63901700	-1.16166700	-1.87178000
O	-0.83333200	-2.92385800	-0.10159500	C	-2.02427200	-0.33379400	-0.91244000
C	-0.35560900	-3.79029400	0.92679800	C	-2.77311900	0.60772700	-0.20128300
H	-1.23481000	-4.34324800	1.26914300	C	-4.15072000	0.74309300	-0.38552800
H	0.39535100	-4.49280100	0.54273100	H	-5.84806000	-0.00835600	-1.48492400
H	0.06964700	-3.22484100	1.76430900	H	-4.52856300	-1.64334900	-2.78248300
C	-1.60682700	0.47355400	1.05647600	H	-4.71657900	1.48931600	0.16518800
H	-1.61884700	1.55598800	1.22632000	C	-0.52715100	-0.28796700	-0.53350500
C	-2.13196500	-0.11071600	2.35658400	O	0.35473600	-0.43848500	-1.48192600
F	-3.36082200	0.38177400	2.67813600	N	-0.31525000	-1.36678200	0.61672600
F	-1.31254000	0.19481600	3.40357700	H	-1.13219200	-1.33332900	1.23686800
F	-2.24808800	-1.46204600	2.33951300	O	-0.36794900	-2.66586200	0.00046600
C	-0.18353500	-0.05139500	0.74159200	C	-0.24295800	-3.68562900	0.99627800
H	1.73065200	-2.31918600	0.14941400	H	-0.31128300	-4.62884800	0.44858400
H	0.07040900	-0.86649500	1.41992000	H	0.72227900	-3.62375000	1.51065200
C	0.94901200	0.95088200	0.87932800	H	-1.06316000	-3.62726300	1.72532700
C	0.79444000	2.38075700	0.45360000	C	-1.89890100	1.48009400	0.68308100
C	-0.09476000	2.78358400	-0.55829400	H	-2.08948600	2.53730700	0.47013900
C	1.60608100	3.34616800	1.07576800	C	-2.18301700	1.33386800	2.16610700
C	-0.16408400	4.12490100	-0.94078900	F	-3.45243000	1.70559000	2.47866200
H	-0.69610100	2.04512100	-1.07463400	F	-1.35559800	2.10919100	2.91721600
C	1.52493400	4.68868600	0.70340800	F	-2.03508300	0.05802600	2.63252900
H	2.29314600	3.03164000	1.85554900	C	-0.44840500	1.10671400	0.30559000
C	0.64035200	5.08055300	-0.30909700	H	0.18739900	0.98431800	1.18486200
H	-0.84439600	4.42314500	-1.73401700	C	0.15859100	2.15848200	-0.61921100
H	2.14931800	5.42722200	1.19904100	C	1.64174500	2.24622400	-0.76995900
H	0.57888400	6.12475300	-0.60441700	C	2.52061800	1.35008800	-0.14019400
C	-1.50744700	-1.67817400	-3.40673300	C	2.17376500	3.25991700	-1.58809500
H	-1.39255300	-2.73801500	-3.14001000	C	3.89992900	1.45939700	-0.32920100
H	-2.02315700	-1.64086800	-4.37233100	H	2.13684800	0.55926000	0.48735400
H	-0.50645400	-1.25142400	-3.51938400	C	3.55111900	3.37277400	-1.77441500

H	1.49396300	3.95155600	-2.07545700	F	1.32019800	-3.12709300	0.87542100
C	4.41909700	2.46988800	-1.14572900	F	2.47016400	-1.41668200	1.58648400
H	4.56816200	0.75506200	0.15895700	C	0.15644300	-0.78635400	-0.43679100
H	3.94948500	4.16058900	-2.40821400	H	-0.10499400	-0.72239400	0.95560600
H	5.49288700	2.55512900	-1.29126000	C	-0.90761900	-1.64950300	-0.98927700
C	-1.87521200	-2.15767600	-2.71376800	O	-0.65532700	-2.76137200	-1.48092700
H	-2.51836800	-2.57717300	-3.49523400	C	-2.33951700	-1.19436400	-0.96592600
H	-1.00618800	-1.68157300	-3.17594400	C	-3.12732900	-1.41684400	-2.10648900
H	-1.49221700	-2.97679300	-2.09759300	C	-2.92731600	-0.62256100	0.17231300
O	-0.57505900	2.92583400	-1.24376700	C	-4.47345900	-1.04333200	-2.12177400
K	2.05867900	-2.34045100	-1.76085600	H	-2.67408800	-1.87288100	-2.98208700
C	2.80572000	-1.66340000	1.86041200	C	-4.28253000	-0.28071100	0.16874100
C	3.88694900	-1.47614600	2.90266600	H	-2.33235300	-0.46936000	1.06530500
H	4.79157100	-2.01832500	2.62123700	C	-5.05612900	-0.47771500	-0.98128100
H	4.11508000	-0.40880000	3.00364700	H	-5.06854400	-1.20024300	-3.01772200
H	3.53059900	-1.82623800	3.87755500	H	-4.73441500	0.14101800	1.06326300
O	2.99291100	-2.31247400	0.82149400	H	-6.10646100	-0.19797400	-0.98664000
O	1.67308600	-1.07055900	2.15284300	C	1.22903700	3.59246600	-1.30076200
H	0.83134500	-1.23042000	1.39040700	H	0.83823100	3.84250800	-0.30655600
NH ₂ OMe				H	1.80338800	4.45273300	-1.65943000
C	-1.18047400	-0.20604000	-0.00001500	H	0.36500500	3.44153800	-1.95364200
H	-2.00332700	0.51550600	0.00013200	C	-0.28564900	0.32506700	2.82188700
H	-1.24048700	-0.83720000	0.89655500	C	-0.22482900	0.18997200	4.33316800
H	-1.24056700	-0.83693100	-0.89676300	H	0.75326700	-0.21507900	4.61893500
O	0.01293000	0.57543200	0.00007700	H	-0.36840300	1.15958200	4.81509600
N	1.15362700	-0.31153300	-0.00002600	H	-0.98466300	-0.51734100	4.68180500
H	1.69389600	-0.01366300	-0.81537800	O	-0.28280400	-0.80802600	2.18182100
H	1.69450000	-0.01419700	0.81510800	O	-0.32924300	1.44086600	2.27241900
TS13				K	-2.11924900	2.90116900	0.85036200
C	4.31810300	1.33039200	-1.33813100	INT16			
C	3.48523100	2.45602700	-1.41160800	C	4.35275400	1.50645700	-0.81813300
C	2.09743900	2.36021500	-1.23646500	C	3.54821800	2.60712700	-0.49354800
C	1.58090700	1.07315400	-0.98290000	C	2.18159000	2.46660400	-0.19933000
C	2.41254800	-0.05194100	-0.91117400	C	1.65518400	1.16304800	-0.25222100
C	3.79050400	0.05979100	-1.08631600	C	2.46208900	0.06123800	-0.56921000
H	5.38862400	1.44890200	-1.48446500	C	3.81612600	0.21266200	-0.85174800
H	3.92628300	3.42996800	-1.61075900	H	5.40420500	1.66120200	-1.04688100
H	4.43781800	-0.80970800	-1.03354000	H	3.99241900	3.60011300	-0.47262300
C	0.16555500	0.65544600	-0.79805000	H	4.43960000	-0.64272900	-1.09426700
O	-0.81418100	1.40058600	-0.93847600	C	0.24328000	0.70185500	-0.05710700
C	1.59000500	-1.30194700	-0.65688200	O	-0.69597700	1.47132200	0.27272000
H	1.61562700	-1.96753400	-1.52846800	C	1.63456200	-1.21449800	-0.51262200
C	2.16015200	-2.13969400	0.47993800	H	1.75505600	-1.83951600	-1.40611200
F	3.32014600	-2.75708500	0.09525000	C	2.12365600	-2.07361100	0.65627000

F	3.41289700	-2.49199400	0.46415800	H	0.75663800	1.56006200	1.12321400
F	1.39405200	-3.19562100	0.85417800	H	0.92189500	1.71191300	2.88132600
F	2.11658200	-1.39925000	1.84094700	O	0.01877100	-3.41932700	-0.40760900
C	0.21562200	-0.70560700	-0.33105200	C	-1.90897000	-2.05707400	-0.35208000
C	-0.90738500	-1.52716100	-0.60221700	C	-2.64983500	-2.84863900	-1.24616800
O	-0.82031400	-2.75215800	-0.89188200	C	-2.57466200	-1.13145200	0.46886900
C	-2.30029700	-0.93885900	-0.62041300	C	-4.03463000	-2.69857900	-1.34284500
C	-2.66159100	0.04650800	-1.55138900	H	-2.13016500	-3.56841300	-1.87194700
C	-3.28231900	-1.46239800	0.23373100	C	-3.96648200	-1.01303600	0.39700100
C	-3.98104900	0.50300400	-1.62627200	H	-2.00591000	-0.52036400	1.16482100
H	-1.90341600	0.46011600	-2.21062300	C	-4.69768600	-1.78305000	-0.51592500
C	-4.59978700	-0.99126200	0.17728600	H	-4.59651900	-3.29831200	-2.05406400
H	-3.01083600	-2.23745000	0.94614700	H	-4.47988300	-0.31318900	1.05224200
C	-4.95361300	-0.00883100	-0.75615000	H	-5.77747000	-1.67456200	-0.57914200
H	-4.25028200	1.26095000	-2.35779700	C	1.00432900	2.55542100	-2.75186100
H	-5.34836100	-1.39436000	0.85488300	H	1.48203700	3.35584600	-3.32563000
H	-5.97746300	0.35248600	-0.80797400	H	0.30013900	2.02667500	-3.40303800
C	1.33839300	3.67140800	0.14474100	H	0.40848800	3.00921700	-1.95112900
H	0.89832500	3.57429100	1.14342700	H	0.14498100	-0.58968800	1.05052500
H	1.93981200	4.58642400	0.11623400	F	-0.44132500	3.68344500	1.88824200
H	0.49943900	3.78006000	-0.55084600	F	-1.58536300	2.43955100	3.27164100
K	-2.83855500	1.93477700	1.66223600	F	-1.84012900	2.18791900	1.12496200
TS14				O	-0.72486800	0.51662400	-1.42188500
C	4.37263500	0.95783300	-1.86156300	K	-2.97188800	1.81489800	-1.59937900
C	3.40531700	1.81778100	-2.40304700	INT17			
C	2.03658800	1.61453100	-2.18366700	C	4.61295600	-0.02534000	-1.45511100
C	1.68710500	0.50271900	-1.39075700	C	3.91005900	0.89363200	-2.24927000
C	2.65040200	-0.35443800	-0.84361400	C	2.51134500	0.93047600	-2.26212500
C	4.00746400	-0.13945600	-1.07355400	C	1.85478400	0.00161500	-1.42691100
H	5.42408300	1.14900500	-2.05967100	C	2.55426700	-0.91297100	-0.62436400
H	3.72505100	2.66431100	-3.00600300	C	3.94585200	-0.94325700	-0.63568700
H	4.76213800	-0.79846900	-0.65675900	H	5.69932200	-0.02290500	-1.47801300
C	0.33575800	0.03761900	-1.00969600	H	4.46465200	1.59446400	-2.86783600
C	1.98396600	-1.46245300	-0.04747500	H	4.50153300	-1.65009700	-0.02911200
H	2.13016300	-2.43151000	-0.53823700	C	0.41114900	-0.17801900	-1.24614000
C	2.59245100	-1.62967000	1.33588900	C	1.59612700	-1.80900800	0.14458200
F	3.85132800	-2.15940500	1.25509900	H	1.62036300	-2.82744600	-0.25866000
F	1.87468000	-2.47536600	2.11627300	C	1.91577900	-1.93221800	1.62360500
F	2.71759400	-0.46451300	2.01833300	F	3.10410100	-2.55377300	1.83642800
C	0.48350700	-1.10501200	-0.04059800	F	0.96790300	-2.66263000	2.26956200
C	-0.42860300	-2.27491900	-0.27307100	F	1.97914200	-0.73048200	2.24953300
O	-0.23454000	0.10373400	2.23227900	C	0.20255800	-1.19004600	-0.08923000
C	-0.90277300	2.41404000	2.09548300	C	-0.89743800	-2.18312300	-0.46159300
C	0.22648800	1.38474900	2.08342200	O	-1.18777700	3.15902300	-0.05280500

C	0.03956900	2.58752100	1.94813600	C	0.30990400	-1.15776600	-0.83972500
C	0.05024000	3.04596900	0.48406100	O	0.48433800	-0.52886200	-1.90334100
H	0.64523700	3.98999600	0.51266300	C	-0.92365300	-1.99857500	-0.61734700
H	0.71356000	2.29743500	-0.01248300	C	-2.03118000	-1.78834900	-1.45106800
O	-0.60615800	-3.23373200	-1.02441900	C	-0.99623900	-2.98517000	0.37752300
C	-2.31552300	-1.79622700	-0.22304200	C	-3.18194600	-2.57097900	-1.31593600
C	-3.30007600	-2.32866900	-1.07679400	H	-1.97454200	-1.01654900	-2.21233000
C	-2.70027300	-0.93182300	0.81780300	C	-2.14905400	-3.76291500	0.52023500
C	-4.64045600	-1.98739100	-0.90574700	H	-0.14579000	-3.14698800	1.03120100
H	-2.99651700	-2.99332200	-1.87955300	C	-3.24432100	-3.56587300	-0.33170900
C	-4.04796400	-0.61124300	1.00228300	H	-4.02731600	-2.40727700	-1.98010400
H	-1.96575300	-0.51419100	1.49684500	H	-2.18931600	-4.53053700	1.28913600
C	-5.01742000	-1.12941300	0.13649700	H	-4.13485000	-4.18126500	-0.22987200
H	-5.39155500	-2.38670400	-1.58143100	C	-3.51404000	2.50201400	-0.74816300
H	-4.33692300	0.04739200	1.81626800	H	-3.82280400	2.56595500	0.30116800
H	-6.06284100	-0.86634300	0.27251900	H	-4.11122500	3.21076900	-1.33166400
C	1.75078800	1.91888200	-3.10589000	H	-3.75419900	1.48629100	-1.08201900
H	2.43559800	2.59658200	-3.62410000	C	3.84631600	-1.75801300	-0.37649700
H	1.13363600	1.40490800	-3.85173300	C	2.54590100	-2.06635800	-1.09525100
H	1.06403700	2.51135700	-2.49069300	H	2.50474100	-1.44598400	-1.99549500
H	-0.09241200	-0.57849300	0.76799300	H	2.57233800	-3.12633700	-1.38039500
F	1.30236400	2.45870200	2.46262800	O	1.46400800	-1.80320300	-0.23283700
F	-0.56114600	1.36884300	2.12051900	H	0.29555600	-0.45538400	1.57200900
F	-0.62085000	3.44498600	2.77724300	F	4.90512800	-2.13349100	-1.14438100
O	-0.50006900	0.34596900	-1.87177600	F	3.96341300	-2.41343900	0.80668400
K	-2.80218100	1.83054800	-1.52706700	F	4.00139100	-0.43690700	-0.10752900
TS15				O	-2.29387300	0.37114200	1.04390000
C	-0.21623500	4.12048400	-1.85780800	K	-4.49662900	-0.82179200	1.52491700
C	-1.58402500	3.85420100	-1.69110300	INT18			
C	-2.03907900	2.78632200	-0.90258900	C	0.84271000	3.07785400	-0.64930200
C	-1.05416200	1.99454900	-0.28416400	C	-0.41839200	3.11169300	-0.04227400
C	0.31319500	2.25856300	-0.45342100	C	-1.08814700	1.94056000	0.35953600
C	0.75205900	3.32009500	-1.23947200	C	-0.43053200	0.71829500	0.13428600
H	0.09204800	4.95710400	-2.47980700	C	0.83777300	0.68941600	-0.47297300
H	-2.31188700	4.48898100	-2.19217500	C	1.48680900	1.85178800	-0.87409200
H	1.81123200	3.52225500	-1.37217400	H	1.32343000	4.00664100	-0.94660500
C	-1.20341200	0.79778600	0.59015800	H	-0.89966400	4.07405100	0.12392700
C	1.13432800	1.23551300	0.31313300	H	2.46527300	1.81555600	-1.34521600
H	1.91833400	0.80770800	-0.32025500	C	-0.86684200	-0.69664500	0.42787100
C	1.86241500	1.85485200	1.49376300	C	1.29222700	-0.75759100	-0.60792200
F	2.81434000	2.75053900	1.09788100	H	1.49847900	-1.00121400	-1.66259200
F	2.51055000	0.91744700	2.23876000	C	2.61452400	-1.01314900	0.10015900
F	1.04126500	2.52414700	2.34862900	F	3.65383500	-0.33007400	-0.47091800
C	0.09873800	0.21262100	0.74064000	F	2.96487700	-2.33198200	0.04772700

F	2.61199900	-0.66874200	1.41409700	C	-1.18781700	2.98777100	1.52398700
C	0.14388800	-1.53347300	-0.01602500	C	-0.38539000	2.62725800	0.42868200
C	-2.46315800	2.03038100	0.98425100	C	-0.48953100	1.29911700	-0.02269100
H	-2.55693700	1.36154500	1.84304800	C	-1.35423500	0.38334500	0.59757200
H	-2.67876300	3.05758200	1.30023300	C	-2.13223600	0.74926200	1.69266400
H	-3.24242800	1.73259700	0.27034000	H	-2.64386600	2.39065400	2.99713900
H	0.13123600	-2.61637100	0.04534300	H	-1.13787400	4.00727200	1.90090200
O	-2.00173300	-0.99080800	0.97130200	H	-2.79229800	0.03518500	2.17686600
K	-3.93727900	-1.63376400	-0.65148000	C	0.22667200	0.60434200	-1.14431200
INT19				C	-1.25260600	-0.97267800	-0.08427100
C	-1.82872500	2.17169600	2.16333000	H	-1.05459700	-1.76150300	0.65410500
C	-0.88772700	3.00227800	1.54196600	C	-2.55311500	-1.36754100	-0.76117700
C	-0.13374300	2.57695700	0.43329000	F	-3.57430400	-1.53741500	0.13044000
C	-0.37593400	1.27508100	-0.03922600	F	-2.43310600	-2.55363900	-1.42464000
C	-1.32773700	0.44741000	0.58017400	F	-2.99099300	-0.45993500	-1.67419600
C	-2.05541500	0.87326100	1.68673400	C	-0.10791100	-0.78017900	-1.06789900
H	-2.38671100	2.53948900	3.02087200	H	1.16874900	-1.19159800	-0.31235800
H	-0.73072100	4.00712300	1.92965600	C	0.54842800	3.63076000	-0.20588400
H	-2.78225000	0.22277400	2.16506300	H	0.39185200	3.69396700	-1.28699600
C	0.25243200	0.52279000	-1.18451700	H	0.40614100	4.62465500	0.23200600
C	-1.36873200	-0.90107100	-0.12253600	H	1.59597200	3.34059800	-0.06116100
H	-1.19624600	-1.71209100	0.59994000	C	2.13396300	-1.97128400	1.32877900
C	-2.73079600	-1.19200500	-0.72919200	C	3.49412000	-2.18385000	1.96256300
F	-3.70820000	-1.31530500	0.21882000	H	3.97699600	-1.21361000	2.12751200
F	-2.73014900	-2.36922400	-1.41995100	H	3.39515000	-2.70673000	2.91580000
F	-3.16056700	-0.23841400	-1.59700900	H	4.13732300	-2.75905400	1.28793700
C	-0.27303000	-0.77819000	-1.15870300	O	1.07933500	-2.28832400	1.88095800
H	1.20680000	-1.31603200	-0.26895600	O	2.19671700	-1.40815700	0.13417600
C	0.89658300	3.49548300	-0.18371100	H	-0.01713600	-1.41869500	-1.94493700
H	0.86238200	3.46077800	-1.27519700	O	1.05964900	1.16132600	-1.91504500
H	0.74438700	4.52810000	0.14989400	K	3.65768600	0.61780700	-1.21858100
H	1.91257700	3.19936800	0.10864300	INT20(5a)			
C	2.03364900	-2.05389100	1.35396700	C	1.14902100	1.28735100	2.37420500
C	3.37873500	-2.36232800	1.96489500	C	2.15075000	1.70663300	1.48502800
H	3.95697500	-1.43675600	2.06542500	C	2.03204700	1.51279900	0.10368200
H	3.25057100	-2.82160400	2.94618400	C	0.85338500	0.88159700	-0.34517300
H	3.94371200	-3.03297700	1.30893400	C	-0.14761200	0.45928800	0.54102100
O	0.95999800	-2.22938400	1.91517600	C	-0.00945300	0.65381800	1.91420500
O	2.13692400	-1.55499100	0.11573500	H	1.28314100	1.45071100	3.44034600
H	-0.15287300	-1.49158600	-1.96890200	H	3.04323800	2.18701400	1.87869200
O	1.15897900	1.00528300	-1.94377700	H	-0.77163600	0.31756700	2.60914000
K	3.69668800	0.46988400	-1.27022100	C	0.46339200	0.54517800	-1.72882200
TS16				O	1.09390300	0.77654800	-2.75572100
C	-2.04408000	2.07045500	2.14883300	C	-1.27545800	-0.24806800	-0.19465400

H	-1.31301800	-1.29548800	0.12777400
C	-2.63974600	0.34029700	0.09671700
F	-2.98636000	0.22074400	1.40749100
F	-3.61597500	-0.28266400	-0.61855300
F	-2.72492800	1.66513000	-0.20677800
C	-0.89725900	-0.14496100	-1.69032200
H	-0.80142000	-1.13357000	-2.14452500
C	3.11716900	1.94786200	-0.84681200
H	2.73260000	2.65892600	-1.58639800
H	3.94555600	2.41543900	-0.30543600
H	3.50452300	1.09376100	-1.41387400
C	1.02894900	-2.71803000	0.10263300
C	2.29186200	-2.30732100	0.88062700
H	2.11766500	-1.32897400	1.34503000
H	2.50113900	-3.02114200	1.68528300
H	3.16286900	-2.22468200	0.22340800
O	0.03852200	-3.11470300	0.79161900
O	1.04900100	-2.59770600	-1.15773200
H	-1.61297600	0.43978100	-2.27823100

6. Cartesian coordinates of the structures (optimization in 1,2-dichloroethane)

1a				C	-3.77737300	-1.37204400	0.13966300
O	-3.04775100	-0.83041600	0.05290500	H	-4.77040200	0.20651600	1.23256100
C	-0.87604700	0.05783700	0.47643200	H	-2.55300100	-2.74068500	-0.99689600
C	0.58195400	-0.15983400	0.18451400	H	-4.60050700	-2.07316500	0.24806900
C	1.10964000	-1.45826100	0.26066400	C	0.86517400	1.01965900	-0.41288400
C	1.41673200	0.93857700	-0.11973700	H	1.49749300	1.71723200	-0.95568800
C	2.47041900	-1.68800500	0.04397600	INT1			
H	0.45876500	-2.29050200	0.51747200	Rh	1.09104900	-0.39979200	-0.45477400
C	2.77590400	0.68209800	-0.34768200	C	1.24888700	-0.78545100	-2.61393900
C	3.30398100	-0.61075800	-0.26492700	H	0.94208100	-0.02476400	-3.31807400
H	2.87108100	-2.69511300	0.11687100	C	2.54050500	-0.88229100	-2.02238400
H	3.43291800	1.51225900	-0.59625400	H	3.37943400	-0.23084800	-2.22708700
H	4.36396200	-0.77271900	-0.44239200	C	2.51944000	-1.97458000	-1.07630700
O	-1.29396700	0.87813400	1.29492600	H	3.35064700	-2.30744300	-0.46943700
C	-3.85057600	0.09414100	-0.70930300	C	1.20742300	-2.52234500	-1.08440900
H	-4.87414800	-0.07217900	-0.36589900	H	0.85123200	-3.33105500	-0.46016200
H	-3.54367500	1.12370100	-0.50151300	C	0.40333200	-1.77986700	-2.01801100
H	-3.77108200	-0.12167000	-1.78088100	H	-0.63587000	-1.96106500	-2.25514600
C	0.88334100	2.34997700	-0.21251000	O	-0.08642100	1.28116900	-0.64901700
H	-0.03258300	2.39798000	-0.81246000	O	1.17790200	2.27603500	-2.24234800
H	0.63108000	2.74009000	0.77939300	C	0.22487300	2.25907500	-1.45094800
H	1.62514200	3.01439500	-0.66659900	C	-0.72256200	3.44403100	-1.31146000
N	-1.70739700	-0.70996300	-0.29213600	H	-0.49943700	3.96526100	-0.37267200
H	-1.36802900	-1.48288300	-0.85399500	H	-0.59127700	4.13725300	-2.14559500
2a				H	-1.76038700	3.10341600	-1.25592000
C	-0.56374200	1.44202700	-0.28387900	O	0.52296900	-1.18149000	2.57662600
O	-0.80137000	2.65062100	-0.28244200	C	-1.37311900	-1.20491600	1.15376300
C	1.38947300	-0.04588100	0.20096200	C	-2.43730200	-0.28565000	0.68268500
H	0.79912600	-0.74052000	0.79060000	C	-2.46304100	1.04736700	1.13454600
C	2.85017400	-0.37291300	0.15830500	C	-3.46039800	-0.76738900	-0.17534100
F	3.38913800	-0.38340800	1.40794500	C	-3.49306200	1.90781700	0.76475600
F	3.05352500	-1.61653900	-0.35848200	H	-1.68205300	1.42489400	1.78466000
F	3.58093500	0.48976600	-0.58329800	C	-4.46520500	0.13059500	-0.55965700
C	-1.65062700	0.43435300	-0.13173300	C	-4.49384800	1.44808200	-0.09401400
C	-2.82281500	0.81459200	0.54772600	H	-3.50331300	2.92961100	1.13212300
C	-1.55952700	-0.85576600	-0.68503100	H	-5.24638700	-0.21409200	-1.23264700
C	-3.87482400	-0.08767200	0.69246300	H	-5.29638000	2.11215900	-0.40427800
H	-2.88893000	1.81498100	0.96418300	O	-1.50976600	-2.40615700	1.31119200
C	-2.62425500	-1.75070400	-0.55539500	C	1.39412600	-2.29415300	2.34501100
H	-0.67516400	-1.15160000	-1.23996200	H	1.71741000	-2.58229400	3.34813300

H	0.86102100	-3.12295200	1.87491000	H	-4.88885800	0.29611300	-1.39035800
H	2.26147500	-1.99043300	1.75230200	H	-4.75810400	2.61280100	-0.53102200
C	-3.51545500	-2.18738800	-0.68871100	O	-1.88112000	-2.17736400	1.86171100
H	-2.53610800	-2.55104700	-1.01216400	C	0.95963500	-3.05569900	1.65584100
H	-3.85141400	-2.87317700	0.09668800	H	1.36623900	-3.62059700	2.49871800
H	-4.21046700	-2.26045900	-1.53087800	H	0.05005000	-3.54177600	1.29574500
O	2.38920900	0.77917000	0.68935100	H	1.71289400	-2.99598000	0.86388700
C	2.05375900	1.66157900	1.57759400	C	-3.45750500	-1.87360300	-0.66434800
O	0.91773100	1.81149300	2.07309100	H	-2.50999600	-2.41724400	-0.71276900
C	3.19510600	2.57676200	1.99413000	H	-4.10742700	-2.44638300	0.00784900
H	4.14675500	2.03834800	2.00500900	H	-3.91341700	-1.88088200	-1.66009400
H	3.27702400	3.38750100	1.25948600	O	2.50330800	0.33156900	0.63684200
H	2.99395600	3.01378400	2.97523700	C	2.31590500	0.97141200	1.71593400
N	-0.07026000	-0.61471900	1.40983600	O	1.20042800	1.01880400	2.34541800
H	-0.04705500	0.40167400	1.63650600	C	3.47005000	1.75135100	2.29113400
TS1				H	4.41506900	1.42629300	1.85238200
Rh	0.91698400	-0.39648200	-0.58038800	H	3.31888600	2.81227900	2.05724100
C	0.77640500	-0.30579800	-2.77216300	H	3.49335100	1.64620500	3.37911600
H	0.55221400	0.63402400	-3.25665200	N	-0.03856900	-0.86922000	1.34454200
C	2.07601800	-0.75329700	-2.41446900	H	0.43678000	0.22004800	1.85268100
H	3.00114700	-0.22722600	-2.60787600	INT2			
C	1.93933100	-2.01230700	-1.71437900	Rh	-0.64364100	0.14023800	0.78073800
H	2.75017000	-2.60986100	-1.31958900	C	-0.04473900	1.53258100	2.42480800
C	0.55453300	-2.31478800	-1.63753000	H	-0.17771400	2.60104600	2.34289300
H	0.12015900	-3.18041800	-1.15520400	C	-0.97562500	0.60661400	2.93766900
C	-0.18287700	-1.24398800	-2.25775400	H	-1.95569200	0.84269700	3.33264200
H	-1.25653800	-1.18112900	-2.36676600	C	-0.43507600	-0.72882900	2.76998000
O	0.15035400	1.49840200	-0.30176000	H	-0.91255900	-1.65268800	3.06898200
O	1.50619000	2.50439400	-1.81421400	C	0.85559300	-0.59610600	2.18093000
C	0.63083400	2.52982100	-0.93809400	H	1.51227600	-1.41075200	1.91301400
C	-0.00974300	3.83425200	-0.47994100	C	1.08497800	0.79129300	1.90136900
H	0.23507300	4.00826800	0.57416700	H	1.96012200	1.21324300	1.42776200
H	0.35225000	4.67006300	-1.08268300	O	-0.93017200	1.50842900	-0.80875400
H	-1.09929200	3.76084800	-0.55155700	O	0.14978300	3.30165500	0.02720300
O	0.68674700	-1.75991800	2.19776200	C	-0.53308200	2.76082800	-0.84298600
C	-1.42358300	-1.14723300	1.37709500	C	-0.96928400	3.48880700	-2.10477800
C	-2.31118700	-0.09557200	0.78796700	H	-2.04729600	3.37572700	-2.26233500
C	-2.22629700	1.22142500	1.26036300	H	-0.71326000	4.54802400	-2.03956300
C	-3.29141200	-0.45622000	-0.16261100	H	-0.46345900	3.04620700	-2.97100400
C	-3.11683200	2.19532500	0.80835600	O	-1.19305900	-2.05832800	-1.17709100
H	-1.46267100	1.48606500	1.98354500	C	1.03491700	-1.49335300	-1.33883400
C	-4.14503700	0.54885200	-0.63795100	C	2.17659400	-0.57967300	-0.97285800
C	-4.07116000	1.85904700	-0.15455100	C	2.17352100	0.74667500	-1.42165500
H	-3.05199300	3.20977000	1.19142800	C	3.27364300	-1.08233300	-0.24403900

C	3.24147000	1.59939100	-1.13659700	H	-4.23550300	1.42130400	2.76617800
H	1.31689900	1.10750200	-1.97989000	O	-1.36720900	2.03786700	-1.19497200
C	4.32820800	-0.20625100	0.05371600	C	0.75031400	1.93492500	-0.22098500
C	4.31948000	1.12189900	-0.38507700	C	1.65187000	0.96613500	0.50791400
H	3.22134500	2.62958600	-1.48111600	C	1.06264700	0.18432900	1.53084800
H	5.17038000	-0.57296300	0.63690900	C	3.00179100	0.78454400	0.14917600
H	5.15066100	1.77823400	-0.14005600	C	1.82126200	-0.79802300	2.19842400
O	1.22861100	-2.42950900	-2.14244500	H	0.08063000	0.47933900	1.91891000
C	-1.27983700	-3.22578800	-0.35417700	C	3.72828400	-0.19911300	0.83458800
H	-2.11176700	-3.81023200	-0.75749400	C	3.15251100	-0.98885900	1.84322200
H	-0.35277300	-3.80725200	-0.40967800	H	1.36517900	-1.38219500	2.99259600
H	-1.49283000	-2.94708400	0.68568600	H	4.76900600	-0.36461400	0.56488900
C	3.34302800	-2.52747100	0.19818000	H	3.75443700	-1.74075600	2.34604800
H	2.35604000	-2.94169400	0.43002500	O	1.01132700	3.14439500	-0.34662100
H	3.76002200	-3.15407100	-0.59974900	C	-1.45702900	1.87120500	-2.61285300
H	3.98273800	-2.63864000	1.08039600	H	-1.66185800	0.82301600	-2.86619200
O	-2.72492000	-0.39038500	0.45014000	H	-2.29425000	2.49752000	-2.93136500
C	-3.39741500	-0.33177300	-0.59796200	H	-0.53161800	2.19808400	-3.10221600
O	-3.06280700	0.37567500	-1.64840600	C	3.63918900	1.58936100	-0.95849300
C	-4.67159800	-1.10946700	-0.73542000	H	3.04109300	1.54043600	-1.87640800
H	-5.05270400	-1.38981200	0.24767400	H	3.70804600	2.64715300	-0.68471400
H	-5.41763500	-0.53888600	-1.29404200	H	4.64455500	1.21962500	-1.18262000
H	-4.44693900	-2.02195700	-1.30144900	TS2			
N	-0.14562600	-1.21458400	-0.74148700	Rh	-0.90495000	-0.47949400	-0.09652200
H	-2.19075300	0.87259100	-1.47121600	N	-0.00080300	1.15431600	-0.94577800
INT3				C	-0.49754200	-2.41995900	-1.04813400
Rh	-0.52687400	-0.72493900	-0.16753600	H	0.50852300	-2.78999800	-1.19429800
N	-0.32418400	1.26512900	-0.68012800	C	-1.34165700	-2.67624700	0.09831800
C	1.01074500	-2.07179500	-1.00411900	H	-1.07705400	-3.26063000	0.96895900
H	2.06877700	-1.90247600	-0.85313000	C	-2.56832300	-2.00341100	-0.11762800
C	0.14711500	-2.86379700	-0.13851100	H	-3.39214600	-1.95298400	0.58353700
H	0.45868400	-3.37639200	0.76199600	C	-2.52161300	-1.34544100	-1.39915800
C	-1.16043300	-2.80762800	-0.65576100	H	-3.31713400	-0.76646900	-1.84879500
H	-2.04310100	-3.24871400	-0.21113600	C	-1.24549400	-1.63193800	-1.97510200
C	-1.14683400	-1.95270300	-1.82431100	H	-0.87955300	-1.26850200	-2.92654000
H	-1.99899700	-1.71936600	-2.44905300	O	-1.93549800	0.88641700	1.14383600
C	0.22253300	-1.55990600	-2.06187500	O	-0.15842800	1.23745600	2.46403000
H	0.56720900	-0.91490200	-2.85948300	C	-1.36876700	1.45478300	2.12654500
O	-2.33726600	-0.25558400	0.71615800	C	-2.16481000	2.44812800	2.93790100
O	-1.72531200	1.31560700	2.22818300	H	-1.72758700	3.44372000	2.80314300
C	-2.57702200	0.66902700	1.60056400	H	-3.20876300	2.46286100	2.62074700
C	-4.06502700	0.92283100	1.80893600	H	-2.09501900	2.19571500	4.00048900
H	-4.42189800	1.57697800	1.00378300	O	-0.75206100	2.21990400	-1.45183600
H	-4.63558400	-0.00915400	1.75940900	C	1.32163400	1.39821300	-0.77300400

C	1.94587200	0.27424400	0.00975500	C	1.21160900	-1.41044100	-1.82573100
C	1.05475700	-0.45032700	0.84309900	H	1.34791000	-1.43800000	0.85959700
C	3.31143500	-0.05457400	-0.06688600	C	3.52509300	-0.69715000	-1.66139200
C	1.54848300	-1.52360200	1.61113100	C	2.55264200	-1.54237400	-2.20317200
H	0.32807700	0.35644300	1.61872900	H	0.46499900	-2.08013000	-2.24411200
C	3.75806200	-1.13878900	0.70994800	H	4.56299000	-0.81231700	-1.96531300
C	2.89898600	-1.86305200	1.54434100	H	2.84071200	-2.30731300	-2.92097400
H	0.88074400	-2.06410400	2.27710400	O	2.05487000	2.22174100	1.29174800
H	4.80786800	-1.41950300	0.65999500	C	-0.88508000	3.33633400	1.30333800
H	3.28936800	-2.68544600	2.13875500	H	-1.53487300	3.26619300	0.42269900
O	1.94379400	2.39970900	-1.17430400	H	-1.40368900	3.86908900	2.10535400
C	-1.11360700	1.98544100	-2.81564400	H	0.04302900	3.85582500	1.04340000
H	-1.75775900	1.10102000	-2.89736900	C	4.29415700	1.16496500	-0.15317900
H	-1.66747700	2.87388000	-3.13048600	H	4.09689500	2.22532100	-0.33868800
H	-0.22076100	1.85636800	-3.43884400	H	4.36612300	1.05653900	0.93358800
C	4.29089000	0.68365300	-0.95032800	H	5.25926500	0.90057500	-0.59887800
H	3.90471900	0.79970400	-1.96769400	INT5			
H	4.47421500	1.69532700	-0.57388900	Rh	-0.14589900	0.63737400	0.55544600
H	5.24579800	0.14897900	-0.99433900	N	-1.49378400	1.27642600	-0.83603400
INT4				C	-0.39067900	1.17817300	2.76702800
Rh	-1.06100700	-0.09064100	-0.27061300	H	-1.15573400	0.71237300	3.37180200
N	0.01231700	1.21938600	0.86181800	C	0.94450000	0.71764200	2.60041600
C	-1.88722600	-0.17109800	-2.31962500	H	1.39395800	-0.13172000	3.09676400
H	-1.23853100	-0.42336100	-3.14785900	C	1.60533800	1.63830900	1.72002900
C	-2.65300200	-1.07566700	-1.54702300	H	2.64253200	1.58850600	1.42007200
H	-2.72884100	-2.14484900	-1.69719700	C	0.68212000	2.64789200	1.33164100
C	-3.38996800	-0.29980200	-0.56073800	H	0.89187000	3.47734300	0.67032600
H	-4.05365300	-0.71235700	0.18914500	C	-0.56671300	2.35174200	1.96408300
C	-3.05229000	1.04908000	-0.70683300	H	-1.48454400	2.91636000	1.86641500
H	-3.41567500	1.86685300	-0.09881400	O	-1.10359000	2.12910400	-1.86753900
C	-2.04552000	1.14380700	-1.75115700	C	-2.73652200	0.73069500	-0.93642600
H	-1.61003200	2.05724500	-2.13571500	C	-2.91390000	-0.31272500	0.12033800
O	-0.94604400	-1.50273300	1.40913200	C	-1.78216100	-0.59116800	0.89639200
O	1.24691200	-1.98948400	1.67251500	C	-4.11388400	-1.03632300	0.31786900
C	-0.02931400	-2.05665500	2.02581600	C	-1.80204900	-1.58495200	1.87334900
C	-0.27044900	-2.87464800	3.25904400	C	-4.12053800	-2.02624000	1.31121800
H	0.20911000	-2.38291000	4.11287600	C	-2.98465200	-2.30172500	2.07850000
H	-1.34082100	-2.96962500	3.44252400	H	-0.91857000	-1.81351200	2.46266600
H	0.18663300	-3.86271300	3.14583800	H	-5.03154900	-2.59494300	1.48234200
O	-0.60324600	2.03067300	1.82532500	H	-3.01865500	-3.07997100	2.83758300
C	1.34524100	1.39611400	0.68439900	O	-3.58384900	1.05908300	-1.78328400
C	1.83928400	0.41667500	-0.34613700	C	2.53613900	0.60614100	-1.09960100
C	0.84502700	-0.42257100	-0.90176500	O	2.77607000	1.62983600	-1.74070800
C	3.19773400	0.29301900	-0.72124500	C	0.60949000	-1.09269400	-0.57037800

H	1.21957700	-1.71405000	0.07302800	C	-0.88067400	-1.61449000	1.90173400
C	-0.26495600	-1.97216600	-1.42865300	C	-3.21034100	-2.25204400	2.02138300
F	0.54686500	-2.68534000	-2.27654200	C	-1.90749000	-2.32413800	2.52230100
F	-0.95656200	-2.89533600	-0.72328100	H	0.13670600	-1.68901900	2.27421300
F	-1.13922500	-1.31030600	-2.21444900	H	-3.99930300	-2.81825800	2.51014300
C	3.66977900	-0.14099700	-0.45573900	H	-1.69173000	-2.94225100	3.38973700
C	4.92469300	-0.03160100	-1.08467100	O	-3.68612000	0.13018200	-1.65004500
C	3.56876000	-0.91188700	0.71589300	C	2.33999600	0.45936800	-1.27290100
C	6.04127300	-0.68799200	-0.56780000	O	2.67464700	1.28848000	-2.12425000
H	5.00865800	0.56496100	-1.98721000	C	0.35944400	-1.06327900	-0.50594700
C	4.69089400	-1.55321300	1.24387900	H	1.04257500	-1.58549200	0.15400800
H	2.63287300	-0.98770400	1.25367500	C	-0.26919600	-2.11557100	-1.41590500
C	5.92817500	-1.45037700	0.60029700	F	0.74315500	-2.65484900	-2.15737600
H	6.99871700	-0.60327100	-1.07420800	F	-0.84048400	-3.14424800	-0.75333800
H	4.59627600	-2.13042700	2.15934000	F	-1.17432500	-1.63226200	-2.28804700
H	6.79811800	-1.95805200	1.00778600	C	3.41017500	-0.20387100	-0.44806900
C	1.12265200	0.09363600	-1.13975300	C	4.66829400	-0.35897600	-1.05895900
H	0.61630900	0.49425200	-2.01318800	C	3.24312400	-0.66178100	0.86982000
C	-5.36435500	-0.78796800	-0.49415700	C	5.72209100	-0.96915800	-0.37823700
H	-5.69123000	0.25404400	-0.41942300	H	4.80445700	-0.00326100	-2.07513500
H	-5.19061900	-0.97641500	-1.55834300	C	4.30205800	-1.25689000	1.55872100
H	-6.17588100	-1.43752600	-0.14888000	H	2.30089400	-0.52444700	1.38431900
C	-1.48098800	3.48511600	-1.59108600	C	5.54298300	-1.41918600	0.93485200
H	-1.02204200	3.83135700	-0.65820200	H	6.68272100	-1.09177100	-0.87093900
H	-1.10059800	4.07164600	-2.43138700	H	4.15573100	-1.58961400	2.58262300
H	-2.57074100	3.57069700	-1.52910000	H	6.36440600	-1.88951400	1.46843500
TS3				C	0.89389200	0.09733400	-1.19803500
Rh	-0.15108800	1.02799500	0.39722200	H	0.39888600	0.37470100	-2.12536100
N	-1.72037400	1.11292700	-0.92130800	C	-4.96992600	-1.39820800	0.43325100
C	-0.50980200	1.94483200	2.48289300	H	-5.32208300	-0.36460400	0.35866300
H	-1.25795600	1.56058800	3.16359200	H	-5.07276600	-1.82896600	-0.56730800
C	0.85639700	1.50993800	2.39544200	H	-5.62236600	-1.94423900	1.12240700
H	1.32847000	0.77911400	3.03875700	C	-2.17449200	3.17497900	-1.91398000
C	1.49418100	2.25370700	1.35952400	H	-1.56575700	3.73398100	-1.19335600
H	2.52992200	2.16382200	1.06008200	H	-2.11630900	3.65626000	-2.89375900
C	0.52197300	3.11988900	0.76673600	H	-3.21554800	3.13406800	-1.57423200
H	0.69933200	3.82741300	-0.03203100	INT6			
C	-0.71544500	2.92641100	1.48308000	Rh	0.61688200	-1.05340600	-0.10314000
H	-1.65277900	3.42384700	1.27106300	N	2.05795700	-0.06053100	-1.20627400
O	-1.65284800	1.85625900	-2.10357700	C	1.29743000	-2.85615200	1.18245600
C	-2.72484800	0.20146000	-0.86635000	H	2.04105000	-2.77882500	1.96503900
C	-2.49933200	-0.73188100	0.28999700	C	-0.12587400	-2.61437500	1.34303000
C	-1.17826800	-0.81654400	0.78900000	H	-0.61935800	-2.36906300	2.27500800
C	-3.53587100	-1.46019700	0.90632700	C	-0.75426200	-2.80052000	0.08967600

H	-1.81294200	-2.72244600	-0.11470400	H	2.92963200	-1.09978500	-4.14283200
C	0.27968400	-3.04584000	-0.88424300	H	3.78229000	-1.41488100	-2.59346500
H	0.12203400	-3.24992800	-1.93531900	O	0.70778700	1.15681000	0.00000100
C	1.53929300	-3.14498000	-0.16934700	TS4			
H	2.50656000	-3.32698000	-0.61913700	Rh	-0.02562500	-1.51257700	-0.02060300
O	2.23616400	-0.01254000	-2.59187200	N	1.94665800	-0.94033900	-0.73510000
C	2.45988100	1.00579300	-0.50617200	C	-1.75849100	-2.80183000	-0.55925000
C	1.80518100	0.87806200	0.86946300	H	-2.67217200	-2.40705800	-0.97753700
C	0.42782000	1.19348000	1.08429100	C	-0.59566300	-3.18889800	-1.30254800
C	2.65323700	0.56942600	1.97928300	H	-0.49128500	-3.18015700	-2.37895700
C	-0.05002600	1.23651000	2.41799100	C	0.35815100	-3.73458800	-0.35550400
C	2.12630200	0.60326700	3.26277900	H	1.34717200	-4.09291200	-0.60485700
C	0.78234700	0.95152000	3.48533500	C	-0.16587000	-3.58910800	0.93780100
H	-1.08632700	1.50736100	2.59813000	H	0.33877800	-3.83488400	1.86338200
H	2.76595200	0.36529800	4.10885200	C	-1.47385000	-2.96765500	0.82227700
H	0.39577500	0.99479200	4.49973500	H	-2.13424100	-2.71615400	1.64189400
O	3.22687600	1.92944700	-0.80671100	O	2.31782700	-1.94228300	-1.68667300
C	-1.99751500	-0.22181600	-1.37921200	C	2.13329700	0.35416200	-1.24545200
O	-2.17492000	-0.69707500	-2.50785100	C	2.07457400	1.40855100	-0.16771100
C	-0.58931800	1.51565100	-0.02361300	C	0.87455600	1.94989900	0.31241800
H	-1.55261800	1.62323300	0.47893500	C	3.31917600	1.79270000	0.38605500
C	-0.41517800	2.87726200	-0.68787000	C	0.92625400	2.86663900	1.37458200
F	-1.52967100	3.18523200	-1.40968400	C	3.33263000	2.72194600	1.43018400
F	-0.25334900	3.86789500	0.22994300	C	2.14141900	3.25146400	1.93193500
F	0.62878800	2.95439500	-1.54068800	H	0.00023500	3.28306900	1.76069500
C	-3.14510400	-0.24457200	-0.40310100	H	4.28399900	3.01994900	1.86360700
C	-4.44523900	-0.14381100	-0.92767900	H	2.16218700	3.96001900	2.75550500
C	-2.98478400	-0.37988200	0.98640600	O	2.43260200	0.60229700	-2.40523400
C	-5.55645400	-0.16269900	-0.08336500	C	-2.24437200	0.05070200	-1.19537700
H	-4.57071600	-0.04428800	-2.00139800	O	-2.62830000	-0.33562900	-2.30639000
C	-4.09651100	-0.41772800	1.83069900	C	-0.49889200	1.66563400	-0.28716500
H	-1.99396000	-0.48648600	1.41226200	H	-1.22705700	1.83772100	0.50804300
C	-5.38538800	-0.30251700	1.29900900	C	-0.80438700	2.78339400	-1.30723100
H	-6.55480000	-0.07111500	-0.50260300	F	-2.07297900	2.69904900	-1.79168700
H	-3.95450600	-0.53783500	2.90139400	F	-0.69661300	4.02611300	-0.76395400
H	-6.25028200	-0.32390100	1.95658000	F	0.02615100	2.75392300	-2.37817600
C	-0.66905500	0.36353100	-1.03895900	C	-3.26643300	0.24567600	-0.10360700
H	-0.16979100	0.59276100	-1.97948400	C	-4.59812200	0.47538900	-0.48860900
C	4.09867000	0.21460900	1.73663600	C	-2.95617100	0.19193200	1.26722100
H	4.18479600	-0.58161000	0.98723800	C	-5.59689800	0.65462900	0.46963400
H	4.65197700	1.07707000	1.34909100	H	-4.83550900	0.51792000	-1.54696200
H	4.58018600	-0.12352500	2.65861700	C	-3.95774900	0.35840200	2.22644300
C	2.80928800	-1.23296500	-3.06513100	H	-1.94026100	-0.00186600	1.59368600
H	2.13624200	-2.07675000	-2.87158100	C	-5.27936700	0.59383900	1.83172700

H	-6.62047600	0.84139400	0.15582800	H	1.91379100	4.17609600	2.59526800
H	-3.70455100	0.30306900	3.28199200	O	2.33967900	0.50952000	-2.36970600
H	-6.05595100	0.72918900	2.57999500	C	-2.23577300	-0.09235700	-1.20472400
C	-0.78555000	0.29482700	-0.94904600	O	-2.62844600	-0.56229800	-2.28066800
H	-0.30632800	0.24763600	-1.92931900	C	-0.52362300	1.61403800	-0.41766100
C	4.61397500	1.19079300	-0.10994000	H	-1.28322800	1.81894700	0.33860900
H	4.65075100	0.11411900	0.09692300	C	-0.81671700	2.65742400	-1.51687700
H	4.73133000	1.32035600	-1.19077100	F	-2.06758700	2.51435700	-2.03193300
H	5.47254700	1.65234600	0.38623300	F	-0.74962000	3.93522100	-1.05387400
C	3.73563300	-2.15131400	-1.67899700	F	0.04710600	2.57703300	-2.55860900
H	4.08172600	-2.44386700	-0.67933700	C	-3.25441200	0.17088600	-0.12454800
H	3.90445800	-2.97142600	-2.38159100	C	-4.58783500	0.36973100	-0.52196900
H	4.27103000	-1.25886200	-2.01912800	C	-2.94043200	0.20621100	1.24586800
O	2.61464200	-1.05865400	1.68518200	C	-5.58617700	0.60593600	0.42430100
H	2.39077300	-1.08244600	0.53337400	H	-4.82769900	0.34222100	-1.58025300
C	1.58673700	-0.62287000	2.33381500	C	-3.94319100	0.42823100	2.19307300
O	0.43106000	-0.53341900	1.83456600	H	-1.92283300	0.03835000	1.58141100
C	1.81403600	-0.16668500	3.74821500	C	-5.26654900	0.63273400	1.78712300
H	2.32606100	0.80188200	3.71472500	H	-6.61096800	0.76789200	0.10061800
H	0.86548900	-0.05340300	4.27538700	H	-3.68874700	0.43948500	3.24985700
H	2.46439600	-0.87331300	4.27156100	H	-6.04282000	0.81192100	2.52654700
INT7				C	-0.77537000	0.19862400	-1.00195700
Rh	0.05258200	-1.55284200	-0.01000500	H	-0.31344500	0.11594200	-1.98897400
N	2.11568100	-0.94138300	-0.58137700	C	4.59697100	1.32385300	0.03920400
C	-1.25064800	-3.00666400	-1.06706100	H	4.69528800	0.28946600	0.39098800
H	-1.85376000	-2.70313600	-1.91052900	H	4.74049000	1.32213400	-1.04655600
C	0.08455000	-3.47470600	-1.12440000	H	5.41496500	1.89677600	0.48474000
H	0.67875600	-3.59179000	-2.02010500	C	4.07745600	-1.97039900	-1.41928300
C	0.52734000	-3.77196600	0.22547600	H	4.49112100	-2.06972200	-0.40900300
H	1.50716000	-4.13388700	0.50635700	H	4.34246600	-2.84628000	-2.01479200
C	-0.52262200	-3.43312700	1.09947400	H	4.45061100	-1.06403800	-1.90412200
H	-0.48425400	-3.46968800	2.18104500	O	2.38451200	-0.92856100	2.14502800
C	-1.62373800	-2.90859300	0.32044600	H	2.47464500	-0.98193000	0.40431700
H	-2.58266100	-2.59032200	0.70608500	C	1.28137600	-0.44399800	2.48972500
O	2.63778100	-1.98608500	-1.38217800	O	0.21086700	-0.44317500	1.76632200
C	2.18139100	0.35836000	-1.17714900	C	1.14573900	0.25471200	3.82958200
C	2.05750700	1.45597400	-0.15952800	H	1.47652100	1.29226900	3.70529900
C	0.81327600	1.97752600	0.22424400	H	0.10855600	0.26166500	4.17315800
C	3.25929700	1.90735400	0.43218500	H	1.79157200	-0.22360600	4.57074800
C	0.78527800	2.95555900	1.22994600	TS5			
C	3.18981500	2.90016300	1.41368100	C	-1.57921200	-0.99577400	-1.88163900
C	1.95838700	3.41719800	1.81898800	H	-2.02373100	-0.25850700	-1.23075800
H	-0.17150400	3.35967900	1.54758300	Rh	-0.30353800	-2.48677700	-1.09455700
H	4.10799000	3.25819500	1.87193800	C	-0.29907100	-0.88567000	-2.55856200

H	0.41979000	-0.07077100	-2.47164600	C	-4.25660500	1.39201500	1.55965600
C	-0.07184100	-2.10092800	-3.25130500	H	-5.31219900	1.63761400	1.40749800
H	0.81682600	-2.35932000	-3.81214200	H	-4.19162200	0.32159600	1.78663500
C	-1.20736400	-2.96560100	-3.01821500	H	-3.90820700	1.93748300	2.44232900
H	-1.30065900	-3.98819700	-3.36353200	C	1.71088100	-1.76842300	1.02169100
C	-2.14908800	-2.27527100	-2.20251600	O	1.51583700	-2.31268500	-0.09749700
H	-3.08783600	-2.66271200	-1.83150600	C	2.69102000	-2.36168600	1.98687700
O	-0.91105400	0.10084100	3.36971300	H	2.26051600	-2.35619300	2.99274100
C	-1.36570200	1.74621800	1.70118900	H	2.96337800	-3.37500800	1.69011000
C	-2.04694200	1.91311200	0.35922300	H	3.58500200	-1.72758900	2.00254500
C	-1.33144500	2.25227800	-0.80782100	O	1.12495100	-0.68317800	1.40957600
C	-3.45278200	1.73821000	0.32234700	H	0.87272200	0.03015300	0.65087700
C	-2.04685800	2.39790000	-2.00763500	N	-1.40844600	0.46490300	2.12845100
C	-4.12404400	1.89470600	-0.89714900	H	-1.83837000	-0.29719700	1.59997700
C	-3.42708800	2.21855100	-2.06052700	C	-2.01347500	-2.80431100	1.31129500
H	-1.50558500	2.64714600	-2.91628400	O	-0.93025100	-3.20336800	0.70638600
H	-5.20268100	1.76280100	-0.92980800	C	-2.34960200	-3.58829300	2.56475300
H	-3.95583900	2.33094400	-3.00324800	H	-2.09564100	-4.64555000	2.45310400
O	-0.88816500	2.67881600	2.35144400	H	-1.75342500	-3.18290500	3.39163400
C	2.24241700	1.06087700	-0.86575200	H	-3.40733300	-3.47098200	2.80997900
O	2.20260200	0.86336600	-2.12018100	O	-2.69657500	-1.83064400	0.95043800
C	1.15528100	1.59128500	-0.11773000	INT8(3a)			
C	0.18393400	2.45411400	-0.90803300	C	-3.65058300	-2.03904000	-0.98882800
H	1.35767000	1.93325600	0.89411400	C	-4.31786100	-0.83445700	-0.75656600
H	0.43196500	2.27497700	-1.95977000	C	-3.63159500	0.28603600	-0.27202700
C	0.54606400	3.93841400	-0.74147800	C	-2.25148500	0.16093200	-0.01298400
F	1.83493400	4.17309800	-1.11979900	C	-1.57092700	-1.05239900	-0.22454300
F	-0.22470600	4.75210900	-1.52631400	C	-2.28455000	-2.14819700	-0.72802400
F	0.42695700	4.40946500	0.52093100	H	-4.19653800	-2.89698000	-1.37133500
C	3.49131200	0.60928500	-0.14065100	H	-5.38411000	-0.76031200	-0.95478400
C	4.27511500	-0.40225800	-0.72089500	H	-1.77715600	-3.08925100	-0.91162800
C	3.91696500	1.17197400	1.07432600	C	-1.49766200	1.35400500	0.52425000
C	5.44233600	-0.85240100	-0.10104700	O	-1.22663200	1.51595600	1.71398800
H	3.94588200	-0.83369400	-1.66071300	N	-1.12847900	2.22047300	-0.45628600
C	5.09000700	0.73097100	1.69385000	H	-1.38892400	2.10296300	-1.43025300
H	3.34044800	1.96712400	1.53639500	O	-0.39696800	3.36120200	-0.17757900
C	5.85558800	-0.28547600	1.11078500	C	-1.26465100	4.45487200	0.19934200
H	6.02831700	-1.64505700	-0.55983000	H	-0.59128200	5.29244500	0.39223900
H	5.40676900	1.18307200	2.63028900	H	-1.94815800	4.69861000	-0.62167100
H	6.76542100	-0.63086300	1.59511500	H	-1.82371200	4.19998000	1.10436300
C	-1.92744200	0.24316800	4.38268400	C	-0.07325700	-1.15269500	0.04483500
H	-1.44718600	-0.06822000	5.31333500	H	0.26734900	-0.24081900	0.53926600
H	-2.25196300	1.28601300	4.45622400	C	0.25372400	-2.24350100	1.06439500
H	-2.78165800	-0.40790300	4.16349300	F	-0.50172900	-2.12825300	2.18296300

F	1.55358900	-2.16555200	1.45863600	H	-3.97681300	1.24843300	-3.67500800
F	0.07143800	-3.50358300	0.58964100	H	-2.42427700	3.18952300	-3.64358800
C	0.72033900	-1.34480800	-1.27551100	O	-3.70643900	-0.31441200	1.15323300
H	0.46111600	-2.30247400	-1.73251600	C	1.98553000	1.86002800	0.41168300
H	0.39483200	-0.55562000	-1.96276400	O	2.07074600	2.98569100	0.90293100
C	2.24360600	-1.29723300	-1.14860000	C	0.66350100	1.15357100	0.25955200
O	2.90309300	-2.28839900	-1.45051800	C	-0.56441100	2.08627300	0.45208600
C	2.90442900	-0.04864800	-0.66531400	H	0.66667300	0.89508800	-0.80678100
C	4.24012900	-0.12078700	-0.22857500	H	-0.19709000	3.10068900	0.25911700
C	2.23922900	1.18932600	-0.62937800	C	-1.08443400	2.25443700	1.88353400
C	4.89093800	1.01834600	0.24157500	F	-0.11827100	2.75255500	2.69873500
H	4.74914700	-1.07921800	-0.25365000	F	-2.10541100	3.16404500	1.89698100
C	2.89227900	2.33146000	-0.16207300	F	-1.55120000	1.14797000	2.49425700
H	1.21494700	1.28134500	-0.97165400	C	3.21868000	1.22034800	-0.16480400
C	4.21764100	2.24730700	0.27621100	C	4.08095700	2.04475200	-0.90915800
H	5.91936300	0.95111900	0.58571800	C	3.54942000	-0.13148800	0.00776100
H	2.35710400	3.27574200	-0.13575800	C	5.23288500	1.51940700	-1.49635800
H	4.72486800	3.13416800	0.64679100	H	3.83294500	3.09525200	-1.02903400
C	-4.35728100	1.59091900	-0.02640300	C	4.71581600	-0.65217200	-0.56072600
H	-5.43778200	1.46262500	-0.13816200	H	2.91894400	-0.78109800	0.59891200
H	-4.16380600	1.97236000	0.98277100	C	5.55368000	0.16715400	-1.32320100
H	-4.03829100	2.36780900	-0.73196000	H	5.88187800	2.16340100	-2.08378600
TS6				H	4.96716000	-1.69806700	-0.40518300
N	-1.56789400	-1.04627400	0.70170600	H	6.45418700	-0.24176100	-1.77369200
C	-0.18185200	-0.81774600	-2.57178100	C	-2.15748900	-3.17090600	1.47508800
H	-0.63810600	0.08923800	-2.94734700	H	-2.23605300	-3.72368100	2.41511600
Rh	0.16027800	-1.20280000	-0.42382500	H	-3.14067900	-3.10078200	0.99600500
C	1.23950100	-1.06310700	-2.40370500	H	-1.44649800	-3.67576800	0.80898000
H	2.03353700	-0.35221800	-2.59405800	C	-4.37773900	-0.61769400	-1.76948700
C	1.40410500	-2.36107800	-1.88078500	H	-4.68592000	-0.83312000	-2.79770000
H	2.34299700	-2.81643800	-1.59385400	H	-3.97616300	-1.53583700	-1.32842500
C	0.09276000	-2.95200700	-1.71407100	H	-5.27272000	-0.36646300	-1.18916100
H	-0.11485400	-3.94934200	-1.35003800	C	1.12752900	-1.48845000	2.37175000
C	-0.87104900	-2.00386800	-2.19084200	O	1.03590700	-2.09916700	1.26330900
H	-1.94338800	-2.13961600	-2.19086600	C	1.45042100	-2.28071300	3.60700000
O	-1.67665400	-1.87240000	1.83276600	H	0.50650400	-2.48121900	4.12832600
C	-2.64721100	-0.26141000	0.50278600	H	1.91668100	-3.23235600	3.34543000
C	-2.51801800	0.72222300	-0.63690400	H	2.09349700	-1.70303300	4.27518000
C	-1.63110200	1.82016000	-0.61111400	O	0.95404800	-0.22893800	2.49300300
C	-3.38559800	0.52508600	-1.73635100	H	0.76522300	0.26997000	1.40827500
C	-1.62357600	2.70286300	-1.70400200	INT9			
C	-3.32803700	1.41187700	-2.81784600	N	-0.75506300	-1.17216300	1.15863400
C	-2.45554600	2.50085000	-2.80363500	C	-0.12978100	-0.98713200	-2.25204700
H	-0.94419500	3.55146200	-1.69713300	H	-0.77333500	-0.12871800	-2.36978400

Rh	0.65141200	-1.68363500	-0.32556900	H	-1.96201800	-2.87021600	2.78048400
C	1.30193800	-0.96720300	-2.30605200	H	-0.47784400	-3.59685800	2.06032400
H	1.90944100	-0.07814000	-2.40716700	C	-3.62859500	-2.32119600	-0.29884600
C	1.78873000	-2.29310700	-2.10659500	H	-4.07844500	-2.96949400	-1.05769100
H	2.82593100	-2.59741800	-2.06348400	H	-2.74237100	-2.82354000	0.10327400
C	0.64388700	-3.14763300	-1.94164600	H	-4.34014900	-2.22644100	0.53018700
H	0.67217900	-4.20904900	-1.72877100	C	2.25803400	-1.71684400	1.64266100
C	-0.53491600	-2.35056400	-2.03982800	O	1.75160800	-2.79835500	1.19206500
H	-1.54873800	-2.71171300	-1.96267900	C	3.08507500	-1.70150600	2.89202000
O	-0.37102500	-1.55742300	2.46716100	H	2.40956700	-1.54769200	3.74214500
C	-1.96125900	-0.55318600	1.16218400	H	3.59924000	-2.65655500	3.02598300
C	-2.46567400	-0.05927200	-0.17276400	H	3.80449900	-0.87920000	2.86635700
C	-2.24643800	1.24441400	-0.66316500	O	2.00656500	-0.63930000	1.00780300
C	-3.30185400	-0.95930100	-0.87419400	H	0.35260100	2.84934500	1.11924400
C	-2.82974500	1.59980400	-1.89155200	TS7			
C	-3.85440400	-0.57065100	-2.09845000	Rh	-2.18998900	-1.26244900	-0.07962500
C	-3.61332500	0.70388200	-2.61392200	N	-1.17887200	0.18149400	-1.45719100
H	-2.65098400	2.59307700	-2.29337100	C	-4.09389000	-0.71188000	0.84412500
H	-4.47970100	-1.27019500	-2.64809200	H	-4.22363600	0.18131500	1.43533300
H	-4.03924400	1.00019400	-3.56863000	C	-4.31347900	-0.85520300	-0.56257000
O	-2.69829900	-0.43058500	2.15748300	H	-4.62650900	-0.07027000	-1.23810000
C	0.94057000	2.12391800	-0.80226400	C	-4.00027200	-2.19594200	-0.94158300
O	0.47549300	2.11157300	-1.94170400	H	-4.06476100	-2.62216500	-1.93323300
C	0.02060700	2.08592200	0.40732400	C	-3.62275600	-2.90062500	0.25648300
C	-1.45047200	2.35452300	0.03055100	H	-3.28296100	-3.92762000	0.30200000
H	0.14763400	1.12321300	0.91289100	C	-3.69100200	-2.00065400	1.35112100
H	-1.43932500	3.18763800	-0.67818700	H	-3.42687400	-2.21332300	2.37616200
C	-2.17214700	2.95589400	1.24096100	O	-1.20941900	-0.21017400	-2.83250200
F	-1.72096000	4.22934100	1.46670000	C	-1.17917800	1.59190800	-1.33676400
F	-3.51159800	3.05506300	1.05246800	C	-0.93928500	2.14493400	0.04394100
F	-1.97759100	2.28468200	2.39713600	C	0.37196500	2.31430400	0.52530100
C	2.41722300	2.18133700	-0.58508000	C	-2.04787900	2.60675800	0.78077500
C	3.25673300	2.27469200	-1.71125000	C	0.55225500	2.85117900	1.80692300
C	2.99437400	2.14660700	0.69554800	C	-1.83080900	3.13879200	2.05654600
C	4.64114000	2.32616800	-1.56153400	C	-0.54178800	3.24298600	2.57686400
H	2.80794900	2.31181800	-2.69929800	H	1.55363700	2.97482700	2.20486900
C	4.38105600	2.20322800	0.84587700	H	-2.68215900	3.47443100	2.64355700
H	2.37311200	2.05001200	1.57757000	H	-0.38579700	3.64511100	3.57408800
C	5.20664800	2.29097400	-0.27966200	O	-1.34437100	2.33930200	-2.29188400
H	5.27949000	2.39802600	-2.43794600	C	3.37264400	0.10194200	-0.57129900
H	4.81621900	2.17061000	1.84088900	O	3.49664800	0.37972100	-1.75712100
H	6.28614600	2.33271000	-0.16031500	C	1.59415600	1.97500400	-0.32951300
C	-0.86669700	-2.86395900	2.77664300	H	1.28891000	1.58789800	-1.30517400
H	-0.48760500	-3.09057800	3.77749100	C	2.35161100	3.26941400	-0.66062100

F	3.31187300	3.10852400	-1.59733900	C	1.89858700	-1.37415700	-0.33017100
F	1.50865300	4.22534400	-1.13480500	H	1.58796400	-2.36958800	-0.61453800
F	2.97560700	3.80578700	0.42869400	C	2.19115600	-0.29723600	-1.21844500
C	4.08847400	-1.07642000	0.01827800	H	2.19312100	-0.34418400	-2.29962700
C	4.87768800	-1.87023600	-0.83200600	C	2.48653300	0.87285100	-0.41716300
C	3.97230700	-1.43523200	1.37242000	H	2.73218000	1.85638600	-0.79618400
C	5.52858500	-3.00213000	-0.34440800	C	2.34807400	0.51132800	0.94675500
H	4.95995300	-1.59150100	-1.87769000	H	2.45412100	1.17793000	1.79331600
C	4.62427400	-2.56994600	1.86196100	C	-1.33986200	2.03000100	0.09899100
H	3.37466600	-0.84125900	2.05516100	O	-0.77247300	1.76508700	-1.01243800
C	5.40025600	-3.35719300	1.00476300	O	-0.91788100	1.41643600	1.13763100
H	6.13111100	-3.61109700	-1.01296200	C	-2.48490000	2.99649900	0.18033700
H	4.52402700	-2.83906700	2.90984500	H	-3.42104500	2.44476100	0.03081600
H	5.90363000	-4.24198100	1.38542700	H	-2.51783400	3.46926900	1.16504100
C	-3.43860700	2.62224600	0.19173500	H	-2.40246600	3.75339700	-0.60359200
H	-4.20168400	2.60389800	0.97606400	O	-1.28891500	-0.90308900	-0.41983700
H	-3.58871000	3.53731700	-0.39493300	C	-1.44816600	-2.10919900	0.04970100
H	-3.61592100	1.78341300	-0.48288800	O	-0.62946100	-2.72928900	0.74374100
C	-2.49176000	-0.12234100	-3.46160400	C	-2.78993600	-2.71990800	-0.33862200
H	-3.15928300	-0.90613300	-3.09486600	H	-3.60495200	-2.11364400	0.07240500
H	-2.94274900	0.86390300	-3.33078000	H	-2.90074800	-2.72092100	-1.42842800
H	-2.28576200	-0.29208200	-4.52142500	H	-2.86901200	-3.74124700	0.04016700
O	0.89466600	-1.13956700	-1.14080700	HOAc			
H	-0.07566600	-0.38627000	-1.17853500	C	1.39645900	-0.11929600	-0.00000400
C	0.51020800	-2.33752700	-0.92247400	H	1.67732500	-0.70296000	-0.88322700
O	-0.68887400	-2.65973500	-0.66730800	H	1.67735700	-0.70281800	0.88330400
C	1.55642300	-3.42121100	-0.95616000	H	1.92591700	0.83395900	-0.00008600
H	2.16565400	-3.34096700	-0.04815100	C	-0.08888900	0.12166400	0.00001600
H	1.09348400	-4.40878700	-0.99354100	O	-0.63569600	1.21068200	-0.00000400
H	2.22284500	-3.27332100	-1.80965700	O	-0.78742600	-1.03798200	-0.00000300
C	2.47448000	0.91219500	0.35636300	H	-1.74104000	-0.82399100	-0.00000600
H	3.08625600	1.36118600	1.14779900	KOAc			
H	1.79493000	0.21115800	0.84885600	C	-2.60195500	-0.00741300	-0.00011000
C	-0.90460000	-0.50635500	2.53461200	H	-2.96430400	-0.56221600	-0.87388700
O	-2.00723800	-0.37675500	3.08140200	H	-3.02190000	1.00203100	-0.01322500
C	0.38850200	-0.41860300	3.33914600	H	-2.96291800	-0.53764000	0.88951100
H	0.87154700	0.54312700	3.14231000	C	-1.06923900	0.01165900	-0.00041600
H	0.17228000	-0.49041500	4.40744800	O	-0.47863500	1.13601600	0.00003100
H	1.08058000	-1.21250000	3.04200600	O	-0.47961500	-1.11470500	0.00000900
O	-0.69588400	-0.72741200	1.26713900	K	2.03380400	-0.00516500	0.00002300
CpRh(OAc) ₂				TS8			
Rh	0.42151300	0.20995400	-0.06127000	Rh	0.61688200	-1.05340600	-0.10314000
C	1.95548100	-0.87802300	1.01157100	N	2.05795700	-0.06053100	-1.20627400
H	1.74861800	-1.44616300	1.90726000	C	1.29743000	-2.85615200	1.18245600

H	2.04105000	-2.77882500	1.96503900	H	4.65197700	1.07707000	1.34909100
C	-0.12587400	-2.61437500	1.34303000	H	4.58018600	-0.12352500	2.65861700
H	-0.61935800	-2.36906300	2.27500800	C	2.80928800	-1.23296500	-3.06513100
C	-0.75426200	-2.80052000	0.08967600	H	2.13624200	-2.07675000	-2.87158100
H	-1.81294200	-2.72244600	-0.11470400	H	2.92963200	-1.09978500	-4.14283200
C	0.27968400	-3.04584000	-0.88424300	H	3.78229000	-1.41488100	-2.59346500
H	0.12203400	-3.24992800	-1.93531900	INT10			
C	1.53929300	-3.14498000	-0.16934700	C	-3.54671900	-2.06210700	-1.03826900
H	2.50656000	-3.32698000	-0.61913700	C	-4.20681200	-0.84639800	-0.85141700
O	2.23616400	-0.01254000	-2.59187200	C	-3.52340200	0.27615100	-0.36738400
C	2.45988100	1.00579300	-0.50617200	C	-2.15127400	0.14445800	-0.06270500
C	1.80518100	0.87806200	0.86946300	C	-1.47849200	-1.08162200	-0.22656200
C	0.42782000	1.19348000	1.08429100	C	-2.19210300	-2.17861600	-0.72839900
C	2.65323700	0.56942600	1.97928300	H	-4.09005700	-2.92309300	-1.41793100
C	-0.05002600	1.23651000	2.41799100	H	-5.26653000	-0.76576000	-1.08015600
C	2.12630200	0.60326700	3.26277900	H	-1.69285500	-3.13192100	-0.86724900
C	0.78234700	0.95152000	3.48533500	C	-1.40650600	1.34073600	0.47926800
H	-1.08632700	1.50736100	2.59813000	O	-1.06309300	1.46036300	1.65546000
H	2.76595200	0.36529800	4.10885200	N	-1.17074300	2.28395100	-0.47208800
H	0.39577500	0.99479200	4.49973500	H	-1.35035400	2.13000500	-1.45865800
O	3.22687600	1.92944700	-0.80671100	O	-0.40626500	3.40462300	-0.19460600
C	-1.99751500	-0.22181600	-1.37921200	C	-1.24548100	4.50348300	0.22348000
O	-2.17492000	-0.69707500	-2.50785100	H	-0.55461300	5.32810900	0.41119100
C	-0.58931800	1.51565100	-0.02361300	H	-1.94896900	4.77104000	-0.57275300
H	-1.55261800	1.62323300	0.47893500	H	-1.78320900	4.24248800	1.13992000
C	-0.41517800	2.87726200	-0.68787000	C	0.00441300	-1.22785000	0.12067400
F	-1.52967100	3.18523200	-1.40968400	H	0.37935800	-0.29066100	0.53275700
F	-0.25334900	3.86789500	0.22994300	C	0.20142100	-2.21409100	1.28195200
F	0.62878800	2.95439500	-1.54068800	F	-0.59863200	-1.92834100	2.33969300
C	-3.14510400	-0.24457200	-0.40310100	F	1.48036300	-2.17855000	1.73761400
C	-4.44523900	-0.14381100	-0.92767900	F	-0.05031000	-3.50736000	0.93924300
C	-2.98478400	-0.37988200	0.98640600	C	0.84446200	-1.65154400	-1.06323700
C	-5.55645400	-0.16269900	-0.08336500	H	2.38247600	-2.48072900	-2.76984500
H	-4.57071600	-0.04428800	-2.00139800	H	0.45413500	-2.48275100	-1.64715100
C	-4.09651100	-0.41772800	1.83069900	C	2.05039000	-1.15141400	-1.39552000
H	-1.99396000	-0.48648600	1.41226200	O	2.80403700	-1.67682300	-2.41899000
C	-5.38538800	-0.30251700	1.29900900	C	2.75919100	-0.02361400	-0.74004600
H	-6.55480000	-0.07111500	-0.50260300	C	4.07176400	-0.20444400	-0.27210700
H	-3.95450600	-0.53783500	2.90139400	C	2.14576400	1.22836300	-0.58776400
H	-6.25028200	-0.32390100	1.95658000	C	4.74279300	0.84237800	0.36343900
C	-0.66905500	0.36353100	-1.03895900	H	4.55596700	-1.16863000	-0.39710600
H	-0.16979100	0.59276100	-1.97948400	C	2.81570300	2.27488100	0.05108200
C	4.09867000	0.21460900	1.73663600	H	1.14723600	1.38863100	-0.97843000
H	4.18479600	-0.58161000	0.98723800	C	4.11485100	2.08312200	0.53124700

H	5.75389600	0.68920700	0.73149500	C	-4.69118700	0.35601900	-1.67733100
H	2.31476200	3.23117100	0.16852200	H	-4.54358100	-1.79827100	-1.71189400
H	4.63757600	2.89493600	1.03024400	H	-4.60788800	2.49921000	-1.41238100
C	-4.25802500	1.58464200	-0.16316400	H	-5.50359600	0.39388700	-2.39851600
H	-3.99172700	2.32233700	-0.92945900	C	3.58718700	2.17903900	-0.67455000
H	-5.34004600	1.43039400	-0.21158200	H	3.53690600	2.63137500	0.32230200
H	-4.02369300	2.03141800	0.80953700	H	4.61493100	2.30443000	-1.02644000
TS9				H	2.93768600	2.75443200	-1.34022100
C	3.85667300	-1.59502900	-1.06977500	INT11			
C	4.17011400	-0.23872300	-1.00827800	C	2.37052800	-1.06304800	2.79418400
C	3.20549700	0.71852600	-0.66044000	C	2.62751400	-2.07126200	1.85352200
C	1.91127900	0.26631400	-0.32706900	C	2.00067100	-2.08431500	0.60217600
C	1.59197300	-1.10515800	-0.38356800	C	1.10318000	-1.02746700	0.34213200
C	2.56547900	-2.03030200	-0.76768900	C	0.84970500	-0.01257000	1.27801200
H	4.61762200	-2.31693000	-1.35314000	C	1.47568900	-0.02207400	2.52153700
H	5.17678900	0.09286300	-1.24936300	H	2.87695200	-1.09262100	3.75517900
H	2.33490200	-3.08704300	-0.82213400	H	3.33209800	-2.86106700	2.10094300
C	0.74327000	1.21312600	-0.11699900	H	1.28378200	0.75100300	3.25766600
O	0.09735200	1.67788500	-1.04458000	C	0.31936900	-0.79103600	-0.87841800
N	0.73544100	2.11994600	1.19079300	O	0.23624800	-1.49183200	-1.87689400
H	1.62775600	2.09991500	1.70083700	N	2.58535900	0.47571300	-2.75484900
O	0.28103700	3.44882500	1.02243700	H	3.06674500	0.75096900	-3.61530400
C	1.14067400	4.30339600	0.24734700	O	3.54734500	-0.34198100	-2.04985100
H	0.63936400	5.27159400	0.29387100	C	4.07421800	0.40079600	-0.95338900
H	2.13314300	4.38192300	0.70212900	H	4.75038000	-0.28418900	-0.43332500
H	1.19832900	3.96174700	-0.78678500	H	4.63553800	1.27872500	-1.30175300
C	0.15273400	-1.46213400	0.00944000	H	3.27637600	0.72134800	-0.27452000
H	-0.49197700	-1.42252800	-0.87685300	C	-0.17187700	0.98402700	0.75029700
C	0.02477200	-2.88760600	0.55401200	H	-1.10124300	0.91833300	1.32647700
F	0.19940100	-3.83197800	-0.41353000	C	0.26622900	2.43547800	0.86889700
F	-1.20243400	-3.12184900	1.08586100	F	0.40450300	2.81555700	2.16541400
F	0.92423900	-3.15727200	1.53507000	F	-0.65002900	3.26703900	0.30967800
C	-0.26842100	-0.44253300	1.02721800	F	1.45024700	2.67957500	0.25546000
H	-0.06573600	1.74861900	1.81645100	C	-0.39041900	0.57388100	-0.72927000
H	0.36266200	-0.43945300	1.91605100	H	1.87674900	-0.20399400	-3.03676500
C	-1.46922800	0.27684900	1.17627000	H	0.16917200	1.24475100	-1.39056700
O	-1.50710000	1.16763200	2.10360700	C	-1.82942700	0.58384200	-1.24991200
C	-2.58610900	0.25650600	0.18572400	O	-2.08006100	1.22267600	-2.26635300
C	-3.09735700	-0.92528900	-0.37539700	C	-2.89841900	-0.17341400	-0.53255000
C	-3.15219100	1.48873400	-0.18939900	C	-2.62206900	-1.16040700	0.43048600
C	-4.14806400	-0.87498400	-1.29667900	C	-4.23905100	0.11009400	-0.85438600
H	-2.70511600	-1.88699100	-0.06865500	C	-3.66273100	-1.85183500	1.05343500
C	-4.18948800	1.53937600	-1.12054000	H	-1.60172100	-1.41721000	0.69508500
H	-2.75710200	2.40000000	0.24708000	C	-5.27751100	-0.57200100	-0.22369000

H	-4.44923600	0.87172300	-1.59842100	H	2.91911900	-4.29694300	-0.57905300
C	-4.99124800	-1.55641300	0.73118600	H	1.23506900	-3.93673000	-0.12610000
H	-3.43495300	-2.61889000	1.78799300	INT13			
H	-6.30866700	-0.33965600	-0.47480200	C	-2.69947400	-3.37630200	0.62098900
H	-5.80065000	-2.09093700	1.22096700	C	-3.60572300	-3.04013400	-0.38622600
C	2.29098900	-3.14955400	-0.41948200	C	-3.62748700	-1.75255700	-0.93415300
H	2.72228700	-2.69515700	-1.31889200	C	-2.70650600	-0.79706200	-0.44983600
H	2.99239100	-3.88992800	-0.02289300	C	-1.77734800	-1.12862900	0.55839200
H	1.37371700	-3.65997500	-0.73190800	C	-1.79303300	-2.42687800	1.08858200
INT12(4a)				H	-2.69786400	-4.37876400	1.04029700
C	4.24999800	-0.79005800	0.90921000	H	-4.30386200	-3.78683000	-0.75623700
C	3.84345800	-2.02910400	0.39087800	H	-1.09886500	-2.69975400	1.87656400
C	2.55133000	-2.22764500	-0.10951900	C	-2.76815900	0.58754100	-1.05583900
C	1.68539900	-1.11389400	-0.06327100	O	-3.74895700	1.32825200	-0.95454300
C	2.09105100	0.12632200	0.44847300	N	-1.64765300	0.88754100	-1.76079100
C	3.37903500	0.30417900	0.94585800	H	-0.80053800	0.32253900	-1.64846700
H	5.26126000	-0.68172100	1.29195500	O	-1.44205200	2.14544200	-2.32372300
H	4.54761900	-2.85719700	0.38191100	C	-1.26318000	3.17160800	-1.30975300
H	3.70113300	1.25839700	1.34974000	H	-1.07747200	4.08642500	-1.87769100
C	0.28192400	-1.04568500	-0.49499600	H	-2.17460600	3.27707400	-0.71618200
O	-0.38695900	-1.91944500	-1.02412000	H	-0.39894700	2.93361100	-0.68202400
C	0.96865500	1.14767700	0.38701200	C	-0.78026700	-0.11188500	1.11706500
H	0.76291700	1.55640000	1.38079100	H	-0.78631100	0.80180600	0.52200500
C	1.30447600	2.33701200	-0.49818300	C	-1.21994400	0.36080800	2.50147100
F	2.37699400	3.02688900	-0.03517200	F	-2.50151600	0.80893500	2.49421800
F	0.26812300	3.21458200	-0.55998400	F	-0.45022300	1.38823700	2.94420700
F	1.58841300	1.97690700	-1.77758700	F	-1.14960300	-0.61260700	3.44864800
C	-0.25520000	0.37533200	-0.15398300	C	0.67459500	-0.61091200	1.17756600
H	-0.63775800	0.81319300	-1.07864800	H	1.30906200	0.15510000	1.64377200
C	-1.39264000	0.26819100	0.87643200	H	0.76307400	-1.50785200	1.79941400
O	-1.13762400	0.41161800	2.06844500	C	1.28331700	-0.89347300	-0.17811900
C	-2.77356200	-0.02935000	0.40622000	O	0.68288100	-0.65231200	-1.23238400
C	-3.08462900	-0.28592600	-0.94133700	C	2.64608800	-1.49086900	-0.22922900
C	-3.80584000	-0.05361000	1.36511500	C	3.49571400	-1.51540500	0.89112500
C	-4.40041200	-0.56177700	-1.31953900	C	3.09512400	-2.03761900	-1.44641700
H	-2.30855000	-0.29999200	-1.69700300	C	4.77326200	-2.06938800	0.79037200
C	-5.11788700	-0.32319900	0.98453200	H	3.18077400	-1.07767800	1.83165900
H	-3.56119000	0.14333400	2.40383500	C	4.36713100	-2.59872300	-1.54183600
C	-5.41802700	-0.57845700	-0.36067800	H	2.43119700	-2.02672400	-2.30528400
H	-4.62882600	-0.76476000	-2.36195800	C	5.21036500	-2.61227200	-0.42285300
H	-5.90696400	-0.33580000	1.73124300	H	5.42833100	-2.07240000	1.65688400
H	-6.44160400	-0.78978800	-0.65846100	H	4.70212200	-3.02688100	-2.48260200
C	2.11462200	-3.55976300	-0.65984600	H	6.20424500	-3.04558000	-0.49689500
H	1.82216800	-3.47264100	-1.71243000	C	-4.61253600	-1.41172100	-2.03046900

H	-5.36291900	-0.69677400	-1.67737700	C	4.53165900	-2.36982100	0.43844900
H	-4.11362800	-0.94991000	-2.89110100	H	3.12830300	-1.23485500	1.60423100
H	-5.12852100	-2.31097400	-2.38024300	C	3.89797400	-2.82273400	-1.85325800
C	2.00351200	2.56035200	1.04017800	H	1.98219300	-2.03386800	-2.46421700
C	1.36604000	3.90442000	1.41787300	C	4.81975800	-2.94132200	-0.80623600
H	1.93080100	4.40305200	2.21112200	H	5.24698400	-2.44859300	1.25303300
H	1.28171100	4.56362100	0.54763900	H	4.11231400	-3.26831000	-2.82143600
H	0.35196900	3.71414600	1.79290700	H	5.75490100	-3.47384600	-0.95923400
O	2.70082000	1.96757900	1.90573900	C	-4.77768700	-0.71573700	-2.11044900
O	1.73782500	2.10759600	-0.12233300	H	-5.47429600	-0.01031400	-1.64537400
K	1.94699000	1.65321200	-2.64008600	H	-4.25281000	-0.16758500	-2.90246000
TS10				H	-5.35757300	-1.51652700	-2.57949600
C	-2.95300200	-3.17801800	0.16508500	C	2.60400300	2.14645000	1.11351900
C	-3.85560200	-2.63634300	-0.75463700	C	3.62945400	3.12012800	1.66495600
C	-3.81119700	-1.27942700	-1.09219100	H	4.54520500	2.57479000	1.92203900
C	-2.83654000	-0.46303000	-0.47528500	H	3.86303000	3.89302400	0.92950700
C	-1.92697400	-0.99698300	0.45986600	H	3.25516600	3.58083300	2.58514500
C	-1.99471400	-2.36402500	0.76404300	O	2.17580500	1.27254100	1.97648700
H	-2.99662900	-4.23579900	0.41109100	O	2.22981300	2.20145500	-0.07199400
H	-4.59657400	-3.27732100	-1.22630500	K	1.81557000	1.73840200	-2.63591700
H	-1.29078200	-2.78800800	1.47279200	INT14			
C	-2.78345400	0.99352700	-0.87867100	C	-3.25822800	-3.05865200	-0.05928000
O	-3.69921100	1.79638700	-0.67766400	C	-4.10041700	-2.38024900	-0.94573700
N	-1.62683000	1.28302400	-1.52873400	C	-3.94110200	-1.01129300	-1.18395700
H	-0.81503800	0.64119300	-1.45878600	C	-2.91144000	-0.32285300	-0.50229800
O	-1.29278800	2.59732900	-1.86942600	C	-2.06060700	-0.99625700	0.39678500
C	-0.99178500	3.39825800	-0.69847700	C	-2.24293400	-2.37180600	0.60093900
H	-0.75045700	4.38792200	-1.09351900	H	-3.39136900	-4.12419800	0.10917200
H	-1.86602000	3.45837300	-0.04505900	H	-4.88390000	-2.92333700	-1.46880800
H	-0.12758500	2.98741000	-0.16592900	H	-1.57781300	-2.90209100	1.27505900
C	-0.87888400	-0.13258500	1.17281700	C	-2.74365100	1.15317200	-0.78836300
H	-0.92389700	0.88726500	0.78591100	O	-3.60347700	2.00092700	-0.52544700
C	-1.26421000	0.04438500	2.63984100	N	-1.56283000	1.40906400	-1.40499500
F	-2.54750600	0.47693100	2.77699500	H	-0.77570400	0.71625500	-1.37230500
F	-0.48124800	0.96348100	3.26021300	O	-1.14200500	2.72749500	-1.62709300
F	-1.16306400	-1.10105300	3.37010500	C	-0.80410700	3.40039300	-0.39055900
C	0.55993500	-0.64031700	1.05717300	H	-0.48192000	4.39954100	-0.69348200
H	1.43327600	0.44182500	1.50264400	H	-1.68091100	3.46914600	0.25854000
H	0.82342000	-1.41592300	1.77655000	H	0.01804900	2.88249700	0.11537800
C	1.09610300	-0.82672700	-0.24993100	C	-0.93576300	-0.27982200	1.15845700
O	0.58523500	-0.33586400	-1.30304600	H	-0.91243800	0.76862100	0.85320800
C	2.39635800	-1.56391200	-0.40653900	C	-1.27055900	-0.18675400	2.64292900
C	3.32728500	-1.69024500	0.63961800	F	-2.50452100	0.34464600	2.85615600
C	2.70058100	-2.13177200	-1.65606400	F	-0.38910200	0.61426200	3.30218200

F	-1.24984700	-1.38616500	3.28584600	C	-2.53496100	-2.64354900	-1.23588500
C	0.43685500	-0.89411700	0.95384600	H	-2.93446400	-3.66029900	-1.16000100
H	1.67642200	0.52567500	1.53272700	H	-2.85023900	-2.04849300	-0.37289300
H	0.77717700	-1.60802500	1.69727000	H	-2.89804600	-2.16671900	-2.15509800
C	1.04444500	-0.86618900	-0.29021000	C	1.32797000	1.35673800	0.19029800
O	0.58025900	-0.22708600	-1.31860800	H	1.30123200	1.58497900	1.26301100
C	2.34656800	-1.59524000	-0.49936900	C	1.68664400	2.67426300	-0.48312300
C	3.24637100	-1.87560600	0.54504300	F	2.84258300	3.22435900	-0.00636200
C	2.69188300	-1.99777500	-1.80147600	F	0.72510600	3.61798300	-0.28929600
C	4.44616700	-2.54746600	0.29596800	F	1.84666500	2.55695700	-1.83052400
H	3.02387500	-1.55088300	1.55703200	C	-0.03878400	0.88779200	-0.25241800
C	3.88773600	-2.67621800	-2.05207900	H	-0.21641600	0.97887100	-1.31894700
H	2.00296000	-1.78209300	-2.61230300	C	-1.15325100	1.06621000	0.62338200
C	4.77237100	-2.95310600	-1.00361200	C	-2.54176400	0.87607800	0.08515800
H	5.13083400	-2.74617900	1.11689800	C	-2.88209700	1.10739400	-1.25818000
H	4.12843300	-2.98992300	-3.06512600	C	-3.54387400	0.42980100	0.96509600
H	5.70588400	-3.47569200	-1.19635600	C	-4.18733600	0.89507400	-1.70980700
C	-4.84541500	-0.29905600	-2.16560300	H	-2.13305700	1.46439000	-1.95725000
H	-5.49237400	0.42198200	-1.65487300	C	-4.84463800	0.20217400	0.51375800
H	-4.26776500	0.26406800	-2.90882600	H	-3.28204700	0.25200000	2.00340400
H	-5.47848100	-1.01453900	-2.69949900	C	-5.17148100	0.43556200	-0.82807700
C	2.82649100	2.06374800	1.19789200	H	-4.43445900	1.08487100	-2.75126500
C	3.82094200	2.96139500	1.88801700	H	-5.60290300	-0.15814900	1.20460700
H	4.63524900	2.36046400	2.30673000	H	-6.18455000	0.26250600	-1.18241100
H	4.22119900	3.69117200	1.18293700	C	1.93099600	-3.51154300	-0.79858500
H	3.33356700	3.47851900	2.72182700	H	2.68121100	-4.30190900	-0.69110700
O	2.31894500	1.14190500	2.01291900	H	1.10260900	-3.71095100	-0.11363100
O	2.50835900	2.16950500	0.01698800	H	1.51918400	-3.58103200	-1.81380200
K	1.83104100	1.79060100	-2.56168300	O	-1.00889600	1.21112100	1.86854700
TS11				K	0.01497700	-0.77941200	3.45280000
C	4.52369300	-0.74369000	-0.32767200	INT15			
C	3.93508900	-1.99085800	-0.56162800	C	4.40875400	0.07556200	1.46448500
C	2.54258700	-2.15168700	-0.54691300	C	3.68584200	-0.58117600	2.47050200
C	1.74522400	-1.01288200	-0.30260200	C	2.32588100	-0.88802300	2.31999600
C	2.33113600	0.23812700	-0.08170100	C	1.70331300	-0.51298600	1.11598700
C	3.72524200	0.37484800	-0.08095400	C	2.42782000	0.12618800	0.11147200
H	5.60634500	-0.64501000	-0.33543500	C	3.78136500	0.43912300	0.27111200
H	4.56698700	-2.85617600	-0.75112300	H	5.45979500	0.30679000	1.61861300
H	4.18835900	1.33737500	0.10612900	H	4.19017700	-0.85653000	3.39492800
C	0.22754300	-1.13748600	-0.13640200	H	4.33223000	0.95248700	-0.51151700
O	-0.18532500	-1.62066700	0.96260600	C	0.20692600	-0.64887000	0.77895900
N	-0.50924400	-1.50501800	-1.35314500	N	-0.21642200	-2.11202700	0.68492300
H	0.12262000	-1.56153400	-2.15068600	H	-0.31469100	-2.41387700	1.65658200
O	-1.11441200	-2.79528500	-1.26384200	O	0.85592500	-2.92775700	0.16043300

C	0.38364300	-3.81239700	-0.85473900	C	-2.82067800	0.55508900	-0.21813100
H	1.26683300	-4.36427200	-1.18835500	C	-4.19888400	0.66839100	-0.41149000
H	-0.36259500	-4.51434100	-0.46000300	H	-5.87346900	-0.09394900	-1.53772100
H	-0.04534500	-3.26299600	-1.70068100	H	-4.51467900	-1.68647900	-2.84780700
C	1.55675400	0.45948900	-1.08626300	H	-4.78217400	1.39451800	0.14778400
H	1.56050900	1.53824500	-1.27900500	C	-0.55291500	-0.28048300	-0.55924300
C	2.05294100	-0.14998500	-2.38630100	O	0.32769000	-0.35432500	-1.51896000
F	3.27310100	0.33868900	-2.74536200	N	-0.29227200	-1.39945300	0.54258100
F	1.20893500	0.13453300	-3.41962300	H	-1.13233000	-1.45912100	1.12993700
F	2.17198200	-1.49982100	-2.34512500	O	-0.21807000	-2.66372800	-0.13935000
C	0.14290900	-0.06170800	-0.72535200	C	-0.04939900	-3.71985800	0.80995100
H	-1.69888600	-2.34186200	-0.10733300	H	-0.01328700	-4.63578000	0.21451600
H	-0.13613700	-0.87924300	-1.39087800	H	0.88416100	-3.60562700	1.37181700
C	-0.98983500	0.94521100	-0.83108300	H	-0.90240700	-3.76995400	1.50160700
C	-0.80819000	2.38112900	-0.43505500	C	-1.97338900	1.42049500	0.69829100
C	0.10157900	2.78948100	0.55583300	H	-2.17927300	2.48081000	0.51629200
C	-1.61151400	3.34642300	-1.06766800	C	-2.26741900	1.21345300	2.17218300
C	0.19991300	4.13762000	0.90693900	F	-3.55022400	1.53171700	2.48796300
H	0.69710900	2.05092700	1.07887200	F	-1.47108900	1.98620200	2.95903000
C	-1.50066500	4.69542700	-0.72720400	F	-2.07976600	-0.07423500	2.58923600
H	-2.31404400	3.02668700	-1.83149300	C	-0.51405700	1.07893100	0.33452200
C	-0.59519100	5.09359900	0.26404000	H	0.10201000	0.92704500	1.22203400
H	0.89682100	4.44101300	1.68368900	C	0.11364600	2.15665900	-0.54211100
H	-2.11732700	5.43420300	-1.23218400	C	1.59741100	2.17246300	-0.72814900
H	-0.50972500	6.14309300	0.53366300	C	2.48146400	1.52474600	0.14893700
C	1.57696400	-1.61394400	3.41331400	C	2.12027800	2.86113800	-1.83698000
H	1.45840100	-2.67739200	3.16306300	C	3.85866000	1.55341800	-0.08469200
H	2.11669000	-1.56214100	4.36509600	H	2.10775700	0.99324300	1.01482000
H	0.57788100	-1.18771400	3.54438800	C	3.49374200	2.88109900	-2.07709800
O	-2.46641900	-2.57600300	-0.75179000	H	1.43449900	3.36009400	-2.51427100
O	-3.84789200	-1.55428200	0.70783800	C	4.36857400	2.22480200	-1.20079700
C	-3.64058600	-2.09237900	-0.37974400	H	4.53206500	1.04817700	0.60275000
C	-4.70336500	-2.25504700	-1.43825300	H	3.88403000	3.40445100	-2.94603800
H	-5.69359900	-2.08319400	-1.01279800	H	5.43952400	2.23963900	-1.38617800
H	-4.51830700	-1.51803400	-2.22915300	C	-1.85454400	-2.16034900	-2.75892100
H	-4.65058500	-3.24861200	-1.89319300	H	-2.45395100	-2.51054500	-3.60671500
O	-2.08736300	0.57149400	-1.24533300	H	-0.93722100	-1.69299700	-3.12524600
O	-0.62379400	-0.07008200	1.64635700	H	-1.54787900	-3.02862800	-2.16652000
K	-3.02324200	0.64510400	2.05306900	O	-0.59252600	2.97800700	-1.12483900
TS12				K	2.35017900	-1.88866900	-1.70484700
C	-4.80347400	-0.16169300	-1.35767400	C	2.77522300	-1.51339700	1.95281400
C	-4.02965000	-1.06524400	-2.09726800	C	3.78201800	-1.27098500	3.05647800
C	-2.64182700	-1.18495100	-1.91426200	H	4.74989300	-1.70354400	2.79660000
C	-2.04827900	-0.35957200	-0.93938700	H	3.89113800	-0.19382200	3.22590500

H	3.41881700	-1.71032900	3.99220700
O	3.06382500	-2.13180300	0.91836200
O	1.59000800	-1.00659900	2.19002600
H	0.80857400	-1.20681400	1.37841400
NH ₂ OMe			
C	-1.18034000	-0.20614600	0.00000400
H	-2.00356300	0.51496700	-0.00004000
H	-1.23913600	-0.83710900	0.89648200
H	-1.23911900	-0.83719000	-0.89642100
O	0.01287500	0.57548600	-0.00002700
N	1.15345000	-0.31123600	0.00000500
H	1.69349200	-0.01459900	-0.81526800
H	1.69321400	-0.01442300	0.81540100