

Supporting Information

Insights into the synergistic influence of [Emim][OAc] and AgOAc
for the hydration of propargylic alcohols to α -hydroxy ketones in the
presence of CO₂

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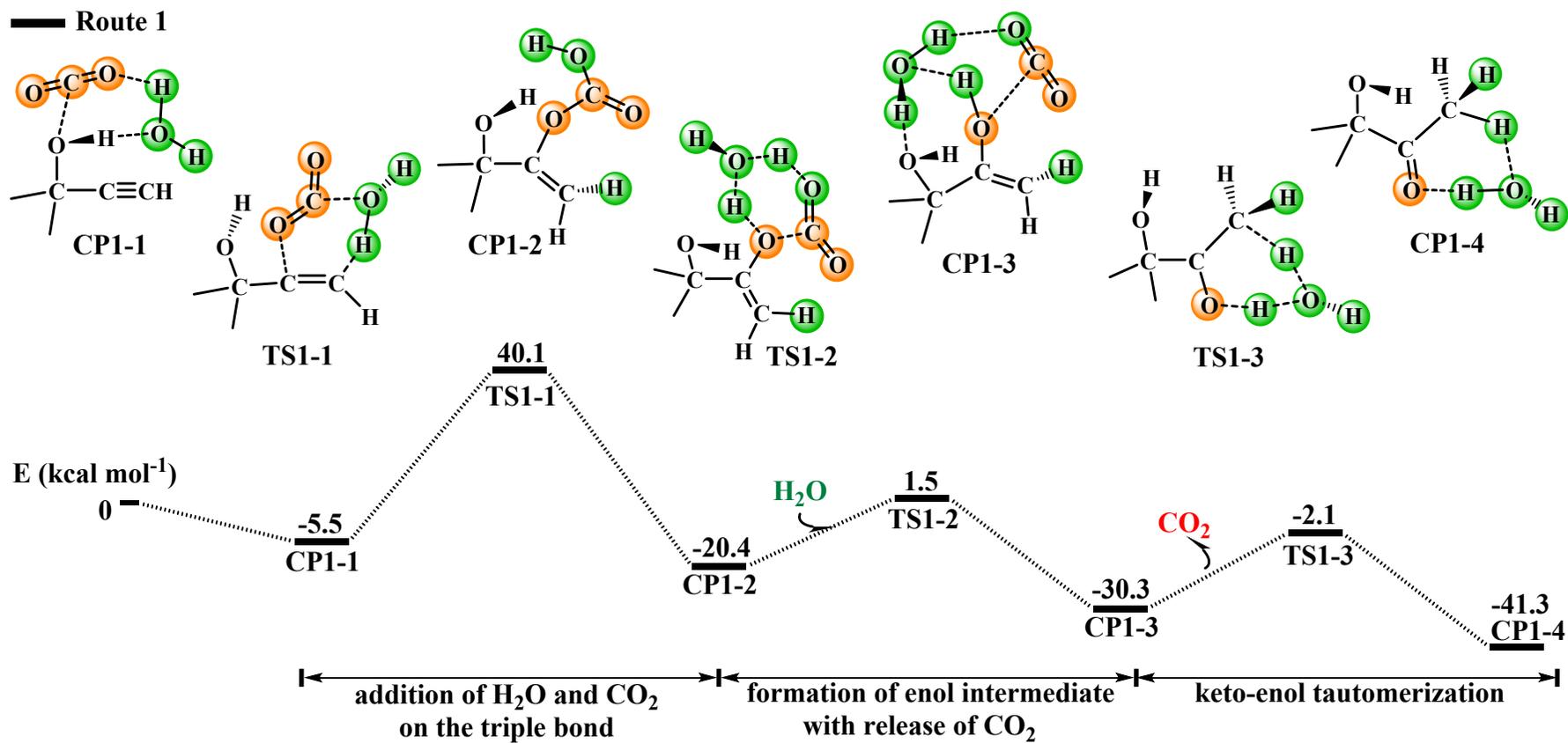


Fig. S1 The energy profile along with the schematic structures of all transition states and intermediates involved in Route 1 calculated at the M06/6-311+G(2d,2p) (PCM)/B3PW91/6-31G(d,p) level.

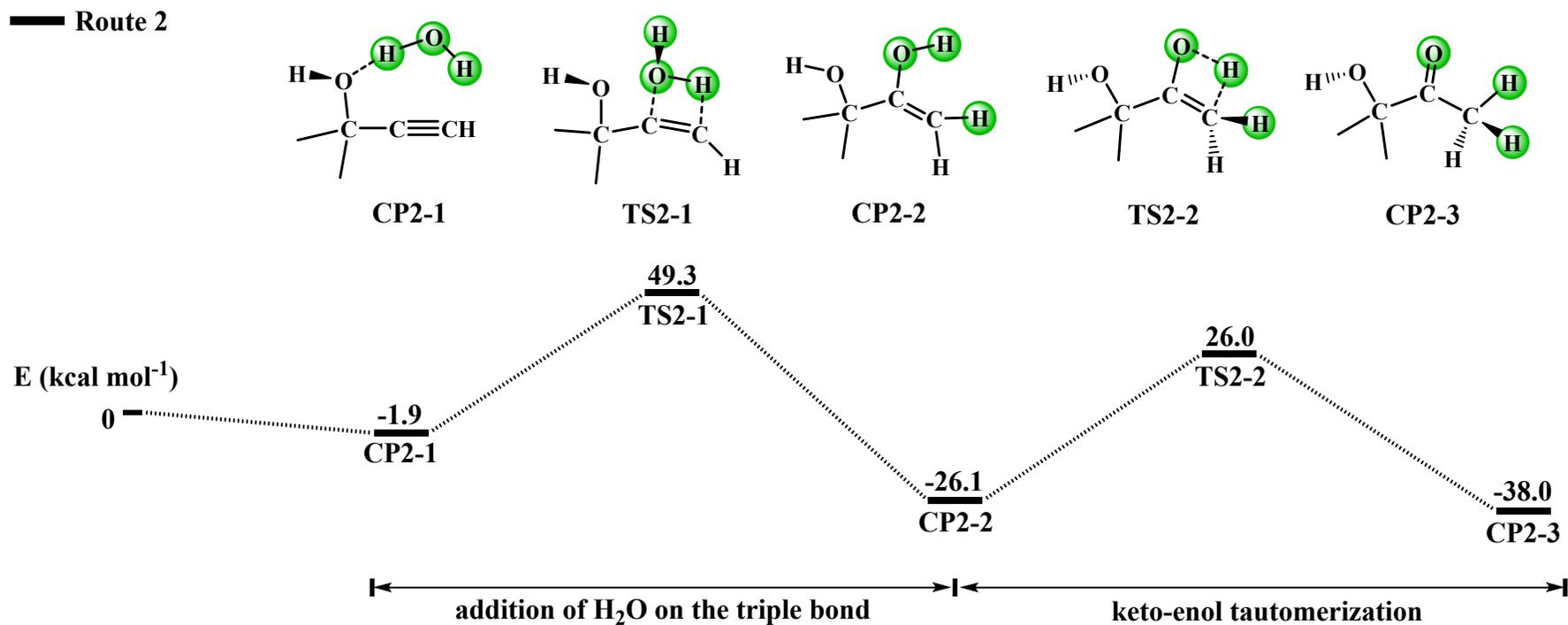
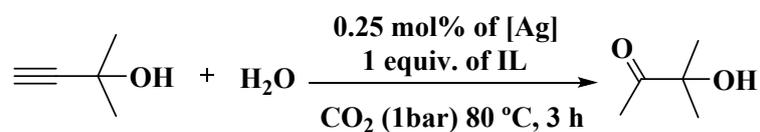


Fig. S2 The energy profile along with the schematic structures of all transition states and intermediates involved in Route 2 calculated at the M06/6-311+G(2d,2p) (PCM)/B3PW91/6-31G(d,p) level.

Table S1 Experimental results by Li et al.¹ Hydration of propargylic alcohol promoted by different ILs/Ag salts catalyst in the presence of CO₂.



Entry	Ag salt	IL	Yield
1	AgCl	/	/
2	/	[Emim][OAc]	/
3 ^[a]	AgCl	[Emim][OAc]	8%
4	AgCl	[Emim][OAc]	70%
5	AgBr	[Emim][OAc]	67%
6	AgI	[Emim][OAc]	58%
7	AgOAc	[Emim][OAc]	79%
8	AgCF ₃ COO	[Emim][OAc]	73%
9	AgNO ₃	[Emim][OAc]	72%
10	Ag ₂ CO ₃	[Emim][OAc]	62%
11	Ag ₂ O	[Emim][OAc]	45%
12	AgOAc	[Emim][Br]	/
13	AgOAc	[Emim][NO ₃]	/
14	AgOAc	[Emim][OTf]	/
15	AgOAc	[Emim][BF ₄]	/
16	AgOAc	[N ₄₄₄₄][OAc]	47%
17	AgOAc	[DBUH][OAc]	25%
18	AgOAc	[DBUH][2-methyl-Im]	2%
19 ^[b]	AgOAc	[Emim][OAc]	95%

^[a]In the absence of CO₂; ^[b]6 h.

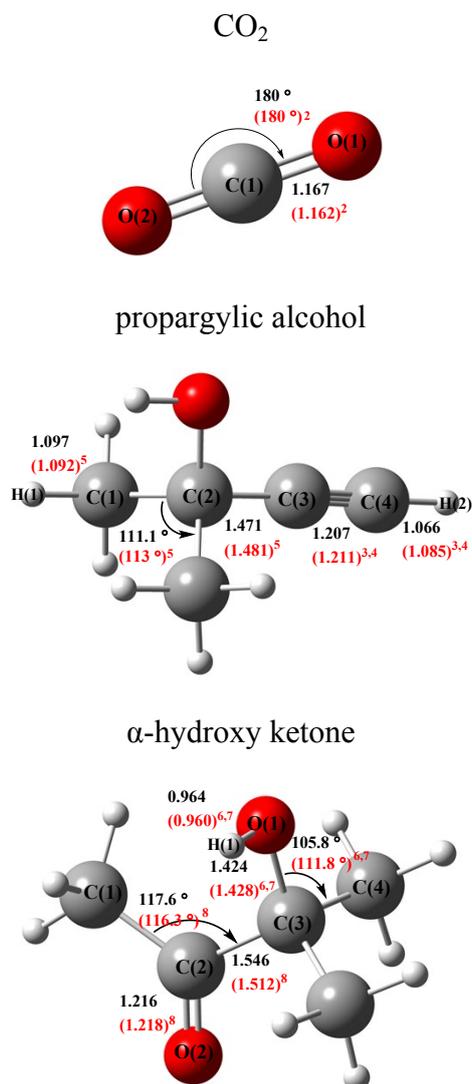


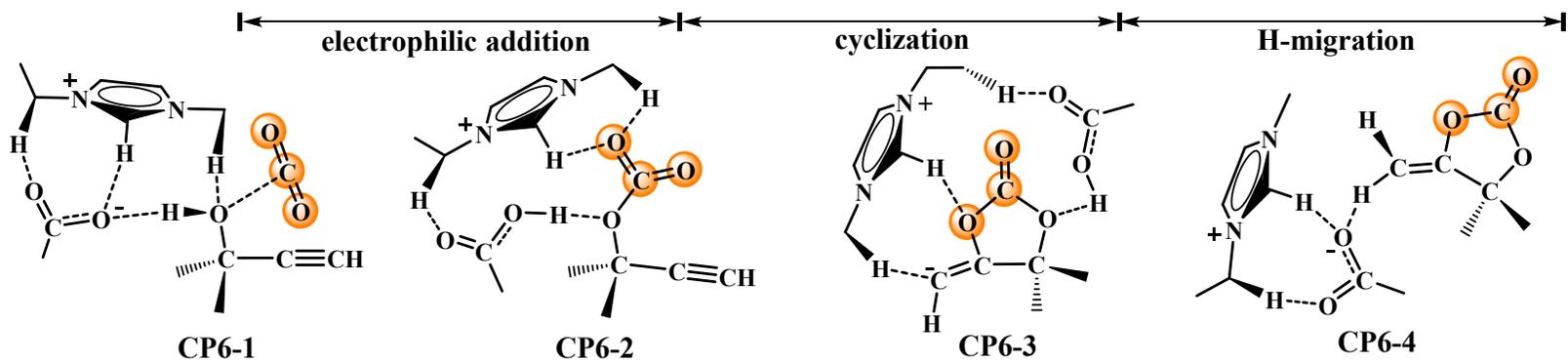
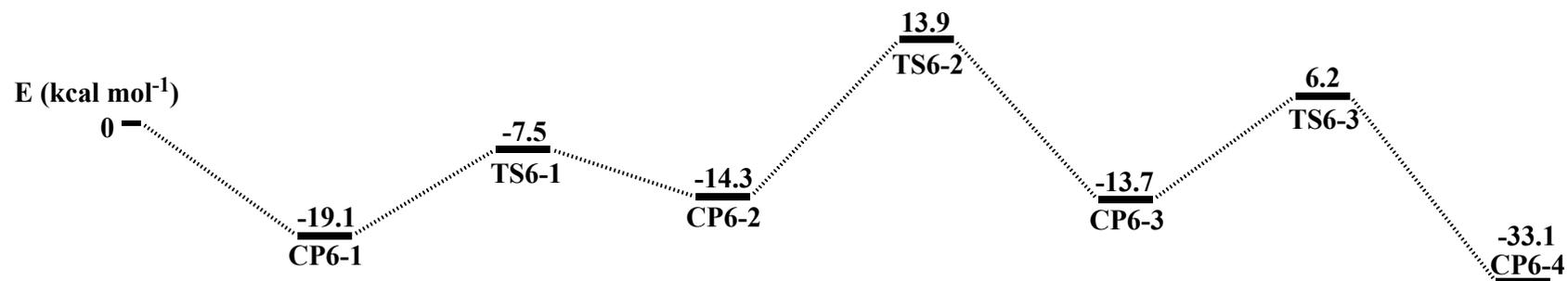
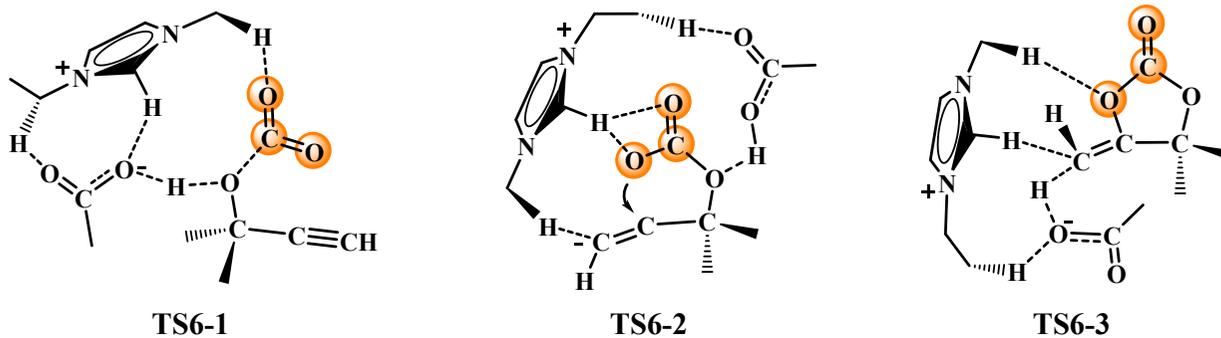
Fig. S3 Geometric data of CO₂, propargylic alcohol, and α -hydroxy ketone (the theoretical and experimental values are shown in black colour and red colour, respectively; bond lengths in Å and bond angles in degrees). Note that the experimental values of 2-propynal,^{3,4} 2-methyl propanenitrile,⁵ 2-propen-1-ol^{6,7} and 2-butanone⁸ are employed due to the absence of experimental values for propargylic alcohol and α -hydroxy ketone, respectively.

Table S2 The experimental FT-IR characteristic peaks and theoretical vibrational frequencies (in cm^{-1}) of CO_2 ,² propargylic alcohol,¹ and α -hydroxy ketone.¹

	Theoretical value	Experimental value
CO_2	647, 2460	667, 2350
propargylic alcohol	3049, 2246, 3166	3000, 2150, 3300
α -hydroxy ketone	3049, 1822, 3187	3000, 1713, 3300

Route 6

A



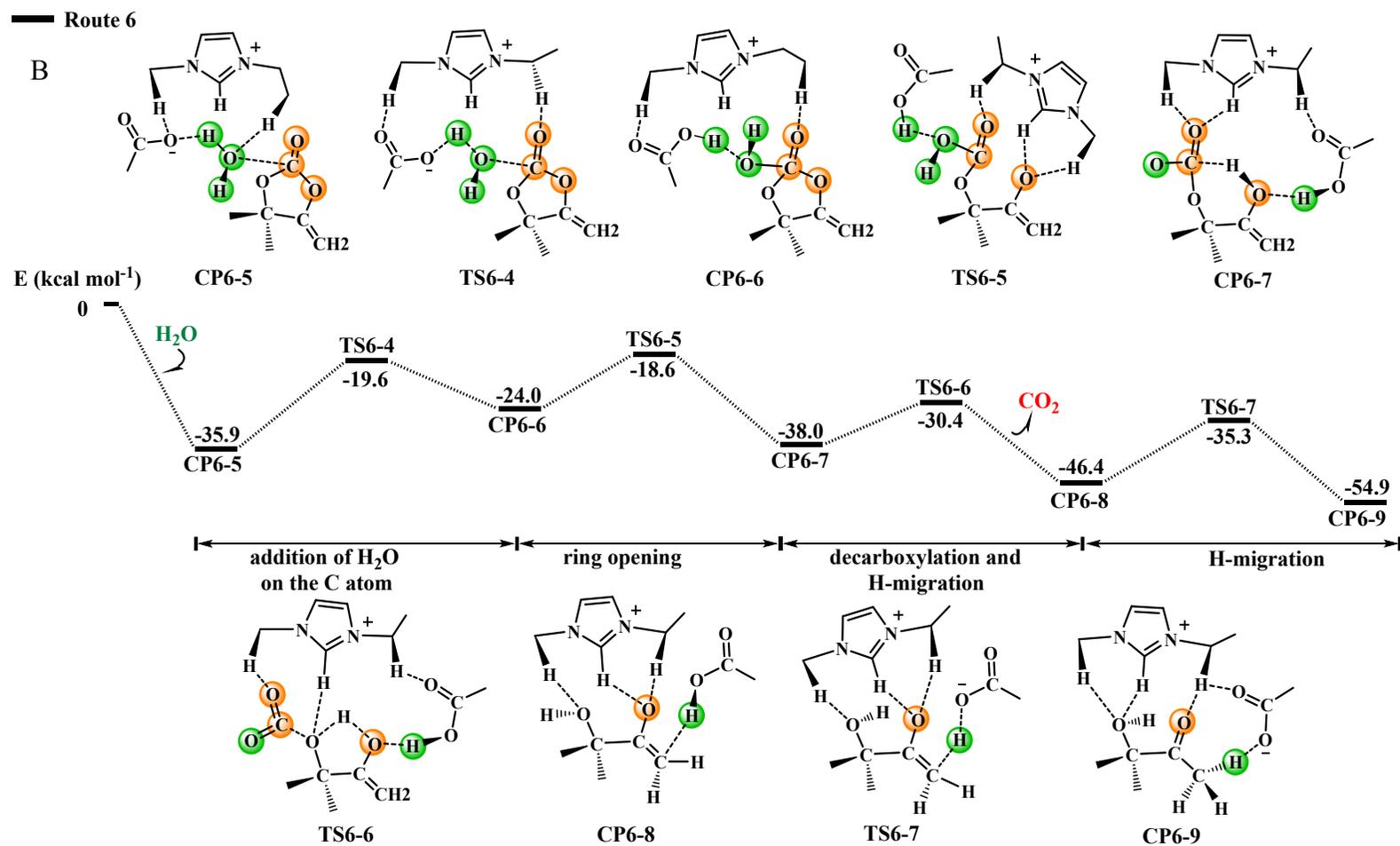


Fig. S4 The energy profiles along with the schematic structures of all transition states and intermediates involved in Route 6 calculated at the M06/6-311+G(2d,2p) (PCM)//B3PW91/6-31G(d,p) level. (A) represents the steps to form the cyclic carbonates. (B) presents the following steps to form the final product.

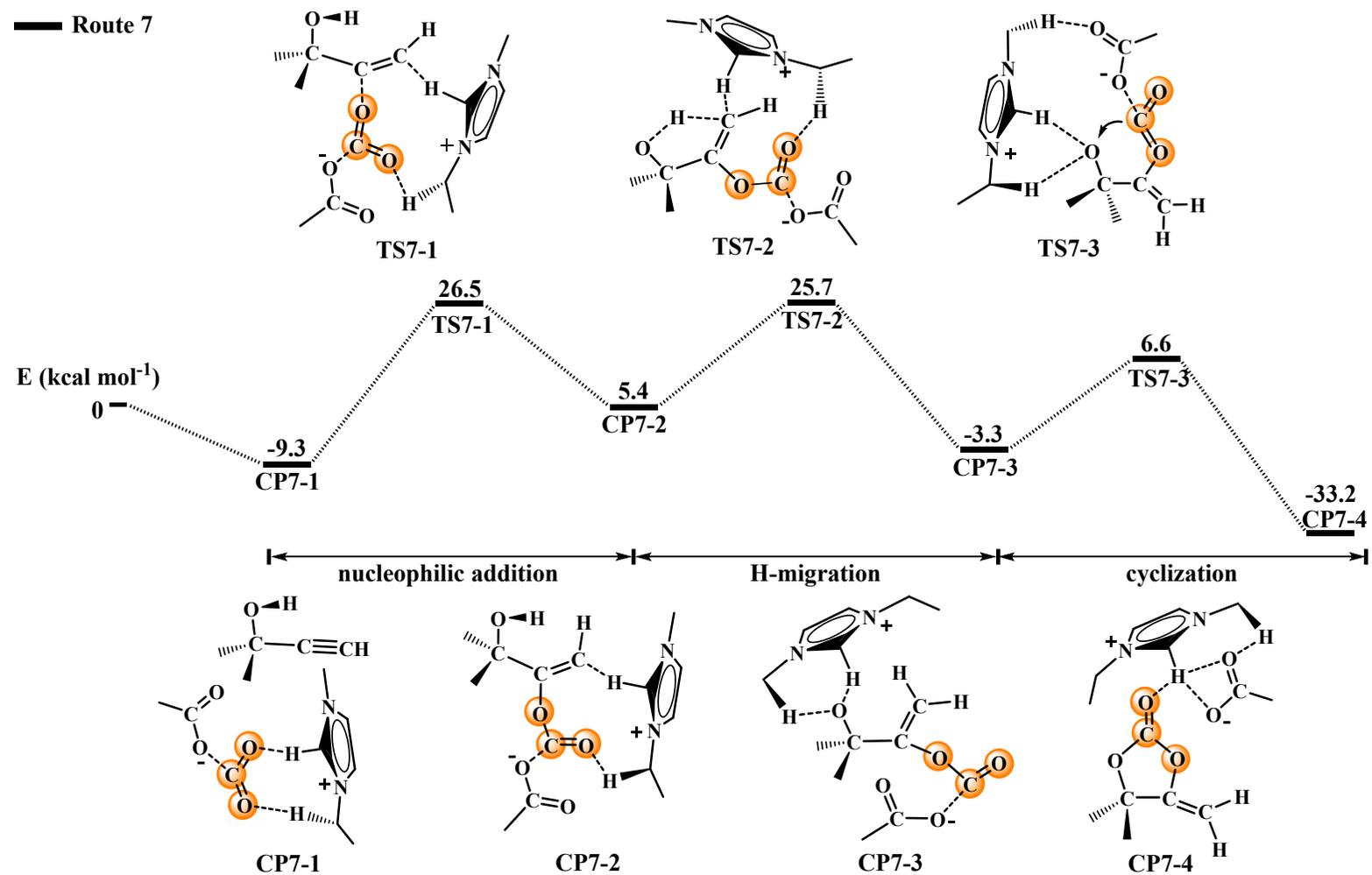
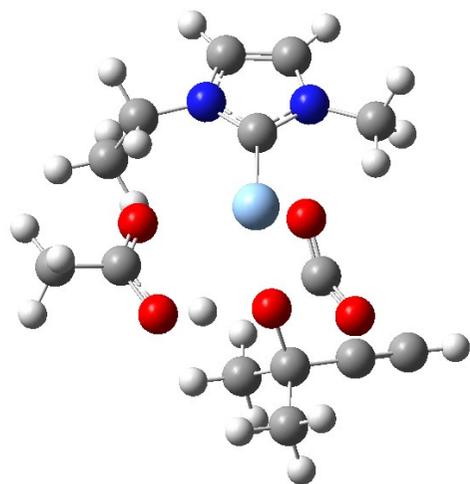
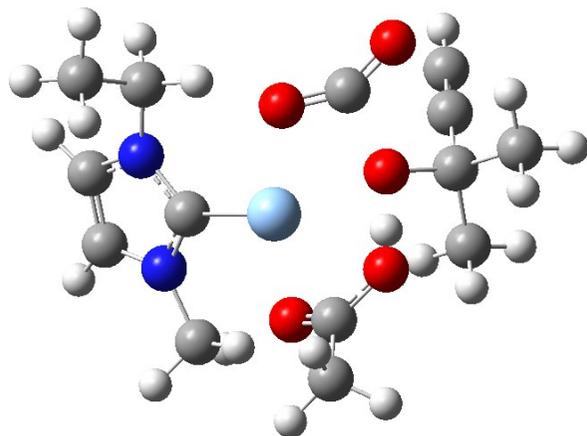


Fig. S5 The energy profile along with the schematic structures of all transition states and intermediates involved in Route 7 to form the cyclic carbonates calculated at the M06/6-311+G(2d,2p) (PCM)//B3PW91/6-31G(d,p) level.

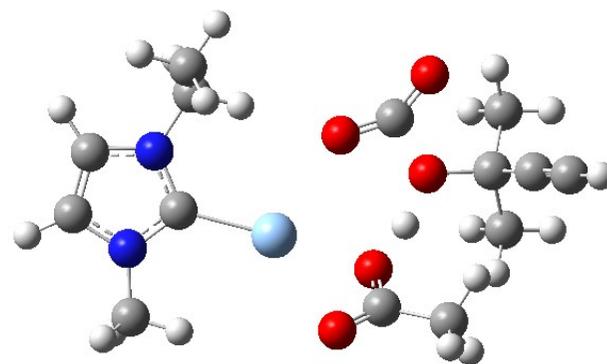
A



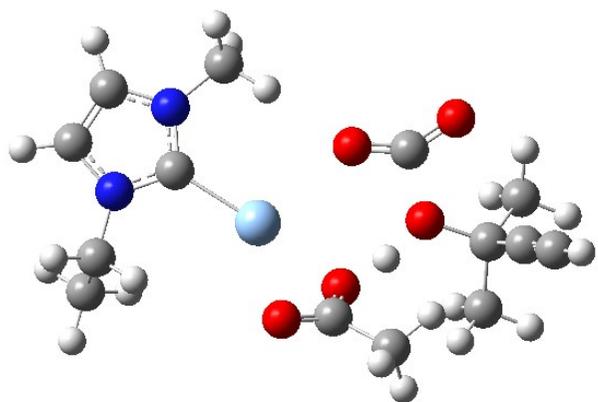
TS9-1(a) 1.7 kcal mol⁻¹



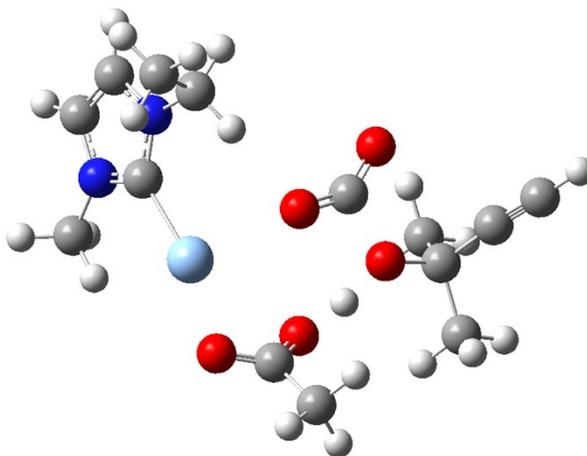
TS9-1(b) 2.1 kcal mol⁻¹



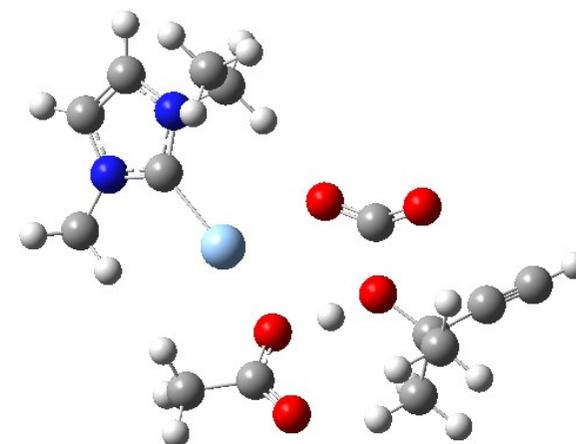
TS9-1(c) 7.6 kcal mol⁻¹



TS9-1(d) 7.6 kcal mol⁻¹

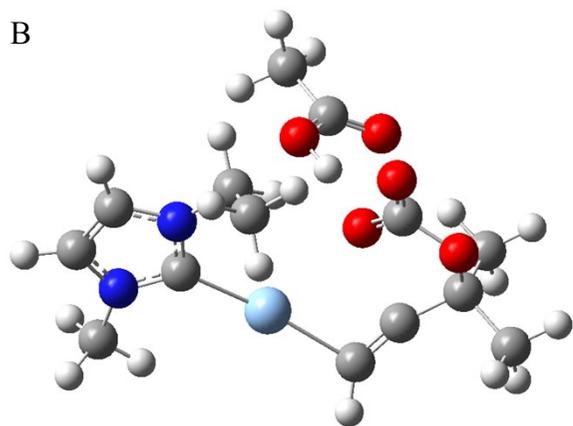


TS9-1(e) 8.2 kcal mol⁻¹

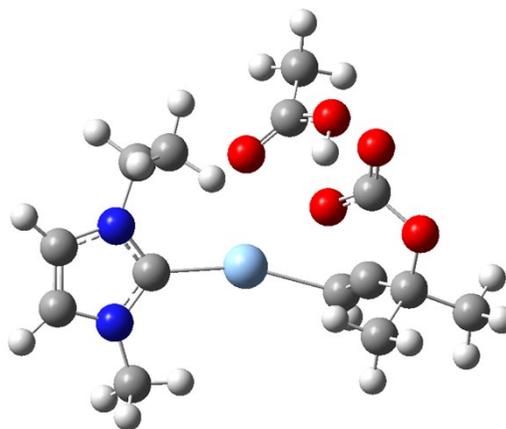


TS9-1(f) 8.7 kcal mol⁻¹

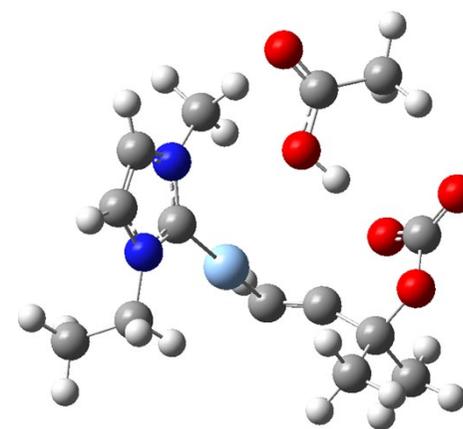
B



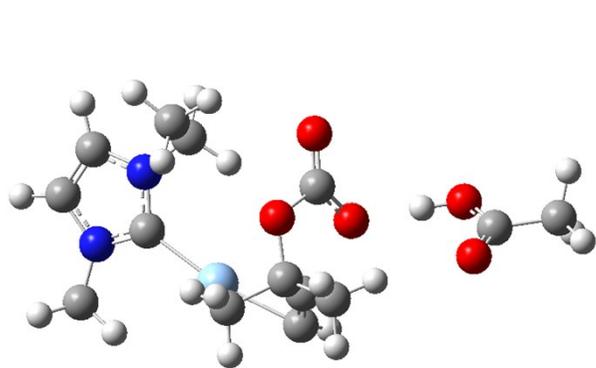
TS9-2(a) 8.2 kcal mol⁻¹



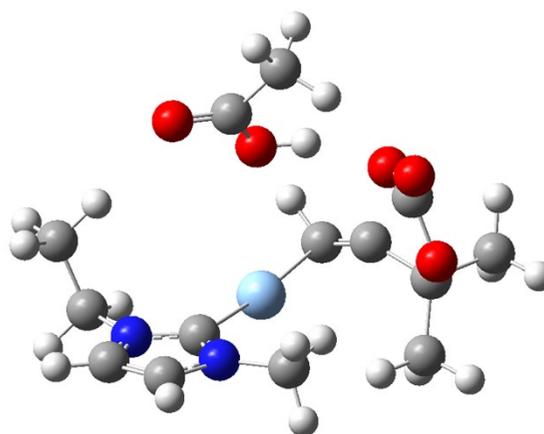
TS9-2(b) 9.4 kcal mol⁻¹



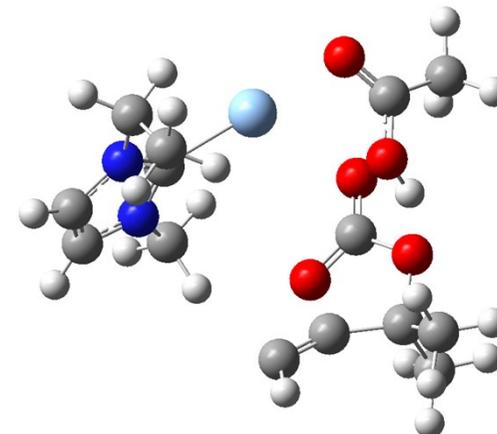
TS9-2(c) 10.4 kcal mol⁻¹



TS9-2(d) 12.9 kcal mol⁻¹



TS9-2(e) 15.9 kcal mol⁻¹



TS9-2(f) 36.4 kcal mol⁻¹

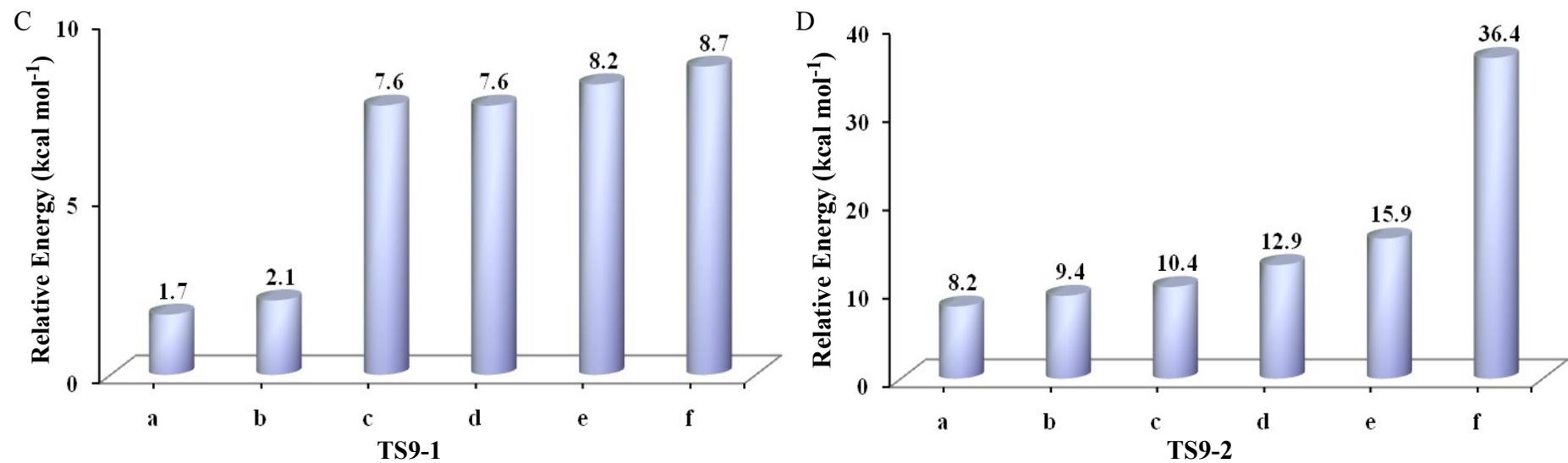


Fig. S6 Different configurations for (A) TS9-1, (B) TS9-2 in the Route 9, relative energy of different configurations for (C) TS9-1 and (D) TS9-2.

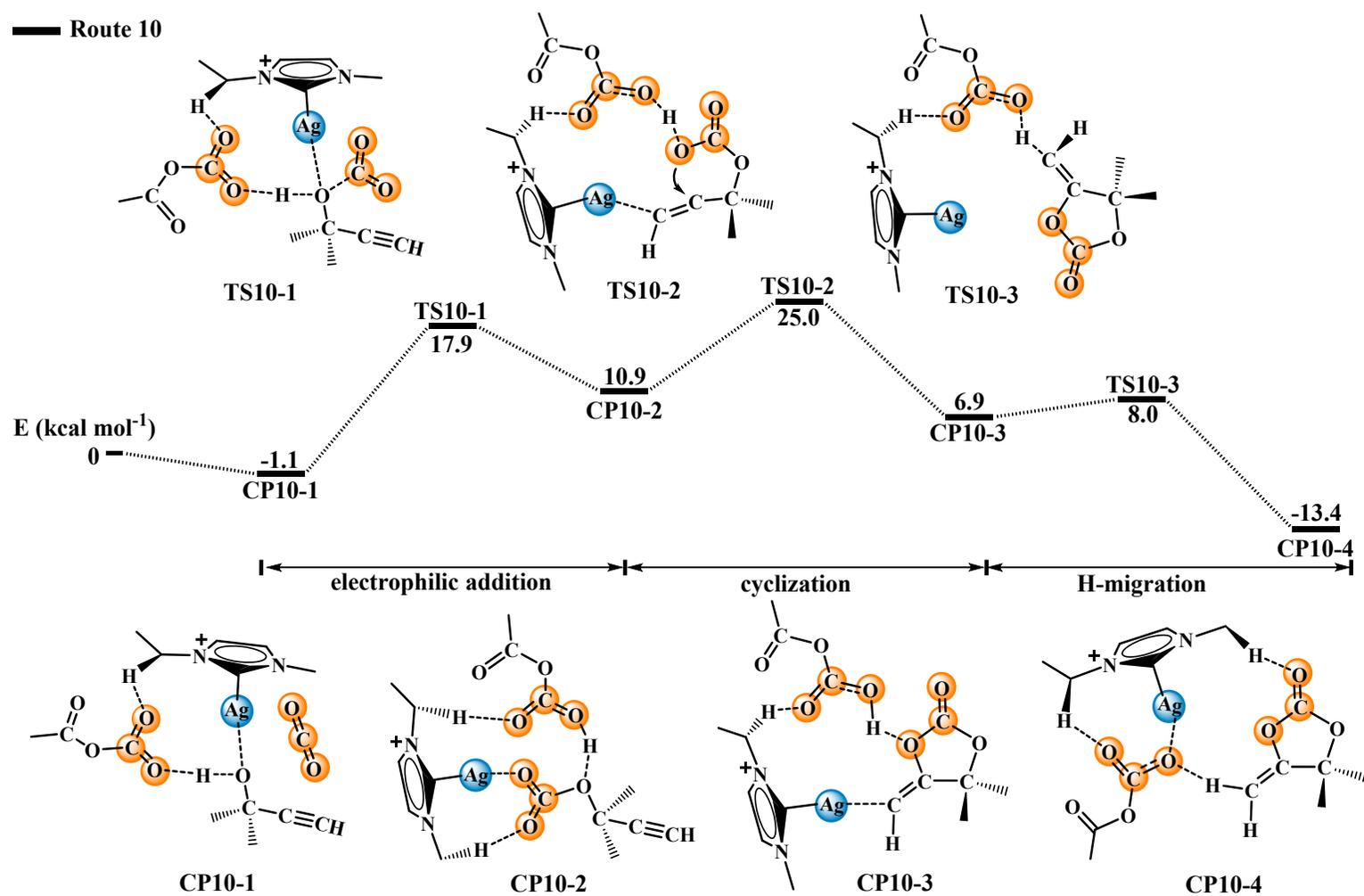


Fig. S7 The energy profile along with the schematic structures of all transition states and intermediates involved in Route 10 calculated at the M06/6-311+G(2d,2p)-LANL2DZ (PCM)//B3PW91/6-31G(d,p)-LANL2DZ level.

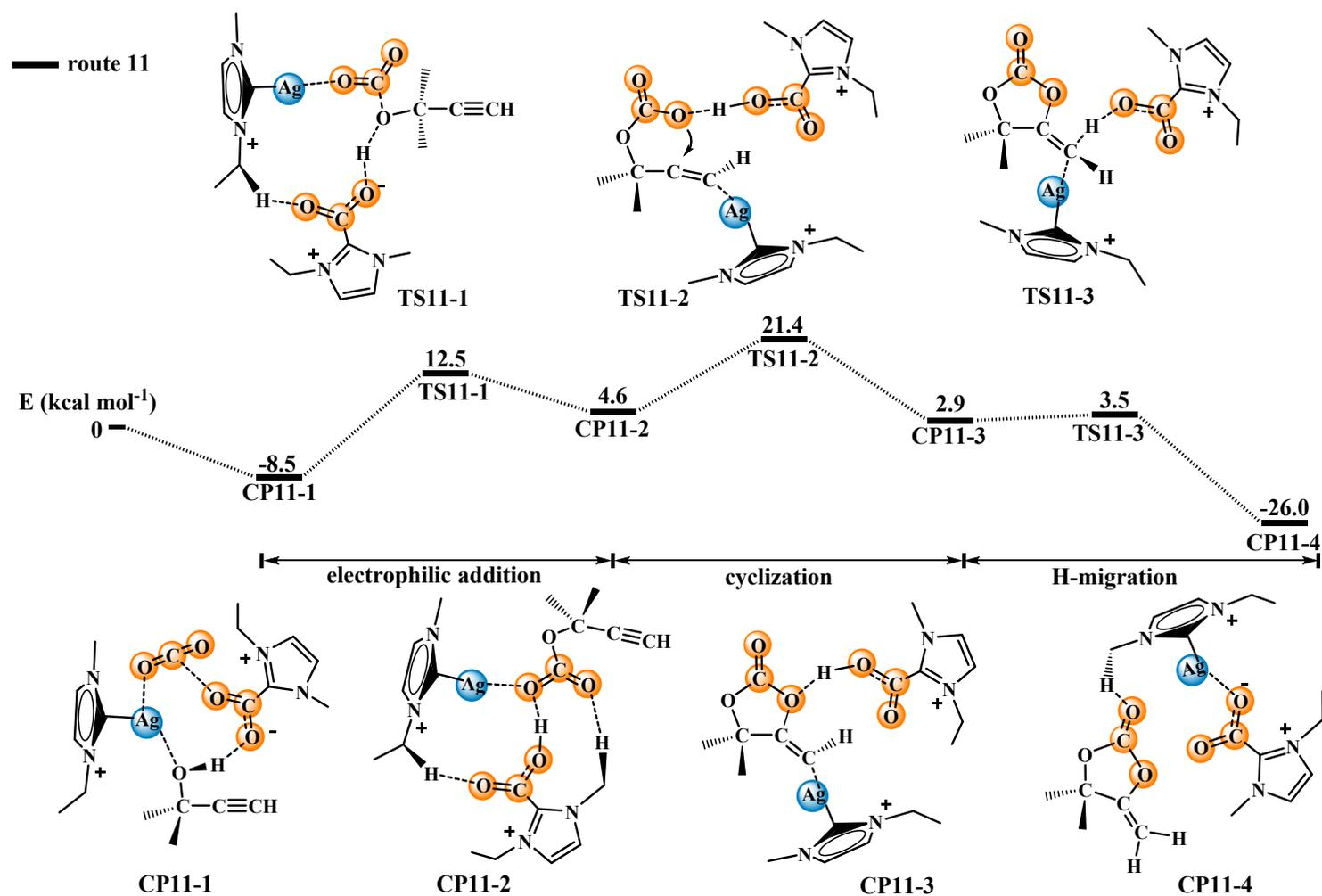


Fig. S8 The energy profile along with the schematic structures of all transition states and intermediates involved in Route 11 calculated at the M06/6-311+G(2d,2p)-LANL2DZ (PCM)//B3PW91/6-31G(d,p)-LANL2DZ level.

Table S3 The enthalpies to form NHC-Ag, AcO-COO⁻, and NHC-CO₂.

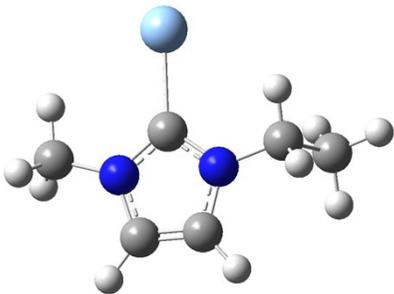
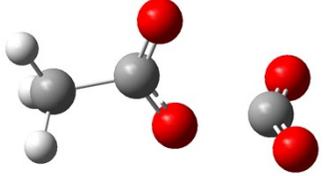
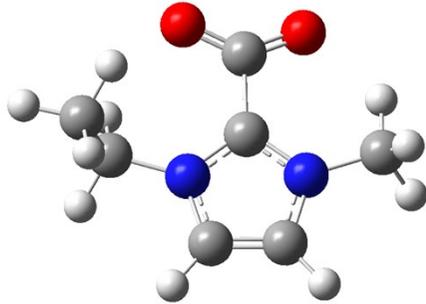
name	NHC-Ag	AcO-COO ⁻	NHC-CO ₂
optimize structures			
ΔH (kcal mol ⁻¹)	-80.67	-14.63	-13.89

Table S4 The barrier heights (in kcal mol⁻¹) of the rate-limiting step for Route 9 and Route 10.

Methods	TS9-2	TS10-2
M06/6-311+G(2d,2p)-LANL2DZ (PCM)//B3PW91/6-31G(d,p)-LANL2DZ	19.13	26.06
M06/6-311+G(2d,2p)-SDD (PCM)//B3PW91/6-31G(d,p)-SDD	16.87	24.85
M06/6-311+G(2d,2p)-LANL2DZ (PCM)//M06/6-31G(d,p)-LANL2DZ	18.12	27.40
M06/6-311+G(2d,2p)-SDD (PCM)//B3LYP/6-31G(d,p)-LANL2DZ	19.62	24.61
M06/6-311+G(2d,2p)-LANL2DZ (SMD)//B3PW91/6-31G(d,p)-LANL2DZ	17.09	26.09

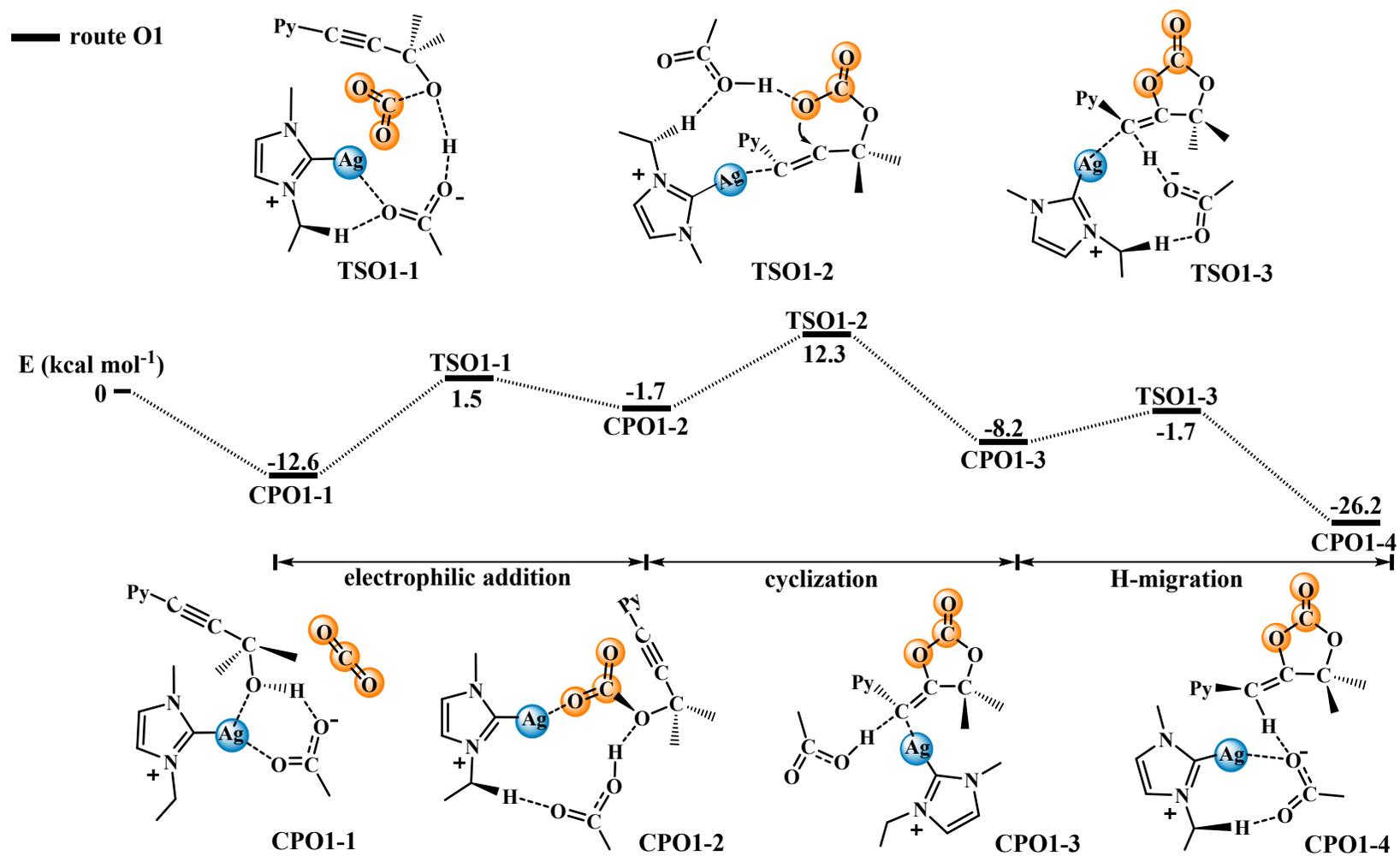


Fig. S9 The energy profile along with the schematic structures of all transition states and intermediates involved in Route O1 calculated at the M06/6-311+G(2d,2p)-LANL2DZ (PCM)//B3PW91/6-31G(d,p)-LANL2DZ level.

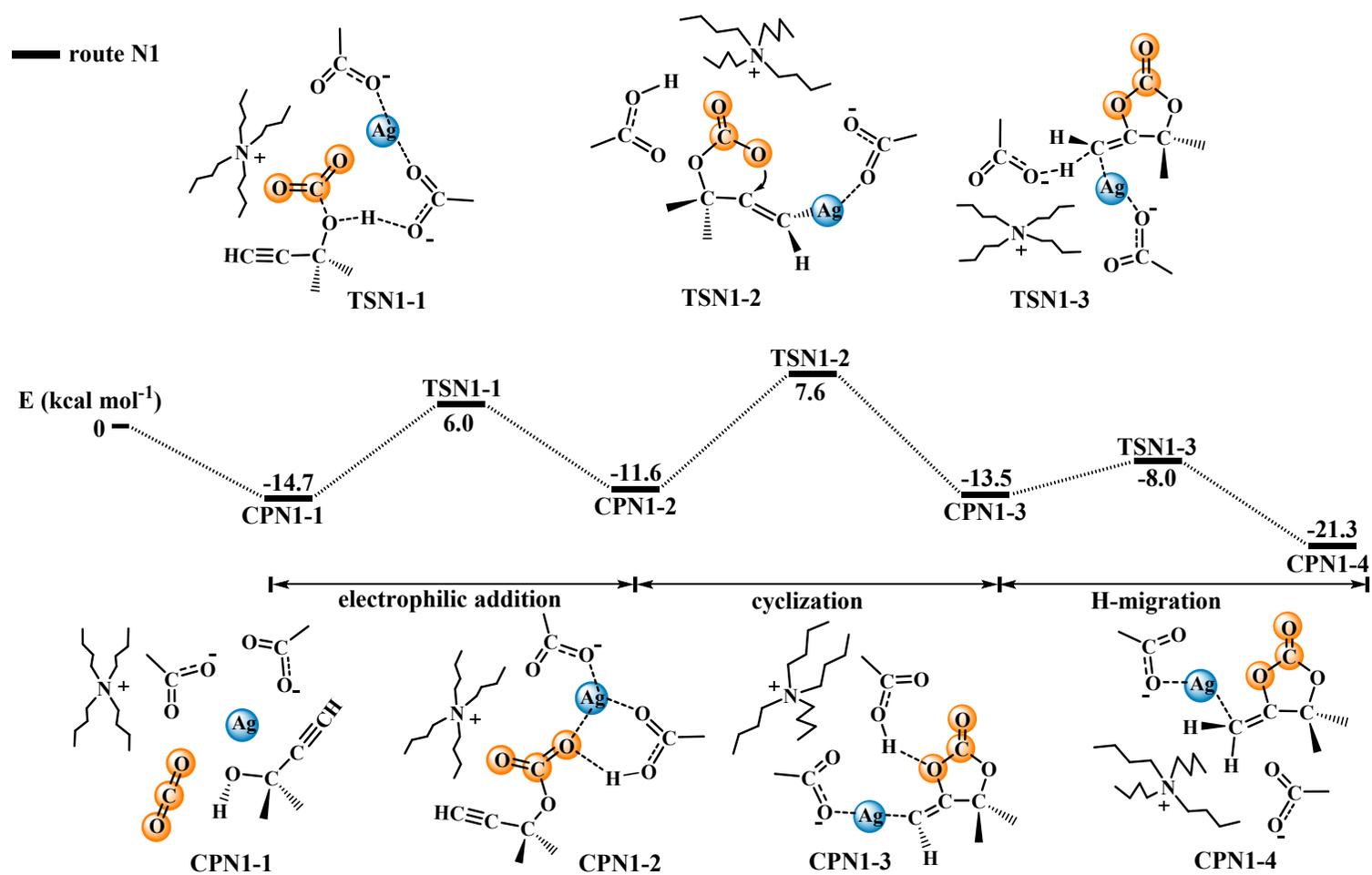


Fig. S10 The energy profile along with the schematic structures of all transition states and intermediates involved in Route N1 calculated at the M06/6-311+G(2d,2p)-LANL2DZ (PCM)//B3PW91/6-31G(d,p)-LANL2DZ level.

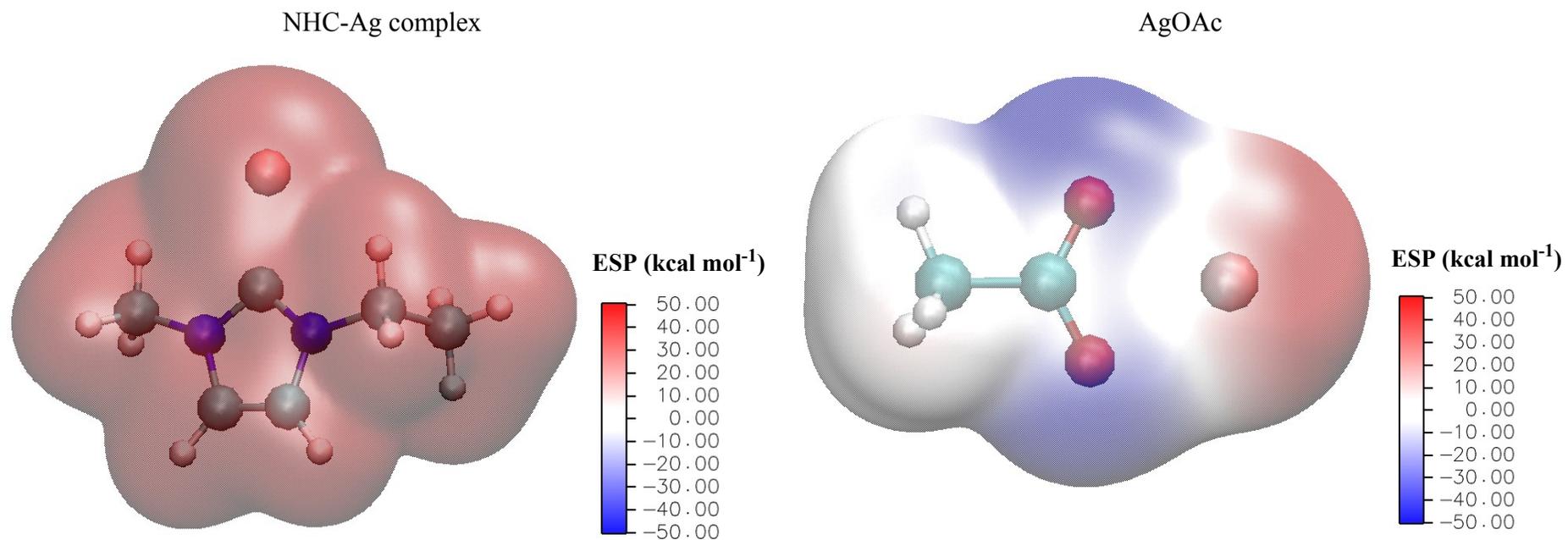


Fig. S11 The ESP mapped onto a surface of electron distribution for NHC-Ag complex and AgOAc. Blue colour represents the negative electrostatic potential and red colour represents the positive electrostatic potential.

References

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- 5 K. Kuchitsu (ed.). Landolt-Bornstein: Group II: Atomic and Molecular Physics Volume 15: Structure Data of Free Polyatomic Molecules. Springer-Verlag, Berlin, 1987.
- 6 F. Vanhouteghem, W, Pyckhout, C, van Alsenoy and L, van den Enden, *J. Mol. Struct.*, 1986, **140**, 33-48.
- 7 K. Kuchitsu(ed.). Landolt-Bornstein: Group II: Atomic and Molecular Physics Volume 21: Structure Data of Free Polyatomic Molecules. Springer-Verlag, Berlin, 1992.
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Table S5 Following are the cartesian coordinates of the optimized intermediates and transition states, along with the calculated absolute energies (in hartree).

CO ₂		HF=-188.5640509	
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16748800
O	0.00000000	0.00000000	-1.16748800
H ₂ O		HF=-76.4266426	
O	0.00000000	0.00000000	0.11863500
H	0.00000000	0.75790700	-0.47454100
H	0.00000000	-0.75790700	-0.47454100
propargylic alcohols		HF=-270.3959778	
C	2.37383400	-0.00002400	-0.03247100
H	3.43954300	-0.00000700	-0.06813000
C	1.16766100	-0.00005300	0.02335300
C	-0.30345700	-0.00000400	0.03772500
O	-0.69254500	0.00001200	1.41259400
H	-1.65792200	0.00011300	1.42421400
C	-0.82533200	1.26712900	-0.65658200
H	-0.49071200	1.31783300	-1.69634400
H	-1.92196200	1.26955500	-0.65070700
H	-0.46960500	2.15415800	-0.12773800
C	-0.82542800	-1.26710100	-0.65657400
H	-0.46976600	-2.15415800	-0.12773200
H	-1.92205700	-1.26944400	-0.65068600
H	-0.49082100	-1.31783200	-1.69633900
[Emim][OAc]		HF=-573.0218024	
C	-2.94253400	-0.78045300	-0.18041300
C	-2.70253700	0.54139700	-0.37234800
N	-1.70780100	-1.36582200	0.04017300

H	-3.86568100	-1.33968400	-0.18952000
H	-3.37931800	1.35640100	-0.57907500
N	-1.33354300	0.71020000	-0.26548900
C	-0.63939000	1.99291600	-0.37487900
H	-1.00470300	2.49823100	-1.27595300
H	0.42050500	1.75970900	-0.51360100
C	-0.84254200	2.86670500	0.85631900
H	-0.30129500	3.80950500	0.73385300
H	-1.89889000	3.10167900	1.02476700
H	-0.45514500	2.36620900	1.74816900
C	-1.49607700	-2.77906400	0.28744000
H	-1.86201200	-3.37694600	-0.55253100
H	-0.42531200	-2.94409800	0.40456400
H	-2.01063100	-3.09310700	1.20051700
C	2.78515600	-0.13195800	-0.08659900
O	2.47945300	0.99805700	-0.44398400
O	1.93084700	-1.08053600	0.23904900
C	4.22460800	-0.58477400	0.02785900
H	4.39648800	-1.44639800	-0.62417100
H	4.89565900	0.22883300	-0.24703500
H	4.43202700	-0.90971200	1.05181600
C	-0.69762800	-0.45877100	-0.00787000
H	0.93097900	-0.75742200	0.13783800

NHC-Ag/OAc⁻

HF=-718.265285

C	2.94083900	1.90313800	0.03338600
C	3.53978600	0.70124900	-0.16711500
C	1.30936100	0.35062700	-0.12348000
N	1.58043500	1.66675300	0.05823700
H	3.36119800	2.89004000	0.14987000
H	4.58277100	0.43880600	-0.25436800
N	2.52492800	-0.23165900	-0.26389500
C	2.72909900	-1.66781700	-0.43112300
H	3.51429500	-1.80977100	-1.18099800

H	1.79852200	-2.06571700	-0.84336100
C	3.08301500	-2.36444000	0.87630900
H	3.22401500	-3.43506500	0.70118500
H	4.00704000	-1.96623700	1.30675800
H	2.27932000	-2.23870900	1.60712300
C	0.56781800	2.69906200	0.24152200
H	0.62780500	3.42829500	-0.57078800
H	-0.42202100	2.23524800	0.23731200
H	0.72396400	3.20629100	1.19719100
C	-3.30159600	0.02672000	0.08818900
O	-2.76110100	1.14079700	0.22780600
O	-2.66628900	-1.07485000	-0.11693100
C	-4.81441400	-0.10402300	0.15409700
H	-5.08976700	-0.80493500	0.94794900
H	-5.28049000	0.86480100	0.33824700
H	-5.18885200	-0.52215200	-0.78527700
Ag	-0.63361000	-0.42683400	-0.13465900

AgOAc

HF=-374.2416895

C	-1.50953700	0.00992200	-0.00699100
O	-0.91337900	-1.10975200	-0.00515800
C	-3.02647800	-0.00507700	0.00356100
H	-3.36952400	-0.40893900	0.96072400
H	-3.42916400	0.99813200	-0.13396400
H	-3.39185300	-0.67284000	-0.78023500
O	-0.91467200	1.12759600	-0.00482700
Ag	1.10704300	-0.00187600	0.00114700

NHC-Ag/NHC-CO₂

HF=-1022.2279321

C	4.92277400	-1.46322100	0.24072000
C	5.22331900	-0.13961700	0.23006500
C	2.97943300	-0.32525000	0.14299300
N	3.54623000	-1.55481900	0.18527300
H	5.56136400	-2.33157200	0.28998800

H	6.17560400	0.36661900	0.26373200
N	4.02191100	0.53813600	0.17326300
C	3.90454100	1.99459700	0.09426300
H	4.59978200	2.42299700	0.82276500
H	2.89222400	2.24475400	0.42181000
C	4.17492500	2.52858400	-1.30593300
H	4.07733600	3.61782300	-1.31141400
H	5.18564200	2.27995800	-1.64218500
H	3.46212300	2.11507600	-2.02498300
C	2.81451300	-2.81267200	0.19126700
H	3.00026300	-3.35219600	1.12335900
H	1.74848900	-2.59908800	0.10657100
H	3.12500200	-3.43023500	-0.65496500
Ag	0.93112200	0.09950300	0.05152600
C	-5.51152800	-0.73390600	-0.26808600
C	-5.37449400	0.62185100	-0.25696100
C	-3.34653200	-0.26732200	-0.15586400
N	-4.25110700	-1.26939400	-0.20632400
H	-6.39470400	-1.35104300	-0.31929300
H	-6.11698100	1.40356500	-0.29513300
N	-4.03245700	0.89483300	-0.19132800
C	-3.49011000	2.26683400	-0.12184800
H	-4.21063700	2.89683500	-0.64960800
H	-2.54765600	2.26667300	-0.66605800
C	-3.28961800	2.72592000	1.31442800
H	-2.93530700	3.76035300	1.31288100
H	-4.22115000	2.68722400	1.88633600
H	-2.53627700	2.10884300	1.80878200
C	-3.97936000	-2.71006800	-0.20502700
H	-4.94033400	-3.22296100	-0.24453600
H	-3.36984400	-2.97317100	-1.06789600
H	-3.43687300	-2.98404000	0.69817300
C	-1.84963000	-0.46672800	-0.08383800
O	-1.44563800	-1.63188400	-0.08566100

O	-1.17214300	0.60958500	-0.02725400
2-methyl-4-(pyridin-2-yl)but-3-yn-2-ol		HF=-517.3820118	
C	-0.07522400	0.07450000	-0.00012000
C	-1.28712200	0.07863700	-0.00031600
C	-2.75650800	0.03792300	-0.00011800
O	-3.20179700	1.39436000	-0.00364200
H	-4.16688300	1.36686700	-0.00332700
C	-3.25147600	-0.68096000	-1.26553900
H	-2.87830500	-1.70778400	-1.31291600
H	-4.34759600	-0.71645800	-1.26710700
H	-2.91663900	-0.14155500	-2.15430300
C	-3.25126500	-0.67428700	1.26917300
H	-2.91642600	-0.13006700	2.15499700
H	-4.34738100	-0.70995100	1.27103000
H	-2.87792700	-1.70077900	1.32204800
C	1.35619200	0.04059600	-0.00003400
C	2.02546900	-1.19483100	0.00031400
C	3.33632100	1.18700400	-0.00033100
C	3.41425100	-1.20191500	0.00037300
H	1.45419400	-2.11718600	0.00054100
H	3.83201900	2.15681900	-0.00059300
H	3.95849000	-2.14221800	0.00066800
C	4.09162500	0.01452800	0.00004100
H	5.17616900	0.05872400	0.00006600
N	2.00444000	1.22022100	-0.00037400

[N ₄₄₄₄][OAc]/AgOAc	HF=-1288.5130197		
C	2.76300600	2.07166000	0.16055600
O	2.29114900	0.92611400	-0.01229200
O	2.09447900	3.15505000	0.21910800
C	4.27016500	2.21768800	0.33130900
H	4.57545200	1.72700400	1.26152900
H	4.78332700	1.70540300	-0.48769000

H	4.57243900	3.26502400	0.36223800
Ag	-0.01243300	2.95766700	-0.00069200
C	0.16661500	-1.01719000	1.20137800
C	1.21210000	-2.85007800	-0.16722800
C	-0.15632000	-1.01871400	-1.20116900
C	-1.18744100	-2.85950500	0.16813700
C	0.36731400	-1.69549500	2.54869000
C	0.36205400	-0.64247000	3.66423000
C	0.59872100	-1.24611800	5.04592800
C	2.51612300	-2.19014500	-0.59287900
C	3.68639500	-3.16135600	-0.40040500
C	5.00843000	-2.58644900	-0.90242000
C	-2.49681600	-2.20986600	0.59312700
C	-3.65896100	-3.19096300	0.40166500
C	-4.98599300	-2.62596300	0.90177600
C	-0.35257500	-1.69898100	-2.54812100
C	-0.35694700	-0.64615800	-3.66384200
C	-0.59058200	-1.25187300	-5.04515000
H	-0.73177200	-0.39286500	1.19607100
H	1.00289800	-0.35279000	0.96026600
H	1.33637300	-3.35935700	0.79205800
H	0.91742800	-3.61349200	-0.89383600
H	0.73740200	-0.38773400	-1.19623500
H	-0.99742400	-0.36040300	-0.96003200
H	-0.88666800	-3.62001500	0.89529200
H	-1.30748900	-3.37044900	-0.79080200
H	-0.42027700	-2.43223800	2.75497200
H	1.32350700	-2.23233300	2.58427400
H	-0.59663500	-0.10897000	3.65200400
H	1.13083200	0.11029400	3.45078500
H	-0.17443700	-1.98046700	5.29929800
H	1.56860400	-1.75335700	5.09947300
H	0.58690900	-0.47299100	5.82004500
H	2.46070100	-1.90453700	-1.64988800

H	2.70135800	-1.25758600	-0.04806200
H	3.47820100	-4.10802000	-0.91907700
H	3.77786200	-3.41263900	0.66519500
H	4.96437800	-2.37057600	-1.97537100
H	5.25133500	-1.65122100	-0.38800300
H	5.83322200	-3.28654400	-0.73715600
H	-2.68980900	-1.27944200	0.04733100
H	-2.44376800	-1.92261200	1.64983200
H	-3.44338000	-4.13500900	0.92208600
H	-3.74769300	-3.44480400	-0.66356200
H	-5.80494100	-3.33303900	0.73715400
H	-5.23607700	-1.69365600	0.38552000
H	-4.94448300	-2.40786900	1.97438000
H	-1.30441100	-2.24359100	-2.58272700
H	0.44078800	-2.42936000	-2.75495100
H	0.59755400	-0.10517100	-3.65287800
H	-1.13133800	0.10056600	-3.44950300
H	-0.58535400	-0.47886400	-5.81945700
H	-1.55671700	-1.76633500	-5.09754900
H	0.18775100	-1.98050800	-5.29918600
N	0.00871100	-1.94370400	0.00021000
C	-2.78088100	2.04784100	-0.16098600
O	-2.12191200	3.13719000	-0.21722200
O	-2.29888600	0.90586300	0.00770500
C	-4.28954900	2.18134400	-0.32878400
H	-4.60057400	3.22614000	-0.35867800
H	-4.59266700	1.68834600	-1.25848000
H	-4.79680700	1.66465900	0.49114900

Route 1	CP1-1	HF=-535.4066021	
C	-1.04700300	0.23779700	1.13233900
C	-1.30481100	-0.40965600	-0.17724900
O	-0.20495100	-0.19189900	-1.05050900
C	-1.41512700	-1.92448900	0.00888800

H	-2.24145400	-2.17751500	0.67788600
H	-1.58974100	-2.38586000	-0.96707700
H	-0.48584700	-2.32256300	0.42115400
C	-2.59092000	0.16698900	-0.78768400
H	-2.49283200	1.24524100	-0.94329700
H	-2.76595300	-0.30964900	-1.75632800
H	-3.45424100	-0.01112100	-0.13989900
H	-0.08730800	0.77835500	-1.12725900
O	0.32298000	2.50039600	-0.59434300
H	1.26768300	2.31795300	-0.50761000
C	-0.82705300	0.79257000	2.18673000
H	-0.64753500	1.24326300	3.13707900
H	-0.02234300	2.35021600	0.29810900
C	2.46242200	-0.56274700	-0.01304500
O	2.65043000	0.58144200	-0.17236500
O	2.33835600	-1.70632700	0.16813700

Route 1	TS1-1	HF=-535.3308051	
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C	-0.00376000	1.94012700	0.29072000
H	-0.21135100	2.98528700	0.46496100
C	-0.68337400	0.89948200	0.14103000
C	-1.66639500	-0.19072000	-0.01742900
C	-1.59969500	-1.18522800	1.14819800
H	-1.76048200	-0.68853200	2.10979700
H	-2.38042400	-1.93630700	1.00060600
H	-0.62567700	-1.67616900	1.15793800
C	-3.03240500	0.52570700	-0.05754100
H	-3.07215700	1.22865000	-0.89207300
H	-3.78985100	-0.24648100	-0.21749000
H	-3.24581900	1.04646900	0.87881800
O	-1.51053700	-0.82502100	-1.26114600
H	-0.58189300	-1.11453900	-1.28599600
C	2.17283200	-0.43639000	-0.06622000
O	3.17490600	-1.00800100	0.28204700

O	0.99387900	-0.71995300	-0.33341100
O	2.36220900	1.07518000	-0.21937100
H	1.24364400	1.59797500	0.09242700
H	3.13713300	1.30815200	0.31351400

Route 1	CP1-2	HF=-611.869792	
C	0.54385700	-2.20490800	-0.17009600
H	1.50878600	-2.65448100	-0.36701200
C	0.46123300	-0.88980500	0.02875500
C	1.61222500	0.11071000	0.03070100
C	1.75518400	0.76369500	1.40508800
H	2.02975200	0.01489600	2.15238300
H	2.53445200	1.52999300	1.36704800
H	0.81692700	1.23225800	1.70860600
C	2.93370800	-0.50263500	-0.42087600
H	2.84677500	-0.95438700	-1.41476800
H	3.69280500	0.28241300	-0.46201900
H	3.27434600	-1.27422800	0.27446600
O	1.27165200	1.19680300	-0.86544300
H	1.18760600	0.81871500	-1.75075400
C	-1.97716100	-0.63034900	0.07720300
O	-2.30164700	-1.78207100	-0.03706200
O	-0.69198600	-0.17297400	0.27089000
O	-2.78723800	0.40876000	0.05244200
H	-0.33268800	-2.83596900	-0.13620100
H	-2.25112400	1.25356900	0.03071800
O	-1.18835800	2.52820700	-0.15532000
H	-0.33799200	2.10102500	-0.38638000
H	-1.36330400	3.17615900	-0.84478300

Route 1	TS1-2	HF=-611.8287978	
C	-0.61644200	2.01516100	-0.69627700
H	-1.56323700	2.53489600	-0.62540100
C	-0.51678600	0.73338200	-0.34344300

C	-1.64625600	-0.17342500	0.12848000
C	-1.39884800	-0.64315700	1.56211000
H	-1.39691400	0.20776400	2.24806200
H	-2.18649700	-1.34095900	1.85933100
H	-0.44018100	-1.15935700	1.64398600
C	-3.02092800	0.47859800	0.00669100
H	-3.21172700	0.81842200	-1.01714100
H	-3.78483100	-0.25586300	0.27498000
H	-3.12118200	1.33918700	0.67367300
O	-1.60725000	-1.36831600	-0.67375600
H	-1.85131900	-1.10714600	-1.57116500
C	2.10488900	0.62840000	0.18063700
O	2.08564200	1.78488000	0.45954500
O	0.67802500	0.05289100	-0.41235500
O	2.88148600	-0.33879200	0.17041700
H	0.25195800	2.57724900	-1.01269200
H	2.23262600	-1.55938500	-0.08463600
O	1.38549900	-2.18319900	-0.27917400
H	0.76264300	-1.22656400	-0.41362800
H	1.48765700	-2.64171000	-1.12198400

Route 1	CP1-3	HF=-611.883187	
C	-0.49355700	-2.22166000	-0.16692100
H	-1.30258500	-2.80632100	0.24766000
C	-0.58104300	-0.89318600	-0.31318100
C	-1.78702700	-0.05775600	0.11037500
C	-2.34563600	0.73588700	-1.07061100
H	-2.72457900	0.04985000	-1.83232000
H	-3.16511800	1.37515200	-0.73028300
H	-1.58359700	1.36948500	-1.52923200
C	-2.89377800	-0.87748600	0.76725100
H	-2.51969500	-1.43155800	1.63439500
H	-3.68233800	-0.20038300	1.10560200
H	-3.32815900	-1.59533200	0.06681400

O	-1.33918900	0.94008600	1.06881100
H	-0.97786100	0.45878500	1.82455500
C	3.13884000	-0.25041600	0.23154600
O	3.42598000	-1.29829800	-0.18655000
O	0.44804100	-0.21641500	-0.88286200
O	2.89700600	0.80487900	0.67700000
H	0.39781400	-2.74381000	-0.49642200
H	1.32157000	2.44809400	0.09859000
O	0.46241100	2.45510000	-0.34071900
H	0.36758800	0.76141000	-0.77808700
H	-0.18383900	2.21951800	0.35253100

Route 1	TS1-3	HF=-423.2656739	
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C	-1.08056500	1.34032900	-0.23851200
H	-0.56533500	2.20567500	0.16256100
C	-0.36060000	0.12934200	-0.32225100
C	1.11244600	0.00763600	0.08128800
C	1.21484900	-0.78733200	1.38344400
H	0.74045100	-1.76399300	1.26804400
H	2.26698700	-0.92425300	1.64794100
H	0.72577100	-0.24232700	2.19586700
C	1.86888500	-0.69252900	-1.05557600
H	1.81775900	-0.10218300	-1.97802400
H	2.92009800	-0.80224600	-0.77494700
H	1.44027300	-1.67510300	-1.26266900
O	1.68516500	1.27647500	0.35649200
H	1.64705700	1.79453000	-0.45716700
O	-0.94660200	-0.97151300	-0.62777000
H	-1.75562800	1.55306000	-1.06953900
O	-3.02262700	-0.22020100	0.26803200
H	-3.13302800	-0.63514600	1.13328300
H	-2.12946300	-0.76550800	-0.28311000
H	-2.23252100	0.69474000	0.35336500

Route 1	CP1-4	HF=-423.3326674	
C	-0.89737600	1.45256400	-0.08451800
H	-0.44475700	2.08017100	0.68820900
C	-0.28986800	0.07684800	-0.07160300
C	1.24637700	-0.04556600	0.00891200
C	1.59153700	-0.46919600	1.43908100
H	1.10837100	-1.41778000	1.68272500
H	2.67577800	-0.57731200	1.53061000
H	1.26475800	0.29084800	2.15500700
C	1.73609500	-1.07512800	-1.00998100
H	1.53285000	-0.74047100	-2.03478400
H	2.81442000	-1.22022800	-0.90129400
H	1.22312000	-2.02804200	-0.86726900
O	1.87732100	1.21382200	-0.18504500
H	1.88254300	1.40404000	-1.13050600
O	-0.96707000	-0.94048600	-0.09677000
H	-0.67388300	1.94354100	-1.03940300
O	-3.76453300	-0.23316400	-0.03670300
H	-4.00166200	-0.42560200	0.87604700
H	-2.88800600	-0.64264200	-0.13650800
H	-1.97985700	1.37496700	0.03396200

Route 2	CP2-1	HF=-346.834476	
C	-0.22079300	2.33505500	0.05918400
H	-0.55344500	3.34813800	0.08923300
C	0.16212500	1.19008200	0.01590000
C	0.66027500	-0.19387200	-0.00160000
O	-0.01839100	-0.84363200	-1.09413000
H	0.22801200	-1.77724900	-1.05877600
C	2.17079200	-0.19793900	-0.26733800
H	2.70772800	0.33935100	0.51895500
H	2.54072800	-1.22928300	-0.29015700
H	2.38515300	0.27439700	-1.22852300
C	0.30917700	-0.89327500	1.31813900

H	-0.77744700	-0.92608900	1.42973000
H	0.70190300	-1.91730500	1.30977900
H	0.75024100	-0.36877000	2.16982200
O	-2.71491800	-0.52225800	-0.05249000
H	-1.93635300	-0.68471500	-0.60913200
H	-2.66950800	0.42835100	0.09631600

Route 2	TS2-1	HF=-346.7497618	
C	1.74575600	1.30778100	0.15113600
H	1.56528400	2.37646700	0.22399400
C	0.80925300	0.41362900	0.07969400
C	-0.62213200	0.00037900	-0.01422400
O	-0.69554900	-0.83614300	-1.18186300
H	-1.57729900	-1.22754400	-1.20109900
C	-1.06427100	-0.79171200	1.22046300
H	-0.98430600	-0.18171600	2.12423900
H	-2.11055800	-1.10588300	1.11655000
H	-0.43905800	-1.67877700	1.34155400
C	-1.47569600	1.25578400	-0.21220400
H	-1.17254500	1.77467100	-1.12417000
H	-2.53213000	0.97825600	-0.29927700
H	-1.37356100	1.94049600	0.63426000
O	1.72352900	-0.97973500	0.01754500
H	2.43480700	-0.13805200	0.03350900
H	1.60805800	-1.32605900	-0.88420200

Route 2	CP2-2	HF=-346.8773937	
C	1.70899800	1.18275900	0.10786400
H	1.25508000	2.16106700	0.18945900
C	0.96906000	0.07864400	-0.02200600
C	-0.55900400	0.03338300	-0.02031800
O	-0.87248600	-1.08887600	-0.87094400
H	-1.75476500	-1.39962000	-0.63941300
C	-1.05348800	-0.25883800	1.40166800

H	-0.80978800	0.56843600	2.07279200
H	-2.14280700	-0.39487900	1.41278200
H	-0.57993500	-1.16524000	1.78923400
C	-1.20287200	1.29144600	-0.59166700
H	-0.83700000	1.47924500	-1.60338400
H	-2.29072500	1.16818500	-0.62946000
H	-0.99168800	2.16726000	0.02753900
O	1.53983900	-1.15186200	-0.07760900
H	2.78970600	1.11258400	0.14836300
H	0.84693000	-1.73549500	-0.43273800

Route 2	TS2-2	HF=-346.7877075	
C	-0.88554100	-0.06159400	-0.04834500
C	0.62355400	-0.00940000	-0.02281200
O	1.09215600	-1.16940500	-0.68953300
H	2.05479200	-1.16214000	-0.62955300
C	1.12579700	1.25630300	-0.72750600
H	0.76603500	2.16428200	-0.23766300
H	2.22112100	1.27282600	-0.70383100
H	0.80679100	1.26511300	-1.77302200
C	1.05141100	-0.03018200	1.45674100
H	0.70668200	-0.95331300	1.92916400
H	2.14526800	0.00747500	1.52000200
H	0.64909000	0.82575700	2.00491700
O	-1.50092500	-1.18359700	-0.16201500
C	-1.84872300	0.98056300	0.05544900
H	-2.42360300	-0.33575500	-0.31470400
H	-2.41326500	0.92316900	0.98960300
H	-1.64174400	2.00245600	-0.25369000

Route 2	CP2-3	HF=-346.8949671	
C	-0.92374000	0.27736600	-0.02478300
C	0.59490600	-0.00274400	-0.01719600
O	1.21392300	1.20851300	-0.40397400

H	2.16630300	1.06824100	-0.34572700
C	1.01350600	-0.37252800	1.41573800
H	0.52177800	-1.28032100	1.77752100
H	2.09496700	-0.55203400	1.44791100
H	0.78117900	0.45147100	2.09567100
C	0.95398500	-1.11884900	-1.00726100
H	0.66012400	-0.83662900	-2.02237000
H	2.03854600	-1.27941900	-1.00164000
H	0.48222600	-2.07249200	-0.75404700
O	-1.35414200	1.40586300	-0.09788000
C	-1.85884600	-0.91415800	0.06766500
H	-2.84239100	-0.56415000	0.38409800
H	-1.95972600	-1.37488200	-0.92203600
H	-1.50011800	-1.68931000	0.75047300

Route 3	CP3-1	HF=-721.1086945	
C	-1.89043700	0.73530300	0.04353400
C	-3.01896400	-0.21745400	-0.01938800
C	-3.52346300	-0.51404000	1.39959300
H	-3.88001500	0.39446300	1.89197100
H	-4.35742200	-1.22389500	1.35205100
H	-2.72404700	-0.95171800	2.00219100
C	-4.13147200	0.36562300	-0.90225100
H	-3.75597400	0.53955100	-1.91293700
H	-4.96550800	-0.34312100	-0.95354300
H	-4.50967200	1.30759400	-0.49584000
O	-2.47930200	-1.39800000	-0.61512900
H	-3.16258600	-2.07947000	-0.58691700
O	1.51181000	3.06268300	0.20577500
H	2.02186900	2.22645900	0.18152300
H	1.76529000	3.50432100	-0.61108900
C	-1.05289300	1.62724000	0.10819200
H	-0.28893600	2.40774100	0.16870200
Ag	0.32280200	-0.23817700	-0.01194800

C	3.00502500	-0.58929900	-0.04104100
O	2.74391500	0.62549900	-0.24183900
C	4.45696500	-1.02128500	0.01685200
H	4.99725000	-0.61210400	-0.84073000
H	4.91650300	-0.60258200	0.91798000
H	4.54887600	-2.10745400	0.03752700
O	2.11784200	-1.48793000	0.12340800

	Route 3	TS3-1	HF=-721.0430991
C		-0.93039700	0.72215500
H		-1.01550200	1.80465200
C		-1.99474300	-0.06765600
C		-3.48490900	0.16856700
O		-3.91706800	-0.76771400
H		-4.87554700	-0.85405400
C		-4.12899500	-0.18199800
H		-3.77732600	0.49161700
H		-5.21951800	-0.08302700
H		-3.88497300	-1.20759000
C		-3.81807100	1.59314300
H		-3.37303500	1.81054000
H		-4.90379900	1.71355500
H		-3.45260900	2.32222600
O		-1.68001500	-1.44843200
H		-0.34761500	-1.08104500
H		-2.19785200	-1.88859100
C		3.59964100	0.10184700
O		2.95974100	-1.00246600
C		5.10898400	0.03746900
H		5.45370300	-0.59332400
H		5.44848900	-0.43207900
H		5.54023100	1.03478700
O		3.00761900	1.20787900
Ag		1.01136300	-0.02538200

Route 3	CP3-2	HF=-721.1505364	
C	-1.90977300	-0.74333000	-0.16529000
C	-2.55146600	0.61289800	0.11912100
O	-1.95753700	1.48006600	-0.84060000
H	-2.31684900	2.36495200	-0.70462700
C	-4.06556900	0.50256500	-0.12253300
H	-4.52985300	-0.21699600	0.55909200
H	-4.53367600	1.47770100	0.05013700
H	-4.26117600	0.19590100	-1.15119200
C	-2.26996100	1.11737800	1.53448900
H	-1.19539000	1.21304600	1.71624700
H	-2.71620700	2.11066400	1.65185700
H	-2.71011700	0.47132500	2.29969600
O	-2.19526000	-1.16203000	-1.41130200
C	-1.21749500	-1.50430600	0.74309300
H	-1.79740900	-2.02854000	-1.56743300
H	-1.19247900	-1.22468000	1.78978800
H	-0.96957400	-2.53934800	0.51493700
C	3.15736800	0.32500400	-0.05978900
O	2.28274200	0.93477400	-0.75406300
C	4.59931100	0.77100500	-0.20528700
H	4.94011800	0.55912500	-1.22358100
H	4.66781200	1.85282900	-0.06212300
H	5.24379200	0.25620000	0.50792300
O	2.87915100	-0.62475700	0.72209700
Ag	0.61369700	-0.34050800	0.06015700

Route 3	TS3-2	HF=-721.0744051	
C	2.12435700	-0.32125900	-0.03174100
C	3.58182600	0.10647200	0.02585700
O	4.34306800	-1.07945200	-0.01759100
H	5.27230800	-0.82876000	0.03998800
C	3.90245600	1.00257000	-1.18245100

H	3.31600500	1.92499300	-1.18116500
H	4.96144500	1.28078800	-1.14773000
H	3.72322900	0.46374600	-2.11687500
C	3.81897400	0.85423000	1.35119800
H	3.58388600	0.20856800	2.20155100
H	4.87659000	1.13278200	1.41498700
H	3.23000200	1.77218400	1.42185700
O	1.80159900	-1.51186900	-0.03545500
C	0.98594900	0.64285200	-0.08736400
H	0.45770300	-0.97199900	-0.06387700
H	0.99751300	1.35936500	0.74147300
H	1.00011700	1.21522600	-1.02269400
C	-3.63672000	0.13396100	0.03264900
O	-3.06299700	-1.00580800	0.02191100
C	-5.14778300	0.15847500	0.07234500
H	-5.54491700	-0.39033200	-0.78646800
H	-5.49698400	-0.35676100	0.97201000
H	-5.52120900	1.18277200	0.06398900
O	-2.98617900	1.21423700	0.01269700
Ag	-1.05093600	-0.09347300	-0.03133000

Route 3	CP3-3	HF=-721.1612217	
C	-1.82553800	0.21904900	-0.15829100
C	-3.33581500	0.19010900	0.09735300
O	-3.68240100	-1.16646100	0.26578600
H	-4.62058200	-1.19786600	0.48498900
C	-3.61837300	0.97677400	1.39126600
H	-3.32169800	2.02672800	1.32399800
H	-4.69491000	0.95204300	1.59507300
H	-3.09861600	0.51411500	2.23451000
C	-4.08818100	0.79071400	-1.10054000
H	-3.89215500	0.20736200	-2.00451000
H	-5.16496800	0.75582600	-0.90120600
H	-3.82243300	1.83473100	-1.28574600

O	-1.17864900	-0.81624600	-0.02506000
C	-1.18043400	1.50804800	-0.57986400
H	-0.14291500	1.56019700	-0.22816600
H	-1.15344600	1.52476500	-1.67739500
H	-1.73356300	2.39077600	-0.25409500
C	3.22756000	0.71940900	0.10100600
O	3.18813800	-0.55643600	-0.05265000
C	4.62045000	1.32300100	0.14474600
H	5.19155500	0.86830300	0.95942700
H	5.14948900	1.09225100	-0.78464000
H	4.57130100	2.40329100	0.28442300
O	2.22180300	1.45082800	0.21150300
Ag	1.05412300	-0.86358800	-0.04930500

Route 4	CP4-1	HF=-919.8852712	
C	-2.29685000	2.46745300	-1.05066600
C	-1.78030700	2.74858100	0.17687700
C	-1.03079800	0.76114300	-0.43994500
N	-1.81915200	1.22610600	-1.41437100
H	-2.95648200	3.03575200	-1.68665300
H	-1.91024000	3.60517100	0.81871600
N	-0.99074300	1.67592000	0.53244800
C	-0.31030500	1.48533800	1.82122500
H	0.16368900	2.43756200	2.07684200
H	0.48482500	0.75964800	1.64357600
C	-1.27014000	1.00704000	2.90131000
H	-0.71549800	0.85785000	3.83242100
H	-2.05480400	1.74644000	3.09200100
H	-1.72583100	0.05729800	2.60167600
C	-2.13632400	0.49539300	-2.64076800
H	-1.32552700	0.60985700	-3.36404400
H	-2.28106700	-0.55744600	-2.36790100
H	-3.05575500	0.90813600	-3.05726600
C	-2.66453900	-1.95200900	0.19823300

O	-1.96336200	-1.69896100	1.22134000
O	-2.23222200	-2.05641800	-0.98690800
C	-4.15687500	-2.19354700	0.42254200
H	-4.73793700	-1.91623400	-0.46054100
H	-4.31374400	-3.26368800	0.59837200
H	-4.51550400	-1.65582800	1.30338900
C	3.24974200	0.87270800	-0.32151800
C	3.94764500	-0.41502800	-0.10993100
C	3.55581000	-1.02801000	1.23414600
H	2.49933100	-1.30456200	1.22486700
H	4.15547800	-1.92864400	1.39387000
H	3.75905800	-0.32683600	2.04743300
C	3.61651000	-1.37697000	-1.25724400
H	3.88029500	-0.93585000	-2.22481200
H	4.19348300	-2.29660200	-1.12237400
H	2.55070500	-1.61961200	-1.25122400
O	5.35503900	-0.17516400	-0.03392300
H	5.62158500	0.22448100	-0.87097500
O	0.34581200	-1.85520600	-0.09900200
H	-0.30097700	-1.87533200	0.65201800
H	-0.28569600	-2.17866100	-0.77303300
C	2.72827300	1.94402500	-0.53471500
H	2.28864200	2.89668300	-0.72320500
H	-0.50194300	-0.20448600	-0.41901500

	Route 4	TS4-1	HF=-919.8297654	
C		3.71777500	-0.61460200	-1.02028500
C		3.36891200	-1.52029300	-0.06585300
C		1.50989100	-0.68018000	-0.92439300
N		2.54723900	-0.11292400	-1.54766100
H		4.68695700	-0.28771600	-1.36173100
H		3.97726600	-2.13601200	0.57651900
N		1.99054500	-1.54784000	-0.02977800
C		1.15265000	-2.34777600	0.87551900

H	1.37999500	-3.40249900	0.68778800
H	0.12094800	-2.16059300	0.56777800
C	1.36297100	-1.96909800	2.33395100
H	0.68957900	-2.56542400	2.95654800
H	2.38693900	-2.17563200	2.66269300
H	1.13774700	-0.90753600	2.47700100
C	2.42726200	0.98127000	-2.50727300
H	1.68464000	0.71741600	-3.26156100
H	2.10288000	1.87042200	-1.95714300
H	3.39425800	1.13026700	-2.98830800
C	1.17836600	1.88127900	0.97400000
O	0.47403100	1.08470200	1.67293300
O	0.93366900	2.21737500	-0.21435200
C	2.39819500	2.48204900	1.66739200
H	3.03568900	3.01767000	0.96124100
H	2.05756400	3.18299800	2.43657600
H	2.97102600	1.70331000	2.17929500
C	-2.32612900	-0.33805300	-0.67871300
C	-3.72738200	-0.17470900	-0.16352200
C	-3.81166300	-0.30086000	1.35567800
H	-3.28154000	0.51997000	1.83985100
H	-4.86295800	-0.27857800	1.65817100
H	-3.37943900	-1.25198000	1.67676000
C	-4.36935300	1.12946700	-0.65005700
H	-4.33516300	1.18797100	-1.74375600
H	-5.41709400	1.15191600	-0.33478300
H	-3.84544100	1.99565100	-0.24376000
O	-4.46256800	-1.29193800	-0.67444700
H	-4.35073600	-1.27804900	-1.63340700
O	-1.59365500	1.21523300	0.19749300
H	-0.88278800	0.98852800	0.89968800
H	-0.98102800	1.62181600	-0.44842000
C	-1.48616000	-0.93746400	-1.40797100
H	-1.65947900	-1.82069100	-2.01014700

H	0.42185300	-0.54702600	-1.13866600
Route 4	CP4-2	HF=-919.9313511	
C	2.77180300	-1.98862200	-1.34267100
C	2.70705800	-2.37962600	-0.04155900
C	1.04079300	-0.97252400	-0.41127000
N	1.71915800	-1.12177900	-1.55004000
H	3.46215200	-2.25596800	-2.12663200
H	3.32883700	-3.05571800	0.52302900
N	1.61553700	-1.74120600	0.51641500
C	1.21566700	-1.76377600	1.92704400
H	1.22838100	-2.80637900	2.25936500
H	0.18214700	-1.39958400	1.95834600
C	2.12341100	-0.88343300	2.77486400
H	1.75716800	-0.86481200	3.80507000
H	3.15305100	-1.25414000	2.78573800
H	2.12751300	0.13682600	2.38321100
C	1.45002700	-0.32815300	-2.74052700
H	0.44771200	0.08972000	-2.64491800
H	2.17076900	0.48963800	-2.79752100
H	1.51081200	-0.96085100	-3.62786000
C	1.36311400	2.65548000	0.01069700
O	0.07073300	2.79520200	-0.04284000
O	1.98267000	1.59987400	-0.15166000
C	2.08649200	3.95567900	0.30127000
H	3.16421700	3.79349100	0.33336800
H	1.84290500	4.69444100	-0.46801500
H	1.74207600	4.36524700	1.25550500
C	-1.99310600	0.31597500	0.40205900
C	-3.25322000	-0.38833600	-0.12105100
C	-4.20219900	0.65782400	-0.70319800
H	-3.69074300	1.23128100	-1.47981900
H	-5.08649400	0.17464400	-1.13131100
H	-4.52461100	1.34162200	0.08626900

C	-2.87085100	-1.42376700	-1.18690800
H	-2.21350300	-2.19145600	-0.75876600
H	-3.77199700	-1.91990000	-1.55975200
H	-2.34533200	-0.95089800	-2.01911700
O	-3.97348100	-1.03502500	0.92587600
H	-3.31989900	-1.54512200	1.42140700
O	-1.19063400	0.76063500	-0.55316900
H	-0.46926200	1.86073900	-0.24609000
H	0.16302600	-0.30672500	-0.31359900
C	-1.75685100	0.42445700	1.73472100
H	-2.50908300	0.13467600	2.45829500
H	-0.89983400	0.98756500	2.09270100

	Route 4	TS4-2	HF=-919.9179622	
C		3.58321900	-2.16423300	-0.31725000
C		4.07664900	-0.98473900	0.14678900
C		1.86816700	-0.86605500	0.20704500
N		2.20984400	-2.06981900	-0.26835400
H		4.08520800	-3.05143900	-0.66897700
H		5.09272800	-0.64899300	0.27811300
N		2.99416900	-0.19225700	0.46898100
C		3.07534100	1.17443800	1.00471100
H		3.67169600	1.12660000	1.92139200
H		2.05583200	1.47994900	1.24107400
C		3.66383400	2.14559400	-0.00613200
H		3.73184200	3.13657600	0.45077100
H		4.66816100	1.85527800	-0.33103900
H		3.00514800	2.21927300	-0.87362600
C		1.25363500	-3.10348000	-0.66321000
H		0.25972900	-2.74587400	-0.36383100
H		1.30328600	-3.25238900	-1.74413800
H		1.50332700	-4.03404100	-0.14931100
C		-0.57088000	2.66966400	-0.35312600
O		0.42709500	2.00991200	-0.06258300

O	-1.61397000	2.21171600	-0.98897000
C	-0.69502100	4.13697800	0.00668200
H	-1.56695100	4.28685900	0.65024600
H	0.20394800	4.48321200	0.51778500
H	-0.86014600	4.72819400	-0.89871300
C	-1.83461400	-0.89882500	-0.27219400
C	-3.24251500	-0.80462700	0.36592100
C	-3.81420200	-2.21711200	0.47492500
H	-3.13951800	-2.84772400	1.05893800
H	-4.79582700	-2.19059900	0.95891300
H	-3.93282700	-2.64998700	-0.52284600
C	-3.12879000	-0.15209600	1.74793300
H	-2.78470100	0.88406800	1.65099700
H	-4.10656600	-0.14456200	2.23978100
H	-2.40628500	-0.68984700	2.36485000
O	-4.16264100	-0.07538100	-0.44130500
H	-3.77355300	0.79725100	-0.58726000
O	-0.92119100	-1.36207700	0.48031800
C	-1.65596600	-0.39931000	-1.56928000
H	-1.53289900	1.11893200	-1.20580900
H	-0.71141200	-0.62300300	-2.06451400
H	-2.52816600	-0.32948200	-2.21419900
H	0.82236700	-0.56426800	0.35045400

	Route 4	CP4-3	HF=-919.9531005	
C		3.42711800	-2.19350900	-0.16283200
C		3.86312800	-1.11884900	0.54822700
C		1.81142300	-0.68222400	-0.15773500
N		2.14968500	-1.90244500	-0.59239500
H		3.90693600	-3.13151700	-0.39237800
H		4.79525700	-0.94713500	1.06154900
N		2.84535100	-0.18998100	0.53505200
C		2.86398800	1.14022200	1.16787100
H		2.95946600	0.98760400	2.24747800

H	1.88410500	1.58087200	0.94167900
C	3.98936900	2.00796300	0.62577000
H	3.95188900	2.98422900	1.11661300
H	4.98111900	1.58215800	0.80996900
H	3.87139800	2.16782500	-0.44931900
C	1.31687800	-2.76594700	-1.42600200
H	0.26540300	-2.54606800	-1.21562900
H	1.55101900	-2.59906700	-2.48038000
H	1.52671800	-3.80458000	-1.16621100
C	-0.59672400	2.39746500	-0.67348400
O	0.16302700	1.54105300	-0.11937800
O	-1.81260400	2.25297100	-0.93366400
C	0.04663600	3.73754500	-1.03769000
H	0.30204700	4.27771000	-0.11912200
H	0.97933300	3.57656000	-1.58790300
H	-0.63354600	4.35108800	-1.63047300
C	-2.22688100	-1.14204200	-0.32537000
C	-2.98547600	-0.43907600	0.81374500
C	-4.09803900	-1.39918100	1.25982000
H	-3.68438700	-2.33392100	1.64834700
H	-4.68218200	-0.90951000	2.04460600
H	-4.77535500	-1.62375700	0.42994800
C	-2.03047800	-0.13727200	1.97386700
H	-1.24837100	0.54878600	1.63565700
H	-2.59576900	0.33304100	2.78386300
H	-1.55891100	-1.05135200	2.34522900
O	-3.62336300	0.72109400	0.34802200
H	-2.93460600	1.31517200	-0.04701700
O	-1.31948800	-1.93136000	-0.08578400
C	-2.65966500	-0.82402200	-1.72963200
H	-2.28695400	0.17971700	-1.96970900
H	-2.25593500	-1.55997000	-2.42819900
H	-3.74852900	-0.76528200	-1.80176300
H	0.87637500	-0.12210600	-0.30832400

Route 5	CP5-1	HF=-1065.1065269	
C	3.67913600	-1.20436000	-1.22466200
C	3.64127800	-1.76876000	0.01009400
C	1.56436700	-1.01600200	-0.46023300
N	2.40157500	-0.75343700	-1.49108200
H	4.49182500	-1.09317400	-1.92552600
H	4.41427500	-2.24388800	0.59369800
N	2.33880500	-1.64626600	0.45515600
C	1.89075900	-1.98628800	1.80361700
H	2.30479800	-2.96744200	2.06082600
H	0.80356400	-2.08861300	1.74944000
C	2.28544200	-0.92236100	2.82150200
H	1.87438800	-1.17920100	3.80287700
H	3.37384300	-0.85779300	2.92079900
H	1.90661400	0.06124600	2.52173800
C	2.02100900	0.04139000	-2.65280400
H	1.11600700	-0.37610200	-3.09960900
H	1.83799600	1.07261800	-2.32949200
H	2.82800400	0.00415700	-3.38666500
C	1.76192600	2.46550400	0.35698800
O	1.17111400	2.11826800	1.42239200
O	1.23252200	2.54367300	-0.79268500
C	3.24965100	2.78889000	0.46437300
H	3.55668700	3.47285400	-0.32978700
H	3.48018100	3.21374700	1.44387900
H	3.82727700	1.86289600	0.35911800
Ag	-0.46353500	-0.32333800	-0.24831800
C	-3.00045300	-1.03893300	-0.25971400
C	-4.07315800	-0.07370100	0.10558500
C	-3.87498100	0.43038200	1.53418500
H	-2.94688100	1.00105100	1.60256000
H	-4.71649400	1.07940300	1.79163100
H	-3.85436800	-0.40832100	2.23444900

C	-4.10360700	1.08923400	-0.89040500
H	-4.22803800	0.72386400	-1.91620500
H	-4.95074200	1.73548000	-0.64287500
H	-3.17735000	1.66536700	-0.82332900
O	-5.30876400	-0.78589000	0.10524700
H	-5.51003800	-1.01978700	-0.80928200
O	-1.08382500	1.85637500	0.19454800
H	-0.42496700	1.95417300	0.94909400
H	-0.44287400	2.23570800	-0.47105800
C	-2.25736000	-1.95001800	-0.59455400
H	-1.75264800	-2.84270600	-0.89368800

	Route 5	TS5-1	HF=-1065.0770796
C		4.29613400	0.05850700
C		4.45480300	-0.73424200
C		2.23654800	-0.56737100
N		2.93626200	0.14956400
H		5.02330300	0.55283300
H		5.34623600	-1.05584200
N		3.18538300	-1.10843200
C		2.88157300	-1.86154200
H		3.65861500	-2.62364100
H		1.93469700	-2.37690300
C		2.77659600	-0.96003200
H		2.52301200	-1.55927300
H		3.72680100	-0.45352500
H		1.99804400	-0.20389400
C		2.30911100	0.93589700
H		1.93097800	0.27999200
H		1.48924900	1.51415700
H		3.05277600	1.61301000
C		0.53059400	2.10892100
O		0.22094500	1.26920700
O		0.07487100	2.10460800

C	1.54927600	3.18515800	1.08484400
H	1.35585800	4.10222300	0.52388700
H	1.54507400	3.38392800	2.15838500
H	2.54964000	2.82987200	0.81055700
Ag	0.09653800	-0.64171300	-0.32236400
C	-2.95030600	-0.68445900	-0.17088700
C	-4.39369200	-0.31469000	-0.06586600
C	-4.83116500	-0.09447900	1.37871200
H	-4.32721800	0.77839700	1.79292500
H	-5.91358100	0.06141600	1.39820500
H	-4.59532600	-0.97500600	1.98121800
C	-4.77190700	0.86391700	-0.96385400
H	-4.44878600	0.68687300	-1.99600800
H	-5.86045100	0.97342100	-0.95129500
H	-4.30806500	1.78431900	-0.60965900
O	-5.06721100	-1.50228500	-0.49843800
H	-4.91268500	-1.59117000	-1.44761800
O	-2.32393400	1.32623100	0.56883500
H	-1.66410400	1.09582600	1.25776900
H	-1.68381000	1.64997600	-0.10768100
C	-1.94739800	-1.39377200	-0.42162600
H	-1.88740600	-2.42739300	-0.73688500

	Route 5	CP5-2	HF=-1065.1267496	
C		4.48968300	1.19973200	0.55787900
C		4.84566600	0.10332000	-0.15843000
C		2.59336200	0.06259000	0.07813100
N		3.11515100	1.15661800	0.68695100
H		5.08681800	1.99949700	0.96784700
H		5.81269700	-0.23588400	-0.49620800
N		3.67487100	-0.57236900	-0.44329900
C		3.60992700	-1.83913600	-1.16706400
H		4.29341300	-1.77334900	-2.02028700
H		2.59349600	-1.92078300	-1.56038900

C	3.94420500	-3.03506400	-0.28504600
H	3.88292200	-3.95773400	-0.86972300
H	4.95530400	-2.96039800	0.12711300
H	3.23630200	-3.10736800	0.54533600
C	2.33318300	2.13915100	1.42328400
H	1.32058000	2.18176400	1.01964200
H	2.29372800	1.87731100	2.48469900
H	2.79958100	3.12104700	1.31478700
C	-1.55725500	3.12433000	-0.41871700
O	-0.80040200	2.63005900	0.40758300
O	-2.71644000	2.58810300	-0.76641400
C	-1.27311300	4.40919600	-1.15061400
H	-2.09563000	5.11365500	-0.99901400
H	-0.33810000	4.84262800	-0.79749800
H	-1.20973800	4.21237600	-2.22500600
Ag	0.56702600	-0.61212200	0.00355900
C	-2.51680100	-0.84659300	0.22637600
C	-3.90810000	-1.46504700	0.11377000
C	-4.41897100	-1.86801400	1.49881400
H	-4.46210400	-0.99778500	2.15855200
H	-5.41988400	-2.30483600	1.41881600
H	-3.74602600	-2.61083300	1.93466900
C	-4.89111000	-0.49365100	-0.56021900
H	-4.52468300	-0.19653000	-1.54972400
H	-5.85559500	-0.99399300	-0.68889400
H	-5.04288000	0.41187800	0.03310900
O	-3.85220800	-2.66850800	-0.64154800
H	-3.34220600	-2.46358400	-1.43581800
O	-2.61106800	0.43836200	0.77327900
H	-1.70020400	0.73724100	0.95158900
H	-2.82833300	1.73549600	-0.25268000
C	-1.34923300	-1.40718600	-0.10260100
H	-1.45755600	-2.43572300	-0.45031100

Route 5	TS5-2	HF=-1065.0683143	
C	-4.01112600	2.08196800	0.43125000
C	-4.73533000	0.93862000	0.52964000
C	-2.57794900	0.35159100	0.19337500
N	-2.69892800	1.70144900	0.22600100
H	-4.31186600	3.11606500	0.49763600
H	-5.79021000	0.78338500	0.69524200
N	-3.84115100	-0.10445300	0.38623900
C	-4.21517300	-1.51654200	0.37319100
H	-4.96297300	-1.67086300	1.15784900
H	-3.32152100	-2.07982200	0.65385300
C	-4.73774500	-1.97102000	-0.98338100
H	-5.00292800	-3.03158700	-0.94380600
H	-5.62890000	-1.40866700	-1.27842700
H	-3.97336200	-1.83649600	-1.75375100
C	-1.59953500	2.64180400	0.06793000
H	-0.66099200	2.09832800	-0.04394800
H	-1.75929400	3.25763500	-0.82106600
H	-1.53317900	3.28692100	0.94792700
C	2.88342100	2.92944900	-0.21388800
O	4.03881900	2.55695700	-0.25573700
O	1.82820100	2.14096300	-0.41587200
C	2.47480700	4.35574300	0.07750300
H	1.83916900	4.39016000	0.96779000
H	3.36270400	4.96697600	0.23642000
H	1.89260900	4.75742700	-0.75739900
Ag	-0.81840400	-0.78789100	-0.11101300
C	2.17432400	-1.36774100	-0.31170800
C	3.44927600	-1.78851500	0.38539700
C	4.47447800	-2.25245300	-0.65010500
H	4.69180800	-1.44571100	-1.35301700
H	5.39701100	-2.55117300	-0.14315900
H	4.08595200	-3.11300600	-1.20141800
C	3.99668900	-0.61508800	1.21007900

H	3.26979700	-0.31313200	1.97365700
H	4.90975000	-0.93743000	1.71956700
H	4.21918900	0.25580000	0.58822800
O	3.19758700	-2.91166400	1.22294100
H	2.44325800	-2.67443800	1.77722900
O	2.19002700	-0.31608300	-1.14192000
H	1.02194900	-0.92621400	-1.33040700
H	2.11853800	1.19999100	-0.65851400
C	0.94091800	-1.95990300	-0.31659800
H	0.79961400	-3.00111000	-0.02997900

Route 5	CP5-3	HF=-1065.1662775	
C	-3.20537300	2.64320200	0.75731000
C	-4.17262400	1.69817500	0.87361600
C	-2.28475100	0.65922100	0.19092700
N	-2.06327400	1.98857200	0.33907400
H	-3.23120200	3.70601000	0.94179800
H	-5.20511100	1.77951800	1.17641600
N	-3.58838100	0.49544800	0.52689300
C	-4.29730500	-0.78086700	0.47078600
H	-4.91456700	-0.86159600	1.37154200
H	-3.53483000	-1.56220100	0.52136500
C	-5.14022100	-0.92791400	-0.78925800
H	-5.64640000	-1.89764000	-0.78647300
H	-5.90412600	-0.14722900	-0.85537700
H	-4.51134500	-0.87129600	-1.68214600
C	-0.79131400	2.65383500	0.09641200
H	-0.04464300	1.91728200	-0.19878600
H	-0.89848200	3.38781600	-0.70624300
H	-0.45300100	3.15626400	1.00615300
C	3.69380500	2.41111700	-0.19330900
O	4.51896400	1.74622600	0.40117100
O	2.66155400	1.90795100	-0.86973200
C	3.72575700	3.92091200	-0.25985400

H	2.76485900	4.33963200	0.05320300
H	4.52420100	4.30078600	0.37689100
H	3.89562800	4.23942400	-1.29303500
Ag	-0.87816100	-0.81003000	-0.45150500
C	1.81801400	-1.56031700	-0.63063700
C	2.34312400	-2.05809300	0.73759700
C	3.64634700	-2.81533600	0.47973800
H	4.36446200	-2.15998900	-0.01728400
H	4.06568000	-3.16112900	1.42938500
H	3.45904800	-3.68773600	-0.15329300
C	2.57687900	-0.87397000	1.67871900
H	1.63653800	-0.33620400	1.86156300
H	2.94419400	-1.24597200	2.64009600
H	3.30299100	-0.16838500	1.26794700
O	1.45881300	-2.99865900	1.34045500
H	0.60199600	-2.56095800	1.42725200
O	2.44917600	-0.65068000	-1.20714400
H	0.54864800	-2.05028100	-2.25651200
H	2.70871100	0.90391000	-0.89591600
C	0.62786000	-2.16997400	-1.17387000
H	0.41268300	-3.17540200	-0.81666300

	Route 5	TS5-3	HF=-1065.1449686	
C		-4.70518300	-1.32853600	-0.08445400
C		-4.72463900	0.02830900	-0.08499700
C		-2.55896400	-0.61226700	-0.11524100
N		-3.37457200	-1.69885900	-0.10141700
H		-5.50990100	-2.04732800	-0.08135700
H		-5.55167600	0.72136100	-0.07766400
N		-3.40821800	0.44404800	-0.10814900
C		-2.99257100	1.84795800	-0.06710000
H		-3.63996000	2.39887800	-0.75774000
H		-1.96594900	1.90010900	-0.43987700
C		-3.07056400	2.42946400	1.33854000

H	-2.75900500	3.47772300	1.31852800
H	-4.08522100	2.38362800	1.74772300
H	-2.39873000	1.89091100	2.01244200
C	-2.91465400	-3.07582400	-0.11694100
H	-1.82410000	-3.06996200	-0.10328900
H	-3.28384700	-3.60882900	0.76347300
H	-3.26168800	-3.58363800	-1.02114200
C	1.14778500	2.66815200	-0.31107300
O	0.18074100	1.89591700	-0.41847000
O	2.23330600	2.43081400	0.34472300
C	1.11771300	4.03182500	-0.97685300
H	1.98767700	4.14192200	-1.63063400
H	0.20196100	4.16178800	-1.55488400
H	1.18974400	4.81357900	-0.21446100
Ag	-0.44108600	-0.60355100	-0.13574800
C	2.51830300	-0.73384300	0.49834800
C	3.96518600	-0.96592800	0.01391400
C	4.33635000	-2.42477200	0.27808300
H	3.63598400	-3.09028100	-0.23153600
H	5.35068900	-2.61868200	-0.08387300
H	4.30795500	-2.63158200	1.35186900
C	4.05965900	-0.62927400	-1.47864400
H	3.82256800	0.42782100	-1.64537600
H	5.07779800	-0.81688500	-1.83273700
H	3.35285700	-1.22678000	-2.05761700
O	4.90226000	-0.18853500	0.74819400
H	4.67549300	0.73959700	0.60716000
O	1.61569700	-1.26197800	-0.22268800
C	2.28889800	0.11612800	1.59502200
H	2.22505500	1.36161800	0.89568900
H	1.29373300	0.05784500	2.04073900
H	3.10918900	0.24964000	2.29599600

Route 5 CP5-4

HF=-1065.1859296

C	2.88796100	-2.72607400	-0.49279400
C	3.68964700	-2.15824700	0.44440400
C	2.17776800	-0.60692500	-0.19259600
N	1.97803800	-1.76091900	-0.87171600
H	2.88208400	-3.72198300	-0.90748100
H	4.52676900	-2.55968600	0.99402000
N	3.23664500	-0.86484000	0.61508600
C	3.85626700	0.11566300	1.50224400
H	4.06885800	-0.38144600	2.45434300
H	3.10233500	0.88375000	1.69182300
C	5.11700600	0.72906500	0.90720400
H	5.54291300	1.45518000	1.60580400
H	5.87664600	-0.03201200	0.70423600
H	4.88804600	1.24590200	-0.02893100
C	0.89376300	-1.98375700	-1.81990400
H	0.02724100	-2.42941300	-1.32130400
H	0.60339600	-1.02079300	-2.24153200
H	1.24967400	-2.63223300	-2.62355500
C	-1.34505300	2.64416200	-0.25142200
O	-0.11009200	2.95772100	-0.29689500
O	-1.76019300	1.45801100	-0.24857700
C	-2.34636200	3.78147900	-0.19544700
H	-2.92921100	3.70350400	0.72752400
H	-1.85198800	4.75227000	-0.23583600
H	-3.05082000	3.68852800	-1.02719200
Ag	0.99016000	1.12031700	-0.27182900
C	-2.73359700	-1.68447600	-0.31957000
C	-3.52180600	-1.04827500	0.84357900
C	-4.70521600	-1.97715300	1.14266900
H	-4.35976500	-2.96413700	1.46208200
H	-5.30840200	-1.53091700	1.93902300
H	-5.34442000	-2.09026300	0.26150900
C	-2.61932800	-0.90178900	2.07204800
H	-1.82382000	-0.18075300	1.86241800

H	-3.21119000	-0.53136200	2.91440500
H	-2.16140100	-1.85683900	2.34026200
O	-4.07265000	0.18964500	0.45490900
H	-3.32057900	0.78228800	0.22987800
O	-1.86558900	-2.52054300	-0.11747100
C	-3.09386200	-1.22750600	-1.71141800
H	-2.63627500	-0.24448300	-1.87165400
H	-2.71334900	-1.93845200	-2.44765600
H	-4.17194900	-1.08691300	-1.81949600

	Route 6	CP6-1	HF=-1032.0230194	
C		2.78316200	-2.78084900	0.12069900
C		3.86134200	-1.95190700	0.16674100
C		2.04547200	-0.69416400	-0.00411300
N		1.66603000	-1.97884100	0.01239600
H		2.71516200	-3.85632700	0.16241900
H		4.91435500	-2.16795900	0.25342300
N		3.37995500	-0.66259200	0.09110200
C		4.17943600	0.57254900	0.08709800
H		4.94299600	0.45792400	0.86241200
H		3.49218700	1.37900600	0.38607100
C		4.80634100	0.83808300	-1.27384500
H		5.39502100	1.75824300	-1.22317700
H		5.47032900	0.02763400	-1.59280400
H		4.03476800	0.97635700	-2.03636200
C		0.28357000	-2.44943500	-0.04273200
H		0.03466400	-2.96361700	0.88727300
H		-0.39270500	-1.59760200	-0.16692400
H		0.17073800	-3.13563700	-0.88506600
C		0.80670200	2.47882500	0.64232100
O		1.99861300	2.57079200	0.97795700
O		0.31798200	1.52562500	-0.07310900
C		-0.17478200	3.56312700	1.07211200
H		-1.04975500	3.11555100	1.55365200

H	0.30246700	4.26955500	1.75279600
H	-0.53358000	4.10238000	0.18877900
C	-4.34170300	-1.66169300	-1.65412300
H	-5.03866900	-2.45418900	-1.80509600
C	-3.55778000	-0.75880900	-1.47665500
C	-2.61048400	0.35584400	-1.28877100
O	-1.80345400	0.03230200	-0.16343800
C	-1.73649000	0.50517300	-2.54596900
H	-2.33909300	0.78092200	-3.41629800
H	-0.98470500	1.27923100	-2.36613400
H	-1.22431900	-0.43576500	-2.76529000
C	-3.39167100	1.65185000	-1.01749400
H	-3.98081800	1.54428800	-0.10442100
H	-2.68357500	2.47582200	-0.88541800
H	-4.06190400	1.89435400	-1.84750300
C	-3.01896700	-0.94300100	2.24153000
O	-3.80193900	-0.07898300	2.27759300
O	-2.26021000	-1.83138700	2.27033900
H	-1.09197400	0.73300300	-0.08076800
H	1.37371300	0.20650400	-0.07158400

	Route 6	TS6-1	HF=-1032.0033105	
C		-4.19049900	1.64379000	-0.27055500
C		-4.42913700	0.38058400	-0.71771600
C		-2.35166100	0.45251800	0.02632400
N		-2.89031800	1.66784600	0.18633400
H		-4.82598300	2.51403900	-0.23333400
H		-5.31481900	-0.06089800	-1.14595500
N		-3.27543500	-0.34331700	-0.52232400
C		-3.07164500	-1.76694800	-0.84770500
H		-4.07019100	-2.20717200	-0.91221700
H		-2.53492800	-2.19506200	0.01017500
C		-2.28640700	-1.95007900	-2.13674600
H		-2.22564800	-3.01760600	-2.36692000

H	-2.75685700	-1.44280200	-2.98506600
H	-1.26670700	-1.57968000	-2.00715800
C	-2.22404700	2.82772000	0.77404500
H	-2.73573200	3.10764500	1.69752100
H	-1.18367600	2.57094100	0.98901100
H	-2.26116600	3.65895800	0.06685100
C	-0.21871900	-1.78588200	1.46973100
O	-1.35307200	-2.22668600	1.67308600
O	0.11565300	-1.19214400	0.35463600
C	0.86162400	-1.91079300	2.52702400
H	1.33325300	-0.93983500	2.69951600
H	0.43544300	-2.29878100	3.45230400
H	1.64411900	-2.59213900	2.17749200
C	5.46140300	0.89125400	-0.28624200
H	6.40285100	1.36416300	-0.12415200
C	4.37481000	0.39286700	-0.46010200
C	3.09582000	-0.29563600	-0.70508700
O	2.14870900	0.10319600	0.29236800
C	2.57805600	0.02340900	-2.11540100
H	3.29607000	-0.30668700	-2.87180800
H	1.63173800	-0.50255100	-2.27933400
H	2.41995000	1.09702900	-2.22295900
C	3.31623300	-1.80922400	-0.54250200
H	3.68924000	-2.02735100	0.46084400
H	2.37093900	-2.33811300	-0.69526400
H	4.04724000	-2.16794900	-1.27223900
C	1.56644000	1.80055200	0.44321300
O	2.22057100	2.51464800	-0.25192000
O	0.65532500	1.69502500	1.22745400
H	1.20825600	-0.55773600	0.33261800
H	-1.33422600	0.13278500	0.26733900

Route 6

CP6-2

HF=-1032.0188827

C

-3.84539700

-1.94384700

0.20467300

C	-4.10335200	-0.66609600	0.59723900
C	-2.19814400	-0.66031200	-0.52692200
N	-2.65502200	-1.91711000	-0.48921700
H	-4.39889100	-2.85614600	0.36025700
H	-4.92245500	-0.25446900	1.16496900
N	-3.06839600	0.11527000	0.12891600
C	-2.89643400	1.55622800	0.37763600
H	-3.84635700	2.03937000	0.13006200
H	-2.14203400	1.92285400	-0.31868600
C	-2.46807900	1.85280500	1.80536800
H	-2.30262600	2.92836200	1.89500900
H	-3.22259700	1.54143700	2.53493400
H	-1.51760000	1.36343300	2.02740900
C	-1.97179200	-3.05765200	-1.09778500
H	-2.40575200	-3.26989200	-2.07798500
H	-0.90552200	-2.80787200	-1.17985400
H	-2.09446100	-3.92470600	-0.44674300
C	0.43142500	3.03181800	-0.33820100
O	-0.51678100	3.76736700	-0.14328000
O	0.72896900	2.07116700	0.54755100
C	1.32856000	3.11615800	-1.54725700
H	1.25976300	2.16794900	-2.09087000
H	1.01585000	3.94765900	-2.17810400
H	2.37068800	3.25366900	-1.24221100
H	1.35167300	1.41042700	0.16380200
H	-1.25285000	-0.33757800	-1.02182700
C	2.54210900	-1.38707000	1.54994100
C	3.15683000	-0.78925000	0.35178500
O	2.18270000	-0.07222500	-0.43896800
C	4.14372100	0.29801300	0.79622800
H	4.93865600	-0.13910200	1.40556500
H	4.58782600	0.76890700	-0.08549800
H	3.63258800	1.06144600	1.38818600
C	3.86844700	-1.84796000	-0.49650600

H	3.15848700	-2.60995100	-0.81505300
H	4.30592900	-1.36500000	-1.37584900
H	4.66949000	-2.31478700	0.08392200
C	1.05153000	-0.75200600	-0.97693700
O	0.92283300	-1.95950400	-0.74736500
O	0.31232800	0.04608400	-1.60014200
C	2.12852700	-1.83257100	2.59457800
H	1.73602500	-2.24579300	3.49526500

	Route 6	TS6-2	HF=-1031.9738842	
C		-3.89335700	-0.32201100	0.52307900
C		-3.52424300	0.97187600	0.73908800
C		-2.17865400	0.11520900	-0.78264400
N		-3.04598600	-0.83677700	-0.43135900
H		-4.67268600	-0.91694400	0.97132000
H		-3.92917500	1.71674100	1.40379600
N		-2.44914700	1.22324800	-0.08296800
C		-1.67134100	2.47285500	-0.17448700
H		-2.23738500	3.17881000	-0.79096200
H		-0.75269000	2.21335800	-0.70363100
C		-1.35146200	3.05634600	1.19103400
H		-0.63112300	3.86705000	1.05986200
H		-2.24127800	3.44747200	1.69424600
H		-0.87002500	2.30898200	1.82500000
C		-2.97307000	-2.24006300	-0.83743800
H		-3.97753300	-2.66308800	-0.78605000
H		-2.59917600	-2.29217000	-1.85891500
H		-2.25685900	-2.75953500	-0.15970900
C		2.16458100	2.78691700	0.04105900
O		1.75223600	3.91322100	0.21171900
O		1.70531200	1.77864100	0.80693100
C		3.18288500	2.40362300	-1.00419300
H		2.72356500	1.69466000	-1.70098700
H		3.51392100	3.29599100	-1.53404700

H	4.04288400	1.90892100	-0.54130100
H	1.99260500	0.90854100	0.46410700
H	-1.35320300	0.01483800	-1.48004500
C	0.45988700	-2.55711700	0.50152300
C	1.89521600	-2.12676100	0.50367000
O	1.93130000	-0.84732000	-0.20751300
C	2.39773400	-1.87209100	1.91777600
H	2.33963200	-2.79667800	2.49722400
H	3.43912600	-1.53592600	1.90316600
H	1.78231700	-1.11701700	2.41224100
C	2.79083200	-3.10089700	-0.26165800
H	2.40064400	-3.26013000	-1.26965800
H	3.81126000	-2.71065900	-0.32990300
H	2.81371300	-4.06557600	0.25249500
C	0.86959300	-0.76455200	-1.07688500
O	0.09451700	-1.78573400	-1.02564100
O	0.72731700	0.25152200	-1.75422200
C	-0.52004900	-3.15343900	1.05382400
H	-0.44936200	-3.64493600	2.01935200

	Route 6	CP6-3	HF=-1032.0205792	
C		-3.89932400	0.64813500	-1.50090800
C		-3.34853100	1.78959800	-1.06760200
C		-2.35168900	0.08645600	0.09953600
N		-3.53586200	-0.40221100	-0.62114200
H		-4.62742800	0.48893800	-2.28260000
H		-3.50956000	2.80173800	-1.40966400
N		-2.59384400	1.53449100	0.09501100
C		-1.56625900	2.45058000	0.56148000
H		-1.70205800	3.39503000	0.02411800
H		-0.55895200	2.09129100	0.30042600
C		-1.65693700	2.70965800	2.06238000
H		-0.86771900	3.39772300	2.38202900
H		-2.62770700	3.14192200	2.32100800

H	-1.54227600	1.78559300	2.63791100
C	-3.52988500	-1.76494100	-1.10004300
H	-2.72337600	-1.99250000	-1.81635900
H	-3.44019600	-2.45542500	-0.25505100
H	-4.48816100	-1.96867200	-1.58625300
C	3.72906800	1.72913400	-0.34285000
O	4.17934600	2.49166700	0.47164400
O	2.41674500	1.37272100	-0.28006000
C	4.50889200	1.10742900	-1.47788600
H	4.11042500	1.44714300	-2.44043700
H	5.55365400	1.40516300	-1.40007300
H	4.43018400	0.01549000	-1.45086200
C	-1.05550300	-0.25107100	-0.62896100
H	-0.98018500	0.16243200	-1.63293200
C	-0.01588000	-0.95499500	-0.19066400
C	0.29708300	-1.68702900	1.10779400
O	1.58047300	-2.30259800	0.79464100
C	0.52817300	-0.73997500	2.28066200
H	-0.41550900	-0.28251500	2.58757500
H	0.93588500	-1.29772700	3.12824600
H	1.22661000	0.05328300	2.00387300
C	-0.66833300	-2.81767300	1.43737700
H	-0.78502300	-3.49076900	0.58483600
H	-0.28553400	-3.38898100	2.28734200
H	-1.64911700	-2.41769300	1.70483200
C	2.03382900	-1.90047800	-0.39394900
O	1.10231000	-1.10343200	-1.00824100
O	3.09226900	-2.16806100	-0.88143400
H	2.19477600	0.73979700	-0.97900800
H	-2.33816200	-0.30855500	1.12338200

	Route 6	TS6-3	HF=-1031.9865576	
	C	-1.07107100	-3.44744500	-0.40239900
	C	-2.15969000	-2.82991700	-0.91220300

C	-1.15435500	-1.37561400	0.47290600
N	-0.51464500	-2.59007900	0.53657800
H	-0.64718000	-4.41676900	-0.60930000
H	-2.87504600	-3.16250800	-1.64728300
N	-2.27331400	-1.59454000	-0.29366200
C	-3.28218600	-0.59363300	-0.60920900
H	-3.94996100	-1.05379000	-1.34279900
H	-2.78470500	0.24886000	-1.10234700
C	-4.06827800	-0.12045300	0.60549800
H	-4.84319000	0.58148700	0.28531500
H	-4.54881300	-0.96147600	1.11389900
H	-3.42508300	0.41542300	1.30677600
C	0.70800600	-2.82750000	1.26303700
H	1.53411700	-2.26593300	0.81208400
H	0.59501600	-2.52447500	2.30703300
H	0.93589100	-3.89368500	1.23519700
C	-1.89025700	2.76086400	-0.07625800
O	-2.71578300	3.46670700	0.45975600
O	-1.34460500	1.72052200	0.56816200
C	-1.38470800	3.02053000	-1.48354200
H	-1.09720000	2.10454300	-2.00644300
H	-2.14777600	3.56127100	-2.04453700
H	-0.49433900	3.65596600	-1.42691200
C	0.14519000	-0.18849700	-0.68561000
H	0.01560500	-0.73284500	-1.62681300
C	1.43655700	0.06593600	-0.43023000
C	2.12683800	0.90154400	0.63733700
O	3.50423100	0.45070500	0.52363900
C	2.10167600	2.38911400	0.27907800
H	1.08876500	2.77725100	0.40101100
H	2.77690200	2.93972200	0.94051500
H	2.42045300	2.54487600	-0.75532500
C	1.65626100	0.67018200	2.06182800
H	1.78578100	-0.37330200	2.35527200

H	2.23298300	1.29251300	2.75179300
H	0.60316800	0.95066300	2.14860600
C	3.68053600	-0.18074700	-0.65418800
O	2.48165900	-0.36267100	-1.27305000
O	4.73073300	-0.55212100	-1.09039300
H	-0.78386100	1.07319800	-0.02877100
H	-1.19281900	-0.71997000	1.33143500

	Route 6	CP6-4	HF=-1032.0501833
C		-3.19063300	-2.81899600
C		-4.18396800	-2.04508800
C		-2.43341800	-0.73355200
N		-2.11356600	-1.98400900
H		-3.16054700	-3.87235400
H		-5.18671200	-2.29809700
N		-3.69366500	-0.75831500
C		-4.41121400	0.41990700
H		-5.40200000	0.41659600
H		-3.84566800	1.29048800
C		-4.50995700	0.40704500
H		-5.05219000	1.29752700
H		-5.04206200	-0.47211400
H		-3.51549100	0.43421200
C		-0.82529600	-2.37551200
H		-0.95800400	-2.74593400
H		-0.16793300	-1.50570300
H		-0.37683000	-3.15707400
C		-1.31617500	2.43745900
O		-2.54127500	2.53438500
O		-0.62738300	1.36046800
C		-0.54521200	3.69592200
H		0.18175500	3.47770500
H		-1.22942000	4.48098900
H		0.01266300	4.06413200

C	2.07732500	0.02436500	-1.73335800
H	2.28415400	-0.43264700	-2.69494400
C	2.90817900	-0.15714600	-0.71276000
C	2.85339800	0.40792500	0.69472800
O	4.04299500	-0.18095000	1.28958700
C	2.99964300	1.92402500	0.71586500
H	2.11298100	2.37093400	0.25966600
H	3.08664900	2.27777200	1.74715000
H	3.88520200	2.23928400	0.15808800
C	1.63436600	-0.05562400	1.47940100
H	1.56655700	-1.14748200	1.47635200
H	1.70877300	0.28445500	2.51662400
H	0.73621800	0.37295200	1.02262800
C	4.70029400	-0.94025000	0.39972400
O	4.04369500	-0.93428300	-0.80316500
O	5.70934100	-1.54646200	0.60206700
H	1.19203800	0.64372900	-1.59855400
H	-1.74248600	0.16875700	-0.36698200

Route 6	CP6-5	HF=-1108.4880094	
C	-4.67335300	-0.74919300	1.38459800
H	-4.60781300	-1.57115900	2.08664800
C	-3.76442200	-0.58620500	0.43246300
C	-3.65897700	0.46831700	-0.65424600
C	-4.79196700	0.36966300	-1.67002200
H	-5.73916700	0.64300400	-1.19698400
H	-4.60794900	1.05405800	-2.50270200
H	-4.88195200	-0.64733700	-2.06082900
C	-3.46202500	1.87528500	-0.10931400
H	-2.57944500	1.88724100	0.53647300
H	-3.32555700	2.57829000	-0.93623000
H	-4.34541500	2.17754600	0.46122700
O	-2.42990000	0.06383800	-1.32172800
H	-5.49480000	-0.04993900	1.47929100

C	-1.91340600	-1.01667100	-0.74018800
O	-0.90371200	-1.57581000	-1.08133300
O	-2.70871200	-1.45587800	0.26943200
O	-0.83219100	0.78514800	1.40452000
H	-0.78397500	1.08305700	2.31778300
H	0.02544600	1.11579300	0.98098200
C	4.33469900	-1.02997100	-0.62715300
C	3.81330100	-1.93824300	0.24127000
C	2.14106700	-0.90482300	-0.75937800
N	3.27599300	-0.41119400	-1.25351300
H	5.35698800	-0.77170600	-0.85098800
H	4.29304200	-2.63507500	0.90941500
N	2.44057700	-1.85573300	0.13184200
C	1.46506900	-2.61830600	0.92109500
H	1.89490600	-3.61350500	1.06925700
H	0.56788400	-2.71702800	0.30650900
C	1.13553100	-1.93821700	2.24247000
H	0.46936600	-2.58672000	2.81979100
H	2.03690200	-1.75800700	2.83639300
H	0.61826400	-0.99111800	2.06180000
C	3.36591200	0.74973000	-2.13321300
H	4.27947800	0.66521500	-2.72434500
H	2.50374600	0.75004100	-2.80045700
H	3.35635100	1.65589600	-1.49455700
C	2.03903000	2.53477800	0.51495700
O	3.08954900	2.89089100	-0.05101200
O	1.39880400	1.45040000	0.28693000
C	1.46010000	3.44553200	1.60353000
H	1.65842400	3.00542400	2.58826900
H	1.92006800	4.43444700	1.56782900
H	0.37442800	3.53307400	1.49672000
H	1.14071900	-0.61176500	-1.03528500

Route 6 TS6-4

HF=-1108.4598511

C	4.88865700	-1.12473200	-0.97042200
H	4.92935300	-1.83341000	-1.78884100
C	3.74321500	-0.85853200	-0.34558400
C	3.48913800	0.09723800	0.81214300
C	4.23981900	-0.31676000	2.07581600
H	5.31890800	-0.21128900	1.93175100
H	3.93734700	0.31851000	2.91394500
H	4.02145700	-1.35739200	2.32786100
C	3.75546900	1.55279500	0.43717700
H	3.16202100	1.81747300	-0.43890400
H	3.48129100	2.20795900	1.26994500
H	4.81673800	1.69954200	0.21418000
O	2.08707700	-0.09890800	1.06300800
H	5.80614000	-0.63803400	-0.66290000
C	1.52129400	-0.82473100	0.04489200
O	0.46165400	-1.42732600	0.20865400
O	2.56694000	-1.46638700	-0.65956600
O	1.23839800	0.51732700	-1.14294300
H	1.15615700	0.03497000	-1.97514700
H	0.11150800	1.01470200	-0.86359900
C	-4.38933600	-0.26938800	1.03616000
C	-4.25802800	-1.39348800	0.28048000
C	-2.23431400	-0.69393600	0.83048200
N	-3.11847900	0.14381600	1.37343300
H	-5.26754900	0.26656200	1.35844000
H	-5.00070400	-2.03049400	-0.17225200
N	-2.90592600	-1.64321300	0.17004800
C	-2.27135900	-2.69978800	-0.62887400
H	-2.76691800	-3.64321900	-0.38077000
H	-1.22824000	-2.74339600	-0.30809100
C	-2.34901300	-2.39333700	-2.11783200
H	-1.85106100	-3.18895300	-2.67892000
H	-3.38215500	-2.32191100	-2.47163300
H	-1.83943600	-1.45055400	-2.33168000

C	-2.77910300	1.39173500	2.05191500
H	-3.54053100	1.59721600	2.80612000
H	-1.81036900	1.27237100	2.53607700
H	-2.71561800	2.19087900	1.29880000
C	-1.23302700	2.63870400	-0.87782000
O	-2.20958100	3.22702500	-0.41715800
O	-0.91430400	1.42042400	-0.52854000
C	-0.35733300	3.29678700	-1.93191600
H	-0.67487900	2.95336000	-2.92323700
H	-0.47816500	4.37970900	-1.89056800
H	0.69205200	3.01854500	-1.80887000
H	-1.14446100	-0.65000600	0.86659000

	Route 6	CP6-6	HF=-1108.469948	
C		4.74974300	-1.57757400	-0.22139800
H		5.05094700	-2.25109500	-1.01485000
C		3.48242800	-1.17444100	-0.10288900
C		2.90394300	-0.22503600	0.94163200
C		3.07997800	-0.75280800	2.36384900
H		4.13871500	-0.79105600	2.63563700
H		2.56567900	-0.09677500	3.07420400
H		2.66184600	-1.75873400	2.44888500
C		3.46361800	1.19088200	0.79217500
H		3.31193600	1.54428900	-0.22936000
H		2.95658900	1.87067900	1.48506100
H		4.53546600	1.20670200	1.01213800
O		1.50629000	-0.24658400	0.64056900
H		5.50107200	-1.24393600	0.48428800
C		1.28499600	-0.80847200	-0.64655800
O		0.20252100	-1.43177900	-0.81382300
O		2.48685000	-1.58516700	-0.91567400
O		1.41985100	0.38697400	-1.56414400
H		1.31224600	0.00043400	-2.44395800
H		0.09194600	1.22104600	-1.19743800

C	-3.91655700	0.00737900	1.50582100
C	-4.19516000	-1.07280900	0.72482700
C	-2.00891700	-0.72931300	0.66688000
N	-2.55118600	0.19858800	1.45686300
H	-4.56415300	0.64579400	2.08519100
H	-5.13121100	-1.55881800	0.50021900
N	-2.99204500	-1.51697100	0.21846800
C	-2.77411600	-2.60777700	-0.74166500
H	-3.52645600	-3.37377600	-0.53339900
H	-1.78281200	-3.01404300	-0.53071100
C	-2.83176800	-2.11554200	-2.18004200
H	-2.70784500	-2.96451800	-2.85842800
H	-3.78529200	-1.62901100	-2.40684100
H	-2.00998600	-1.41725100	-2.35342100
C	-1.81134200	1.29445900	2.07576800
H	-2.13544900	1.40344900	3.11268300
H	-0.75117800	1.04665700	2.03930400
H	-1.97695000	2.21299600	1.50415900
C	-0.68153500	2.99296400	-0.82156900
O	-1.49642700	3.64691200	-0.19656100
O	-0.73378200	1.66369600	-0.82170700
C	0.40778000	3.62042200	-1.66363300
H	0.15102800	3.51448500	-2.72340200
H	0.49021300	4.68026100	-1.42447600
H	1.36497100	3.11575100	-1.50905200
H	-0.95967900	-0.86126900	0.32776800

Route 6	TS6-5	HF=-1108.4607283	
C	-2.83827800	1.65283400	1.22792400
H	-3.16046100	0.84850300	1.88166100
C	-1.54268800	1.76807200	0.86556100
C	-0.98077700	2.92629300	0.04095700
C	-1.94080800	3.53712900	-0.96796500
H	-2.77682400	4.02514300	-0.46013900

H	-1.42267400	4.28903200	-1.57059500
H	-2.33499100	2.76717000	-1.63449500
C	-0.41084700	3.99921800	0.97822100
H	0.20757300	3.54379600	1.75924500
H	0.18843200	4.72039600	0.41312600
H	-1.22014300	4.53368100	1.48365200
O	0.08863600	2.34162100	-0.73196800
H	-3.57427400	2.39574600	0.94636200
C	0.69852400	1.19575600	-0.24931900
O	0.72663200	0.16659300	-0.91488300
O	-0.56674800	0.93902600	1.17366900
O	1.81925900	1.47438900	0.51600000
H	1.73498300	2.36639600	0.87363800
H	3.43591200	0.85018600	-0.11087700
C	-1.66283100	-3.82327700	0.65359900
C	-1.84997600	-3.55547500	-0.66827700
C	-1.25792900	-1.67075000	0.32027600
N	-1.29746500	-2.63227600	1.24787000
H	-1.74890700	-4.74423600	1.20776100
H	-2.13431300	-4.20141100	-1.48370200
N	-1.58870800	-2.21385200	-0.85227700
C	-1.68116500	-1.45288600	-2.10912700
H	-1.45498300	-2.15339100	-2.91742400
H	-0.88410100	-0.70334700	-2.05976000
C	-3.05157000	-0.81295100	-2.27959500
H	-3.07612100	-0.26204200	-3.22405400
H	-3.85189300	-1.55953200	-2.29997000
H	-3.24821600	-0.10538400	-1.46807800
C	-0.96857800	-2.40772100	2.65011000
H	-0.09330500	-2.99926500	2.92678600
H	-0.74795100	-1.34661600	2.77462400
H	-1.81646700	-2.68488500	3.28007800
C	4.57959100	-0.69100100	-0.28675700
O	5.64131100	-1.16055300	-0.62447900

O	4.34896000	0.62910100	-0.38476700
C	3.44119100	-1.50863400	0.28840400
H	2.49740100	-1.26863500	-0.21265800
H	3.67920100	-2.56813000	0.19295300
H	3.31548900	-1.26055100	1.34843300
H	-0.97770300	-0.62077900	0.53165500

Route 6	CP6-7	HF=-1108.4923261	
C	3.65709700	-2.38036500	0.30450000
H	4.51430300	-2.21250900	-0.33767900
C	2.52232900	-1.71021700	0.11837700
C	1.25799600	-1.76482000	0.97223700
C	1.05369200	-3.10050700	1.67902100
H	1.83621500	-3.25457500	2.42845900
H	0.09145900	-3.08253600	2.20065000
H	1.05675700	-3.91915500	0.96174800
C	1.32444500	-0.62650300	2.00196900
H	1.45811000	0.33799000	1.50409200
H	0.39314600	-0.59878200	2.57687900
H	2.16014700	-0.78437300	2.68928400
O	0.14258900	-1.39487400	0.13663300
H	3.73927500	-3.12384300	1.08577200
C	-0.32550900	-2.31286200	-0.90152600
O	0.29335500	-3.34608800	-1.08822900
O	2.43020400	-0.75170200	-0.86709800
O	-1.33654900	-1.81449200	-1.46203300
H	3.29637100	0.68633100	-0.83989600
H	1.47846600	-0.53302600	-0.91032100
C	-4.70036300	0.90969000	0.21898500
C	-3.86508000	1.96394600	0.42836000
C	-2.65792400	0.29590900	-0.38710900
N	-3.92794600	-0.11394000	-0.28779600
H	-5.76082100	0.80585300	0.38567100
H	-4.06397100	2.95180100	0.81160600
N	-2.60138200	1.55945700	0.04509100

C	-1.37386000	2.36724900	0.08954200
H	-1.49867600	3.20338500	-0.60528000
H	-0.56446500	1.74172400	-0.28648700
C	-1.04564600	2.85801500	1.48965900
H	-0.08163600	3.36929300	1.44925100
H	-1.79523800	3.55608500	1.87574500
H	-0.95518900	2.01896900	2.18415300
C	-4.37045100	-1.45298700	-0.67067100
H	-5.12440800	-1.37902500	-1.45734600
H	-3.49297800	-1.99486800	-1.03675900
H	-4.79330200	-1.96141300	0.19863400
C	2.92639000	2.53713600	-0.57269300
O	1.74125300	2.36733300	-0.32822800
O	3.77543800	1.56075800	-0.85584600
C	3.59435800	3.88803500	-0.58627200
H	4.05239200	4.06544400	-1.56336700
H	2.86591900	4.66811900	-0.36805100
H	4.39849800	3.90985200	0.15493500
H	-1.86025100	-0.38716800	-0.79062900

	Route 6	TS6-6	HF=-1108.4775786	
C		2.92045800	-2.67091800	1.00374200
H		3.90281100	-2.69765600	0.54532200
C		1.91864500	-1.98278000	0.45319800
C		0.48262800	-1.79837700	0.99141800
C		-0.10148500	-3.10950300	1.52408000
H		0.47814400	-3.48905700	2.37129700
H		-1.12718600	-2.93785600	1.87005100
H		-0.11282600	-3.87231500	0.74436500
C		0.53631200	-0.75057700	2.12054300
H		0.98327000	0.17808700	1.75184500
H		-0.47647000	-0.53849000	2.48467600
H		1.13867500	-1.10530000	2.96271500
O		-0.27906700	-1.26912400	-0.07189500

H	2.77198100	-3.22453300	1.92252100
C	-1.06157000	-2.45734000	-1.50674400
O	-0.29287200	-3.34392200	-1.65016800
O	2.06509600	-1.25911300	-0.69337400
O	-2.05473000	-1.84348300	-1.75509000
H	3.20666300	-0.09734600	-0.75377500
H	1.09760800	-0.99254200	-0.83608500
C	-4.15615800	1.83327800	-0.00542500
C	-3.13956300	2.73201400	-0.10270600
C	-2.24511500	0.70632200	0.01267100
N	-3.57824900	0.58285800	0.06400700
H	-5.22520500	1.97428500	0.01090900
H	-3.15509300	3.80653000	-0.18953900
N	-1.96483500	2.00976100	-0.08899300
C	-0.60447500	2.56291300	-0.17259300
H	-0.54362800	3.14711300	-1.09551600
H	0.08376600	1.72286100	-0.27060500
C	-0.24351200	3.40530400	1.03969600
H	0.80007900	3.70856000	0.93622100
H	-0.86908700	4.29958400	1.12680100
H	-0.33637500	2.82193600	1.95981500
C	-4.28726300	-0.68609200	0.18106300
H	-5.20636200	-0.63332200	-0.40443000
H	-3.64822900	-1.46881200	-0.22764800
H	-4.52998700	-0.88833400	1.22715000
C	3.55972500	1.77309100	-0.49381500
O	2.40784600	2.06752700	-0.21087600
O	3.96823300	0.55515900	-0.80284700
C	4.68902100	2.77300800	-0.53000800
H	5.15680800	2.77026800	-1.51858200
H	4.31537400	3.76931000	-0.29577400
H	5.45943800	2.48498200	0.19115700
H	-1.48450500	-0.12470200	0.04530900

Route 6	CP6-8	HF=-1108.5026951	
C	0.34869500	-1.48644200	2.08580400
H	1.39456000	-1.74534700	1.95418300
C	-0.44879500	-1.27578600	1.01556300
C	-1.97573300	-1.03807200	1.14384300
C	-2.68286100	-2.36824700	1.43202800
H	-2.38485000	-2.77118200	2.40458800
H	-3.76837100	-2.22602400	1.41867800
H	-2.42061800	-3.10324600	0.66503200
C	-2.32996700	0.01192800	2.19199600
H	-1.80224800	0.94947500	1.99264600
H	-3.40730600	0.20724700	2.17376000
H	-2.06079500	-0.32252300	3.19735400
O	-2.41471700	-0.55308400	-0.12805800
H	-0.05303300	-1.51382300	3.09240100
C	-4.80155800	0.35626900	-1.15410200
O	-5.45233600	-0.12987400	-0.31689500
O	-0.05340700	-1.25815900	-0.25095000
O	-4.21325000	0.87606300	-2.02053300
H	1.01048100	-2.12187900	-0.65489000
H	-1.67891800	-0.87427800	-0.70364300
C	0.91274100	3.56469300	-0.60892000
C	2.08968800	3.35663000	0.04140700
C	1.13328300	1.38662900	-0.27308100
N	0.33236900	2.32793000	-0.78890800
H	0.44621100	4.47262200	-0.95604800
H	2.84352900	4.05064600	0.37716100
N	2.20785500	1.99786800	0.23593300
C	3.29254400	1.32533300	0.96601800
H	4.20373800	1.89522900	0.76295500
H	3.40048000	0.33986100	0.50652200
C	2.99748000	1.24249000	2.45673800
H	3.82448200	0.73432200	2.96105300
H	2.88484900	2.23507200	2.90464600

H	2.08423100	0.66507600	2.63143900
C	-0.94369500	2.06666500	-1.45256400
H	-0.77439900	1.80237800	-2.49859600
H	-1.46125500	1.25200500	-0.93861400
H	-1.55193600	2.96988700	-1.40091100
C	2.87471700	-2.17508100	-1.26387100
O	3.07932100	-0.97339300	-1.09751600
O	1.74911600	-2.78957600	-1.01033800
C	3.94040900	-3.10400700	-1.80271100
H	3.58621400	-3.57943500	-2.72202400
H	4.85930900	-2.55189400	-1.99991100
H	4.13203000	-3.90460800	-1.08218100
H	0.91254300	0.30601600	-0.28935800

	Route 6	TS6-7	HF=-919.9185502
C		-1.90589300	-0.86094300
C		-2.50153600	-0.98249700
C		-3.94317900	-0.49962100
H		-4.62690000	-1.07790100
H		-4.25434700	-0.61196700
H		-4.04351400	0.55644200
C		-2.36591100	-2.41866900
H		-1.34369600	-2.76562000
H		-2.61057600	-2.47461500
H		-3.04383700	-3.07790600
O		-0.74406100	-1.35440700
C		3.23152300	0.64492200
C		3.56234400	-0.05209100
C		1.40365900	-0.34825400
N		1.88778200	0.43865900
H		3.82770600	1.27203300
H		4.50572300	-0.16020100
N		2.40848000	-0.65737700
C		2.26330500	-1.52115100

H	2.85552400	-1.06625000	-2.27064800
H	1.20180400	-1.48222000	-1.73999600
C	2.70812800	-2.94974500	-1.19344300
H	2.59622600	-3.54594700	-2.10329100
H	3.75537600	-3.00201700	-0.87880100
H	2.08470400	-3.40162200	-0.41762400
C	1.07520700	1.08988300	2.52685400
H	1.66242900	1.17382300	3.44249100
H	0.77646700	2.07243700	2.15115000
H	0.18798800	0.47918300	2.69720700
C	-0.34594000	2.52033300	-0.74482000
O	0.46462600	2.98053200	0.04359800
C	-0.11055300	2.50708500	-2.23953800
H	-0.90048300	3.06561600	-2.75047800
H	0.85999600	2.94838500	-2.46594700
H	-0.15647600	1.47757100	-2.60888700
O	-1.49945400	2.00319300	-0.34249500
C	-2.55743200	-0.07942300	-1.76914900
H	-1.93151500	1.29282600	-1.02705100
H	-2.15351100	-0.10284300	-2.77975400
H	-3.62260300	0.11491000	-1.69021600
O	-1.65741000	-0.18846800	1.48922600
H	-1.66082300	0.71121800	1.11521100
H	0.36857000	-0.69009500	0.38085000

	Route 6	CP6-9	HF=-919.9505424	
C		-1.95881100	-1.34579400	-0.62706900
C		-2.28586200	-0.99444600	0.85402600
C		-3.69069700	-0.42416100	1.05689300
H		-4.47190700	-1.13812900	0.77247700
H		-3.81945400	-0.18395300	2.11643500
H		-3.82275800	0.49842100	0.48616900
C		-2.07104900	-2.23604200	1.71565000
H		-1.08058900	-2.65530100	1.52617600

H	-2.14664800	-1.95578400	2.77027400
H	-2.82055200	-3.00592600	1.50392500
O	-0.91988200	-1.94385300	-0.87359500
C	3.47774100	0.69775700	1.03205500
C	3.67004400	-0.06311400	-0.07878800
C	1.52390200	-0.13827000	0.43972000
N	2.13975000	0.61988200	1.34677500
H	4.16982800	1.28727300	1.61157900
H	4.56332300	-0.27601900	-0.64347800
N	2.43726800	-0.57965300	-0.42896600
C	2.16632300	-1.47496300	-1.55809600
H	2.66079600	-1.04526800	-2.43435400
H	1.08759800	-1.45691000	-1.72481800
C	2.63754100	-2.89731600	-1.29158800
H	2.43161500	-3.51762900	-2.16825900
H	3.71208100	-2.94264800	-1.08839300
H	2.10013300	-3.32571300	-0.44182800
C	1.42717000	1.41943600	2.33591500
H	2.04867400	1.52568700	3.22658900
H	1.18918500	2.38129100	1.87733900
H	0.49324100	0.91028300	2.57581300
C	-0.67749500	2.51257000	-0.75521300
O	0.49264400	2.32880300	-0.36084300
C	-0.94499000	3.61659100	-1.77796500
H	-1.68537100	4.31777100	-1.38011100
H	-0.02712800	4.15194600	-2.02768700
H	-1.37517300	3.18460400	-2.68767400
O	-1.71106800	1.85682700	-0.38613400
O	-1.31754500	-0.03279300	1.23677500
H	-1.44933900	0.80184200	0.62884100
H	0.45485200	-0.35491000	0.45959000
C	-2.84604400	-0.84724600	-1.73313300
H	-3.89247000	-1.12505300	-1.57728100
H	-2.78794500	0.24986400	-1.71839600

H	-2.49093500	-1.22921500	-2.69166900
Route 7	CP7-1	HF=-1032.0095735	
C	2.74061800	-1.79281400	1.90137600
C	3.50089800	-1.64519400	0.78066700
C	1.59766300	-0.57821100	0.45296000
N	1.56126400	-1.11745800	1.67544200
H	2.94031600	-2.30344200	2.82969600
H	4.49285600	-1.99901000	0.54975700
N	2.77128800	-0.88620900	-0.10635200
C	3.20474000	-0.43858000	-1.44418500
H	4.28347500	-0.61159400	-1.48262500
H	3.00692600	0.64028600	-1.49134700
C	2.47009800	-1.16976400	-2.55671900
H	2.87892200	-0.84952200	-3.51937200
H	2.58179900	-2.25600400	-2.47952700
H	1.41175900	-0.89890800	-2.53820000
C	0.43270500	-1.00343700	2.59648500
H	0.00655600	-0.00421300	2.49413500
H	-0.31871700	-1.75734500	2.35127800
H	0.79888400	-1.15331800	3.61266300
C	-0.58305800	2.83478300	0.73387000
O	-0.27300000	1.83616400	1.37476200
O	-0.14682700	3.11898100	-0.47538600
C	-1.52831400	3.88900500	1.25887200
H	-1.09916100	4.88455100	1.12216500
H	-2.46217300	3.85586400	0.68909100
H	-1.73947700	3.70873200	2.31300400
C	0.76752100	2.08175000	-1.09477600
O	1.93807800	2.43354600	-1.10246500
O	0.15638000	1.07658000	-1.48086700
C	-1.31864300	-3.14165400	-0.03142200
H	-0.59976500	-3.92021000	0.08675400
C	-2.15275300	-2.27779600	-0.18659400

C	-3.20831200	-1.26681900	-0.42401900
O	-4.47300100	-1.92783000	-0.51507700
H	-4.43399300	-2.51098500	-1.28313200
C	-3.32833700	-0.32422300	0.77357000
H	-2.40578600	0.24205900	0.91931800
H	-4.14910700	0.37400400	0.58626000
H	-3.55818200	-0.89242500	1.67855500
C	-2.90573300	-0.48990100	-1.71063500
H	-1.96854700	0.07018900	-1.63450700
H	-2.83044000	-1.17410700	-2.56327300
H	-3.72784600	0.20764300	-1.89798800
H	0.81623400	0.01103200	-0.03077300

	Route 7	TS7-1	HF=-1031.9513112	
C		3.45652400	-0.21425700	1.39249200
C		3.77852200	-0.75564700	0.18696000
C		1.63251700	-1.15099300	0.55519900
N		2.12229900	-0.48283300	1.60161300
H		4.05242900	0.33770500	2.10112500
H		4.71304000	-0.77359100	-0.35069200
N		2.63149900	-1.33767900	-0.31361800
C		2.47793400	-1.91322500	-1.65674600
H		3.47509600	-2.23336800	-1.97287300
H		2.13222700	-1.10734100	-2.30944800
C		1.48920800	-3.06516600	-1.68246600
H		1.43769800	-3.46415500	-2.69931200
H		1.79436000	-3.87288100	-1.01034500
H		0.48971800	-2.71990500	-1.40435900
C		1.29715000	0.00781500	2.69757800
H		1.19770300	1.08961200	2.59835400
H		0.31213300	-0.45189200	2.60673300
H		1.75367400	-0.25995700	3.65278200
C		0.76298700	2.81333900	-0.39294900
O		1.42620900	2.24276400	0.45199800

O	-0.16833900	2.22919400	-1.14869200
C	0.88844700	4.27947000	-0.72319000
H	1.03411900	4.41481200	-1.79801500
H	-0.03787300	4.79554100	-0.45336500
H	1.72300000	4.71119500	-0.17126000
C	-0.43883400	0.80671100	-0.90036500
O	0.09011100	0.02692200	-1.66403000
O	-1.24902400	0.68616100	0.06129800
C	-1.27121000	-1.89969100	0.68574200
H	-1.59596400	-2.89350000	0.97539800
C	-2.07244200	-0.95982000	0.39282000
C	-3.49417500	-0.49823300	0.22605900
O	-4.30475500	-1.65331200	0.46817000
H	-3.97815800	-2.34381900	-0.12271700
C	-3.89940000	0.51022300	1.29916500
H	-3.29608500	1.41478700	1.21535400
H	-4.95741900	0.76391500	1.17985400
H	-3.75608200	0.07133800	2.28970500
C	-3.78660100	0.03890400	-1.17990900
H	-3.27883100	0.98780300	-1.36031900
H	-3.45819600	-0.67475400	-1.94292800
H	-4.86609000	0.18691100	-1.28091300
H	0.55553700	-1.48527800	0.48898400

	Route 7	CP7-2	HF=-1031.9879034
C		4.15423000	0.36557900
C		4.27562300	-0.29487200
C		2.11943200	-0.58809800
N		2.84619100	0.17114100
H		4.87076400	0.95046200
H		5.12087700	-0.40162100
N		3.03425200	-0.85504500
C		2.72813700	-1.69776300
H		3.26024900	-1.29706700

H	1.65813100	-1.59059800	-1.70123200
C	3.09773000	-3.15794100	-1.28102300
H	2.83805900	-3.76050300	-2.15725900
H	4.16980500	-3.27528800	-1.09223500
H	2.55386700	-3.55078300	-0.41749800
C	2.28088000	0.74151100	2.68822100
H	2.29046500	1.83417400	2.64363200
H	1.24752600	0.40582900	2.75782500
H	2.83600500	0.40961600	3.57163000
C	-0.15262600	2.73087400	-0.48508600
O	0.11273200	2.46468100	0.65230200
O	-0.55171600	1.80647500	-1.43574900
C	-0.06554100	4.08232200	-1.13406400
H	0.62006300	4.04288000	-1.98501500
H	-1.04640700	4.37444300	-1.51988700
H	0.28294000	4.81195800	-0.40438700
C	-0.90269300	0.51013200	-1.13415900
O	-0.61045900	-0.38953700	-1.86734700
O	-1.67799700	0.48027800	-0.05029900
C	-1.21957200	-1.62910500	0.94576500
H	-1.58632200	-2.54894400	1.38611100
C	-2.10019100	-0.77124700	0.44950100
C	-3.61346100	-0.91509200	0.40956100
O	-3.97160700	-2.22925000	0.81477000
H	-3.60561400	-2.83707900	0.15944100
C	-4.26007900	0.02250400	1.43020600
H	-3.97570800	1.05974900	1.23675400
H	-5.34918800	-0.06453500	1.37622400
H	-3.93544500	-0.24996700	2.43737900
C	-4.14536200	-0.63922100	-1.00380300
H	-3.97527000	0.39756400	-1.30537200
H	-3.65555200	-1.28783100	-1.73832900
H	-5.22113900	-0.83453200	-1.02327400
H	-0.14786400	-1.41928800	0.91860900

Route 7	TS7-2	HF=-1031.9519949	
C	4.38519500	-0.24897000	-1.33344100
C	3.89581200	-1.50156100	-1.11318500
N	3.53610700	0.63006500	-0.69488500
H	5.24639400	0.08472300	-1.89002900
H	4.25177100	-2.46531600	-1.44103600
N	2.75672000	-1.36129200	-0.34906300
C	1.89757700	-2.43742600	0.17151600
H	1.92765300	-3.24604600	-0.56373000
H	0.87611100	-2.04749000	0.20581000
C	2.34962400	-2.90573400	1.54659700
H	1.69471200	-3.71407700	1.88305500
H	3.37827900	-3.27963100	1.53404700
H	2.27501400	-2.08799700	2.26829900
C	3.62590000	2.08989000	-0.65380000
H	3.67176400	2.47477500	-1.67469600
H	2.72104400	2.45312500	-0.14381300
H	4.52505700	2.38421300	-0.10765500
C	-4.21973400	-0.58203200	-0.86487300
O	-3.65867300	0.08545200	-1.69445500
O	-3.57454700	-1.20035500	0.17073800
C	-5.68973600	-0.88410000	-0.80845200
H	-5.85105200	-1.96458100	-0.76951600
H	-6.11682900	-0.45634600	0.10335400
H	-6.18067900	-0.45918400	-1.68291800
C	-2.20932000	-0.94778300	0.33269400
O	-1.40078500	-1.81057300	0.11589300
O	-2.05419000	0.26837600	0.80081700
C	0.11325400	0.24607300	2.04211900
C	-0.73404500	0.72228600	1.14397100
C	-0.33006400	2.03176700	0.44589000
O	0.97617200	2.25217000	0.92110700
H	0.93541300	1.39919200	1.74421000

C	-0.35916900	1.89463400	-1.08290600
H	-1.36363300	1.65895600	-1.44743600
H	-0.03476500	2.83171400	-1.54880500
H	0.31126700	1.09547600	-1.41827000
C	-1.25501600	3.17884900	0.88368100
H	-2.29611200	2.99898100	0.59400100
H	-1.20535000	3.29173300	1.97015200
H	-0.92361300	4.11661700	0.42452200
H	-0.13237400	-0.63818300	2.63107700
C	2.56087300	-0.06379500	-0.10340900
H	1.74942400	0.37479600	0.48581200

Route 7	CP7-3	HF=-1032.002534	
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C	4.86045300	-0.06800300	-1.10684300
C	4.32481200	-1.30877400	-0.98526300
N	3.92723700	0.80548900	-0.57549100
H	5.80085500	0.25642900	-1.52609400
H	4.71077800	-2.27363600	-1.27768800
N	3.08654400	-1.14052100	-0.38816300
C	2.18265000	-2.23299100	-0.04250100
H	2.12572600	-2.91354700	-0.89910300
H	1.19266600	-1.79458900	0.09551100
C	2.62116800	-2.97925400	1.21135700
H	1.90951300	-3.77869200	1.43816200
H	3.61106900	-3.43051900	1.08837500
H	2.65934600	-2.29923700	2.06692000
C	4.08476000	2.24672300	-0.50724700
H	4.26806700	2.66001300	-1.50364500
H	3.16013000	2.66395500	-0.10698600
H	4.91861000	2.51547500	0.14863300
C	-4.49130000	-0.31373800	-0.85704700
O	-3.98328400	0.60034700	-1.44772900
O	-3.77869800	-1.22688500	-0.11174300
C	-5.94800700	-0.66982700	-0.83421600

H	-6.08580000	-1.70522100	-1.15688400
H	-6.32929900	-0.59236400	0.18818600
H	-6.49588700	0.00649700	-1.48872600
C	-2.43526300	-1.01084700	0.13969800
O	-1.60170900	-1.80955000	-0.17517900
O	-2.29641400	0.11552200	0.83358700
C	-0.45160600	-0.11079800	2.29779900
C	-0.99875000	0.49675000	1.25336200
C	-0.43132000	1.69336400	0.49729100
O	0.87888800	1.93111800	0.94575900
H	0.51027500	0.23703700	2.65109600
C	-0.46951300	1.44503300	-1.01960500
H	-1.49062000	1.31192900	-1.38608600
H	-0.03079600	2.31253100	-1.52159100
H	0.12129500	0.56375100	-1.28305900
C	-1.26123900	2.93426300	0.84897700
H	-2.31255500	2.79649200	0.58191500
H	-1.18531200	3.13941200	1.92020100
H	-0.86762400	3.79590100	0.30175200
H	-0.94438300	-0.93415700	2.80250000
C	2.81741100	0.16427400	-0.11900800
H	1.48167200	1.20630500	0.59409900

Route 7	TS7-3	HF=-1031.9829841	
C	3.72509200	0.59410200	-1.13573500
C	3.97386500	-0.19541400	-0.05878200
C	1.78792500	-0.41901800	-0.58107100
N	2.38482300	0.44145500	-1.43535900
H	4.37814000	1.23653900	-1.70579200
H	4.88535100	-0.37279300	0.49042700
N	2.77550700	-0.80566800	0.25745000
C	2.55323900	-1.68574100	1.40594000
H	3.35730200	-2.42946900	1.42008600
H	1.60885800	-2.20023600	1.21751800

C	2.48051800	-0.91676600	2.71868800
H	2.34040900	-1.61786300	3.54695200
H	3.39925800	-0.35164900	2.90623700
H	1.63209500	-0.22770100	2.70796700
C	1.68184500	1.15513100	-2.49467000
H	1.17748000	0.44111200	-3.14810000
H	0.94929800	1.84299100	-2.06366400
H	2.40971700	1.71668400	-3.08236000
C	-0.97124800	2.58955600	0.10368700
O	-0.46111000	3.22103100	-0.79240200
O	-0.94544600	1.22909700	0.01511000
C	-1.65801400	3.21087400	1.28802600
H	-1.08722900	3.00635700	2.19675400
H	-1.73058700	4.28432500	1.11835500
H	-2.65323600	2.77989600	1.42927800
C	-2.80138700	-0.77811400	-0.19868600
C	-1.60784700	-1.65655600	-0.60619600
O	-0.53396700	-1.22079800	0.18707800
C	-1.91461100	-3.11892000	-0.24833600
H	-2.78442200	-3.49430200	-0.79620400
H	-1.04835400	-3.74375100	-0.48976400
H	-2.11260600	-3.20342000	0.82336100
C	-1.31785900	-1.50834100	-2.10419100
H	-1.12804500	-0.46106700	-2.35125500
H	-0.44180700	-2.10653500	-2.37518800
H	-2.16228400	-1.85504800	-2.70688100
C	-1.29974700	0.41763100	1.13107400
O	-2.55832900	-0.09237100	0.97106300
O	-0.79114500	0.56246200	2.20952900
C	-4.00123200	-0.70276600	-0.76791100
H	-4.77386600	-0.05992200	-0.36262100
H	-4.23702900	-1.30152100	-1.63923600
H	0.43598400	-0.84244200	-0.32457100

Route 7	CP7-4	HF=-1032.0511324	
C	4.24168500	0.26360700	-1.27607700
C	4.23644600	-0.85978100	-0.50992400
C	2.17265800	-0.06643100	-0.55571600
N	2.94393500	0.73601500	-1.29360000
H	5.04195500	0.75466700	-1.80605300
H	5.03406200	-1.53358400	-0.24074500
N	2.93648600	-1.05384200	-0.08325000
C	2.47180400	-2.05619100	0.88221300
H	3.04541400	-2.96981800	0.69831900
H	1.42728600	-2.25937200	0.63544800
C	2.62411000	-1.55660100	2.31314100
H	2.19528000	-2.28935400	3.00326100
H	3.67739700	-1.41584600	2.57636600
H	2.10515000	-0.60003600	2.42962700
C	2.45006100	1.95942300	-1.90905800
H	1.41361000	2.08736000	-1.58561600
H	3.04554600	2.80666000	-1.56262800
H	2.50661900	1.88584000	-2.99793600
C	0.28273800	1.79705100	1.08691900
O	1.41407700	1.50345400	1.53328000
O	-0.21143000	1.37414300	-0.01516100
C	-0.60108700	2.74346900	1.90236600
H	-1.53042200	2.23337700	2.17628700
H	-0.08770700	3.07973800	2.80507500
H	-0.88029900	3.60984900	1.29343300
C	-3.06988600	-0.45638400	0.69733200
C	-3.34286600	-0.14921600	-0.76370100
O	-2.23807200	-0.84081700	-1.41039800
C	-4.63897300	-0.77888400	-1.26077500
H	-5.49406000	-0.30579700	-0.77020700
H	-4.73446400	-0.63499200	-2.34062600
H	-4.66426500	-1.84982400	-1.04289900
C	-3.22931400	1.33391500	-1.08869800

H	-2.24644500	1.69769400	-0.76999500
H	-3.35477700	1.48656600	-2.16510300
H	-4.01618400	1.88680000	-0.56642300
C	-1.43240900	-1.39535500	-0.50244000
O	-1.92485600	-1.21652500	0.75481500
O	-0.43114100	-2.01346000	-0.74171900
C	-3.75572100	-0.12600900	1.78449100
H	-3.42469800	-0.43107700	2.76944300
H	-4.65640100	0.46913500	1.69994500
H	1.11036200	0.14675600	-0.36798300

Route 8	CP8-1	HF=-644.6781773	
C	1.88500100	-0.64996200	0.08975900
C	2.13360400	0.82283500	-0.04381100
O	1.24934400	1.37297700	-0.98805500
C	1.98632300	1.49270700	1.32920700
H	2.66405000	1.05345200	2.06713900
H	2.21964400	2.55548200	1.21969700
H	0.95714900	1.40250800	1.68723700
C	3.54985200	0.99557500	-0.60518400
H	3.62196500	0.53331000	-1.59227200
H	3.74671000	2.06594500	-0.70698400
H	4.29902400	0.55345100	0.05712300
H	0.35578800	1.46566300	-0.58306800
C	1.74614700	-1.86853200	0.16691400
H	1.85618900	-2.93036500	0.23796900
Ag	-0.42486900	-1.08436500	0.00210200
C	-2.35442000	0.83539500	0.00781500
O	-1.25871700	1.43075200	0.16581500
O	-2.47394800	-0.43122900	-0.11669200
C	-3.62799700	1.65254000	-0.06028000
H	-4.50831100	1.03068600	0.10527300
H	-3.58809100	2.46505600	0.66833500
H	-3.69979500	2.10660400	-1.05433600

Route 8	TS8-1	HF=-644.6125578	
C	1.68862900	-0.66934400	0.53940700
C	2.37695200	0.46082500	-0.04159100
O	1.30117000	0.40701900	-0.96512800
C	2.42909200	1.72924200	0.80250600
H	3.14383300	1.62309900	1.62495600
H	2.75333500	2.55851300	0.16602900
H	1.44165200	1.97425800	1.19749900
C	3.70439600	0.14806000	-0.72189000
H	3.62147500	-0.76379800	-1.31670900
H	3.95822200	0.97843400	-1.38793400
H	4.50748900	0.02958300	0.01241600
H	0.06665100	0.84304800	-0.73767400
C	0.95576700	-1.61535900	0.97630000
H	1.17017300	-2.25355200	1.82350500
Ag	-0.94801500	-1.40966600	-0.01987800
C	-1.55561100	1.90535000	-0.03289000
O	-1.04927700	0.87125200	-0.71417800
O	-0.87282500	2.73522500	0.53229200
C	-3.06754800	1.93472800	-0.04438000
H	-3.42101900	2.85794400	0.41427000
H	-3.44214800	1.85497900	-1.06855800
H	-3.46558600	1.08281500	0.51783400

Route 8	CP8-2	HF=-644.6389568	
C	-2.09972300	-0.22428200	-0.00010700
C	-3.31987300	0.55697300	0.00001600
O	-1.95265500	1.14261600	0.00021400
C	-4.08235400	0.78368700	-1.28181900
H	-4.91252200	0.07308800	-1.35923400
H	-4.50326200	1.79552900	-1.30787200
H	-3.43054500	0.64865600	-2.14726900
C	-4.08240100	0.78310000	1.28193700

H	-3.43066300	0.64749600	2.14734800
H	-4.50313700	1.79500200	1.30850300
H	-4.91269900	0.07260600	1.35892200
H	1.18357900	1.39958500	0.00024600
C	-1.32074900	-1.29215100	-0.00034200
H	-1.80867000	-2.26378600	-0.00058500
Ag	0.71595900	-1.05257600	-0.00005800
C	3.02336200	0.93609000	0.00009300
O	2.05708300	1.84352800	0.00002700
O	2.82531900	-0.27682000	0.00046600
C	4.39230600	1.54211000	-0.00018700
H	5.14518900	0.75594800	-0.00119300
H	4.51017500	2.18038000	-0.88044200
H	4.51109600	2.17882000	0.88109100

Route 8

TS8-2

HF=-644.6236572

C	-1.73852300	0.25267300	0.20355100
C	-3.14556400	0.49508900	-0.05094300
O	-2.05671300	0.47735700	-1.08385000
C	-4.11461300	-0.65326500	-0.16328200
H	-4.64587200	-0.78863200	0.78473900
H	-4.85993500	-0.45275800	-0.94082200
H	-3.59506100	-1.58311900	-0.40335100
C	-3.73202700	1.86261000	0.18706500
H	-2.95146700	2.62583000	0.20016200
H	-4.45811700	2.11019300	-0.59503500
H	-4.25331000	1.88348500	1.14995900
H	0.49362400	0.86862900	0.61360200
C	-0.62895400	0.05841300	0.93573000
H	-0.83446400	-0.06711900	1.99973500
Ag	0.85551700	-1.29863100	0.02632200
C	2.50830900	1.17373800	-0.04632600
O	1.41918800	1.65694200	0.43217600
O	2.71905400	-0.02439800	-0.35848500

C	3.61902800	2.18226900	-0.24625900
H	4.52900700	1.68924700	-0.58889300
H	3.30176000	2.92636800	-0.98319700
H	3.80638100	2.71514800	0.69001900

Route 8	CP8-3	HF=-644.6775275	
C	-2.01262500	-0.57047000	0.16422300
C	-2.66840800	0.70322700	-0.04329100
O	-2.45991700	0.00514400	1.28071500
C	-1.88095200	1.97523600	-0.20290200
H	-1.81284300	2.23235200	-1.26504800
H	-2.39259400	2.79621700	0.30951700
H	-0.86557800	1.88299200	0.19015200
C	-4.10732400	0.71923300	-0.48937300
H	-4.60426200	-0.22698400	-0.26622800
H	-4.64686900	1.53007000	0.01002600
H	-4.15815800	0.89503200	-1.56868600
H	-1.40001700	-2.56511000	0.53367000
C	-1.49142900	-1.77192600	-0.20303300
H	-1.46807100	-2.03517600	-1.25582200
Ag	0.46610500	-0.62470400	-0.06073200
C	2.81953000	0.53318900	0.00903400
O	2.74902000	-0.72313400	-0.14919200
O	1.79726400	1.26993300	0.13469900
C	4.19506500	1.16566000	0.06321200
H	4.12787800	2.25399000	0.06729600
H	4.70774500	0.83046200	0.97027200
H	4.79177200	0.82680300	-0.78772700

Route 8	TS8-3	HF=-833.1377308	
C	-1.50385800	-0.26061100	0.60122000
C	-1.66295700	1.17024000	0.57802500
O	-2.92832600	0.25417700	0.33605700
C	-1.81491300	1.85613500	1.91012400

H	-0.81893500	2.17641100	2.23310900
H	-2.44653200	2.74182200	1.80238100
H	-2.24118500	1.19247500	2.66309800
C	-1.19727700	2.03334300	-0.55496900
H	-1.25388800	1.53434200	-1.52156400
H	-1.75963700	2.96947100	-0.57840000
H	-0.13402300	2.23492800	-0.36312300
C	-0.97752700	-1.25849400	1.36529300
H	-0.40249800	-0.93617600	2.23502700
H	-1.45184600	-2.23287000	1.39827500
C	-2.90748400	-0.31624100	-1.18716000
O	-1.75334400	-0.80708800	-1.18759800
O	-3.87733000	-0.16652500	-1.84323600
Ag	1.01372000	-1.09822300	0.22954900
C	2.81662400	0.83535800	-0.37189500
O	1.83805300	1.38463300	0.18707500
O	2.91347800	-0.42420300	-0.58441500
C	3.99030300	1.67506600	-0.84403000
H	4.90734800	1.32820200	-0.35907400
H	4.12798000	1.54069000	-1.92097400
H	3.83067300	2.73044500	-0.62029400

	Route 8	CP8-4	HF=-833.270114	
C		-1.66123300	-0.14228900	0.69962200
C		-2.07580000	1.09959600	-0.07785200
O		-2.99898100	0.53039100	-1.04041200
C		-2.85044000	2.07587800	0.80447200
H		-2.18192400	2.52821500	1.54163600
H		-3.27176500	2.86970700	0.18282300
H		-3.66499900	1.57174600	1.33089700
C		-0.94283000	1.76959700	-0.84435600
H		-0.47692600	1.06620000	-1.53969100
H		-1.33740600	2.61376100	-1.41625800
H		-0.17231800	2.13712700	-0.16091600

C	-0.84666800	-0.25491200	1.78240100
H	-0.48120400	0.64697900	2.26503300
H	-0.84184000	-1.18220600	2.34871200
C	-3.14981700	-0.78535400	-0.85737100
O	-2.35113300	-1.19523000	0.21024800
O	-3.84326400	-1.52854200	-1.47104500
Ag	1.00395000	-0.55986300	0.47657200
C	3.33079200	0.28169900	-0.49255600
O	2.78285400	1.16996800	0.20081600
O	2.81678900	-0.87431500	-0.70294700
C	4.68412600	0.53854100	-1.12697500
H	5.42677500	-0.12118500	-0.66752000
H	4.65004200	0.29158700	-2.19140000
H	4.98702000	1.57691400	-0.98979500

	Route 8	CP8-5	HF=-909.7070242	
C		4.58688900	0.19124200	-1.32999200
H		4.84055900	-0.49096200	-2.13218600
C		3.49693700	0.01171300	-0.59769900
C		2.92958100	0.81852000	0.55571700
C		3.86733300	0.88886600	1.75213900
H		4.74906000	1.48228100	1.49530000
H		3.36224100	1.36673700	2.59559500
H		4.19681800	-0.10883500	2.05260800
C		2.39603500	2.17747600	0.12053300
H		1.62478500	2.05183600	-0.64431600
H		1.95927400	2.69798000	0.97743600
H		3.21477900	2.78382700	-0.27746200
O		1.78398000	-0.00886300	0.93397200
H		5.23998600	1.03355800	-1.13805100
C		1.63833200	-1.01116200	0.08242300
O		0.73985600	-1.82688500	0.10240500
O		2.63740100	-1.05223100	-0.81980800

O	-0.32722400	0.82984600	-1.36874800
H	-0.50823400	0.62020600	-2.29148500
H	-1.17747500	1.25563500	-1.04146800
C	-3.52933600	0.96227200	-0.03067600
O	-3.38889200	-0.25852400	0.32887800
O	-2.64685100	1.70261300	-0.51869400
C	-4.92316700	1.53051200	0.18126000
H	-4.98353400	2.55644900	-0.18326100
H	-5.65826900	0.90571400	-0.33398900
H	-5.16933800	1.50204300	1.24700200
Ag	-1.37983900	-0.98214400	0.12783000

	Route 8	TS8-4	HF=-909.6686307	
C		4.16982300	0.49215600	-1.45004800
H		4.37112500	0.00523800	-2.39663500
C		3.12841700	0.13898700	-0.70263600
C		2.67486600	0.68807500	0.64202600
C		3.69288500	0.42563400	1.74821100
H		4.60430600	1.00308800	1.56910300
H		3.27738200	0.72248900	2.71579400
H		3.95317900	-0.63478300	1.78755200
C		2.26676400	2.15646000	0.56870800
H		1.50322700	2.29366900	-0.19804200
H		1.86949900	2.48198100	1.53495200
H		3.13439800	2.77658300	0.32402600
O		1.51780800	-0.13020200	0.91857000
H		4.84357900	1.27173000	-1.11585400
C		1.18551900	-0.85151200	-0.18994500
O		0.50845200	-1.90152700	-0.08614100
O		2.26889800	-0.86408300	-1.06022600
O		0.14320100	0.35471400	-1.02734000
H		0.14762200	0.08844800	-1.95558900
H		-0.93405700	1.17301300	-0.69878000

C	-2.86916900	1.44452700	-0.12289000
O	-3.13484800	0.26220800	0.17714700
O	-1.72713500	1.88866400	-0.53363800
C	-3.94162900	2.49537300	-0.01682700
H	-4.11666200	2.93676400	-1.00220400
H	-4.86379300	2.06123700	0.36721100
H	-3.59987800	3.29951700	0.64062600
Ag	-1.54565500	-1.24032700	0.18002700

	Route 8	CP8-6	HF=-909.6957858	
C		-2.94924400	-0.65898500	0.38927300
H		-3.43254500	-1.14585900	1.23463900
C		-2.18348700	0.51838700	0.76319100
C		-1.86627600	1.59603500	-0.32495100
C		-1.95323600	1.18499600	-1.78801300
H		-2.98042000	0.91519100	-2.04533900
H		-1.66173600	2.02865800	-2.42141400
H		-1.30264400	0.33854000	-2.01576800
C		-2.74960600	2.80480900	-0.03226400
H		-2.61891800	3.10869700	1.00849300
H		-2.49439900	3.63865600	-0.69300900
H		-3.79935800	2.54259900	-0.19142300
O		-0.50921600	2.09636600	-0.05782300
H		-3.57006200	-0.59959800	-0.50267800
C		0.49602300	1.24236000	0.05413400
O		0.54049000	0.06736000	-0.24251700
O		-1.75873000	0.75343600	1.89322900
O		1.58896300	1.87041100	0.52977400
H		1.35729200	2.78505700	0.74705100
H		3.37167000	1.22576400	-0.04586100
C		4.74027200	-0.12667100	-0.08519900
O		5.78856200	-0.51596400	-0.53604600
O		4.23125700	1.06497600	-0.46718600

C	3.91528300	-0.88708400	0.93243100
H	2.87730600	-0.98697400	0.59955900
H	4.35604900	-1.87088000	1.09012500
H	3.90207900	-0.34471800	1.88435300
Ag	-1.22879300	-1.88023200	-0.15012300

	Route 8	TS8-5	HF=-909.6592462
C		3.69520400	0.02785000
H		3.91744500	-0.90422700
C		2.43098300	0.46863900
C		2.01729500	1.80345000
C		2.92002700	2.30125300
H		3.90833100	2.55242500
H		2.49455600	3.20238600
H		3.02940400	1.53850100
C		1.84263300	2.86718600
H		1.28490500	2.47263300
H		1.33502500	3.75014900
H		2.82080100	3.17396200
O		0.74124100	1.51515000
H		4.52771000	0.60376200
C		-0.08446100	0.61935700
O		-0.53900100	-0.36305400
O		1.33550900	-0.14453900
O		-0.89415700	1.16118000
H		-0.53852800	2.01893800
H		-2.78139700	1.24855200
C		-4.53214600	0.54875900
O		-5.69630600	0.75927400
O		-3.69147100	1.56789400
C		-3.91325900	-0.83325300
H		-2.96748500	-0.86656300
H		-4.61881200	-1.55761300

H	-3.69740100	-1.09420500	-1.09014500
Ag	0.74428200	-2.10479500	0.04353600

Route 8	CP8-7	HF=-909.6825158	
C	-0.20160100	2.27407900	-1.72159300
H	-0.95037900	2.02179200	-2.46427000
C	0.30144500	1.31419100	-0.92234300
C	1.48642000	1.63030000	0.02021400
C	2.80142600	1.50656400	-0.75062800
H	2.85852000	2.29531800	-1.50357900
H	3.65652400	1.59172100	-0.07326000
H	2.86109200	0.54149500	-1.26628800
C	1.39552500	2.97861200	0.72619300
H	0.44608500	3.08797500	1.25000100
H	2.21555300	3.07010700	1.44495900
H	1.49262100	3.79118300	0.00246900
O	1.61217000	0.55911100	1.02603200
H	0.12086600	3.30598400	-1.66077900
C	0.53874200	0.04409600	1.62857100
O	0.49036300	-1.15761400	1.87615400
O	-0.15001800	0.05886200	-0.92806200
O	-0.39910500	0.91531400	1.95292700
H	-1.25472500	0.43303300	1.95664200
H	-1.56738000	-0.11200800	-0.21724000
C	-3.54133200	-0.00630300	0.06381400
O	-4.46816700	-0.07421200	0.83425100
O	-2.28396600	-0.26394100	0.47818800
C	-3.67185400	0.37016600	-1.39474500
H	-3.20192000	-0.38080100	-2.03711700
H	-4.72638300	0.47032500	-1.64943600
H	-3.15765800	1.31942800	-1.57671100
Ag	1.02434800	-1.75331800	-0.42591900

Route 8	TS8-6	HF=-909.6732368	
C	-0.46116300	2.32150000	-1.62677800
H	-1.25771300	2.05428100	-2.31226800
C	0.19881500	1.37132200	-0.95763800
C	1.41739600	1.66996200	-0.07115300
C	2.69544600	1.52910200	-0.90261400
H	2.72594600	2.30921100	-1.66666800
H	3.57856900	1.61621500	-0.26314900
H	2.72824000	0.55801300	-1.40976900
C	1.36354600	3.02851400	0.61901400
H	0.44578400	3.13128300	1.19847100
H	2.22371300	3.12368000	1.28791500
H	1.41815400	3.83729500	-0.11407000
O	1.57574300	0.62069800	0.94046000
H	-0.23689700	3.37286100	-1.50135700
C	0.48905500	0.11215700	1.57226900
O	0.52801600	-1.08874000	1.87322900
O	-0.15873300	0.05522700	-1.07350700
O	-0.50612900	0.91388200	1.76517500
H	-1.38121800	0.41858100	1.37312400
H	-1.17108500	-0.09357500	-0.54814400
C	-3.38509100	-0.01145600	0.11877800
O	-4.12535900	0.40978900	0.98094900
O	-2.08028600	-0.20715500	0.32333000
C	-3.85657600	-0.40447800	-1.26710100
H	-3.74500000	-1.48569500	-1.40114400
H	-4.90468700	-0.13283800	-1.39227300
H	-3.25200700	0.08252500	-2.03840900
Ag	1.06794900	-1.74725900	-0.31059600

Route 8	CP8-8	HF=-909.6983542	
C	-2.26326700	-1.54784000	1.56816900

H	-1.79480800	-2.51903300	1.69201500
C	-2.17331700	-0.88122600	0.41910300
C	-2.82009100	0.45529900	0.04766100
C	-4.06096200	0.19899500	-0.81552000
H	-4.82749600	-0.31574300	-0.23068900
H	-4.45894000	1.15378500	-1.16905500
H	-3.81823900	-0.41636500	-1.68631500
C	-3.17982500	1.31070100	1.25595000
H	-2.33190400	1.45931300	1.92290600
H	-3.51545700	2.29141700	0.91316100
H	-3.99918500	0.83506300	1.80376500
O	-1.88444000	1.07479700	-0.86911000
H	-2.82375800	-1.14220600	2.39975800
C	-0.67223400	1.61242100	-0.35592300
O	-0.68501300	2.48387800	0.48512400
O	-1.44893000	-1.40259900	-0.64631100
O	0.33436900	1.05543500	-0.94528400
H	1.61948600	1.40981500	-0.52062200
H	-1.42561000	-0.65475900	-1.28803000
C	3.31952900	0.60712100	0.19767300
O	2.91088300	-0.56732900	0.32698100
O	2.63808300	1.60697200	-0.24819100
C	4.73578500	0.94474600	0.58003200
H	4.72785900	1.73353400	1.33734400
H	5.25139100	0.06343900	0.95903300
H	5.26127300	1.34172600	-0.29318100
Ag	0.84898000	-1.17979800	-0.17124700

	Route 8	TS8-7	HF=-909.6754392	
C		-2.66205000	-2.09718100	1.01185600
H		-2.27178100	-3.10759100	0.95367200
C		-2.21373400	-1.13979800	0.18711800
C		-2.76780400	0.31475500	0.19333400

C	-4.20228600	0.37234300	-0.32513900
H	-4.86829400	-0.17933000	0.34406300
H	-4.54195800	1.41075700	-0.38940900
H	-4.26557100	-0.08015700	-1.31814800
C	-2.63493800	0.97715400	1.55841900
H	-1.60695600	0.92437900	1.92980400
H	-2.94062800	2.02533300	1.51976800
H	-3.27038700	0.45225600	2.27589200
O	-1.93521700	0.98544000	-0.80339800
H	-3.43804000	-1.89440500	1.74112000
C	-0.61058500	2.12751900	-0.36905900
O	-1.08813000	3.12907200	0.03869300
O	-1.29263300	-1.29550800	-0.77838000
O	0.40282900	1.52180400	-0.67424300
H	1.98529100	1.56197300	-0.18873600
H	-1.46034200	0.12569400	-1.15383600
C	3.46433600	0.40755500	0.30174200
O	2.85352700	-0.66562200	0.24120400
O	2.94864400	1.58771800	0.06651800
C	4.91937500	0.45713800	0.66122200
H	5.06677800	1.13222200	1.50841600
H	5.28049600	-0.54103300	0.90293800
H	5.48515400	0.86631900	-0.18103300
Ag	0.76553600	-1.13439500	-0.25499200

	Route 8	CP8-9	HF=-909.6990907	
C		-1.78350300	-1.20646200	1.79965200
H		-0.95698400	-1.82688700	2.14108800
C		-1.92646700	-0.91966000	0.49151500
C		-3.08844900	-0.09733500	-0.08908100
C		-4.03467700	-1.02935700	-0.85846300
H		-4.53531600	-1.72770600	-0.18003000
H		-4.79118500	-0.43900300	-1.38529900

H	-3.46786400	-1.61130200	-1.59056300
C	-3.85492800	0.73088200	0.93065400
H	-3.18161100	1.36401400	1.51311500
H	-4.56969900	1.37479900	0.40909600
H	-4.41243200	0.08734800	1.61669800
O	-2.48894400	0.81999100	-1.02081500
H	-2.49666700	-0.87017700	2.54173500
C	-0.70748800	2.64609200	-0.08683400
O	-1.53152200	3.33848600	0.34904300
O	-1.10880600	-1.30173800	-0.49594900
O	0.20276400	2.02744300	-0.50065300
H	2.06997400	1.51598500	-0.17954600
H	-1.79642900	0.25881400	-1.41632600
C	3.61951800	0.42391200	0.09718500
O	3.02915700	-0.65622000	0.07275700
O	3.03528700	1.59782600	-0.04439300
C	5.09929600	0.52205700	0.29676400
H	5.30729100	1.10621700	1.19784800
H	5.52820200	-0.47418200	0.38814100
H	5.54908100	1.05383200	-0.54624900
Ag	0.90873000	-1.12423000	-0.14634000

	Route 8	TS8-8	HF=-721.1213929	
C		1.08032200	0.89958100	0.83971000
C		2.05061100	0.26442400	-0.19909600
C		2.93679400	1.25709200	-0.94525500
H		3.59397800	1.79248700	-0.25428600
H		3.55728300	0.71833200	-1.66730300
H		2.34229000	1.99687300	-1.49047100
C		2.89392400	-0.80476300	0.48414700
H		2.25482700	-1.49050200	1.04648300
H		3.46366700	-1.36727600	-0.26132500
H		3.59235800	-0.34177000	1.18701400

O	0.32775800	0.07958900	1.48008800
C	-2.04059000	1.08297500	-0.47063100
O	-2.46105900	-0.04845200	-0.70923700
C	-2.76903800	2.04278300	0.42903800
H	-2.84302100	3.03005400	-0.03336000
H	-3.75827400	1.65540800	0.67065000
H	-2.18758500	2.14899500	1.35183000
O	-0.90375200	1.51453500	-1.00282900
C	0.94967600	2.27708600	0.93128500
H	-0.29250200	2.02213900	-0.31576200
H	0.34740200	2.67480000	1.74504900
H	1.68745000	2.94443000	0.50129400
O	1.24565300	-0.44042200	-1.18702700
H	0.65168700	0.22213000	-1.58063300
Ag	-0.61039500	-1.42474800	0.08590800

Route 8	CP8-10	HF=-721.169758	
C	-2.22582400	-0.38552200	-0.42925700
C	-1.88106700	0.92276000	0.31488900
C	-1.83448400	2.07852700	-0.69737900
H	-2.78230300	2.20190400	-1.22886900
H	-1.62089500	3.00473300	-0.15660900
H	-1.03272800	1.92410600	-1.42551200
C	-2.96165700	1.16361400	1.38497600
H	-2.98979400	0.32905100	2.09168200
H	-2.68478900	2.06373700	1.93925900
H	-3.95917300	1.30767700	0.96262900
O	-1.49105800	-1.36936700	-0.41248400
C	2.58361400	0.88757600	-0.22170500
O	2.69253800	-0.36707600	-0.00774900
C	3.88741700	1.63670500	-0.43239200
H	4.25056000	1.98622500	0.54026900
H	4.64869300	0.98414600	-0.86293000

H	3.72452800	2.51125200	-1.06481300
O	1.51230600	1.54426400	-0.25011200
O	-0.66706600	0.79975300	1.00219900
H	0.11063900	1.18010500	0.49094600
Ag	0.70119400	-1.18870700	0.17706900
C	-3.49978900	-0.46961000	-1.23190600
H	-4.28968800	0.18830900	-0.86805700
H	-3.26770000	-0.17256200	-2.26202900
H	-3.84648900	-1.50437000	-1.25642700

Route 9	CP9-1	HF=-1177.2536983	
C	-4.56973500	-1.98574200	0.15968800
C	-5.01319000	-0.77283800	-0.25959100
C	-2.79294900	-0.59401500	0.10416700
N	-3.21133100	-1.85391200	0.37489000
H	-5.09484300	-2.91628800	0.30981600
H	-6.00050300	-0.44414900	-0.54490600
N	-3.91279000	0.06068800	-0.28959700
C	-3.95105000	1.47834900	-0.65695400
H	-4.53990800	1.56747100	-1.57581600
H	-2.92407200	1.77715400	-0.88576500
C	-4.52582200	2.34882900	0.45241000
H	-4.52751900	3.39486200	0.13332600
H	-5.55374000	2.06644700	0.70173400
H	-3.91518000	2.27083300	1.35624900
C	-2.34446000	-2.92268300	0.84163900
H	-2.51165000	-3.82343000	0.24611500
H	-1.30924500	-2.60441000	0.72054900
H	-2.53957500	-3.14158800	1.89532600
C	0.78038900	2.40710300	-0.35509400
O	-0.32396500	2.71189700	-0.82610100
O	0.99991400	1.29960100	0.28868700
C	1.96710200	3.34188900	-0.47468400
H	2.85328000	2.79500900	-0.80796000

H	1.74209500	4.15816800	-1.16208500
H	2.19642400	3.75962200	0.51157100
Ag	-0.89477400	0.28639100	0.20084600
C	5.25094400	1.09783700	-1.28300300
H	5.67871100	1.63006200	-2.10170300
C	4.76261300	0.48177300	-0.36310800
C	4.16998900	-0.27058300	0.76703100
O	2.84894100	-0.67804200	0.45874400
C	4.97585300	-1.55315800	0.99728300
H	6.01574200	-1.32286800	1.24392100
H	4.52654800	-2.11133800	1.82443600
H	4.95433700	-2.17440500	0.09928000
C	4.17201400	0.60945300	2.02682400
H	3.54791600	1.49310800	1.86985000
H	3.75755900	0.03669700	2.86213200
H	5.18405000	0.93644500	2.28401800
C	1.94909600	-2.57053300	-1.36784900
O	2.99135900	-2.71867700	-1.86995000
O	0.87340700	-2.48369900	-0.91613000
H	2.28078800	0.12204800	0.36853300

Route 9	TS9-1	HF=-1177.2351839	
C	-4.38344000	-1.52940600	-0.10596000
C	-4.58387100	-0.21246400	0.15291200
C	-2.36474000	-0.50998000	-0.15570600
N	-3.02305700	-1.68926200	-0.28897400
H	-5.08161600	-2.34861700	-0.18151000
H	-5.49147600	0.33619500	0.35193600
N	-3.34157800	0.39088800	0.11415600
C	-3.10376500	1.80788600	0.38891800
H	-3.85453900	2.38298700	-0.16351700
H	-2.12156600	2.05570100	-0.01961500
C	-3.15909000	2.12329000	1.87826300
H	-2.97186600	3.18923300	2.03697500

H	-4.13551400	1.88169500	2.31031600
H	-2.39333700	1.55837400	2.41713400
C	-2.38462600	-2.95361400	-0.61047500
H	-2.70244000	-3.30273600	-1.59680200
H	-1.30516400	-2.79988300	-0.61566700
H	-2.63854100	-3.70516200	0.14172100
Ag	-0.29025600	-0.14090200	-0.40097300
C	2.32797100	-0.92344700	-1.54483400
O	1.34398800	-0.60099700	-2.18602600
O	3.37897300	-1.49104800	-1.59112400
H	2.23048700	1.28659000	-0.12664200
C	2.32191000	-2.26314000	1.24790600
C	2.60913600	-0.81767800	1.19650300
O	2.00235500	-0.24979700	0.02591400
C	1.95718500	-0.13948200	2.41152600
H	2.36888300	-0.54057200	3.34222200
H	2.14969400	0.93698100	2.37683800
H	0.87596000	-0.30708600	2.40738400
C	4.12460800	-0.56732500	1.20001300
H	4.58203900	-1.02688200	0.32479600
H	4.31136000	0.51107000	1.17800500
H	4.57586300	-0.98175700	2.10652800
C	1.26889600	2.94802400	-0.36454000
O	0.15530400	2.43031700	-0.34505900
O	2.39867500	2.28900800	-0.22863000
C	1.47487300	4.42821100	-0.55825800
H	1.99349100	4.59819600	-1.50674700
H	0.51542000	4.94435600	-0.56778000
H	2.11357900	4.82604900	0.23488300
C	2.07100200	-3.44298400	1.33536300
H	1.88311600	-4.49095000	1.38862000

Route 9

CP9-2

HF=-1177.2420957

C

-3.93148900

-2.51598200

0.35983200

C	-4.35651000	-1.30591700	-0.08492600
C	-2.10621200	-1.23193900	0.01154600
N	-2.55286800	-2.44927300	0.41328200
H	-4.48224000	-3.40182700	0.63584100
H	-5.35233600	-0.93344500	-0.26759300
N	-3.22898700	-0.53821300	-0.29169200
C	-3.25809600	0.86768000	-0.71488600
H	-3.82150900	0.92265100	-1.65245400
H	-2.22829800	1.16483900	-0.92396600
C	-3.85329400	1.78354900	0.34432800
H	-3.70547100	2.82024400	0.03246900
H	-4.92141800	1.59989900	0.50079000
H	-3.33355800	1.65146800	1.29769500
C	-1.70189700	-3.53501300	0.86434300
H	-1.82741400	-4.41112500	0.22172400
H	-0.66500600	-3.20017600	0.82239500
H	-1.94674800	-3.80560200	1.89496300
C	-0.49716900	3.70096900	-0.19238600
O	-1.58918000	4.22534400	-0.25796200
O	-0.29035900	2.49954500	-0.75795000
C	0.70618500	4.32450700	0.47129200
H	1.42696500	4.62435500	-0.29802700
H	0.39584500	5.20810800	1.02870000
H	1.21195200	3.60503200	1.12563100
Ag	-0.13058400	-0.50838200	-0.13659700
C	1.73320900	-2.61223700	-0.97895200
H	1.02879500	-3.31761100	-1.35731300
C	2.57236500	-1.82611000	-0.59306200
C	3.69419600	-0.95915600	-0.17530900
O	3.35731000	-0.10923000	0.92992700
C	4.80529700	-1.85765200	0.38581500
H	5.15295500	-2.56083400	-0.37527200
H	5.64079100	-1.22936600	0.70535000
H	4.43917500	-2.41709900	1.24957200

C	4.20979000	-0.14243900	-1.36660000
H	3.41810700	0.49294400	-1.76363200
H	5.04205200	0.48212700	-1.02863100
H	4.56710700	-0.80776600	-2.15770600
C	2.38494600	0.87192500	0.82991400
O	1.61893800	0.80518300	-0.21766700
O	2.35125700	1.68819800	1.73145200
H	0.57902800	2.07412200	-0.50971800

Route 9	CP9-2	HF=-1177.2420957	
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C	-3.93148900	-2.51598200	0.35983200
C	-4.35651000	-1.30591700	-0.08492600
C	-2.10621200	-1.23193900	0.01154600
N	-2.55286800	-2.44927300	0.41328200
H	-4.48224000	-3.40182700	0.63584100
H	-5.35233600	-0.93344500	-0.26759300
N	-3.22898700	-0.53821300	-0.29169200
C	-3.25809600	0.86768000	-0.71488600
H	-3.82150900	0.92265100	-1.65245400
H	-2.22829800	1.16483900	-0.92396600
C	-3.85329400	1.78354900	0.34432800
H	-3.70547100	2.82024400	0.03246900
H	-4.92141800	1.59989900	0.50079000
H	-3.33355800	1.65146800	1.29769500
C	-1.70189700	-3.53501300	0.86434300
H	-1.82741400	-4.41112500	0.22172400
H	-0.66500600	-3.20017600	0.82239500
H	-1.94674800	-3.80560200	1.89496300
C	-0.49716900	3.70096900	-0.19238600
O	-1.58918000	4.22534400	-0.25796200
O	-0.29035900	2.49954500	-0.75795000
C	0.70618500	4.32450700	0.47129200
H	1.42696500	4.62435500	-0.29802700
H	0.39584500	5.20810800	1.02870000

H	1.21195200	3.60503200	1.12563100
Ag	-0.13058400	-0.50838200	-0.13659700
C	1.73320900	-2.61223700	-0.97895200
H	1.02879500	-3.31761100	-1.35731300
C	2.57236500	-1.82611000	-0.59306200
C	3.69419600	-0.95915600	-0.17530900
O	3.35731000	-0.10923000	0.92992700
C	4.80529700	-1.85765200	0.38581500
H	5.15295500	-2.56083400	-0.37527200
H	5.64079100	-1.22936600	0.70535000
H	4.43917500	-2.41709900	1.24957200
C	4.20979000	-0.14243900	-1.36660000
H	3.41810700	0.49294400	-1.76363200
H	5.04205200	0.48212700	-1.02863100
H	4.56710700	-0.80776600	-2.15770600
C	2.38494600	0.87192500	0.82991400
O	1.61893800	0.80518300	-0.21766700
O	2.35125700	1.68819800	1.73145200
H	0.57902800	2.07412200	-0.50971800

Route 9	TS9-2	HF=-1177.2266826	
C	-4.69557700	0.20559100	0.06326100
C	-4.08533900	0.44093200	1.25311600
C	-2.50507700	-0.29217400	-0.17635700
N	-3.71139400	-0.24408400	-0.79582000
H	-5.72376600	0.32541400	-0.24097100
H	-4.48215200	0.80165600	2.18940200
N	-2.75120500	0.13492300	1.08449300
C	-1.74389400	0.21309200	2.15032700
H	-1.92374900	1.14079300	2.70152700
H	-0.76506100	0.30234000	1.67682300
C	-1.77364100	-0.99472200	3.07438500
H	-0.94864000	-0.90893800	3.78533000
H	-2.71694400	-1.07092000	3.62544000

H	-1.62969000	-1.91767000	2.50460800
C	-3.93987700	-0.59440900	-2.18492300
H	-4.28131000	0.27826600	-2.74868100
H	-2.99793900	-0.94692600	-2.60634000
H	-4.68729000	-1.38911800	-2.25875600
Ag	-0.60453100	-0.87824400	-0.91678800
H	0.90498300	1.70292900	0.29771100
C	1.35892200	3.42317700	-0.43085600
O	2.49749000	3.12040300	-0.73111400
O	0.48437700	2.59755700	0.14234900
C	0.76659900	4.79302200	-0.66173700
H	0.47630900	5.23683500	0.29535500
H	1.49633100	5.43119400	-1.15907500
H	-0.13914700	4.71400400	-1.27014500
C	1.26461700	-1.74802300	-1.69272800
H	1.16390100	-2.44783000	-2.50469200
C	2.12913100	-1.35074100	-0.88436300
C	3.36207000	-1.17638300	-0.07517000
O	3.01907300	-1.08847600	1.30649400
C	4.18806600	-2.46257800	-0.22064800
H	4.47930700	-2.62232900	-1.26205600
H	5.09229600	-2.36443600	0.38573100
H	3.61970500	-3.32532100	0.13384800
C	4.15909700	0.05380200	-0.51673600
H	3.55691900	0.96228000	-0.45279100
H	5.03233200	0.15059000	0.13509300
H	4.50477500	-0.06464800	-1.54836100
C	1.90319800	-0.30829700	1.58034800
O	1.32554700	0.12153000	0.50489600
O	1.58478600	-0.14605100	2.74259900

Route 9	CP9-3	HF=-1177.2553664	
C	-4.75330500	-1.51777000	0.18708200
C	-4.75523400	-0.18180500	0.42876500

C	-2.66302500	-0.74841000	-0.20568400
N	-3.46682100	-1.84200400	-0.19809900
H	-5.54482700	-2.24850300	0.24896000
H	-5.55038800	0.47506400	0.74564500
N	-3.47399800	0.26728400	0.18123400
C	-3.03989900	1.65869500	0.33877500
H	-3.74790900	2.29318900	-0.20434900
H	-2.06943300	1.74073200	-0.15206200
C	-2.91504400	2.08813100	1.79244000
H	-2.49931300	3.09843700	1.82289600
H	-3.88048200	2.08502300	2.30868300
H	-2.22785600	1.42787200	2.32810600
C	-3.03554200	-3.17977900	-0.56141000
H	-3.61451300	-3.54810100	-1.41269000
H	-1.98188500	-3.13481100	-0.83828000
H	-3.15798700	-3.86326300	0.28331600
C	0.44806200	3.46634500	-0.18403000
O	-0.31768400	4.33785900	0.15767600
O	0.36732800	2.24470100	0.38063000
C	1.53232400	3.64228300	-1.22169200
H	1.40409800	2.92383500	-2.03772300
H	1.49492400	4.65683200	-1.61663000
H	2.51659700	3.45622400	-0.78013900
Ag	-0.59405300	-0.57256800	-0.66841000
C	1.41981800	-0.21751000	-1.12485600
H	1.65539700	0.18917400	-2.11277600
C	2.51851400	-0.50812400	-0.42440000
C	2.70122300	-1.14165600	0.94830000
O	4.14196700	-1.12717700	1.11056100
C	2.09291000	-0.32490700	2.08099800
H	1.00766100	-0.27290400	1.95906400
H	2.31992700	-0.78808600	3.04582100
H	2.48756300	0.69411400	2.08027800
C	2.24375500	-2.59705500	0.97869800

H	2.72711800	-3.16860900	0.18196800
H	2.49235400	-3.05234500	1.94213300
H	1.16148600	-2.64246400	0.82797100
C	4.74082100	-0.63593200	0.00940300
O	3.80885100	-0.27632900	-0.91350300
O	5.92234500	-0.52507100	-0.14396700
H	0.91899200	1.56539900	-0.07239200

	Route 9	TS9-3	HF=-1177.2373547
C		-4.42636900	-2.11815300
C		-4.66663800	-0.80410600
C		-2.48966800	-0.99678800
N		-3.08921000	-2.21377800
H		-5.08232200	-2.97441400
H		-5.57473200	-0.29594300
N		-3.47467100	-0.13756300
C		-3.29672800	1.30796100
H		-4.11236900	1.81247500
H		-2.36310900	1.60120400
C		-3.25144800	1.71269100
H		-3.01660200	2.77845300
H		-4.20038800	1.52948700
H		-2.45812200	1.17065400
C		-2.42013100	-3.45450000
H		-2.88977600	-3.90940400
H		-1.37860400	-3.22779500
H		-2.45989300	-4.15600300
C		-0.15671100	3.27783800
O		-1.24877600	3.79167400
O		0.20535700	2.12872800
C		0.87786600	3.94571700
H		1.18696600	3.26733400
H		0.47069800	4.86144600
H		1.77498400	4.18203500

Ag	-0.48168900	-0.44480100	-0.55287100
C	1.55201300	0.24365500	-1.08414900
H	1.67933000	0.18562700	-2.16811800
C	2.60681500	-0.25402500	-0.41262300
C	2.91694300	-0.24855900	1.07803300
O	4.18990800	-0.94529000	1.12648300
C	3.12399000	1.17011900	1.60146800
H	2.19136800	1.73310000	1.50988900
H	3.43345700	1.13951300	2.65008900
H	3.89889300	1.68075500	1.02317000
C	1.92470000	-1.03523200	1.92315900
H	1.80459400	-2.05146800	1.53815800
H	2.27784800	-1.08913000	2.95703600
H	0.95358700	-0.53239900	1.91106700
C	4.62508100	-1.22747000	-0.11011200
O	3.70406900	-0.80481100	-1.03748600
O	5.65105500	-1.76933800	-0.39080500
H	0.91953900	1.33690100	-0.50279400

Route 9	CP9-4	HF=-1177.283321	
C	-3.26404200	-3.21614200	-0.16222300
C	-4.25133400	-2.31922300	0.09107200
C	-2.33307600	-1.15912800	-0.16903800
N	-2.10094600	-2.48639900	-0.31647000
H	-3.29221900	-4.29111100	-0.25105300
H	-5.30566600	-2.46463400	0.26845600
N	-3.66269400	-1.07033800	0.07938100
C	-4.36585700	0.18480200	0.35486400
H	-5.29031600	0.18375900	-0.23191200
H	-3.73106900	0.99335000	-0.01788400
C	-4.65337400	0.37543100	1.83802200
H	-5.17304300	1.32541000	1.99089500
H	-5.28251600	-0.42605700	2.23806200
H	-3.72092700	0.40353000	2.40850800

C	-0.80162100	-3.06758500	-0.60897200
H	-0.83281700	-3.60618700	-1.55986400
H	-0.07117900	-2.26059700	-0.67719800
H	-0.50601600	-3.75536400	0.18769100
C	-0.50109200	3.17314200	-0.28434100
O	-1.72910500	3.05834500	-0.14312700
O	0.30793600	2.16923900	-0.39595100
C	0.15071200	4.54340400	-0.33271300
H	0.71566500	4.65291600	-1.26333900
H	-0.59953000	5.33147700	-0.26165500
H	0.86502500	4.64152000	0.49073200
Ag	-1.03631800	0.48268000	-0.28688500
C	2.17760700	-0.20314600	-1.61675900
H	1.99094300	-0.88882700	-2.43578400
C	3.06320400	-0.50415000	-0.67196000
C	3.51463200	0.30085000	0.53257800
O	4.57444400	-0.54451800	1.06087000
C	4.11012500	1.64835500	0.14873300
H	3.32004100	2.28263500	-0.26177500
H	4.53130000	2.13670100	1.03210000
H	4.89807600	1.52910300	-0.59917900
C	2.43293200	0.43690400	1.59739700
H	2.02776200	-0.54306600	1.86581600
H	2.85494600	0.89707600	2.49584600
H	1.62727300	1.06986900	1.21249200
C	4.66844200	-1.68813400	0.36718100
O	3.76631100	-1.68886700	-0.66629800
O	5.41724500	-2.59121500	0.59282600
H	1.64851900	0.74353600	-1.57734400

Route 9	CP9-5	HF=-1253.6974148	
C	-3.95991100	-1.21071700	1.94306400
H	-3.48077300	-1.32017100	2.90828400
C	-3.30927900	-1.48142500	0.81885900

C	-3.76734600	-1.39752200	-0.62556400
C	-4.90151400	-2.36596900	-0.94012100
H	-5.80679600	-2.06321200	-0.40673100
H	-5.11185500	-2.35905700	-2.01329600
H	-4.64493700	-3.38431500	-0.63624400
C	-4.05222300	0.02984100	-1.07220900
H	-3.17081200	0.64950700	-0.88219800
H	-4.29559900	0.04427800	-2.13883100
H	-4.90482900	0.42843200	-0.51424800
O	-2.57980200	-1.86194200	-1.32757800
H	-4.98203100	-0.85438600	1.90976100
C	-1.59105600	-2.10978600	-0.46879700
O	-0.48453100	-2.47634300	-0.76233500
O	-2.00849600	-1.93470200	0.81511600
C	5.12658200	-0.18255300	-0.46975300
C	4.77715400	-1.43431200	-0.07792900
C	2.88237600	-0.21595000	-0.20739200
N	3.95490100	0.54559800	-0.54077900
H	6.08997800	0.24082300	-0.70783500
H	5.37962900	-2.31235500	0.09620600
N	3.40487100	-1.43407200	0.07200800
C	2.62336400	-2.58225900	0.53653300
H	3.04153500	-3.47495700	0.06035200
H	1.60419100	-2.45694200	0.16287300
C	2.63724600	-2.71179000	2.05409700
H	2.04216300	-3.57918600	2.35400400
H	3.65239900	-2.84318300	2.44248700
H	2.20111700	-1.82330600	2.51962700
C	3.88330000	1.94124700	-0.93709200
H	4.23424800	2.06364600	-1.96539500
H	2.84337600	2.26286600	-0.87237400
H	4.49185300	2.55579200	-0.26839600
C	-1.35409600	3.96137500	0.51174200
O	-1.47041400	3.35322800	1.57218700

O	-1.15804000	3.39445400	-0.65720100
C	-1.43564300	5.47208700	0.43499300
H	-2.29087500	5.76319100	-0.18291300
H	-1.54323700	5.89453900	1.43427700
H	-0.54023900	5.87373600	-0.04864500
Ag	0.87599300	0.36616200	-0.12508600
O	-1.10089700	1.00642300	-0.07063700
H	-1.13011400	2.32329800	-0.49383000
H	-1.30475800	1.25810900	0.84449100

Route 9	TS9-4	HF=-1253.6826256	
C	-4.57075600	-2.15632400	1.60826100
H	-4.15804900	-2.98013000	2.17842900
C	-3.84465700	-1.52412500	0.68800000
C	-4.24006700	-0.35968900	-0.20849200
C	-5.35500900	-0.73291600	-1.18168600
H	-6.28555100	-0.92459400	-0.63971300
H	-5.52437200	0.08589700	-1.88735300
H	-5.08681000	-1.63036500	-1.74419600
C	-4.56806000	0.90244300	0.58583900
H	-3.71626500	1.18490200	1.20728500
H	-4.79647200	1.72566500	-0.09771700
H	-5.43699100	0.73370300	1.22865900
O	-3.04298400	-0.15297100	-0.97791200
H	-5.59889500	-1.86713300	1.78950200
C	-2.00769600	-0.88696100	-0.46522600
O	-1.02964000	-1.16937200	-1.16618600
O	-2.55908500	-1.86545000	0.39402500
O	-1.32049600	0.21572100	0.79407300
H	-1.48108500	-0.18209700	1.65932800
H	-0.79484700	1.74317100	0.84389000
C	5.00502200	0.64395400	0.23510900
C	5.10807100	-0.61957600	-0.25041300
C	2.91068400	-0.16593200	0.01587000

N	3.65774400	0.89941600	0.39396000
H	5.76370400	1.37448900	0.46933400
H	5.97449800	-1.20707200	-0.51198700
N	3.81785500	-1.09408300	-0.38192400
C	3.47346200	-2.43842300	-0.83720800
H	4.12076400	-2.67864700	-1.68701100
H	2.44622400	-2.38983700	-1.20760100
C	3.60325100	-3.48204800	0.26454600
H	3.33532500	-4.46865100	-0.12468200
H	4.62618700	-3.53429300	0.64996300
H	2.93257200	-3.24807300	1.09608700
C	3.12013200	2.17375200	0.85383600
H	3.22778600	2.93833300	0.08112500
H	2.05834000	2.06282000	1.07379300
H	3.65034600	2.48714400	1.75634700
C	-0.30367900	3.40224900	-0.11553500
O	0.52376100	4.27187900	-0.28566100
O	-0.18363500	2.53991400	0.90541200
C	-1.53141100	3.23230100	-0.98278300
H	-2.41256900	3.56917900	-0.42563700
H	-1.42735500	3.84316900	-1.87936900
H	-1.70216000	2.18614200	-1.25189700
Ag	0.80973200	-0.34278800	-0.02620300

Route 9	CP9-6	HF=-1253.6951642	
C	1.49291800	-3.92756600	-0.26536700
H	0.66462200	-4.18112900	-0.91699200
C	1.92105100	-2.66863700	-0.14272000
C	3.05886500	-2.14379500	0.72827500
C	2.68304500	-2.14559600	2.21254000
H	2.51887900	-3.16770500	2.56755600
H	3.48987000	-1.69317000	2.79737100
H	1.77361200	-1.56124400	2.36515500
C	4.37923600	-2.86255700	0.47666600

H	4.62997100	-2.84705200	-0.58693600
H	5.18177000	-2.37017600	1.03394400
H	4.31954400	-3.90402300	0.80523400
O	3.20221900	-0.80073100	0.25531500
H	1.98068600	-4.72786200	0.27772000
C	1.97172400	-0.36638900	-0.27655000
O	1.17304500	0.23630400	0.55604000
O	1.38071800	-1.62329600	-0.81350000
O	2.25527800	0.43647600	-1.39724800
H	2.94883800	-0.01573900	-1.89634800
H	2.90124900	2.12585700	-1.08927600
C	-4.81711100	-0.70882100	-1.30274500
C	-5.12911000	0.19053500	-0.33523700
C	-2.88731100	-0.07004300	-0.32063900
N	-3.44391100	-0.85509900	-1.27539600
H	-5.44446300	-1.24112100	-2.00071200
H	-6.08233800	0.58883800	-0.02400600
N	-3.93654600	0.57053200	0.24892900
C	-3.82514200	1.49259500	1.37806600
H	-4.51079300	2.32613200	1.19572900
H	-2.80786100	1.89110500	1.35623200
C	-4.11680400	0.81948100	2.71271900
H	-4.01797200	1.54655000	3.52386200
H	-5.13200500	0.41227200	2.74354000
H	-3.41165300	0.00385100	2.89519700
C	-2.69485800	-1.71961200	-2.17403100
H	-2.79036000	-1.36836200	-3.20489000
H	-1.64374900	-1.69772200	-1.88367200
H	-3.06601900	-2.74496300	-2.10182100
C	2.84984400	3.93028600	-0.39121000
O	3.38694700	5.00683100	-0.26817200
O	3.42598400	2.95332000	-1.11061900
C	1.49703300	3.59380500	0.20277200
H	1.48614600	2.59349700	0.64820200

H	1.23148200	4.35252500	0.93938400
H	0.74633500	3.60025300	-0.59663300
Ag	-0.85524200	0.08336200	0.11803500

Route 9	TS9-5	HF=-1253.682481	
C	1.72651800	-3.49226100	-0.79821600
H	0.92416500	-3.66003400	-1.50904500
C	2.04756400	-2.25395900	-0.39945600
C	3.19942400	-1.89133800	0.53708100
C	3.32809600	-2.81722600	1.73949300
H	3.58636300	-3.83170300	1.42444500
H	4.11637900	-2.45452800	2.40592700
H	2.38770600	-2.84863200	2.29370000
C	4.52003200	-1.81197300	-0.24193200
H	4.40996800	-1.21380400	-1.15312700
H	5.30315900	-1.37406300	0.38523200
H	4.83700500	-2.81049800	-0.55525700
O	2.85348500	-0.59780200	1.05764600
H	2.27454200	-4.35473800	-0.43959000
C	1.99113400	0.17245300	0.28186300
O	0.96718100	0.66622400	0.77776400
O	1.44792300	-1.12427500	-0.79540200
O	2.69677700	0.99874500	-0.59391100
H	3.59488400	0.65793800	-0.68380200
H	2.57468600	2.80655000	-0.26292600
C	-5.00715600	-0.33379300	-0.31906000
C	-4.64572000	0.46394100	0.71826100
C	-2.75507100	-0.38661900	-0.16941000
N	-3.83655900	-0.84419300	-0.84653600
H	-5.97922300	-0.56994400	-0.72336900
H	-5.24478700	1.05480900	1.39367400
N	-3.26797900	0.42028800	0.79053700
C	-2.46926500	1.11612300	1.80480400
H	-2.83388300	2.14669500	1.86209900

H	-1.43941200	1.14570900	1.44022800
C	-2.53506800	0.43120400	3.16302100
H	-1.92065300	0.98373600	3.87911300
H	-3.55786300	0.39084500	3.55118300
H	-2.14655500	-0.58901400	3.09933700
C	-3.77591300	-1.74284500	-1.98521800
H	-4.21325700	-1.26840900	-2.86773900
H	-2.72808200	-1.97075200	-2.18236800
H	-4.31212100	-2.67020900	-1.76670700
C	1.54341100	4.41383900	-0.51432400
O	1.44063800	5.61181700	-0.38634300
O	2.66066900	3.77284400	-0.13254100
C	0.46803800	3.53433700	-1.11896500
H	0.28089700	2.66383200	-0.48188700
H	-0.44036100	4.12012900	-1.26019900
H	0.80625800	3.15530100	-2.08984900
Ag	-0.69994800	-0.71433200	-0.44622200

Route 9	CP9-7	HF=-1253.7103157	
C	3.30657100	-0.58829900	-2.01232700
H	3.55021000	0.39844600	-2.39076200
C	2.23310400	-0.75729400	-1.21998200
C	1.78745000	-2.17168700	-0.79208200
C	0.82634400	-2.74410600	-1.83677600
H	1.35765500	-2.89165800	-2.77971300
H	0.41806600	-3.70196700	-1.49927800
H	-0.00677700	-2.05607300	-2.01529000
C	2.93743500	-3.14285300	-0.53726200
H	3.65949200	-2.72322300	0.16332900
H	2.53839300	-4.07640100	-0.12849900
H	3.45079900	-3.37988200	-1.47230000
O	0.94662600	-2.09804700	0.40750200
H	3.95012800	-1.41035300	-2.29840100
C	1.26103100	-1.30836700	1.44015900

O	0.40329100	-0.89419400	2.19506300
O	1.47850100	0.26441500	-0.80308700
O	2.56716500	-1.07754700	1.57139800
H	2.66835800	-0.21623300	2.02118800
H	2.17853800	1.16275800	0.28300700
C	-4.80394700	1.26863400	-0.28186600
C	-4.71592600	0.37596800	0.73698300
C	-2.65776900	0.57656500	-0.15947200
N	-3.53542700	1.37499100	-0.81787300
H	-5.64354700	1.83233500	-0.65788200
H	-5.46760100	0.00772200	1.41783400
N	-3.39872000	-0.03125900	0.79694700
C	-2.88798700	-1.03114500	1.74018400
H	-3.31927900	-0.80301600	2.72014900
H	-1.80509800	-0.89615500	1.81483800
C	-3.22454700	-2.45215200	1.30865000
H	-2.82636200	-3.15847300	2.04239000
H	-4.30485700	-2.61281300	1.23086300
H	-2.76855100	-2.67805800	0.34080100
C	-3.18865200	2.24896600	-1.92423200
H	-3.34698500	3.29503000	-1.64816200
H	-2.13561100	2.09674200	-2.16278500
H	-3.79486900	2.00791200	-2.80143400
C	3.24318300	2.69451900	0.97804000
O	3.71521400	3.27841500	1.92587400
O	2.51076900	1.58216700	1.14343100
C	3.43934500	3.12984500	-0.45938000
H	2.48922000	3.15549500	-1.00075600
H	3.91163300	4.11170600	-0.47916400
H	4.08182100	2.40694900	-0.97271200
Ag	-0.60855500	0.33382700	-0.48906500

Route 9

TS9-6

HF=-1253.6978096

C

-3.41481100

0.61973900

-1.96773200

H	-3.71610000	-0.35524300	-2.33440700
C	-2.27695200	0.76321500	-1.28636000
C	-1.71694900	2.11254100	-0.82419900
C	-0.77662400	2.66311400	-1.90247800
H	-1.34175500	2.88215700	-2.81171200
H	-0.29383300	3.57898100	-1.54915500
H	0.00387900	1.93520400	-2.15004100
C	-2.80107500	3.13328000	-0.48669600
H	-3.48526700	2.73145900	0.26074400
H	-2.32544100	4.03590600	-0.09175400
H	-3.36540600	3.41599900	-1.37950500
O	-0.84003600	1.93585700	0.32004900
H	-4.07652900	1.45554300	-2.15421900
C	-1.21147200	1.12469200	1.36546400
O	-0.31151500	0.69523200	2.07407300
O	-1.49181300	-0.33624800	-1.01192800
O	-2.48198200	0.88287700	1.46497200
H	-2.64017300	-0.20859200	1.42708300
H	-2.01146800	-0.95732800	-0.29433100
C	4.84815400	-1.30208600	-0.27401600
C	4.76954900	-0.43063700	0.76392800
C	2.70864400	-0.59618200	-0.13046100
N	3.57742100	-1.38743400	-0.80853000
H	5.68244300	-1.86389800	-0.66442400
H	5.52571200	-0.08323100	1.45073200
N	3.45593700	-0.01436000	0.83638900
C	2.95527500	0.96917700	1.80326900
H	3.38164700	0.71104800	2.77785700
H	1.86989400	0.84611400	1.87004300
C	3.31302500	2.39523200	1.40665500
H	2.92455400	3.08872100	2.15765800
H	4.39549600	2.54311000	1.33293400
H	2.86037100	2.65192600	0.44486000
C	3.22245600	-2.23196600	-1.93484700

H	3.39459400	-3.28389900	-1.69158300
H	2.16452700	-2.08357800	-2.15328500
H	3.81309500	-1.96020000	-2.81377700
C	-3.57553800	-2.30194300	0.99396400
O	-4.43254800	-2.21462900	1.85024700
O	-2.58669800	-1.42724300	0.85368000
C	-3.51923700	-3.44826000	-0.00076800
H	-2.58374400	-4.00349800	0.12369300
H	-4.36495600	-4.11854400	0.15458500
H	-3.53626000	-3.06765200	-1.02736400
Ag	0.64896300	-0.32306800	-0.43920700

Route 9	CP9-8	HF=-1253.7207518	
C	4.96905700	-0.93134900	0.23826000
H	5.64964200	-0.45680400	-0.45973600
C	3.65623400	-0.72816700	0.15475500
C	2.58142100	-1.24758600	1.10219400
C	2.97569000	-2.52205600	1.83892500
H	3.79872700	-2.31756800	2.53014500
H	2.12201700	-2.86965000	2.42880300
H	3.26706400	-3.30046700	1.13540700
C	2.23204200	-0.13547500	2.10131500
H	1.91957000	0.77214300	1.57744700
H	1.41229100	-0.46525900	2.74686400
H	3.10152000	0.09871100	2.72147100
O	1.35507600	-1.40862400	0.34755200
H	5.38176000	-1.59461300	0.98608900
C	1.27072000	-2.43438500	-0.64469600
O	2.24656000	-3.10770500	-0.91224500
O	3.14738800	0.12862200	-0.79662100
O	0.09720800	-2.47018200	-1.14371300
H	3.45974100	1.78690100	-0.87681800
H	2.17923800	0.03152100	-0.76585700
C	-5.07453300	0.82864000	0.41013600

C	-4.24212400	1.89649200	0.50534200
C	-2.97947000	0.10486900	-0.02442900
N	-4.28333000	-0.25598100	0.08632300
H	-6.14333100	0.75182200	0.53641800
H	-4.44712400	2.93077300	0.73385400
N	-2.97023300	1.43383800	0.23429200
C	-1.76704400	2.26869700	0.26393300
H	-1.95628500	3.15147300	-0.35487200
H	-0.96605500	1.70466000	-0.21517300
C	-1.36405900	2.66305500	1.67672600
H	-0.43145400	3.22928100	1.62712400
H	-2.12542400	3.27989800	2.16516400
H	-1.19251000	1.77418300	2.29031700
C	-4.78904800	-1.60297900	-0.11312500
H	-5.52943300	-1.61429200	-0.91731000
H	-3.95285500	-2.24671700	-0.38765500
H	-5.24465200	-1.97827300	0.80716300
C	2.35512300	3.31472100	-0.67735700
O	1.36004200	2.66607400	-0.39091400
O	3.53717300	2.77658200	-0.94415500
C	2.38482100	4.81858200	-0.76986800
H	2.69886300	5.12131600	-1.77289900
H	1.39943800	5.22756800	-0.54924100
H	3.12185900	5.21861200	-0.06749500
Ag	-1.36060100	-1.12588700	-0.50671100

Route 9	TS9-7	HF=-1253.7074692	
C	4.90339200	0.30730400	0.44578600
H	5.51960700	0.90099000	-0.22012500
C	3.62674300	0.05959700	0.15676500
C	2.60913000	-0.70596000	1.01284300
C	3.22565300	-1.88473200	1.76167500
H	3.95318800	-1.53215300	2.49899100
H	2.43660000	-2.42014700	2.29944800

H	3.71564200	-2.57211500	1.07329900
C	1.96985700	0.27900400	2.00309000
H	1.50174400	1.10968200	1.46578700
H	1.20473100	-0.23824700	2.59367700
H	2.72390500	0.68460400	2.68443900
O	1.55912800	-1.13184600	0.13371800
H	5.35548100	-0.08613400	1.34696000
C	1.64550700	-2.52227100	-0.90048700
O	2.76967600	-2.91379900	-1.02535500
O	3.04239500	0.57591800	-0.97409900
O	0.48927100	-2.68558600	-1.23705500
H	2.62578300	2.19399600	-1.09124800
H	2.19468200	0.07751200	-1.02136000
C	-4.81061700	-0.83891100	-0.41973600
C	-4.72505500	0.45351900	-0.01234200
C	-2.63096400	-0.38337400	-0.04985000
N	-3.52050100	-1.33113500	-0.43658900
H	-5.66367200	-1.43454500	-0.70546700
H	-5.49077000	1.20074400	0.12770100
N	-3.38563800	0.71195200	0.20285800
C	-2.85111800	1.98676900	0.68303000
H	-3.44437900	2.78156700	0.21893200
H	-1.82823000	2.07404600	0.30593500
C	-2.89044700	2.09426300	2.20207200
H	-2.48704200	3.06168700	2.51536600
H	-3.91134700	2.00927400	2.58779000
H	-2.28251300	1.30810500	2.65855900
C	-3.16385800	-2.68735400	-0.82765900
H	-3.60167200	-2.91840400	-1.80189300
H	-2.07744900	-2.76093400	-0.89972200
H	-3.52899900	-3.40391600	-0.08665100
C	1.07223900	3.29407500	-0.91627600
O	0.34636500	2.38840500	-0.53022200
O	2.35276600	3.14564600	-1.21573500

C	0.61140700	4.71670700	-1.10513700
H	0.78660500	5.02797600	-2.13884700
H	-0.44727800	4.80516900	-0.86399800
H	1.19732200	5.38257900	-0.46484700
Ag	-0.55610600	-0.65869700	0.06682400

Route 9	CP9-9	HF=-1065.1525441	
C	-2.75555900	-0.40072500	-0.66436500
C	-2.43417100	-1.57325700	0.29741800
C	-3.55866300	-1.93281900	1.26703800
H	-4.44878600	-2.28342900	0.73692500
H	-3.21569800	-2.73142500	1.93179000
H	-3.84345000	-1.07529800	1.88467000
C	-2.03342700	-2.79649500	-0.52392400
H	-1.25217500	-2.53304600	-1.24205000
H	-1.66416400	-3.58763800	0.13610600
H	-2.89454700	-3.17482000	-1.08221100
O	-1.77828600	0.00505000	-1.42182000
C	4.26264800	0.95317800	0.41086700
C	4.36943700	-0.40040800	0.40055500
C	2.27729300	0.12430700	-0.26958200
N	2.97839200	1.25101300	0.00192000
H	4.98139000	1.71599700	0.66629700
H	5.19624300	-1.04607900	0.65222200
N	3.14782500	-0.88504100	-0.02330200
C	2.80084800	-2.30298700	-0.10273400
H	3.70914200	-2.84543900	-0.38380000
H	2.08490200	-2.40884700	-0.92200700
C	2.21434100	-2.83667000	1.19816200
H	2.01640700	-3.90847800	1.09995800
H	2.90746100	-2.69364900	2.03293900
H	1.27096800	-2.33498900	1.43103100
C	2.44515800	2.60067400	-0.13866600
H	3.13910000	3.30070400	0.32954700

H	2.34088000	2.85426300	-1.19683100
H	1.47540600	2.67469500	0.35985000
C	-1.53103700	2.49123400	0.91422300
O	-0.49501400	2.78299600	1.47766400
C	-2.00047900	3.11568700	-0.37579800
H	-3.01570400	3.50898200	-0.26945000
H	-1.32235400	3.91991500	-0.66102500
H	-2.01770200	2.33772700	-1.15021300
Ag	0.25084500	-0.04861600	-0.76643500
O	-2.33740700	1.54703800	1.43016700
C	-3.98591900	0.20363200	-0.65209700
H	-3.01692300	1.24215000	0.75594300
H	-4.20593100	0.96889500	-1.39085200
H	-4.81879200	-0.20033400	-0.09030900
O	-1.26754500	-1.21806900	1.07029400
H	-1.47572200	-0.38493100	1.52657100

Route 9	TS9-8	HF=-1065.140624	
C	-2.71835700	-0.47524000	-0.77733300
C	-2.43194700	-1.61195900	0.24374400
C	-3.59821500	-1.94436700	1.17273700
H	-4.46612900	-2.31104900	0.61573500
H	-3.28286600	-2.72523700	1.87125300
H	-3.90318200	-1.07124100	1.75617700
C	-1.97558000	-2.85895800	-0.50813500
H	-1.16199500	-2.61408300	-1.19610100
H	-1.62839800	-3.61225300	0.20531500
H	-2.80079600	-3.28085500	-1.08984500
O	-1.75393500	-0.13161000	-1.52770700
C	4.28719700	1.08098000	0.35030400
C	4.43528800	-0.26841700	0.37729500
C	2.31538400	0.17414100	-0.26569700
N	2.98641300	1.32823900	-0.04022100
H	4.98689300	1.87242100	0.56902300

H	5.28531300	-0.88145700	0.63345400
N	3.22079800	-0.80143900	-0.00826100
C	2.91075200	-2.22934900	-0.03066800
H	3.83212800	-2.75970700	-0.29150300
H	2.19655600	-2.38700900	-0.84329200
C	2.34007000	-2.72475800	1.29231600
H	2.16076600	-3.80290300	1.23678100
H	3.03365200	-2.53630500	2.11753500
H	1.38962400	-2.23025100	1.51169600
C	2.41092300	2.65677400	-0.21191500
H	3.02292300	3.37559000	0.33615100
H	2.40106000	2.92935800	-1.27101800
H	1.39520800	2.67008200	0.19304300
C	-1.67973000	2.32834500	0.91808500
O	-0.48763900	2.30720900	1.21684800
C	-2.28656700	3.46496100	0.12022300
H	-3.17746500	3.85097000	0.62328600
H	-1.55903800	4.26503800	-0.02009100
H	-2.60303600	3.08731700	-0.85826500
Ag	0.27741200	-0.06758800	-0.71768700
O	-2.50968900	1.36923000	1.26387100
C	-3.90435100	0.27590700	-0.68884600
H	-3.25845800	1.01785400	0.40561500
H	-4.08550600	0.98297100	-1.49640900
H	-4.79057300	-0.17087800	-0.24838200
O	-1.31521600	-1.17928700	1.03920800
H	-1.57291200	-0.31204300	1.42008100

Route 9	CP9-10	HF=-1065.1804191	
C	2.55523800	-1.15481400	1.19626700
C	2.69141700	-1.37257200	-0.32885200
C	4.12123600	-1.09470600	-0.81530400
H	4.85737900	-1.75255400	-0.34370500
H	4.15674300	-1.26028100	-1.89579800

H	4.39383800	-0.05268700	-0.62694500
C	2.29569400	-2.83215000	-0.60207300
H	1.26296200	-3.00635500	-0.28399500
H	2.35968800	-3.01354000	-1.67869300
H	2.94857500	-3.54481900	-0.08832700
O	1.54002400	-0.67289900	1.67060000
C	-4.46000700	0.88518600	0.51245500
C	-4.55582500	-0.46007900	0.36137900
C	-2.36542600	0.09141800	0.19837900
N	-3.11881800	1.20013000	0.40727300
H	-5.21923800	1.63098700	0.69082700
H	-5.41512800	-1.11271400	0.37562500
N	-3.26705000	-0.92368200	0.17554500
C	-2.91856600	-2.31511500	-0.08775800
H	-3.51353600	-2.94480000	0.58246700
H	-1.86813700	-2.42568900	0.19271100
C	-3.13203800	-2.70565800	-1.54470200
H	-2.85853600	-3.75439600	-1.69531700
H	-4.17723200	-2.58087700	-1.84445400
H	-2.50907400	-2.08934800	-2.19884100
C	-2.58731600	2.55069300	0.53457100
H	-3.10109100	3.21267800	-0.16789100
H	-2.74333200	2.91722100	1.55345500
H	-1.51758800	2.54588600	0.30934100
C	1.76458600	2.61098400	-0.50222700
O	0.57830600	2.34269300	-0.18057800
C	2.21516400	4.06381700	-0.42825400
H	2.20724000	4.48976400	-1.43764200
H	1.54681700	4.65125800	0.20387000
H	3.24142800	4.12472400	-0.05770400
Ag	-0.24588500	0.07103700	-0.03444300
O	2.62874100	1.77920300	-0.91673600
C	3.68463300	-1.58070400	2.10490400
H	4.50729600	-0.86189000	2.01683500

H	3.33470600	-1.59252100	3.13822900
H	4.08565700	-2.56104000	1.83085800
O	1.78777500	-0.55540400	-1.02487300
H	2.14670000	0.44057500	-1.01582700

Route 10	CP10-1	HF=-1365.8065641	
C	1.01171600	4.64839000	-0.16395900
C	2.19656300	3.99164800	-0.07208700
C	0.56538200	2.43508000	-0.07988400
N	0.02795600	3.67822800	-0.16416100
H	0.79066600	5.70211700	-0.23491300
H	3.20819600	4.36543200	-0.03940500
N	1.90232100	2.64412900	-0.02635100
C	2.90469000	1.58283200	0.12674400
H	3.72318300	1.80516600	-0.56572800
H	2.44690900	0.64406600	-0.19590700
C	3.41255000	1.46817500	1.55679500
H	4.10361400	0.62483400	1.61868200
H	3.92641200	2.37790300	1.88552100
H	2.58278900	1.27242600	2.24224100
C	-1.39331100	3.95106900	-0.27242900
H	-1.63133900	4.36435400	-1.25669700
H	-1.93099100	3.01185300	-0.13864600
H	-1.70097600	4.65797300	0.50281600
Ag	-0.37538600	0.54363600	-0.10855800
C	-3.19717900	-0.68279400	-2.30682700
O	-2.63993300	0.34341800	-2.36982900
O	-3.77677500	-1.69489000	-2.28549800
H	-0.97082500	-2.00992400	0.11455300
C	-3.42691600	-0.37600200	1.48088000
C	-2.43881400	-1.46428900	1.40249000
O	-1.68083100	-1.26004000	0.20196900
C	-1.51171500	-1.42027100	2.62566200
H	-2.07449000	-1.57759900	3.55019600

H	-0.75267400	-2.20206200	2.53076300
H	-1.01119100	-0.44859200	2.68499500
C	-3.15631800	-2.81830300	1.30326600
H	-3.78440300	-2.84401800	0.41042400
H	-2.41185200	-3.61704100	1.23414500
H	-3.78145100	-2.99335700	2.18333800
C	-4.24723000	0.50783800	1.57170800
H	-4.98193200	1.27626500	1.65269300
C	3.48779500	-2.68110700	-0.18493800
O	3.61974900	-1.71596500	0.53434200
O	2.31358900	-3.12622300	-0.67113300
C	4.61358300	-3.57817300	-0.63357400
H	4.71103000	-3.52975200	-1.72241100
H	5.54446100	-3.26216300	-0.16331200
H	4.39333800	-4.61718800	-0.37405000
C	1.14321200	-2.30846400	-0.51949100
O	0.19758500	-2.92573300	0.01227000
O	1.21019800	-1.16330000	-0.98332300

Route 10	TS10-1	HF=-1365.7761935	
C	-2.89248200	3.87972600	0.10303700
C	-1.62524000	4.26593900	0.39773600
C	-1.54717500	2.08275500	-0.17256100
N	-2.82248600	2.54329600	-0.24113800
H	-3.81831500	4.43383700	0.10093500
H	-1.23397700	5.22265900	0.70742800
N	-0.82104000	3.15780600	0.21956700
C	0.62058400	3.13669900	0.48144300
H	1.04489800	4.05271800	0.05789300
H	1.04165400	2.29232000	-0.06703500
C	0.94071900	3.01999300	1.96498100
H	2.02429100	2.96218300	2.09223800
H	0.56388300	3.87602300	2.53427900
H	0.50013900	2.10886800	2.38008100

C	-3.96559800	1.74349100	-0.64281500
H	-4.41728100	2.15302400	-1.55054800
H	-3.61961000	0.72867200	-0.84142700
H	-4.71159700	1.71970400	0.15616800
Ag	-0.83679600	0.13322700	-0.61231700
C	-0.78830600	-2.70109400	-1.47382600
O	-0.88576700	-1.68200600	-2.13478200
O	-0.90264500	-3.88783500	-1.48720100
H	1.18916300	-1.92841200	0.04226300
C	-2.13647500	-2.93543800	1.24817300
C	-0.67206300	-2.77595400	1.28252600
O	-0.24317100	-2.10177200	0.08447300
C	-0.29670100	-1.87210800	2.46703400
H	-0.60791700	-2.33076300	3.41003300
H	0.78739100	-1.72650400	2.48995800
H	-0.78672200	-0.89863500	2.37464000
C	0.01633900	-4.14251300	1.41622800
H	-0.22447100	-4.77043600	0.55920900
H	1.10043500	-3.99912900	1.46313800
H	-0.30938500	-4.64101800	2.33395000
C	-3.33982400	-3.05309300	1.25875400
H	-4.39739700	-3.18721500	1.24789200
C	4.47488400	0.76035800	-0.05788200
O	3.89315100	1.64547300	0.51105700
O	3.91518400	-0.45535600	-0.36980000
C	5.91334900	0.77495800	-0.48788100
H	5.96999400	0.70211100	-1.57826500
H	6.38530900	1.69701100	-0.15088200
H	6.43764900	-0.09241100	-0.07775300
C	2.53714000	-0.60389800	-0.38139100
O	2.23376600	-1.78121600	0.06234600
O	1.79961200	0.25984600	-0.81305000

Route 10 CP10-2

HF=-1365.7891002

C	-1.23227200	4.38774500	-0.22539200
C	0.07070200	4.62836100	0.07029500
C	-0.16659500	2.39861200	-0.20434300
N	-1.35547800	3.02173500	-0.38738100
H	-2.06690300	5.06215100	-0.33837300
H	0.59018200	5.55252800	0.27144200
N	0.70448700	3.40133500	0.07293400
C	2.10819200	3.19470600	0.42526600
H	2.68145000	4.02429900	-0.00153000
H	2.42794800	2.27671200	-0.07466700
C	2.32383800	3.09180700	1.92972700
H	3.38607700	2.94120600	2.14311000
H	1.99725000	4.00081100	2.44422800
H	1.77100100	2.24265000	2.34071600
C	-2.60751600	2.35013500	-0.71044000
H	-2.94526800	2.64841600	-1.70686100
H	-2.45956400	1.27059200	-0.68489400
H	-3.36995100	2.61302100	0.02570800
C	-4.63052200	-1.45311500	0.10901500
O	-4.53828300	-0.25881700	0.22035000
O	-3.57475200	-2.32343700	0.19707900
C	-5.90260300	-2.22682800	-0.09250100
H	-6.01024300	-2.98258400	0.69028900
H	-6.75087000	-1.54356500	-0.07695500
H	-5.86403100	-2.75491400	-1.05007100
Ag	0.24211600	0.31788900	-0.24102600
C	-2.27064100	-1.85508400	0.09010000
O	-1.96714800	-1.00009400	-0.72577900
O	-1.51321400	-2.50041800	0.90573800
H	-0.49689900	-2.20093900	0.76929900
C	2.49522500	0.00902600	-2.11038600
H	2.21504100	0.78979600	-2.78090700
C	2.82194100	-0.89948200	-1.37684100
C	3.31556000	-2.02364600	-0.55618600

O	3.01576900	-1.85221500	0.83896900
C	2.77998400	-3.35882200	-1.08703000
H	3.12800700	-3.52349700	-2.11072700
H	3.15836400	-4.16572100	-0.45235300
H	1.69049500	-3.36796100	-1.07376500
C	4.85017000	-2.00770500	-0.59563500
H	5.22961000	-1.06793600	-0.18814100
H	5.22926400	-2.83168200	0.01459400
H	5.20937300	-2.12342000	-1.62140800
C	1.72260600	-1.85602100	1.32759400
O	0.78691800	-1.76011200	0.41524500
O	1.58555200	-1.93495500	2.52729100

Route 10	TS10-2	HF=-1365.7660715	
C	2.85090300	-3.81750300	-0.82907900
C	3.72474600	-2.84847100	-0.45727000
C	1.64651000	-2.07559300	-0.03388100
N	1.58818100	-3.32552800	-0.56165600
H	3.01796900	-4.79560800	-1.25299400
H	4.80259000	-2.82418700	-0.49225200
N	2.97047700	-1.79586100	0.02317900
C	3.54217700	-0.53999200	0.51733400
H	4.17897100	-0.77493100	1.37759400
H	2.71308500	0.07949000	0.86064900
C	4.31881100	0.20550700	-0.55716200
H	4.70928300	1.13245300	-0.13010800
H	5.16398700	-0.37567700	-0.94044200
H	3.65610000	0.46447200	-1.38599000
C	0.35994800	-4.04947000	-0.83208700
H	0.36821800	-5.01521600	-0.31938200
H	-0.47568900	-3.45408500	-0.46311800
H	0.23806200	-4.20943900	-1.90698800
C	2.39141800	3.57595700	0.42548600
O	2.68874500	2.72904500	1.22841900

O	1.28661100	3.53465400	-0.38067000
C	3.13543000	4.85975700	0.18425300
H	2.46913200	5.71189600	0.34468500
H	3.98928900	4.91879200	0.85819400
H	3.47112000	4.90429200	-0.85604800
Ag	0.00307100	-0.84741300	0.59969800
C	0.55383200	2.35903300	-0.52551500
O	1.09046500	1.26812300	-0.57451500
O	-0.69074900	2.66113900	-0.64797500
H	-1.28139700	1.80658300	-0.81266400
C	-1.77070800	-0.28083200	1.76650700
H	-1.62218800	-0.42622100	2.82399800
C	-2.72523600	-0.14391100	0.96943500
C	-4.07654700	-0.33969300	0.38981500
O	-4.42081200	0.68263200	-0.52784500
C	-4.14085400	-1.69812100	-0.32481500
H	-3.94185100	-2.51891300	0.37033800
H	-5.13899200	-1.82354000	-0.75375700
H	-3.40460500	-1.72464900	-1.13149900
C	-5.09446000	-0.26008100	1.53601200
H	-5.04979300	0.72099300	2.01375900
H	-6.09648100	-0.40084200	1.12246200
H	-4.90557500	-1.03529400	2.28285200
C	-3.36783400	1.18231500	-1.28411200
O	-2.21529300	0.70399700	-0.90866800
O	-3.61458800	1.98845300	-2.15065800

Route 10	CP10-3	HF=-1365.7991525	
C	-3.18704600	-3.55102000	-1.02442400
C	-3.97655300	-2.59973000	-0.46376600
C	-1.83166200	-1.98754600	-0.11009900
N	-1.88267100	-3.15820900	-0.79610800
H	-3.43855800	-4.45044700	-1.56475400
H	-5.05108000	-2.51201600	-0.41916600

N	-3.13127100	-1.65556400	0.08359700
C	-3.58592500	-0.47250800	0.81784300
H	-4.44757400	-0.06365600	0.28200800
H	-2.79161600	0.27394300	0.76412600
C	-3.93485100	-0.79203300	2.26516700
H	-4.26650900	0.11892500	2.77140900
H	-4.73669900	-1.53425900	2.33646900
H	-3.05949500	-1.17705900	2.79622700
C	-0.71729900	-3.89487800	-1.25370700
H	-0.73562000	-3.99586400	-2.34212900
H	0.17558300	-3.34032500	-0.96339500
H	-0.69090300	-4.88785900	-0.79644100
C	-2.59885300	3.77968500	-0.84592500
O	-3.33475000	2.83048800	-0.83941700
O	-1.25453500	3.71276200	-0.55286100
C	-2.96083000	5.18916900	-1.21503100
H	-2.31171300	5.54486500	-2.01987900
H	-4.00379900	5.22695200	-1.52684300
H	-2.80234800	5.84679900	-0.35504600
Ag	-0.09166300	-0.91928800	0.47383700
C	-0.76068800	2.60109500	0.10843200
O	-1.32200800	2.07496400	1.03653000
O	0.40494200	2.30533900	-0.41645100
H	0.78411300	1.49959500	0.05038800
C	1.67945300	0.08334800	0.99922600
H	1.79329700	0.55816700	1.97725400
C	2.83095100	-0.01009500	0.33248500
C	4.24207800	0.44231900	0.67999300
O	4.99818700	0.04332000	-0.49110100
C	4.35471000	1.95626000	0.82308900
H	3.76859500	2.29434500	1.68212500
H	5.39870200	2.24609700	0.97464800
H	3.97610400	2.45721500	-0.07142700
C	4.81082300	-0.29820300	1.88591600

H	4.76573200	-1.37895700	1.72911000
H	5.85263300	-0.00916400	2.05356100
H	4.22891700	-0.05542800	2.77918000
C	4.19522600	-0.55868000	-1.38894700
O	2.91607800	-0.59944200	-0.92872300
O	4.54718700	-1.00268200	-2.44319000

Route 10	TS10-3	HF=-1365.7927981	
C	-2.15648900	4.32074300	0.39180200
C	-3.15154400	3.42797700	0.62589600
C	-1.32725900	2.25064500	0.01236900
N	-1.05185400	3.58110800	0.01725200
H	-2.13986200	5.39714500	0.46479600
H	-4.17229700	3.57839400	0.94129000
N	-2.62550400	2.17392000	0.39034300
C	-3.39365700	0.93053800	0.51694500
H	-3.86252600	0.92978300	1.50598600
H	-2.68985400	0.09926300	0.47918300
C	-4.43027100	0.77163400	-0.58457000
H	-4.95271800	-0.17633200	-0.43677100
H	-5.16849000	1.58081600	-0.57930700
H	-3.94579300	0.74176500	-1.56395200
C	0.23845400	4.15691000	-0.31189500
H	0.63596700	4.71444300	0.54070800
H	0.92064900	3.34184300	-0.55604900
H	0.15010400	4.82474900	-1.17346000
C	-3.20939000	-3.35610400	0.44807600
O	-3.57249000	-2.33632500	0.98312400
O	-2.00536400	-3.52605800	-0.15605500
C	-3.99801900	-4.63694400	0.39203200
H	-3.41474000	-5.45463500	0.82433900
H	-4.93374200	-4.51441100	0.93650700
H	-4.20211600	-4.89976100	-0.65024800
Ag	-0.00207400	0.64727800	-0.44471100

C	-1.19909700	-2.39395500	-0.42653200
O	-1.68917800	-1.42823400	-0.99325800
O	0.00151100	-2.60551100	-0.05838100
H	0.69772100	-1.65092800	-0.37118200
C	1.64233400	-0.74682900	-0.85880400
H	1.84998100	-0.90809700	-1.91961100
C	2.76112600	-0.57348100	-0.13746000
C	4.22453100	-0.59443700	-0.54847900
O	4.90307800	-0.33601200	0.70515300
C	4.65887600	-1.96788100	-1.05174300
H	4.13698100	-2.20774500	-1.98179000
H	5.73652800	-1.97462900	-1.23836200
H	4.42301700	-2.74040700	-0.31566700
C	4.58003700	0.52351900	-1.52197200
H	4.31140100	1.49723100	-1.10445700
H	5.65360600	0.51455600	-1.73063600
H	4.03788200	0.38636200	-2.46128800
C	4.01449800	-0.22889100	1.70897200
O	2.74139500	-0.38064700	1.22780800
O	4.27635800	-0.02312800	2.85540500

Route 10	CP10-4	HF=-1365.8316495	
C	1.65281100	4.10386500	-0.07890600
C	0.98365900	4.10624700	1.10283600
C	0.11186800	2.46193800	-0.17105700
N	1.09948500	3.09639200	-0.84302900
H	2.46907000	4.71533100	-0.43033200
H	1.09288800	4.73247900	1.97459000
N	0.05034300	3.09172700	1.02768800
C	-0.91906400	2.77137800	2.07606700
H	-0.41270800	2.89410300	3.03870400
H	-1.16850700	1.71227200	1.96819300
C	-2.17151200	3.63401900	1.99776600
H	-2.86152600	3.35708200	2.79991100

H	-1.93418500	4.69743200	2.10102200
H	-2.68299400	3.48312100	1.04306800
C	1.59115900	2.69655000	-2.15377800
H	2.46751200	2.05303000	-2.04209300
H	0.79925000	2.14691100	-2.66389700
H	1.84080400	3.58699000	-2.73508300
C	-4.64832500	-2.28415300	-0.02598600
O	-5.05407400	-1.18053600	0.25446500
O	-3.34644800	-2.59040400	-0.20771300
C	-5.51026500	-3.50637400	-0.21459400
H	-5.17961200	-4.30715700	0.45263000
H	-6.55021200	-3.25307700	-0.01048200
H	-5.41147900	-3.87416700	-1.24018600
Ag	-1.03526300	0.80571400	-0.71638200
C	-2.42708000	-1.49881500	-0.09751000
O	-2.30850800	-0.84850000	-1.17482200
O	-1.84132500	-1.37576200	0.97374800
H	0.27152100	-2.10179700	1.07692200
C	1.23634400	-2.60237300	1.10839100
H	1.29907800	-3.56614400	1.60163700
C	2.32694300	-2.08645800	0.55981100
C	3.74346300	-2.62752800	0.48573400
O	4.43009100	-1.55803900	-0.22032500
C	4.39293000	-2.78164400	1.85543900
H	3.87541900	-3.55629100	2.42785700
H	5.44252700	-3.06931800	1.74682900
H	4.33832400	-1.84525800	2.41604800
C	3.84805900	-3.89252500	-0.35853500
H	3.40758400	-3.73502500	-1.34616200
H	4.89591200	-4.18144100	-0.47992300
H	3.31227600	-4.71114800	0.12963700
C	3.57684000	-0.57372900	-0.53625500
O	2.32587000	-0.86098900	-0.08972800
O	3.86572200	0.42851400	-1.12913600

Route 11	CP11-1	HF=-1481.2218459	
C	-4.81527600	-2.05845200	1.01330300
C	-4.77944800	-2.30911400	-0.31953200
C	-3.01434600	-0.98905800	0.16981800
N	-3.72920100	-1.25121300	1.29119400
H	-5.50569900	-2.38658600	1.77488700
H	-5.43470400	-2.89717400	-0.94333300
N	-3.67066900	-1.65019100	-0.81469200
C	-3.29854300	-1.62274000	-2.22834300
H	-3.36108300	-2.64673500	-2.61047600
H	-2.24878800	-1.32057900	-2.26789300
C	-4.17032100	-0.67828700	-3.04527800
H	-3.84926200	-0.68782700	-4.09072900
H	-5.22271500	-0.97491100	-3.01438600
H	-4.09167600	0.34568800	-2.66949600
C	-3.41481700	-0.74653600	2.61858800
H	-3.33131400	-1.57670800	3.32418200
H	-2.46377500	-0.21631400	2.57678500
H	-4.19525600	-0.06028600	2.95743400
Ag	-1.27341100	0.20264400	0.00324900
C	1.53541900	5.04626100	0.42946100
H	2.25526900	5.72889300	0.82221000
C	0.71451300	4.27808300	-0.01333600
C	-0.29522700	3.36082200	-0.56777200
O	0.03190600	2.01805900	-0.15673300
C	-1.66888600	3.67800500	0.02281200
H	-1.96402100	4.70078900	-0.22281900
H	-2.41568500	2.99013200	-0.38915400
H	-1.64685600	3.57230600	1.11011200
C	-0.30756800	3.44651100	-2.09797000
H	0.67099400	3.18154900	-2.50677400
H	-1.05737500	2.75638000	-2.49799600
H	-0.55284800	4.45991800	-2.42635200

C	1.07415000	1.11010700	2.73970800
O	2.21051100	1.26815400	2.52982500
O	-0.05818200	0.93933100	2.97497900
H	0.90828700	1.71572300	-0.53769000
C	5.51484800	-1.64171700	-0.65021700
C	4.80857400	-2.79359100	-0.47889200
C	3.36536200	-1.11038300	-0.52623400
N	4.60908200	-0.61106900	-0.68096600
H	6.57568500	-1.47562800	-0.75280200
H	5.13912000	-3.81826200	-0.41164700
N	3.48218300	-2.44797500	-0.40250100
C	2.39842800	-3.42352000	-0.18215900
H	2.69687200	-4.33139200	-0.71339700
H	1.50161600	-3.01499700	-0.64441600
C	2.16668900	-3.68704500	1.29784000
H	1.38723400	-4.44582100	1.40997800
H	3.07056400	-4.05443600	1.79242000
H	1.82999900	-2.77334500	1.79166800
C	4.97937600	0.79729300	-0.84871000
H	6.06462500	0.86223400	-0.76949800
H	4.64356300	1.15547600	-1.82093600
H	4.50549300	1.39721000	-0.07410600
C	2.08575400	-0.29247500	-0.50170500
O	2.21369500	0.86363000	-0.96388500
O	1.08084800	-0.86059900	-0.02018800

Route 11	TS11-1	HF=-1481.1868206	
C	5.58855600	-0.82590000	-0.14489000
C	5.06438700	-1.19873900	1.05026500
C	3.38614100	-0.34083900	-0.18749800
N	4.54705400	-0.30291900	-0.88551700
H	6.59593100	-0.89295000	-0.52568600
H	5.52982100	-1.64903900	1.91334700
N	3.71759500	-0.89778300	1.00171500

C	2.78982600	-1.08807400	2.11714100
H	2.97852000	-2.08135300	2.53739900
H	1.78276600	-1.09190700	1.69251900
C	2.93365100	-0.00853500	3.18215500
H	2.22211200	-0.19051000	3.99268700
H	3.93888700	0.00169500	3.61348000
H	2.73075800	0.98044700	2.76165600
C	4.69330400	0.21072700	-2.23864000
H	5.00932200	-0.58727800	-2.91520400
H	3.73001200	0.60074600	-2.56789400
H	5.43077200	1.01669400	-2.25627500
Ag	1.50129100	0.34138300	-0.79913000
C	-4.09292800	3.80109300	0.11819000
H	-5.08387500	4.02896600	-0.20510300
C	-2.95197000	3.57894100	0.44723700
C	-1.59260700	3.34122100	0.94688400
O	-0.96513300	2.22671100	0.21458500
C	-0.71134000	4.58234600	0.80919700
H	-1.12121000	5.38305400	1.43006000
H	0.29860500	4.35060500	1.16092400
H	-0.67291600	4.92095600	-0.22488700
C	-1.64593300	2.87216000	2.40556700
H	-2.25545900	1.97179600	2.51084800
H	-0.63358100	2.66820200	2.76541100
H	-2.08735100	3.65813600	3.02267500
C	-0.75575600	2.30802200	-1.33419800
O	-1.13110300	3.31406900	-1.86341500
O	-0.23937900	1.22644300	-1.68437200
H	-1.52833000	1.19847900	0.39250500
C	-4.65027900	-3.01466800	-0.47731700
C	-3.76506700	-3.97800400	-0.09513200
C	-2.76408800	-2.01306900	0.10978200
N	-4.01962900	-1.80479200	-0.34206500
H	-5.66659100	-3.09457800	-0.82991400

H	-3.87052500	-5.05053600	-0.04608700
N	-2.60426600	-3.34313300	0.26358900
C	-1.39041800	-4.05912900	0.70336800
H	-1.74295800	-4.93436700	1.25526200
H	-0.85728000	-3.40022600	1.38612000
C	-0.50900500	-4.45192500	-0.47248100
H	0.35334200	-5.01235600	-0.10112500
H	-1.04311300	-5.08697600	-1.18498500
H	-0.14378600	-3.56042500	-0.98639500
C	-4.64910300	-0.52100900	-0.67393100
H	-5.62826600	-0.73942200	-1.09930900
H	-4.74752500	0.08918600	0.22209200
H	-4.03853500	0.01575800	-1.39845000
C	-1.72386600	-0.95231900	0.38661900
O	-2.24496100	0.21158900	0.46308700
O	-0.55024400	-1.30021000	0.50330100

Route 11	CP11-2	HF=-1481.2029094	
C	-1.05165000	-4.03184000	0.92580300
C	-1.71046100	-4.28431200	-0.23443900
C	-1.91738100	-2.08370900	0.20239100
N	-1.19538800	-2.68320800	1.17664500
H	-0.50016100	-4.68792200	1.58101200
H	-1.85259400	-5.20480400	-0.77901900
N	-2.22942700	-3.07861200	-0.66181300
C	-3.06486700	-2.92402900	-1.85214600
H	-2.59690000	-3.49154500	-2.66246800
H	-3.02379000	-1.86772200	-2.12979200
C	-4.50096900	-3.37612900	-1.62290000
H	-5.08407000	-3.23727100	-2.53767600
H	-4.54933700	-4.43441200	-1.35103500
H	-4.96928000	-2.79608800	-0.82252500
C	-0.57679200	-1.98587400	2.29862900
H	0.39502800	-1.57377100	2.00777300

H	-1.23852400	-1.17987100	2.62034000
H	-0.45664600	-2.68593700	3.12721600
Ag	-2.35099400	-0.00905100	0.06501700
C	-3.92830500	1.70441100	-0.25799700
H	-4.84083400	1.27837900	-0.62109900
C	-3.00618300	2.40675900	0.13252200
C	-2.05900700	3.42869300	0.63514900
O	-0.96957300	3.63370400	-0.28335400
C	-2.80597300	4.77123800	0.60999500
H	-3.67417900	4.74019100	1.27189800
H	-2.12188700	5.55251900	0.94993100
H	-3.13179300	5.00771600	-0.40465800
C	-1.56219400	3.11194200	2.04799500
H	-1.01345900	2.17033700	2.07939500
H	-0.89950400	3.91903700	2.37148800
H	-2.40797000	3.05929400	2.73851800
C	-0.02527500	2.70343900	-0.56645500
O	-0.28402400	1.48777900	-0.10273500
O	0.94477800	3.03008000	-1.20725000
H	0.51190000	0.83053700	-0.36324700
C	5.60841000	0.33858500	-1.72993000
C	6.07150500	-0.38841100	-0.67467700
C	3.87231300	-0.19991700	-0.46241300
N	4.24849100	0.44575500	-1.58629900
H	6.13235000	0.78346000	-2.56115300
H	7.07234800	-0.69866300	-0.41826200
N	4.98691100	-0.71302400	0.09957700
C	5.08684600	-1.46549000	1.36434900
H	5.91450300	-2.16757600	1.23137300
H	4.15865300	-2.02179600	1.48083300
C	5.31295300	-0.54614800	2.55479900
H	5.42692200	-1.15071700	3.45888100
H	6.21676400	0.05831900	2.43485900
H	4.45081900	0.11028100	2.68799700

C	3.38647500	1.16369500	-2.53397600
H	4.03971200	1.72954500	-3.19865800
H	2.79717800	0.44683400	-3.10558300
H	2.70706500	1.83032700	-2.00250300
C	2.45792500	-0.30120600	0.08267000
O	1.57832400	0.02933800	-0.76722000
O	2.33500700	-0.67338400	1.25398100

Route 11	TS11-2	HF=-1481.1734269	
C	4.09195000	-1.67453300	2.04904800
C	4.92466500	-1.42539800	1.00675100
C	3.04239800	-0.22261900	0.67326000
N	2.94744600	-0.93482600	1.82260200
H	4.21911800	-2.29772300	2.92069800
H	5.91344200	-1.79891000	0.78972900
N	4.26631100	-0.53431900	0.18205100
C	4.80618600	-0.03874800	-1.08393000
H	5.85804200	0.21459500	-0.91937000
H	4.27636500	0.89065200	-1.30755500
C	4.65284800	-1.04084700	-2.22019400
H	5.07520800	-0.62565300	-3.13959600
H	5.17583700	-1.97677100	-2.00229900
H	3.59733100	-1.26566100	-2.39755100
C	1.82561900	-0.86557900	2.74678200
H	2.00777000	-0.11075800	3.51675700
H	0.91970300	-0.61321800	2.19447700
H	1.69058800	-1.83820300	3.22432100
Ag	1.63829300	1.15890900	-0.12769700
C	0.51067800	2.85087000	-0.79179900
H	1.10853700	3.50906300	-1.41746200
C	-0.66996300	3.14111200	-0.44654300
C	-1.88153700	3.97775800	-0.26417400
O	-3.04666500	3.13940000	-0.39953000
C	-1.90759600	4.65190500	1.10927800

H	-1.06026600	5.33405000	1.21491600
H	-2.83535000	5.22107600	1.21008400
H	-1.85802900	3.90698300	1.90589300
C	-1.94415500	4.99517800	-1.40593100
H	-1.96107400	4.48958500	-2.37335400
H	-2.85892000	5.58334500	-1.29854700
H	-1.08774700	5.67214700	-1.36433200
C	-2.88934400	1.88735600	0.07105600
O	-1.65181800	1.69082500	0.52059300
O	-3.78483600	1.07627700	0.04924300
C	-2.59099400	-4.50848800	-1.32262100
C	-3.52893900	-4.07504900	-0.43331200
C	-1.92011600	-2.55873100	-0.51041900
N	-1.60523600	-3.55689300	-1.36392000
H	-2.55102600	-5.40281500	-1.92438100
H	-4.46169700	-4.51994500	-0.12381000
N	-3.10201600	-2.86924800	0.05920600
C	-3.87587200	-2.07791200	1.04319000
H	-4.92267100	-2.33034600	0.85533300
H	-3.73406900	-1.02224400	0.80692700
C	-3.47539000	-2.40167300	2.47375100
H	-4.10497200	-1.82284300	3.15501900
H	-3.61044100	-3.46232500	2.70675000
H	-2.43537100	-2.12067100	2.64966800
C	-0.42826200	-3.63221900	-2.23134600
H	-0.40871800	-4.62763800	-2.67500000
H	-0.48994400	-2.86826600	-3.00543400
H	0.47525000	-3.46433700	-1.64754200
C	-1.09393200	-1.30910500	-0.31493000
O	-0.27348800	-1.03710800	-1.18692100
O	-1.36148900	-0.67710600	0.76835100
H	-1.42532100	0.56714800	0.64645300

Route 11 CP11-3

HF=-1481.2079782

C	5.34584900	-2.24459200	-0.49421600
C	4.58700100	-2.96454200	0.37008200
C	3.33775600	-1.21829500	-0.33586200
N	4.56558800	-1.18426100	-0.91144400
H	6.35405900	-2.39957800	-0.84620700
H	4.80954300	-3.86628500	0.91934500
N	3.36602100	-2.32355500	0.44910800
C	2.26904900	-2.75323600	1.31410100
H	2.16270300	-3.83723500	1.20176100
H	1.35987100	-2.29020000	0.92269200
C	2.49433000	-2.37575100	2.77272600
H	1.65227000	-2.71903600	3.38080500
H	3.40453200	-2.83326500	3.17138400
H	2.58008600	-1.29125700	2.88475600
C	5.01320600	-0.17435400	-1.85730600
H	5.26639300	-0.63788200	-2.81415200
H	4.20459000	0.54104500	-2.00874000
H	5.88811800	0.34955300	-1.46432700
Ag	1.75188100	0.16942000	-0.61166200
C	0.27179400	1.60318300	-1.01366200
H	-0.11984900	1.64718400	-2.03550700
C	0.00129400	2.72941000	-0.33626100
C	0.38910900	3.17763500	1.06531400
O	-0.41373500	4.37211900	1.23790300
C	0.00141700	2.18877100	2.15533500
H	0.55280700	1.25444700	2.01866400
H	0.24254400	2.59999400	3.13921000
H	-1.06994700	1.97465600	2.11972700
C	1.85868600	3.58364500	1.14620000
H	2.10266000	4.31116900	0.36762300
H	2.06998600	4.02984800	2.12198300
H	2.49269200	2.70329400	1.00848800
C	-1.03852100	4.69378600	0.09295500
O	-0.76419700	3.75305500	-0.86793000

O	-1.74550300	5.63849600	-0.08238100
C	-5.89832600	-1.16241400	-0.32812100
C	-5.56995400	-2.42296400	0.07789500
C	-3.70007700	-1.25545600	-0.09657700
N	-4.73402100	-0.44966700	-0.43072100
H	-6.85950300	-0.72362200	-0.54622700
H	-6.19299200	-3.28065400	0.27856300
N	-4.20976700	-2.46480400	0.21875900
C	-3.47564000	-3.68743000	0.61428900
H	-4.16828300	-4.25324900	1.24212400
H	-2.62611300	-3.37521200	1.21877400
C	-3.02315800	-4.49595000	-0.59204000
H	-2.53519000	-5.40946100	-0.24176300
H	-3.86653000	-4.78499000	-1.22545900
H	-2.30066200	-3.93250800	-1.18602400
C	-4.69046900	0.96073700	-0.84202900
H	-5.70773200	1.25743500	-1.09405400
H	-4.31181700	1.57576000	-0.02703600
H	-4.04160600	1.07764300	-1.70829900
C	-2.23964800	-0.90532300	-0.06559800
O	-1.40324100	-1.76008600	0.14874900
O	-2.06413500	0.36794600	-0.28936400
H	-1.07148200	0.67227500	-0.38910000

Route 11	TS11-3	HF=-1481.2051937	
C	4.87989800	-2.84507500	-0.50178700
C	4.05849200	-3.48384900	0.36924000
C	3.00185100	-1.60360300	-0.30323200
N	4.21673200	-1.70060100	-0.89856700
H	5.85895800	-3.10794200	-0.87148300
H	4.18706100	-4.40963000	0.90842200
N	2.91795700	-2.71182300	0.47280900
C	1.79249200	-3.02456900	1.35183800
H	1.57810900	-4.09312700	1.24643600

H	0.92948900	-2.47560700	0.96711200
C	2.07223300	-2.66551800	2.80564000
H	1.20755100	-2.91987600	3.42558900
H	2.93685300	-3.21033400	3.19581100
H	2.26752900	-1.59455100	2.91048200
C	4.75821500	-0.74037300	-1.84714800
H	4.94336300	-1.22317800	-2.80999300
H	4.03088500	0.06035800	-1.98239900
H	5.69171600	-0.31816600	-1.46670200
Ag	1.57736100	-0.04728700	-0.54789600
C	0.29590500	1.58870000	-0.96022500
H	-0.04515500	1.67541000	-1.99715100
C	0.36027400	2.79515700	-0.36810700
C	0.80844200	3.20569300	1.02711200
O	0.39560700	4.59324500	1.08360200
C	0.09844900	2.45343800	2.14356000
H	0.35248000	1.39117700	2.09439600
H	0.41070300	2.84476600	3.11538400
H	-0.98538800	2.56029400	2.05505700
C	2.32824100	3.16816900	1.17617300
H	2.81073300	3.72603200	0.36919900
H	2.61773500	3.61398900	2.13180100
H	2.67998100	2.13306100	1.14213400
C	-0.04767600	5.00589100	-0.11493100
O	-0.03746500	3.95123100	-1.00048400
O	-0.41434200	6.10432700	-0.39453300
H	-0.92886300	0.83548000	-0.28436200
C	-5.93331400	-0.62890900	-0.15506200
C	-5.69682500	-1.95168800	0.07781200
C	-3.74192600	-0.92018200	-0.03110200
N	-4.71704100	-0.00210000	-0.21860000
H	-6.86130300	-0.09242600	-0.27705400
H	-6.38119400	-2.77716500	0.19738100
N	-4.33992900	-2.11592900	0.15373800

C	-3.69694300	-3.43258600	0.35610300
H	-4.40609200	-4.01715400	0.94744700
H	-2.79648800	-3.26684100	0.94436200
C	-3.37064900	-4.11424600	-0.96405600
H	-2.94708500	-5.10098800	-0.75838500
H	-4.26381400	-4.25148000	-1.58008200
H	-2.63085200	-3.53685600	-1.52226700
C	-4.56749900	1.43896900	-0.45829800
H	-5.56207800	1.84385900	-0.64174100
H	-4.12185900	1.91715300	0.41261900
H	-3.92868900	1.60887600	-1.32315100
C	-2.25400800	-0.68431300	-0.02250200
O	-1.97604500	0.58102100	-0.06615800
O	-1.49253300	-1.63559000	0.02137700

Route 11

CP11-4

HF=-1481.2553557

C	5.34340200	0.53696700	-0.94354300
C	5.64345600	-0.23252700	0.13354900
C	3.42979100	-0.43099100	-0.24834000
N	3.98604100	0.40404600	-1.15784800
H	5.97207500	1.15164500	-1.56895400
H	6.58339400	-0.41092000	0.63247100
N	4.46126400	-0.81814400	0.54056600
C	4.33599500	-1.68569400	1.71132700
H	5.17986900	-2.38246200	1.69989300
H	3.42416100	-2.27165600	1.57001900
C	4.28495100	-0.90331200	3.01689100
H	4.19166200	-1.59449400	3.85934300
H	5.19285400	-0.31149100	3.16552600
H	3.42613100	-0.22624300	3.02961600
C	3.26992900	1.04205000	-2.25333200
H	3.54879400	2.09687100	-2.30551000
H	3.51760200	0.55563200	-3.20076100
H	2.19696100	0.96563100	-2.07345000

Ag	1.41819500	-1.00832000	-0.10803200
C	-2.37848500	2.98198600	-0.15595600
C	-1.05898300	3.57938700	0.29836600
O	-0.10737000	2.73993900	-0.42163400
C	-0.86863300	5.01591000	-0.17020100
H	-1.58959100	5.66854900	0.32927800
H	0.13899800	5.36070000	0.07677100
H	-1.01826800	5.09937100	-1.24940700
C	-0.80785900	3.39823500	1.79007200
H	-0.88515700	2.34357000	2.06283900
H	0.19000000	3.76378100	2.04751600
H	-1.54291600	3.97159800	2.36197600
C	-0.74058800	1.79934000	-1.11997500
O	-2.08948400	1.93215900	-1.00394800
O	-0.21609400	0.94353700	-1.78432700
C	-5.02551700	-1.84515900	0.84499100
C	-4.69882700	-2.60540600	-0.23723900
C	-2.85216300	-1.60691700	0.47251800
N	-3.87414500	-1.23174200	1.26996500
H	-5.97064300	-1.69972400	1.34395000
H	-5.30947600	-3.23815700	-0.86202700
N	-3.35183400	-2.45453200	-0.44974600
C	-2.62927700	-3.08056600	-1.57594100
H	-3.20272200	-3.97454400	-1.83386900
H	-1.65191400	-3.37675000	-1.19930700
C	-2.49766900	-2.13665700	-2.76235900
H	-1.99570000	-2.66256800	-3.57937300
H	-3.47561200	-1.80544200	-3.12397600
H	-1.89599900	-1.26223300	-2.50300900
C	-3.80955500	-0.31149900	2.40724600
H	-4.75139400	-0.39295800	2.95024500
H	-2.97567400	-0.57885900	3.05292300
H	-3.66098900	0.70685100	2.04787600
C	-1.42216900	-1.12583000	0.61524900

O	-1.24656000	-0.12204700	1.31182400
O	-0.57795400	-1.83125900	-0.01462500
C	-3.62621800	3.33093100	0.13320900
H	-4.46972000	2.81032400	-0.30416400
H	-3.82094100	4.16750700	0.79301400

Route O1	CPO1-1	HF=-1424.2412438	
C	1.42605000	3.17338100	1.32276200
C	0.73427900	4.15473800	0.68902000
C	-0.45363300	2.24200000	0.49817700
N	0.68487300	2.01719400	1.19390300
H	2.36857200	3.19669600	1.84674700
H	0.95737400	5.20134700	0.55107800
N	-0.41352000	3.56568100	0.19594800
C	-1.41520400	4.25696200	-0.60918800
H	-1.58297800	5.24230900	-0.16179400
H	-2.34236800	3.68611900	-0.51179300
C	-1.00833600	4.37953300	-2.07215500
H	-1.78994700	4.89866200	-2.63485700
H	-0.07690300	4.94307800	-2.18333400
H	-0.86643600	3.38911900	-2.51363000
C	1.07464000	0.73580200	1.77171500
H	0.91614500	0.75680400	2.85408800
H	0.46773900	-0.05171200	1.32276700
H	2.12750700	0.54390500	1.54727400
Ag	-1.94431000	0.86431100	-0.04917200
C	-1.85031900	-2.57068600	2.56418800
O	-2.08092600	-1.44280900	2.76608000
O	-1.62111300	-3.70523700	2.41482700
H	-1.43772800	-1.87312200	-0.19529500
C	2.85683300	-1.43712500	-0.60286700
C	1.71827600	-1.81627200	-0.78365200
C	0.33256700	-2.26994800	-0.99931300
O	-0.47487100	-1.61832700	-0.03132800

C	-0.11371600	-1.88587800	-2.42177000
H	0.50778100	-2.37195000	-3.17995800
H	-1.15292500	-2.19767800	-2.56196700
H	-0.05074800	-0.80275100	-2.55613700
C	0.25464600	-3.79473300	-0.80502100
H	0.55523100	-4.05800500	0.21145100
H	-0.77973100	-4.11798600	-0.95536200
H	0.89943400	-4.32118200	-1.51550200
C	4.19812800	-0.99684800	-0.38451100
C	5.25672000	-1.56572200	-1.11401700
C	5.64500000	0.37698200	0.74831900
C	6.55060600	-1.12096800	-0.87803000
H	5.04727200	-2.33972600	-1.84469200
H	5.76904400	1.15408400	1.50165300
H	7.38564500	-1.54528800	-1.42865600
C	6.75698100	-0.12611200	0.07535200
H	7.75048600	0.25173400	0.29509800
N	4.39361300	-0.03190800	0.53789200
C	-3.83656600	-1.41645400	-0.67441300
O	-3.70227900	-0.14892400	-0.67334200
O	-2.95058900	-2.26073400	-0.40171400
C	-5.22453600	-1.91677400	-1.03967400
H	-5.93903300	-1.58735400	-0.27871400
H	-5.54046500	-1.47445500	-1.98868000
H	-5.24143700	-3.00505300	-1.10862200

Route O1	TSO1-1	HF=-1424.2189255	
C	-0.69559800	4.12453000	-0.78396500
C	0.31554100	4.56821500	0.00680300
C	0.66070500	2.36738300	-0.37632100
N	-0.46347200	2.78258600	-1.00720600
H	-1.53993300	4.64566100	-1.20772800
H	0.52387600	5.55078600	0.40101800
N	1.13383800	3.47971500	0.24035300

C	2.33063700	3.50307700	1.07492300
H	2.90775100	4.39651700	0.81339700
H	2.92237800	2.62908300	0.79139300
C	2.00600500	3.47644400	2.56315200
H	2.93138500	3.48809200	3.14671500
H	1.40610000	4.34225800	2.86036000
H	1.45015800	2.56966300	2.81739500
C	-1.33554500	1.91130600	-1.78637400
H	-1.69193000	2.45444400	-2.66508800
H	-0.75640300	1.04690200	-2.11400300
H	-2.18382700	1.57064600	-1.18272300
Ag	1.41720700	0.38194000	-0.36525900
C	0.29933100	-2.04901800	-1.82321500
O	0.96717600	-1.18232400	-2.34696500
O	-0.49928900	-2.92161100	-1.99563400
H	2.16924900	-2.37768600	0.01263800
C	-2.58944600	-1.29667300	0.57138500
C	-1.49302600	-1.80490300	0.68730600
C	-0.15312500	-2.38819600	0.88901500
O	0.73702700	-1.90380300	-0.11712700
C	0.38633500	-1.90351100	2.24634400
H	-0.26175700	-2.23495900	3.06303900
H	1.38850700	-2.31327600	2.40462500
H	0.44267200	-0.81105800	2.26476300
C	-0.22284400	-3.92355100	0.86727000
H	-0.57779600	-4.26739000	-0.10372000
H	0.77788100	-4.32901500	1.04794600
H	-0.89348100	-4.28910700	1.65109500
C	-3.91080800	-0.76813400	0.44761900
C	-5.01189700	-1.55863400	0.82302500
C	-5.29141400	0.97129900	-0.12949900
C	-6.29026900	-1.03046800	0.70804000
H	-4.84477700	-2.56490100	1.19193400
H	-5.37094500	1.98606100	-0.51748800

H	-7.15607700	-1.62261900	0.99134400
C	-6.44091900	0.26651300	0.22160200
H	-7.42021100	0.72186500	0.11316700
N	-4.05340200	0.48672200	-0.02535100
C	3.97005100	-1.67109800	0.16460900
O	3.62737400	-0.48860800	0.13404500
O	3.14796800	-2.69048400	0.10576900
C	5.41648200	-2.07940900	0.26817900
H	5.71416800	-2.58178800	-0.65741300
H	6.04490800	-1.20383400	0.42746200
H	5.54738900	-2.79706500	1.08238300

Route O1	CPO1-2	HF=-1424.2269357	
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C	2.06821500	4.18321600	0.83706800
C	3.14256200	3.70844000	0.15488000
C	1.63294600	2.04145500	0.28495800
N	1.15613000	3.14886700	0.90236100
H	1.87578000	5.15498500	1.26447400
H	4.06609400	4.18856200	-0.12875700
N	2.85510600	2.39962400	-0.17480100
C	3.78024600	1.49857200	-0.86986900
H	4.17755400	2.03546000	-1.73737400
H	3.19377400	0.65658600	-1.24371800
C	4.89978500	1.00446000	0.03493500
H	5.50376100	0.27642400	-0.51124500
H	5.54404600	1.82279900	0.37264200
H	4.48638900	0.50234800	0.91435600
C	-0.12184100	3.21156600	1.59565800
H	-0.49315400	4.23831100	1.56562400
H	-0.84143400	2.55448500	1.09982600
H	-0.00580900	2.90478900	2.63910200
C	3.33620300	-2.41085700	-1.12965900
O	4.41936000	-2.00995600	-1.49520300
O	2.21508900	-1.79338000	-1.55473300

C	3.12581100	-3.58823400	-0.21034000
H	2.55476900	-4.36842200	-0.72554600
H	4.09286000	-3.98994800	0.09081000
H	2.54670900	-3.28589100	0.67090300
Ag	0.74524300	0.15830000	0.11892400
C	-3.21842500	-0.45276100	-0.06752900
C	-2.81608800	-1.57867300	0.14281000
C	-2.44947500	-2.98222600	0.39697000
O	-1.31257500	-3.09068000	1.27565700
C	-3.57935900	-3.64959600	1.19384200
H	-4.51069800	-3.63544500	0.62199600
H	-3.30400700	-4.68641100	1.40575100
H	-3.73287100	-3.12781900	2.14089900
C	-2.20293900	-3.72985200	-0.91898400
H	-1.41044300	-3.24385700	-1.48716900
H	-1.91164100	-4.75962500	-0.69021800
H	-3.11654100	-3.74948500	-1.52038300
C	-0.14248200	-2.42542600	1.01308500
O	-0.08027700	-1.81811400	-0.13526200
O	0.72267800	-2.47261300	1.87592100
H	1.40474600	-2.07905800	-1.06345400
C	-3.73758800	0.84227900	-0.37323200
C	-4.99170600	0.94726300	-1.00217800
C	-5.48986500	2.20550900	-1.30957700
H	-5.54704400	0.04567600	-1.23756200
C	-3.50173100	3.12320100	-0.35746100
H	-6.45532600	2.30976900	-1.79679300
H	-2.88222500	3.97757500	-0.08759600
N	-3.00022000	1.92526800	-0.05273700
C	-4.73039500	3.32640100	-0.98184100
H	-5.07629300	4.33128300	-1.20203500

Route O1	TS1-2	HF=-1424.2029315	
C	-4.95420700	-1.09445100	0.09037600

C	-4.76272000	-0.06557900	-0.77483600
C	-2.74122500	-0.64949600	0.02633600
N	-3.70584200	-1.43682800	0.56947800
H	-5.85463400	-1.60504500	0.39484100
H	-5.46722200	0.49605300	-1.36834900
N	-3.40766600	0.18735600	-0.80133600
C	-2.79142000	1.25876700	-1.59498200
H	-3.17666800	1.17627200	-2.61569700
H	-1.71854600	1.06801800	-1.63830200
C	-3.06238600	2.63862800	-1.01558100
H	-2.55287900	3.37742800	-1.63777000
H	-4.13188900	2.87301200	-0.99233100
H	-2.66718900	2.71773900	0.00141700
C	-3.46845900	-2.50184100	1.52712000
H	-3.83576300	-3.45384800	1.13459200
H	-2.39449300	-2.57786500	1.70000000
H	-3.96950400	-2.28199800	2.47377100
C	0.59145200	2.67172700	-2.12804400
O	-0.32627300	2.84123200	-2.90610900
O	0.65404500	1.54661300	-1.39906500
C	1.70969300	3.65829300	-1.90255300
H	2.67107700	3.19933800	-2.15587700
H	1.54827200	4.53836700	-2.52443000
H	1.75266300	3.93488800	-0.84231500
Ag	-0.64996100	-0.74124300	0.39260700
C	1.54602800	-1.27523200	0.51413800
C	1.58118400	-0.26583000	1.29093700
C	1.58235700	0.21468000	2.70837100
O	1.28043900	1.60837000	2.71588100
C	0.52781200	-0.47890000	3.56621100
H	0.69050100	-1.55924300	3.56918600
H	0.59060300	-0.10270000	4.59101300
H	-0.47543700	-0.26487500	3.18487200
C	2.99326900	-0.00092700	3.27863400

H	3.73408600	0.48349600	2.63969000
H	3.03828500	0.43996300	4.27868500
H	3.22679400	-1.06697000	3.34107700
C	1.69429100	2.26102600	1.56967500
O	2.21538600	1.45401000	0.69014900
O	1.51682700	3.45889200	1.47951600
H	1.37939000	1.57070400	-0.71170000
C	2.13646400	-1.79078700	-0.70249200
C	1.39817000	-2.57243700	-1.60972600
C	2.01729300	-3.03710800	-2.76255100
H	0.35899900	-2.80911900	-1.39909800
C	4.02512200	-2.00294600	-1.98803500
H	1.45959400	-3.62691800	-3.48497200
H	5.08410000	-1.77212700	-2.09975700
N	3.44392900	-1.52127200	-0.89117600
C	3.36508400	-2.75007700	-2.96430000
H	3.89490000	-3.09893800	-3.84499300

Route O1	CPO1-3	HF=-1424.2376136	
C	5.26625400	-1.14421900	0.21364100
C	5.17824300	0.20047000	0.04847600
C	3.07237300	-0.59710900	0.21606600
N	3.96962000	-1.61029000	0.31290200
H	6.12539200	-1.79414300	0.27490700
H	5.94842200	0.94757500	-0.06487000
N	3.83403100	0.51329100	0.05553300
C	3.29924900	1.86727600	-0.11698100
H	3.83850000	2.52772200	0.57008700
H	2.25394300	1.83855800	0.19489100
C	3.39146100	2.36797700	-1.55075800
H	2.89330900	3.33863800	-1.61961300
H	4.42831100	2.47957300	-1.88386300
H	2.87832800	1.68104800	-2.22914200
C	3.61579400	-3.00516400	0.50729600

H	4.06145200	-3.38504000	1.43054100
H	2.53014200	-3.07573100	0.57945200
H	3.96112200	-3.60772100	-0.33728100
C	-0.70885000	3.43323900	-0.68521000
O	-0.07674500	4.44376200	-0.87797300
O	-0.06277500	2.24653300	-0.61548100
C	-2.20831700	3.37438300	-0.51528900
H	-2.47590200	2.87438300	0.42113200
H	-2.61215000	4.38610500	-0.52293500
H	-2.66267500	2.79981700	-1.32923800
Ag	0.94779800	-0.64524300	0.26934700
C	-1.16087900	-0.49745900	0.36435500
C	-1.99888500	-0.73829800	-0.65304300
C	-1.72466200	-1.22191200	-2.07258100
O	-3.04189100	-1.17545200	-2.67400000
C	-0.81219300	-0.31858000	-2.89001200
H	0.18246500	-0.28317100	-2.43688000
H	-0.72200000	-0.70167100	-3.91071700
H	-1.20758200	0.69896000	-2.93396600
C	-1.25877300	-2.67636100	-2.08897200
H	-1.94744100	-3.30596600	-1.51955500
H	-1.20827700	-3.04464400	-3.11819100
H	-0.26835500	-2.74955300	-1.63084300
C	-3.97224800	-0.85152500	-1.75526500
O	-3.38403000	-0.61818600	-0.55189600
O	-5.14748000	-0.76916500	-1.96173000
H	-0.64705000	1.47946600	-0.42673300
C	-1.71125500	-0.22812100	1.71471400
C	-1.30792600	0.90298000	2.45087500
C	-1.82805200	1.11763300	3.72081500
H	-0.59118700	1.59630200	2.01938200
C	-3.04639800	-0.91446600	3.45932400
H	-1.53416500	1.99368500	4.29375000
H	-3.73232700	-1.67262100	3.83708900

N	-2.56849500	-1.12849200	2.23262800
C	-2.72319200	0.18855200	4.24708600
H	-3.15196000	0.30758300	5.23726300

Route O1	TS1-3	HF=-1424.2256899	
C	-4.72256200	-0.45775100	-1.99704500
C	-4.93940100	-0.57611200	-0.66264600
C	-2.80694700	0.11371600	-0.93725500
N	-3.41472300	-0.03531400	-2.14300900
H	-5.37616300	-0.63101000	-2.83796000
H	-5.82109600	-0.87372300	-0.11686800
N	-3.76126600	-0.22314800	-0.03535600
C	-3.56579000	-0.22799200	1.41792500
H	-4.31725700	0.43369400	1.86179600
H	-2.58134500	0.20130700	1.60360400
C	-3.62591500	-1.61972900	2.02684600
H	-3.34739600	-1.54257600	3.08050900
H	-4.62192300	-2.06847500	1.95019900
H	-2.90198000	-2.27925800	1.54153600
C	-2.77533100	0.21121300	-3.42170800
H	-3.33500000	0.95994200	-3.98909400
H	-1.76817900	0.58426900	-3.23305900
H	-2.71243900	-0.71207800	-4.00458300
C	-0.29836400	0.03287800	3.35213200
O	-1.25182100	-0.04531700	4.10304300
O	-0.32581400	-0.53704400	2.14640200
C	0.97874600	0.76100300	3.71613600
H	1.18802700	1.55287400	2.99016700
H	0.88203300	1.19020300	4.71321100
H	1.82844700	0.07157400	3.69160600
Ag	-0.79930500	0.69255300	-0.51168900
C	1.50156200	0.11151800	0.20873500
C	2.24352700	-0.91265600	-0.22809900
C	1.99496800	-2.40780500	-0.09634900

O	3.06666400	-2.97199400	-0.89767500
C	2.17307600	-2.89981800	1.33780100
H	1.38361700	-2.48198700	1.96684800
H	2.11604500	-3.99196400	1.37040100
H	3.14395300	-2.58958000	1.73434800
C	0.66945000	-2.85878900	-0.69320000
H	0.58658400	-2.53254400	-1.73331000
H	0.58986500	-3.94947900	-0.65561800
H	-0.15189900	-2.42022800	-0.12132300
C	3.90148400	-2.00921000	-1.32175900
O	3.45400800	-0.78533800	-0.91835300
O	4.89649800	-2.18201300	-1.96340200
H	0.43525700	-0.25425200	1.47190100
C	1.91777400	1.49522400	0.00116800
C	3.20527400	2.03096900	0.19741100
C	3.41765100	3.38793300	0.00475200
H	4.01871400	1.37269300	0.48019200
C	1.11353600	3.61187200	-0.57452900
H	4.40817900	3.81014100	0.15381500
H	0.25096000	4.19801500	-0.88342000
C	2.35611300	4.20503400	-0.39277500
H	2.48609300	5.27031400	-0.55186400
N	0.89525200	2.30943400	-0.36721300

Route O1	CPO1-4	HF=-1424.2672333	
C	4.64724800	2.05742400	1.37210300
C	5.31265700	1.03114800	0.78317100
C	3.10237300	0.61577400	0.56324000
N	3.30002000	1.78364200	1.22552200
H	5.01157100	2.94471500	1.86652900
H	6.37070000	0.85373400	0.66710400
N	4.35331600	0.16542800	0.29531100
C	4.64389100	-1.10752200	-0.37083500
H	5.37902700	-0.91212900	-1.15901100

H	3.71598900	-1.44511200	-0.84266400
C	5.14836200	-2.16370100	0.60329700
H	5.34270900	-3.09421600	0.06272300
H	6.07469100	-1.85788400	1.10076700
H	4.39338500	-2.36789100	1.36762200
C	2.23056500	2.61982900	1.73876800
H	2.34120500	3.64427800	1.37338000
H	1.28331900	2.21286700	1.38446000
H	2.23815700	2.62340000	2.83258400
C	0.56380200	-2.88686300	-1.02620100
O	1.71897700	-2.66401000	-1.42992300
O	-0.11618400	-2.08207900	-0.28376000
C	-0.14224800	-4.17367100	-1.42724100
H	-0.92110300	-3.94456300	-2.16284500
H	0.56204700	-4.87800600	-1.87200500
H	-0.63267800	-4.62814600	-0.56204700
Ag	1.33557500	-0.41656500	-0.01280100
C	-2.16509000	0.31803900	-0.38760800
C	-3.35702800	0.03751600	0.15111600
C	-3.84158100	-1.31281000	0.64074100
O	-5.15075600	-0.96842900	1.17626800
C	-4.03251100	-2.31056800	-0.49589900
H	-3.05448200	-2.56236300	-0.91369000
H	-4.50272000	-3.22260800	-0.11728900
H	-4.66086400	-1.89063700	-1.28587300
C	-2.98073300	-1.88022300	1.76141100
H	-2.87799300	-1.15756400	2.57537100
H	-3.43767400	-2.79249200	2.15609100
H	-1.98879600	-2.11831700	1.36385500
C	-5.42379900	0.32723900	0.99020100
O	-4.36048000	0.94732500	0.36680100
O	-6.42332500	0.89942500	1.30274900
H	-1.47794300	-0.52318500	-0.47421400
C	-1.64146700	1.59436200	-0.86169300

C	-2.41884600	2.74994600	-1.06129200
C	-1.81050800	3.89816800	-1.54989200
H	-3.47881100	2.73335200	-0.83849600
C	0.25126300	2.69896300	-1.59544200
H	-2.39859300	4.79701100	-1.71469400
H	1.32005800	2.63537100	-1.79429900
C	-0.44530800	3.88082700	-1.83219500
H	0.06603800	4.75388100	-2.22529500
N	-0.31496200	1.58720300	-1.12340200

Route N1	CPN1-1	HF=-1747.5022426	
C	-2.90550100	-1.44922900	-2.39182300
O	-3.07726700	-0.93672900	-1.26317900
O	-1.89981900	-2.15212800	-2.74527400
C	-3.96051600	-1.26027600	-3.47347400
H	-4.40743400	-2.22992600	-3.71401200
H	-4.74317100	-0.57425100	-3.14580600
H	-3.49414600	-0.88858200	-4.39021500
Ag	-0.50092100	-2.46408600	-1.16793100
C	5.90386200	-0.15442600	2.29951200
H	6.20943000	-0.29182400	3.31160500
C	5.55770800	0.00270600	1.15048400
C	5.14456000	0.20063300	-0.25815600
O	3.82437300	0.71694300	-0.31641500
C	6.04708100	1.26153400	-0.89806700
H	7.09606900	0.95630100	-0.85998500
H	5.75311300	1.39866900	-1.94243500
H	5.93760600	2.21292700	-0.37174900
C	5.25095400	-1.12942200	-1.01982800
H	4.59179600	-1.88094400	-0.57784600
H	4.95021100	-0.97138700	-2.05880100
H	6.27431200	-1.51573000	-0.99704000
C	2.53527000	1.35047200	-2.71186500
O	1.76592500	1.99393000	-2.11134100

O	3.27063200	0.73697900	-3.37857000
H	3.17518700	0.03228000	-0.02577500
C	-1.34098600	-0.09592200	1.43501900
C	-3.04334500	1.72026700	1.69942500
C	-1.52048100	1.61348500	-0.28705600
C	-0.69243800	2.26369700	1.99146700
C	-1.41544200	-0.58233900	2.87819900
C	-1.46182100	-2.11563100	2.92329900
C	-1.42096400	-2.65802000	4.34946200
C	-4.16790400	0.80816800	1.22785000
C	-5.52918200	1.43794400	1.54437900
C	-6.69297500	0.52317500	1.17127100
C	0.76352200	2.26116400	1.54759500
C	1.61351200	3.03934900	2.56169300
C	3.02999100	3.30187700	2.05679000
C	-1.82023700	3.02270200	-0.77907900
C	-1.65516800	3.09261700	-2.30277500
C	-1.95580900	4.48207700	-2.85870800
H	-0.34075100	-0.26534000	1.02423600
H	-2.04173800	-0.63221100	0.78789600
H	-2.99192200	1.73003200	2.79164600
H	-3.22598600	2.75040200	1.38536200
H	-2.17630100	0.87556800	-0.76068100
H	-0.49505000	1.33260000	-0.53812600
H	-0.77609800	1.94487400	3.03426400
H	-1.10037200	3.27747900	1.93257000
H	-0.54607000	-0.23275100	3.44915600
H	-2.30600500	-0.19563100	3.38979200
H	-0.63260500	-2.53061500	2.33899300
H	-2.37808100	-2.45611600	2.42404000
H	-0.49682600	-2.36596400	4.86112900
H	-2.26166000	-2.28665700	4.94734100
H	-1.46868700	-3.75101400	4.35361200
H	-4.09294500	0.58785700	0.15749300

H	-4.09842600	-0.16218000	1.73237000
H	-5.62405300	2.39030800	1.00508200
H	-5.58649900	1.68668500	2.61343600
H	-6.67365700	0.27528700	0.10516400
H	-6.65076300	-0.41874400	1.72855200
H	-7.65464000	0.99733500	1.39010200
H	0.86351400	2.72987400	0.56302500
H	1.15751300	1.24411000	1.44447500
H	1.65077800	2.47711600	3.50449700
H	1.12503600	3.99589400	2.79785900
H	3.64172900	3.77154800	2.83343700
H	3.01632600	3.97236400	1.19070300
H	3.51933000	2.37695800	1.73945800
H	-1.15267500	3.75928100	-0.31390000
H	-2.84717100	3.32007300	-0.53414000
H	-2.32045500	2.35480800	-2.76809700
H	-0.63363800	2.80041400	-2.56888200
H	-1.83688400	4.50406500	-3.94612500
H	-1.28036700	5.23485800	-2.43702000
H	-2.98238300	4.79187200	-2.63168800
N	-1.64760100	1.38071200	1.21355000
C	1.72799800	-2.14099000	0.69809100
O	0.86095000	-3.02183300	0.38723400
O	1.75951800	-0.97503100	0.22992000
C	2.74796500	-2.58469800	1.73433300
H	3.50903500	-1.82416300	1.91320900
H	2.23028100	-2.80741700	2.67308400
H	3.22027500	-3.51588300	1.40939700

Route N1	TSN1-1	HF=-1747.467408	
C	-2.25654400	-2.92792500	-1.20068900
O	-2.29620700	-1.94303600	-0.42141700
O	-1.20212600	-3.54671100	-1.54636100
C	-3.56081900	-3.47390300	-1.76631200

H	-3.95656600	-4.22722200	-1.07597500
H	-4.30487400	-2.68001700	-1.86175300
H	-3.39505000	-3.95781000	-2.73043100
Ag	0.48290600	-2.58968900	-0.56627100
C	3.73194200	1.86329600	1.63759600
H	3.53865500	2.09188400	2.66060600
C	3.95573400	1.57875600	0.48301700
C	4.33320200	1.23289600	-0.90257800
O	3.51619300	0.16964400	-1.41869000
C	4.19758400	2.44716100	-1.82635400
H	4.87169300	3.24323900	-1.49798900
H	4.47241300	2.14805700	-2.84220400
H	3.17449400	2.82199900	-1.82750700
C	5.78454500	0.72378200	-0.90873000
H	5.87976800	-0.16489800	-0.28223500
H	6.06583200	0.46593400	-1.93376200
H	6.45872400	1.50025400	-0.53624100
C	1.75871400	0.31445500	-1.67279200
O	1.38024300	1.38069500	-1.26020600
O	1.46157400	-0.72122100	-2.19582900
H	3.67523400	-0.76271500	-0.83355700
C	-1.14764300	0.44985300	1.32401300
C	-3.45714100	1.42963300	1.24035600
C	-1.94966100	1.40029200	-0.76439500
C	-1.54562100	2.92424800	1.19540000
C	-0.94160400	0.46082100	2.83292300
C	-0.26286400	-0.84266300	3.27640200
C	0.07039100	-0.84498200	4.76581000
C	-4.27436400	0.26566400	0.69510100
C	-5.53123400	0.05884400	1.54834400
C	-6.44322900	-1.02664500	0.98271100
C	-0.13864300	3.32873800	0.78681700
C	0.20876500	4.69705900	1.38704400
C	1.56260000	5.21533400	0.90841400

C	-2.73578600	2.42033200	-1.57511000
C	-2.62767400	2.09573900	-3.07030000
C	-3.36992000	3.10218400	-3.94528600
H	-0.18499600	0.54346100	0.81598200
H	-1.59106300	-0.48879500	0.97907000
H	-3.39055600	1.37414300	2.32956900
H	-3.94699100	2.37796700	1.00151100
H	-2.28250900	0.37627400	-0.96208000
H	-0.88729200	1.44548400	-1.02046800
H	-1.64983100	2.93240200	2.28430400
H	-2.26713600	3.64422400	0.79959700
H	-0.31649600	1.31097300	3.13473700
H	-1.89088600	0.55702500	3.37538200
H	0.64589400	-1.01152100	2.68679500
H	-0.92857900	-1.68330100	3.04431000
H	0.76789000	-0.03869700	5.02070100
H	-0.82688400	-0.71366600	5.38224100
H	0.53793300	-1.78949000	5.05950600
H	-4.57755100	0.47879600	-0.33705600
H	-3.69330900	-0.66207200	0.64306500
H	-6.09108800	1.00144300	1.63089600
H	-5.23350800	-0.20920100	2.57111800
H	-6.79731000	-0.76374700	-0.02005900
H	-5.91560400	-1.98258000	0.90687400
H	-7.32233200	-1.17519800	1.61724200
H	-0.05480500	3.37925800	-0.30280900
H	0.60522800	2.59257900	1.10596700
H	0.20652600	4.62588200	2.48342100
H	-0.57388800	5.42438900	1.12899600
H	1.81050600	6.16851100	1.38565400
H	1.56153900	5.37466100	-0.17503600
H	2.36176500	4.50189600	1.13230300
H	-2.35073600	3.43424100	-1.40706700
H	-3.79500600	2.43025600	-1.28839500

H	-3.02019400	1.08709100	-3.24959200
H	-1.56919300	2.06473600	-3.35641700
H	-3.28005200	2.84284100	-5.00429700
H	-2.96959200	4.11417800	-3.81726600
H	-4.43784300	3.13389900	-3.70123600
N	-2.02492300	1.56016600	0.74697700
C	3.25271900	-2.19340400	0.84044300
O	2.00666600	-1.99104500	0.89035500
O	4.03708900	-1.77458400	-0.06165100
C	3.88602300	-2.96192200	1.98492300
H	4.07241000	-2.26624400	2.81065500
H	3.20821300	-3.73759800	2.34686100
H	4.84056900	-3.39479900	1.68176200

Route N1	CPN1-2	HF=-1747.4940086	
C	1.45696100	-3.33497300	0.72965800
O	2.70481800	-3.17704100	0.53735500
O	0.58467400	-2.45930800	0.49522400
C	1.01809300	-4.69764400	1.24486100
H	0.12183700	-4.60507100	1.86203700
H	0.77234200	-5.33638900	0.38935100
H	1.81915100	-5.18065600	1.80708400
Ag	2.77243300	-1.07351400	-0.17894200
C	5.21485600	-0.25425600	0.05217400
H	5.67701900	-1.18767900	0.29158600
C	4.77392800	0.85083500	-0.19964100
C	4.34161300	2.23590500	-0.48040800
O	3.07729100	2.52876700	0.13706500
C	5.31595500	3.18551600	0.23137100
H	6.33144200	3.05045700	-0.14950300
H	4.99870500	4.21635200	0.05224200
H	5.30888700	2.99799500	1.30720500
C	4.32145400	2.51889900	-1.98672100
H	3.62780800	1.84958900	-2.49365900

H	4.00410200	3.55424200	-2.14343100
H	5.32328000	2.39186200	-2.40681400
C	1.91584200	1.86291100	-0.20448700
O	2.01635800	0.92085900	-1.07636000
O	0.90611400	2.25387500	0.37337100
H	0.61868500	0.63397300	-1.79153800
C	-2.40441100	0.17516700	2.19686300
C	-2.21131200	1.59952100	0.14547900
C	-4.35944900	0.49386900	0.78776000
C	-2.42817300	-0.82913000	-0.09578200
C	-0.90842200	0.01047700	2.42603200
C	-0.61727500	-0.06685900	3.93006100
C	0.87399800	-0.22963000	4.21491400
C	-2.52899200	2.92279200	0.82798900
C	-1.86436500	4.07629400	0.06483400
C	-2.12911700	5.43125400	0.71553400
C	-3.10765200	-2.15520600	0.21649800
C	-2.51152200	-3.26004700	-0.66582000
C	-3.20457900	-4.60362300	-0.45749300
C	-5.03708100	0.73632700	-0.55361500
C	-6.56137200	0.74542200	-0.39178800
C	-7.28631700	1.02307500	-1.70641300
H	-2.94778800	-0.69738600	2.57060300
H	-2.78088800	1.04626100	2.74073100
H	-1.13131200	1.43649500	0.13717400
H	-2.52616500	1.61075900	-0.89908600
H	-4.58357800	1.31174100	1.47719000
H	-4.73810700	-0.42334200	1.24511300
H	-1.34871400	-0.92408000	0.03074800
H	-2.59894600	-0.54547700	-1.13675000
H	-0.53350100	-0.89991100	1.94370300
H	-0.35080800	0.85050000	1.99610300
H	-1.16959000	-0.90762900	4.37265400
H	-0.98875500	0.84003300	4.42752200

H	1.26476500	-1.14138300	3.75197100
H	1.44326700	0.61539700	3.81381200
H	1.06827500	-0.28668700	5.29059700
H	-3.61059100	3.10706300	0.87794100
H	-2.15225200	2.92761900	1.85788100
H	-2.23395200	4.08507200	-0.96924700
H	-0.78787200	3.88327700	0.01428400
H	-3.20147900	5.65484700	0.76662800
H	-1.73305900	5.46437100	1.73662900
H	-1.64969700	6.23718000	0.15147600
H	-4.18872400	-2.10068000	0.03314700
H	-2.97120900	-2.43467500	1.26907200
H	-1.44366900	-3.33921900	-0.43339500
H	-2.58391200	-2.95794800	-1.71758700
H	-2.75974400	-5.37651000	-1.09188200
H	-4.27213700	-4.55089100	-0.70251300
H	-3.11943400	-4.94181400	0.58183000
H	-4.75502100	-0.03609100	-1.27747300
H	-4.71670600	1.69528700	-0.97540900
H	-6.84667700	1.50201600	0.35162800
H	-6.89098200	-0.22059000	0.01339800
H	-8.37142200	1.02064400	-1.56648900
H	-7.04505300	0.26632500	-2.46034700
H	-7.00514600	1.99931200	-2.11558700
N	-2.85387500	0.36114100	0.75835200
C	-0.50993100	-0.56016200	-2.89847100
O	-0.31396200	0.52913100	-2.16376300
O	-1.63106800	-0.85360300	-3.27739700
C	0.70207500	-1.41793500	-3.18201000
H	1.58380300	-0.81420000	-3.41295300
H	0.91987000	-2.00837300	-2.28337400
H	0.48379800	-2.09906600	-4.00472700

Route N1

TSN1-2

HF=-1747.4686364

Ag	-3.09695900	1.49341700	-0.37606000
H	-0.68585900	-1.09076900	-1.53389900
C	-0.12232700	-1.77540200	-3.25618400
O	-0.97020300	-2.64223700	-3.32757800
O	0.02750600	-0.94135400	-2.22736400
C	0.89704800	-1.51551900	-4.34121800
H	1.91089300	-1.60734100	-3.93963700
H	0.75724000	-2.22676500	-5.15460600
H	0.78681100	-0.49420500	-4.71782500
C	-4.47602200	-0.17423300	-0.61454500
H	-5.48054300	0.20250300	-0.72701500
C	-3.93332400	-1.27270000	-0.37216600
C	-3.74820300	-2.69855000	-0.00284300
O	-2.66336800	-2.81827600	0.92061300
C	-4.99995200	-3.14841900	0.76083300
H	-5.88703900	-3.07034400	0.12714500
H	-4.87421300	-4.19215500	1.06140300
H	-5.14118800	-2.53764800	1.65515500
C	-3.49401500	-3.57290200	-1.23246900
H	-2.62141000	-3.22755400	-1.79067300
H	-3.33108400	-4.60329100	-0.90199100
H	-4.36184000	-3.55308300	-1.89883600
C	-1.58529300	-2.00912900	0.63402000
O	-1.79043900	-1.19329600	-0.33255000
O	-0.58372100	-2.14878000	1.33305800
C	2.29837300	-1.31348200	0.66484400
C	2.46390200	0.71897600	2.12414000
C	2.03962100	0.89686600	-0.33959800
C	4.27161900	0.21540500	0.58373000
C	2.86552400	-2.27527500	1.69953900
C	2.35015100	-3.69531200	1.42970800
C	2.86226800	-4.70293700	2.45521500
C	1.00465200	0.70828200	2.55266700
C	0.88730400	1.18936800	4.00426300

C	-0.56540000	1.23346700	4.47218300
C	4.83426700	-0.27610000	-0.74261000
C	6.35726700	-0.10274600	-0.77740400
C	6.97252100	-0.59485000	-2.08501900
C	2.46749000	2.34118900	-0.55355000
C	1.79473600	2.89724400	-1.81412400
C	2.17760700	4.34937700	-2.08494900
H	2.55262900	-1.64296700	-0.34492900
H	1.20577000	-1.30584900	0.73775000
H	3.08283300	0.15885000	2.83179000
H	2.84585000	1.74377000	2.09744300
H	0.97803000	0.86669700	-0.08787300
H	2.16839200	0.30955900	-1.25043700
H	4.70612100	-0.35383200	1.40871800
H	4.54135400	1.26196200	0.74174000
H	3.96395900	-2.28721100	1.69168400
H	2.55180100	-1.97943700	2.70745000
H	2.65894800	-4.00743100	0.42254300
H	1.25526600	-3.67273500	1.43216600
H	3.95780900	-4.75069900	2.46564000
H	2.53068100	-4.44212100	3.46633800
H	2.48873700	-5.70787200	2.23662500
H	0.41599100	1.37353300	1.91076800
H	0.57031300	-0.29447700	2.46688900
H	1.33209900	2.18983600	4.10030100
H	1.46751100	0.53058500	4.66616600
H	-1.15672100	1.90653500	3.84341500
H	-1.02539900	0.24121600	4.41798200
H	-0.63897000	1.58352400	5.50673600
H	4.39279400	0.27695100	-1.57927800
H	4.59408500	-1.33423400	-0.89603800
H	6.80627700	-0.64373600	0.06610500
H	6.60767000	0.95613400	-0.62994600
H	8.05788100	-0.45806300	-2.08550100

H	6.56840300	-0.04921900	-2.94450600
H	6.77165500	-1.65997800	-2.24314800
H	3.55544900	2.43522600	-0.66596000
H	2.15554100	2.95279700	0.29893600
H	0.71147100	2.81356600	-1.68530500
H	2.06781300	2.27628500	-2.67818300
H	1.68589200	4.72309600	-2.98834700
H	3.25933700	4.46428200	-2.22427200
H	1.87780000	4.99698400	-1.25433400
N	2.77217500	0.13051500	0.75654500
C	-1.34074900	3.61020600	0.41984400
O	-0.54318200	2.64660700	0.43864900
O	-2.55676100	3.55058800	0.04311000
C	-0.86984300	4.99425300	0.85206500
H	-1.59539800	5.43989400	1.53752900
H	0.11217100	4.94931100	1.32657200
H	-0.81575600	5.64724900	-0.02517600

Route N1	CPN1-3	HF=-1747.5055141	
C	0.50766700	2.58231800	-1.05776100
O	-0.59471700	3.09251100	-0.99431800
O	0.70062200	1.36691800	-0.53295700
C	1.70396000	3.25897300	-1.67806900
H	2.26761600	2.58073700	-2.32369300
H	1.37308300	4.13081600	-2.24149800
H	2.38572800	3.59002200	-0.88739400
Ag	2.16765500	-1.72766100	-0.03888300
C	4.10104500	0.52878400	-0.89118900
C	4.86890000	0.68686300	0.41263900
O	5.78112000	1.77517700	0.10548200
C	3.99992900	1.11480100	1.58634100
H	3.26129200	0.33607900	1.79552500
H	4.61477200	1.26952600	2.47769800
H	3.47167400	2.04473100	1.35973500

C	5.70476600	-0.54815200	0.73725600
H	6.34163600	-0.81492700	-0.11038900
H	6.33759500	-0.35726200	1.60918500
H	5.04262300	-1.39196100	0.94964900
C	5.69714300	2.11260800	-1.19319000
O	4.73899400	1.37029600	-1.81353100
O	6.35716400	2.95062800	-1.73657300
C	-2.71072400	-0.10898800	1.44531900
C	-3.52708700	1.69275700	-0.11076700
C	-4.54892300	-0.59081000	-0.06785100
C	-2.27377400	-0.17327700	-1.03125200
C	-1.56058200	0.75582200	1.93556800
C	-1.18748300	0.33092100	3.36136400
C	-0.05646700	1.17726500	3.93919800
C	-4.45287900	2.33878300	0.90974600
C	-4.57623200	3.84242800	0.63373900
C	-5.49438900	4.54755300	1.62849100
C	-2.02252900	-1.65773200	-1.24442400
C	-1.00858500	-1.84453900	-2.38113700
C	-0.69188400	-3.31529900	-2.63842600
C	-5.30357700	-0.47737600	-1.38594100
C	-6.52389100	-1.40601600	-1.37963200
C	-7.33363500	-1.32013000	-2.67080500
H	-2.37809000	-1.15096800	1.42273600
H	-3.56287800	-0.02615400	2.12705600
H	-2.54254700	2.17110900	-0.12487300
H	-3.94143900	1.81125300	-1.11518000
H	-5.19226200	-0.27558100	0.75738700
H	-4.26877800	-1.62919500	0.12411100
H	-1.34391500	0.33561400	-0.77039400
H	-2.65219400	0.28969800	-1.94745700
H	-0.68860300	0.63341500	1.28915000
H	-1.82440800	1.82001900	1.93321800
H	-0.89108100	-0.72282500	3.33461600

H	-2.06957200	0.40574400	4.01416200
H	0.84563400	1.09621600	3.32446500
H	-0.33018400	2.23763200	3.98986000
H	0.20116600	0.85171700	4.95190800
H	-5.45372700	1.88958400	0.87550000
H	-4.07381400	2.19447600	1.92762500
H	-4.95180300	3.99593300	-0.38653200
H	-3.57827800	4.29681500	0.66098000
H	-6.50960100	4.13625300	1.59743200
H	-5.12479500	4.44273200	2.65436800
H	-5.56339400	5.61711800	1.40941500
H	-2.94626300	-2.18673700	-1.51282700
H	-1.61074700	-2.10810200	-0.33407200
H	-0.08358900	-1.31452900	-2.12303100
H	-1.38971100	-1.37976400	-3.30169700
H	0.02382900	-3.42419200	-3.45896600
H	-1.59337600	-3.87892500	-2.90616500
H	-0.25291200	-3.78054000	-1.75026000
H	-4.65751800	-0.74212300	-2.23029500
H	-5.64265100	0.55187400	-1.55290800
H	-7.16679700	-1.15747600	-0.52486600
H	-6.19130400	-2.44012500	-1.22165400
H	-8.19516100	-1.99347500	-2.64007800
H	-6.72692700	-1.59674300	-3.53972900
H	-7.71091200	-0.30541100	-2.83809100
N	-3.27160500	0.20751000	0.05915200
C	3.05452900	-0.23642600	-1.21111800
H	1.60066200	0.96769200	-0.67991500
H	2.79021600	-0.16861700	-2.27123400
C	0.27704300	-3.24802500	1.62477800
O	-0.48005000	-2.26368700	1.47705900
O	1.43521000	-3.38074800	1.10482300
C	-0.16812100	-4.41801400	2.49508400
H	0.50962000	-4.51565900	3.34887600

H	-1.18827000	-4.27639100	2.85636500
H	-0.10025900	-5.35096300	1.92798100

Route N1	TSN1-3	HF=-1747.4915672	
C	0.29566300	2.22835000	-1.59965200
O	-0.81994800	2.73504700	-1.48877500
O	0.69940300	1.25015200	-0.82901700
C	1.26598600	2.71064500	-2.66318100
H	1.52105300	1.89025700	-3.34157100
H	0.81918000	3.52852800	-3.22853700
H	2.20203100	3.04593800	-2.20746500
Ag	2.10551700	-1.51858400	0.07470400
C	4.11869500	0.51550700	-0.85842100
C	4.49852300	1.23392800	0.43063400
O	5.88004200	1.60244800	0.18021500
C	3.69260600	2.51290400	0.63159500
H	2.62806600	2.27446600	0.69438500
H	4.00688600	3.01696100	1.54984800
H	3.84627600	3.19588800	-0.20822400
C	4.48024100	0.33875700	1.66403000
H	5.05358000	-0.57587400	1.49227100
H	4.91351300	0.87407300	2.51405700
H	3.45066100	0.06255000	1.90939900
C	6.27151300	1.18997400	-1.03461400
O	5.23678000	0.54483600	-1.66420400
O	7.35081200	1.34942800	-1.51919600
C	-2.59378800	0.05699700	1.46687400
C	-3.56399100	1.63015600	-0.23867600
C	-4.48905300	-0.66748000	0.12396300
C	-2.28082500	-0.28650700	-1.00032900
C	-1.49440900	1.05533000	1.79913000
C	-0.94955000	0.75238000	3.20090500
C	0.11758100	1.75301200	3.63575400
C	-4.49232700	2.34553400	0.73212200

C	-4.64302300	3.81766800	0.32919400
C	-5.57851900	4.58792200	1.25721600
C	-1.97460800	-1.77515900	-1.05012900
C	-1.01750300	-2.05455800	-2.21680400
C	-0.61161300	-3.52381600	-2.29822100
C	-5.30197900	-0.73248000	-1.16098500
C	-6.48397100	-1.69632400	-1.00298600
C	-7.34826600	-1.77608300	-2.25862500
H	-2.18919400	-0.95715900	1.53302200
H	-3.41454700	0.14927100	2.18520300
H	-2.59709900	2.13477500	-0.34321800
H	-4.00751100	1.62170400	-1.23778300
H	-5.10645800	-0.27601800	0.93631500
H	-4.16229500	-1.66642600	0.42322700
H	-1.36228100	0.28613700	-0.85159900
H	-2.72151700	0.04871600	-1.94364300
H	-0.68034000	0.99933800	1.06999500
H	-1.87313500	2.08417500	1.77642300
H	-0.53840500	-0.26268000	3.19796800
H	-1.77388600	0.76278600	3.92905600
H	0.96769400	1.74482500	2.94586500
H	-0.27492400	2.77618600	3.66321800
H	0.49716200	1.51560800	4.63469500
H	-5.48620600	1.87943400	0.74638200
H	-4.10452800	2.29605300	1.75594500
H	-5.01596100	3.87678700	-0.70173000
H	-3.65340900	4.29030900	0.31990800
H	-6.58662800	4.15822900	1.25622300
H	-5.21367000	4.57556400	2.29017300
H	-5.66423200	5.63424000	0.94933200
H	-2.88402300	-2.37211400	-1.19750500
H	-1.49373600	-2.09894600	-0.12009800
H	-0.12231900	-1.43185600	-2.09637400
H	-1.48345700	-1.74454700	-3.16284500

H	0.05883700	-3.70010200	-3.14514900
H	-1.48509400	-4.17379500	-2.42615700
H	-0.08916100	-3.83657900	-1.38845200
H	-4.67927300	-1.06509800	-1.99887100
H	-5.68663000	0.25985100	-1.42391500
H	-7.10165400	-1.38122000	-0.15135000
H	-6.10642000	-2.69631600	-0.75253700
H	-8.18228400	-2.46994100	-2.11832800
H	-6.76779600	-2.12453800	-3.11960500
H	-7.76940000	-0.79799100	-2.51546400
N	-3.24168800	0.18348200	0.08855600
C	2.94533100	-0.01070700	-1.26351200
H	1.75965500	0.68176600	-1.00390800
H	3.01039400	-0.40283100	-2.28283200
C	0.45962700	-3.10246800	1.82820900
O	-0.30482800	-2.12542200	1.67035600
O	1.59959300	-3.24166500	1.26795100
C	0.05078300	-4.24531800	2.74767900
H	0.78858400	-4.35326900	3.54830000
H	-0.93545500	-4.06959600	3.18024100
H	0.04830200	-5.18602800	2.18906100

Route N1	CPN1-4	HF=-1747.5175256	
C	-0.21488800	2.67404700	-1.42491200
O	-1.41944200	2.91551000	-1.20273700
O	0.42692400	1.63432100	-1.05035300
C	0.58562000	3.72306300	-2.20687600
H	1.16205600	3.24797000	-3.00773800
H	-0.07285800	4.48354600	-2.63102700
H	1.29856400	4.21597700	-1.53546200
Ag	2.20295900	-1.10041000	0.27646800
C	3.97202800	0.26132700	-1.08970700
C	4.31063400	1.56696300	-0.39442500
O	5.62046700	1.25670900	0.15393700

C	4.48327400	2.68583100	-1.42233900
H	3.51198000	2.94459500	-1.84958700
H	4.90475200	3.56683300	-0.93113800
H	5.15553300	2.37946000	-2.22883000
C	3.36128800	1.95345800	0.72419400
H	3.36885400	1.19422200	1.51258800
H	3.66462200	2.90886000	1.16158400
H	2.34751600	2.04719900	0.31442300
C	6.09340900	0.11782300	-0.36675900
O	5.11988500	-0.46816400	-1.16503500
O	7.17133000	-0.35766500	-0.19823100
C	-2.43216200	-0.11117200	1.34546700
C	-3.80727700	1.28068300	-0.23317600
C	-4.25391500	-1.15684700	0.12192300
C	-2.24177400	-0.34196900	-1.13978400
C	-1.51285700	1.06799700	1.62527100
C	-0.82754300	0.85841100	2.98061700
C	0.03872800	2.04894600	3.38290600
C	-4.77026700	1.79176000	0.82830800
C	-5.23045400	3.21123900	0.47315600
C	-6.19633600	3.79218500	1.50221900
C	-1.71305600	-1.76243500	-1.27443900
C	-0.74606900	-1.82983600	-2.46297300
C	-0.11255200	-3.20984400	-2.61815200
C	-5.15338200	-1.33458400	-1.09390500
C	-6.10216200	-2.52170900	-0.89347000
C	-7.05529500	-2.71582400	-2.07006600
H	-1.84991400	-1.03788600	1.35145600
H	-3.19796900	-0.18634700	2.12456000
H	-2.95515400	1.95707400	-0.39949800
H	-4.32555600	1.19624300	-1.19228500
H	-4.85919600	-0.91110000	0.99817600
H	-3.72472100	-2.08603600	0.34806200
H	-1.41817000	0.37398900	-1.02370200

H	-2.79180500	-0.05239200	-2.03961900
H	-0.76046200	1.17684800	0.83488300
H	-2.07418400	2.00824500	1.64874200
H	-0.21626000	-0.04940900	2.92731700
H	-1.58326400	0.68122000	3.76022700
H	0.80791200	2.24568900	2.62972500
H	-0.55988500	2.96100600	3.48611900
H	0.54153700	1.86898800	4.33850700
H	-5.65302000	1.14405000	0.91716700
H	-4.29267400	1.81310700	1.81472100
H	-5.70825600	3.20154700	-0.51544500
H	-4.34984800	3.85724600	0.37638100
H	-7.10144600	3.18074400	1.59258700
H	-5.73426300	3.84891300	2.49404900
H	-6.50663700	4.80394100	1.22413600
H	-2.52470400	-2.48184400	-1.44651500
H	-1.17794600	-2.07333200	-0.37054300
H	0.03076100	-1.06922500	-2.32394800
H	-1.27471500	-1.55847600	-3.38726200
H	0.58328500	-3.23591700	-3.46300500
H	-0.87150200	-3.98104900	-2.79343500
H	0.43992800	-3.49052700	-1.71494200
H	-4.55717400	-1.49960200	-1.99834100
H	-5.74757900	-0.42971100	-1.26600200
H	-6.68152400	-2.37465900	0.02777600
H	-5.51363800	-3.43591800	-0.74137500
H	-7.71837500	-3.56989200	-1.90363800
H	-6.50656500	-2.89759300	-3.00048700
H	-7.68372700	-1.83166700	-2.22274900
N	-3.19514300	-0.08521600	0.02407000
C	2.81747400	-0.10412100	-1.70276100
H	1.97510100	0.60234900	-1.71444500
H	2.82464200	-0.97026400	-2.35986000
C	1.06801000	-2.61793400	2.17297500

O	0.26904500	-2.11933300	1.32155100
O	2.31091200	-2.39373200	2.16143600
C	0.50015600	-3.49651400	3.27085900
H	1.28583900	-4.08957300	3.74007000
H	0.04048000	-2.86019500	4.03483500
H	-0.28020000	-4.14828400	2.87083000
