

## **Supporting Information**

### **Mechanism of Phosphine-Catalyzed Novel Rearrangement of Vinylcyclopropylketone to Cycloheptenone: A DFT Study**

Yong Wu,<sup>†,\*</sup> Mingzhen Li,<sup>†</sup> Lu Jin,<sup>‡</sup> and Xiang Zhao<sup>†,\*</sup>

<sup>†</sup> Department of Chemistry, Institute for Chemical Physics, School of Science, Xi'an Jiaotong University, Xi'an 710049, China.

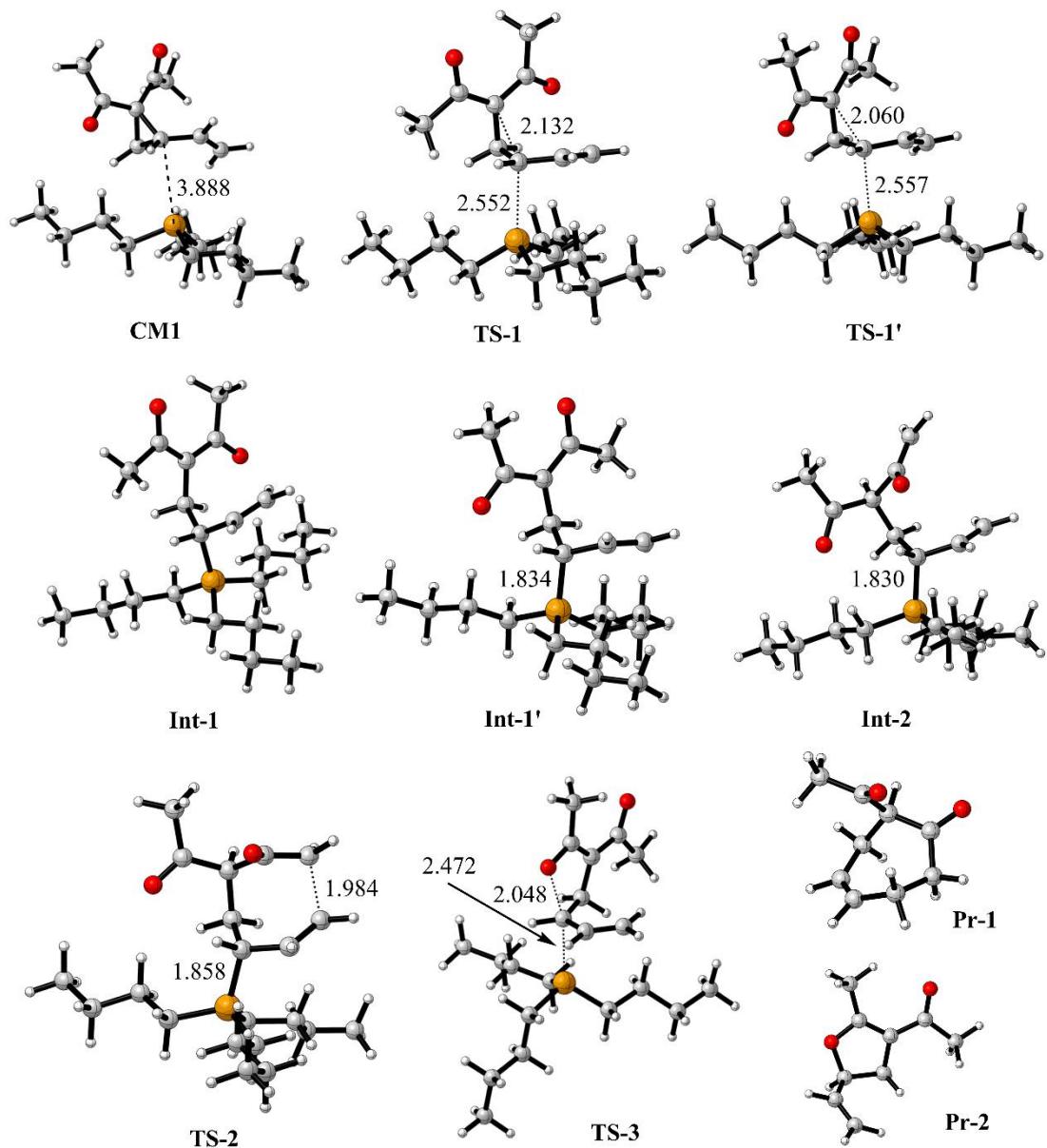
<sup>‡</sup> College of Chemical Engineering, Xinjiang Agricultural University, Urumchi, 830025, China.

# Content

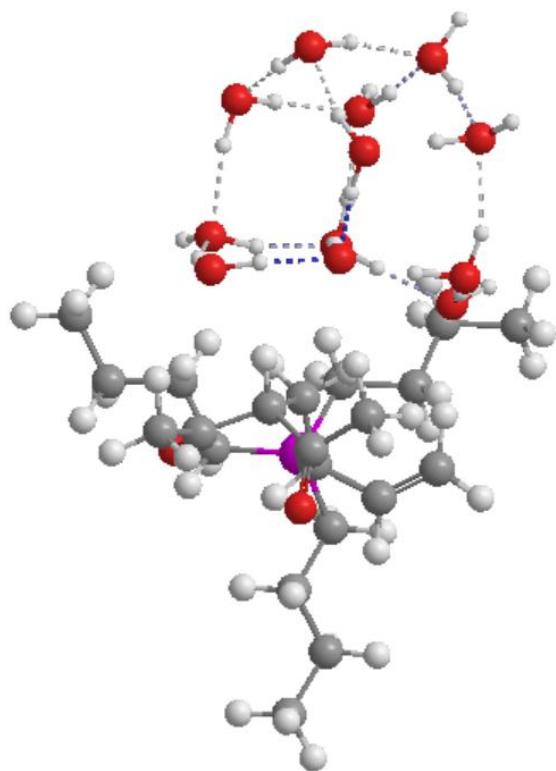
Content.....	2
1. Optimized structures.....	4
Figure S1. Optimized structures (bond length in Å) in route 1.....	4
Figure S2. Optimized water-assisted zwitterionic intermediate.....	5
Figure S3. Relative energies (in parenthesis) and Gibbs free energies (kcal/mol) for the two-water assisted tautomerism. Underlined values are obtained at the ωB97XD/6-31+G(d,p) level. ....	6
Figure S4. Optimized structures (bond length in Å) in channel 2 of route 3.....	7
Figure S5. Optimized structures (bond length in Å) for uncatalyzed reaction in channel 1 of route 3.....	8
Figure S6. Optimized structures (bond length in Å) in route 2.....	9
Figure S7. Optimized structures (bond length in Å) in channel 3 of route 3.....	10
Table S1 Selected Wiberg bond index (WBI) in some optimized geometries.....	11
Table S2. Calculated entropies (cal/(mol K)) and relative entropies <sup>a</sup> .....	12
Table S3. Calculated $\Delta E^\ddagger$ , $\Delta H^\ddagger$ , $\Delta S^\ddagger$ , and $\Delta G^\ddagger$ with (in parenthesis) and without BSSE at 383.15 K.....	12
Table S4. Scanned results at the ωB97XD/6-31+G(d,p) level.....	13
Table S5. Comparative studies on the step from Int-1' to TS-2.....	14
2. Optimized coordinate.....	15
2.1 Reactants and tautomers.....	15
Re-1.....	15
Re-2.....	15
Tau-1.....	16
Tau-2.....	16
2.2 Route 1.....	17
CM1.....	17
TS-1.....	19
TS-1'.....	20
Int-1.....	22
Int-1'.....	23
Int-2.....	25
TS-2.....	26
TS-3.....	28
Pr-1.....	29
Pr-3.....	30
2.3 Channel 2 in route 3.....	30
TS-4.....	31
TS-4' .....	32
Int-3.....	34
Int-3' .....	35
TS-5.....	37

TS-5'	38
Pr-2	40
Pr-2'	40
2.4 Channel 1 in route 3	41
TS-6	41
TS-7	42
2.5 Route 2	42
TS-8	42
Int-4	44
Int-5	45
TS-9	47
2.6 Channel 3 in route 3	48
TS-10	48
Int-6	50
TS-11	51

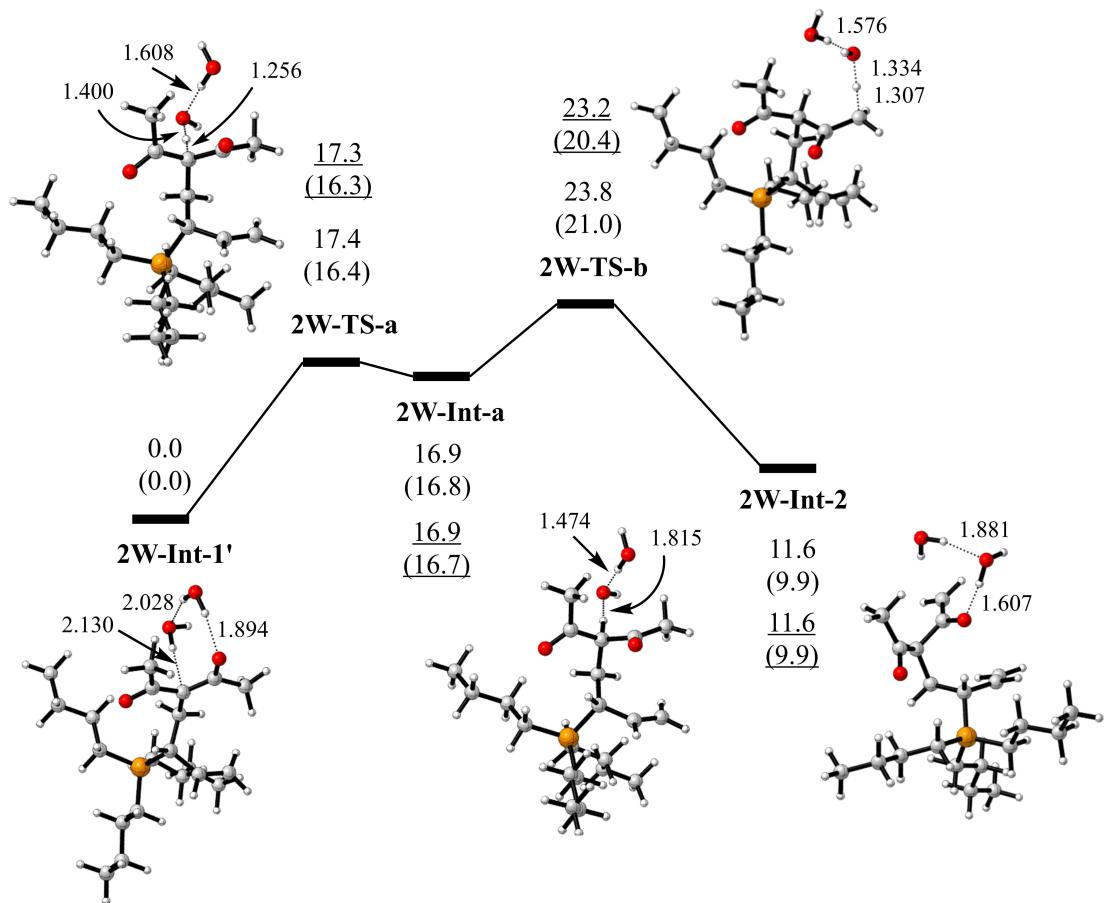
## 1. Optimized structures



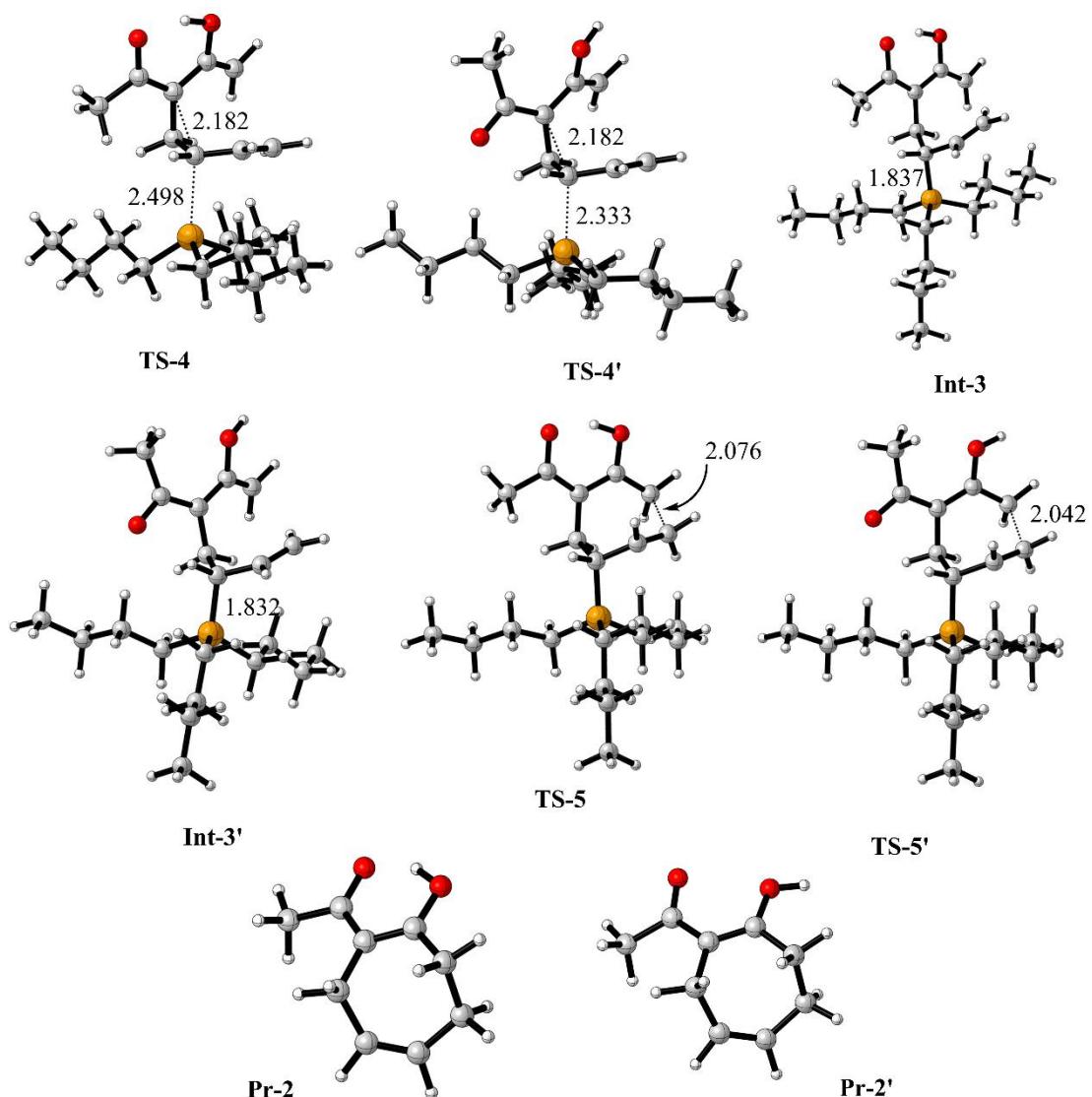
**Figure S1.** Optimized structures (bond length in Å) in route 1.



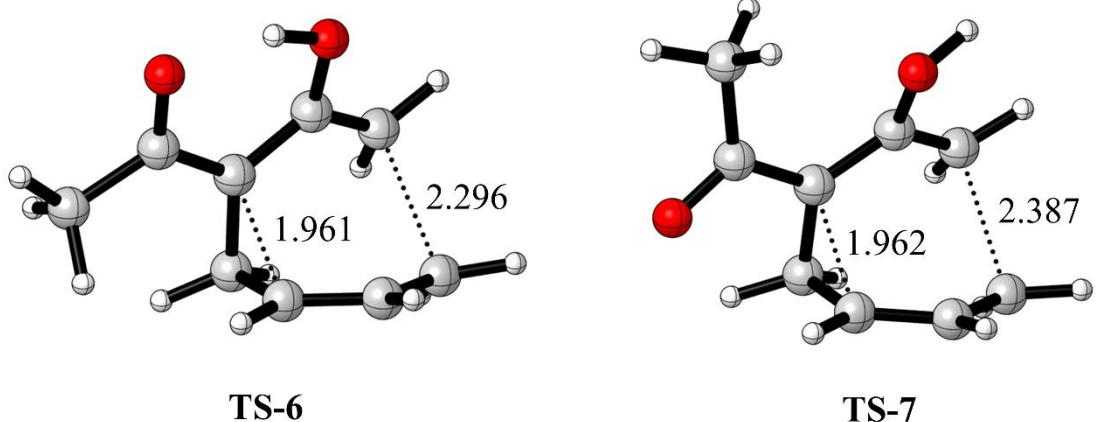
**Figure S2.** Optimized water-assisted zwitterionic intermediate.



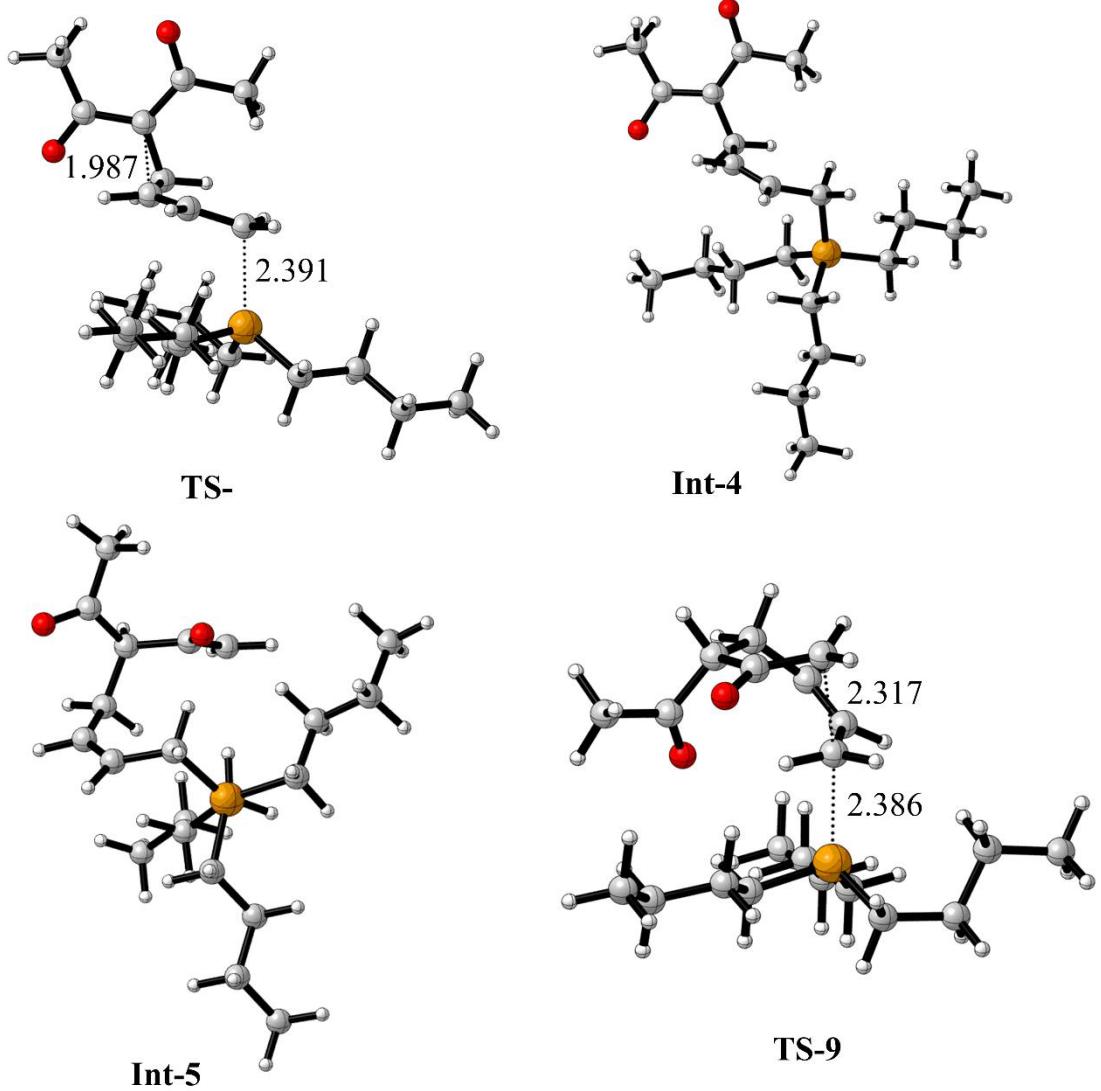
**Figure S3.** Relative energies (in parenthesis) and Gibbs free energies (kcal/mol) for the two-water assisted tautomerism. Underlined values are obtained at the  $\omega$ B97XD/6-31+G(d,p) level.



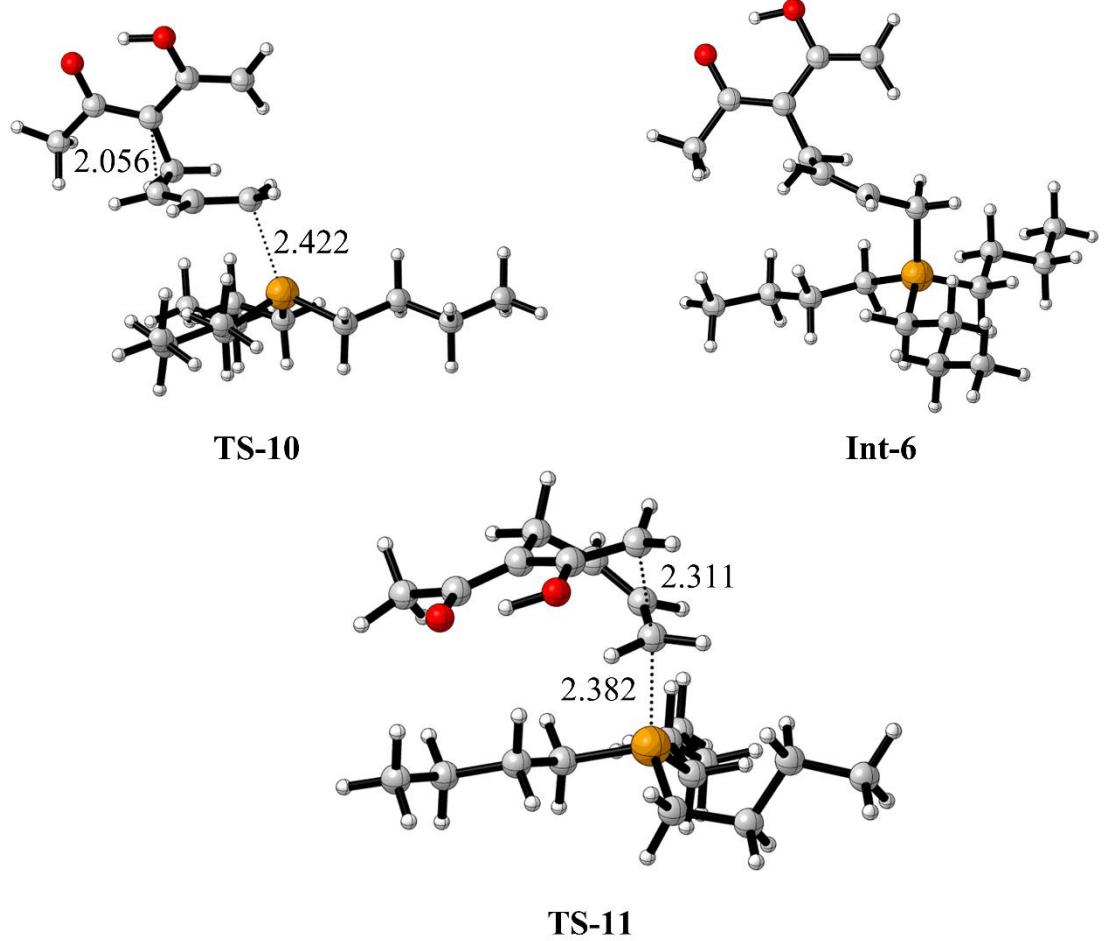
**Figure S4.** Optimized structures (bond length in Å) in channel 2 of route 3.



**Figure S5.** Optimized structures (bond length in Å) for uncatalyzed reaction in channel 1 of route 3.



**Figure S6.** Optimized structures (bond length in Å) in route 2.



**Figure S7.** Optimized structures (bond length in Å) in channel 3 of route 3.

**Table S1** Selected Wiberg bond index (WBI) in some optimized geometries.

	C1-C2	C2-C3	C3-C5	C1-C7	C3-P
<b>Re-1</b>	1.9682	1.0257	0.8786	-	-
<b>Tau-1</b>	1.9586	1.9586	0.8575	-	-
<b>TS-1</b>	1.8500	1.1352	0.2664	-	0.3700
<b>TS-1'</b>	1.8972	1.0945	0.3133	-	0.3620
<b>Int-1'</b>	1.9742	1.0056	0.0185	-	0.9116
<b>Int-2</b>	1.9640	1.0065	-	0.0037	0.9100
<b>TS-2</b>	1.4304	1.0223	-	0.5066	0.8984
<b>TS-4</b>	1.8262	1.1474	0.2296	-	0.3979
<b>Int-3</b>	1.9676	1.0087	-	0.0067	0.9114
<b>TS-5</b>	1.4961	1.0141	-	0.4455	0.9113
<b>TS-6</b>	1.5546	1.3738	0.3925	0.2973	-
<b>Pr-1</b>	1.0268	1.0268	-	1.0032	-
<b>Pr-2</b>	1.0271	1.9391	-	1.0161	-

**Table S2.** Calculated entropies (cal/(mol K)) and relative entropies <sup>a</sup>.

	$S_{\text{trans}}$	$S_{\text{rot}}$	$S_{\text{vib}}$	$S_{\text{total}}$
<b>Re-1</b>	42.214	30.847	46.338	119.399
<b>Cat</b>	43.063	34.39	78.579	156.032
<b>CM-1</b>	44.735	36.832	161.573	243.14
<b>TS-1</b>	44.735	36.668	156.874	238.277
<b>TS-1'</b>	44.735	36.651	156.332	237.718
				-37.15 <sup>b</sup>
$\Delta S^{\ddagger}(\text{TS-1})$				(-18.58) <sup>c</sup>
				[-17.15] <sup>d</sup>
				-37.71 <sup>b</sup>
$\Delta S^{\ddagger}(\text{TS-1'})$				(-18.86) <sup>c</sup>
				[-17.71] <sup>d</sup>

a. Relative to the sum of Re-1 and Cat.

b. Uncorrected values.

c. Scaled by the factor of 0.5.

d. Subtracted by 20 cal/(mol K) from uncorrected values.

e. Discarding the contribution of the translational motion.

**Table S3.** Calculated  $\Delta E^{\ddagger}$ ,  $\Delta H^{\ddagger}$ ,  $\Delta S^{\ddagger}$ , and  $\Delta G^{\ddagger}$  with (in parenthesis) and without BSSE at 383.15 K.

	<b>CM-1</b>		<b>TS-1</b>		<b>TS-1'</b>		
$\Delta E^{\ddagger}$	-2.87	(-2.21)	13.98	(14.64)		14.91	(15.57)
$\Delta H^{\ddagger}$	-3.63	(-2.97)	13.22	(13.88)		14.15	(14.81)
$\Delta S^{\ddagger}$	-32.29	-37.15 <sup>a</sup>	-18.58 <sup>b</sup>	-17.15 <sup>c</sup>	-37.71 <sup>a</sup>	-18.86 <sup>b</sup>	-17.71 <sup>c</sup>
$\Delta G^{\ddagger}$ <sup>d</sup>	8.75	(8.09)	27.46	(21.0)	20.34	(20.45)	19.79
					28.60	(29.26)	21.38
					(22.04)	(21.60)	20.94

a. Uncorrected values.

b. Scaled by the factor of 0.5.

c. Subtracted by 20 cal/(mol K) from uncorrected values.

d.  $\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger}$

**Table S4.** Scanned results at the  $\omega$ B97XD/6-31+G(d,p) level.

Angle (C3-C5-C4)	Energy (hartree)	$\Delta E^b$ (kcal/mol)	Charge(C3)	$\Delta q(C3)^b$	Charge(C1)	$\Delta q(C1)^b$
62.3 <sup>a</sup>	-500.4590932		-0.26614		-0.43361	
65	-500.4583294	0.48	-0.25224	0.0139	-0.43069	0.0029
66	-500.4577193	0.86	-0.24500	0.0211	-0.42815	0.0055
67	-500.4569726	1.33	-0.23794	0.0282	-0.42593	0.0077
68	-500.4560989	1.88	-0.23116	0.0350	-0.42387	0.0097
69	-500.4551194	2.49	-0.22447	0.0417	-0.42191	0.0117
70	-500.454042	3.17	-0.21742	0.0487	-0.41964	0.0140
71	-500.4528845	3.90	-0.21004	0.0561	-0.41687	0.0167
72	-500.4516618	4.66	-0.20216	0.0640	-0.41362	0.0200
73	-500.450396	5.46	-0.19237	0.0738	-0.40855	0.0251
74	-500.4490948	6.27	-0.18384	0.0823	-0.40451	0.0291
75	-500.4477597	7.11	-0.17412	0.0920	-0.39908	0.0345
76	-500.4464105	7.96	-0.16511	0.1010	-0.39424	0.0394
77	-500.445044	8.82	-0.15661	0.1095	-0.38935	0.0443
78	-500.4436608	9.68	-0.14833	0.1178	-0.38465	0.0490
79	-500.4422631	10.56	-0.13927	0.1269	-0.37983	0.0538
80	-500.4408568	11.44	-0.13105	0.1351	-0.37447	0.0591
81	-500.4394443	12.33	-0.12291	0.1432	-0.36897	0.0646
82	-500.4380313	13.22	-0.11479	0.1514	-0.36304	0.0706
83	-500.4366205	14.10	-0.10689	0.1593	-0.35737	0.0762
84	-500.4352082	14.99	-0.09916	0.1670	-0.35164	0.0820
85	-500.4337981	15.87	-0.09133	0.1748	-0.3456	0.0880
86	-500.4324003	16.75	-0.08367	0.1825	-0.3393	0.0943

*a.* Bond angle in the optimized geometry Re-2.*b.* The difference is relative to Re-2.

**Table S5.** Comparative studies on the step from **Int-1'** to **TS-2**.

Method	$\Delta E^\ddagger$ (kcal/mol)	$\Delta G^\ddagger$ (kcal/mol)	$\Delta S^\ddagger$ (cal/mol K)	C3—P <sup>b</sup> (Å)	C1—C7 <sup>b</sup> (Å)
B3LYP	19.0	20.1	-2.69	1.935	1.946
B3LYP-D3	19.3	21.7	-6.33	1.893	1.899
cam-B3LYP	21.5	23.4	-5.08	1.865	1.965
cam-B3LYP-D3	21.8	24.9	-7.89	1.857	1.948
M06	17.6	19.3	-4.43	1.859	2.006
M06-D3	17.9	19.7	-4.77	1.861	1.997
M06-2X	19.8	21.5	-4.45	1.869	1.958
M06-2X-D3	19.9	21.5	-4.10	1.869	1.957
PBE0	15.7	17.6	-4.87	1.873	1.979
PBE0-D3	15.9	18.9	-7.98	1.866	1.953
LC- $\omega$ PBE	20.0	22.2	-5.81	1.837	2.013
$\omega$ -B97XD	19.9	22.8	-7.53	1.858	1.984
B2PLYP-D3 <sup>a</sup>	19.7	22.5	-	-	-

a. At the B2PLYP-D3/6-31+G(d,p)// $\omega$ B97XD/6-31+G(d,p) level including the solvent effect using C-PCM solvent model.

b. Structural parameters in **TS-2**.

## 2. Optimized coordinate

### 2.1 Reactants and tautomers

#### Re-1

E(RwB97XD) = -500.460499331

C	-0.46403700	-0.98216500	1.22046700
C	-0.75177600	-1.19807300	-0.21734300
C	0.31391000	-0.16075300	0.19663500
H	-1.18978100	-0.45094400	1.82684200
H	0.10476700	-1.74545400	1.74004100
H	-0.28703700	-2.07599500	-0.66152600
C	1.74351300	-0.60185100	-0.01261100
C	-0.02650300	1.28908200	-0.05095600
O	0.36359800	1.82782200	-1.07269800
O	2.01161600	-1.79186200	-0.00638100
C	-2.00955800	-0.75666200	-0.87853800
C	-3.18216200	-0.58741800	-0.26824500
H	-3.30585400	-0.76675700	0.79691200
C	-0.84594200	2.03823700	0.96633300
C	2.82174600	0.43731400	-0.17230400
H	2.73013000	1.21745700	0.58985700
H	3.79539400	-0.04699100	-0.09857900
H	2.71930400	0.92709700	-1.14407600
H	-0.41444400	1.92310500	1.96539900
H	-0.89532000	3.09194700	0.69160600
H	-1.93175900	-0.58270300	-1.95034200
H	-4.06127900	-0.27187200	-0.82069900
H	-1.86097800	1.62716300	0.99657900

#### Re-2

E(RwB97XD) = -500.459093226

C	-0.20395500	-1.25624300	1.06472100
C	-0.53272600	-1.25302600	-0.38569800
C	0.33981200	-0.12166000	0.22340900
H	-0.96763200	-0.96147700	1.77629700
H	0.49356700	-2.00179100	1.42900700
H	0.02902800	-1.94141100	-1.01165100
C	1.80188500	-0.07700600	-0.10411200
C	-0.35986500	1.22161600	0.36461200
O	-0.95490600	1.49970800	1.38822400
O	2.36062400	0.98751100	-0.31595400

C	-1.88239400	-0.94086100	-0.93003600
C	-3.00537000	-0.82643400	-0.22151800
H	-3.02616900	-0.96450200	0.85560600
C	-0.33224600	2.15255800	-0.81663800
C	2.60235400	-1.36060700	-0.09300400
H	2.06605900	-2.22159000	-0.49702800
H	3.52364000	-1.20229900	-0.65362500
H	2.86546200	-1.59185300	0.94502100
H	-0.45639000	1.59739100	-1.75075000
H	-1.11810900	2.90140100	-0.71073800
H	-1.91850200	-0.79642700	-2.00848900
H	-3.94635500	-0.58675400	-0.70553800
H	0.64469100	2.64153000	-0.85668100

### Tau-1

E(RwB97XD) = -500.439141637

C	-0.27570700	-1.20212900	1.10564100
C	-0.52362700	-1.24416900	-0.36290900
C	0.30737800	-0.08477200	0.27407500
H	-1.10272400	-0.93656700	1.75334400
H	0.39974700	-1.93367800	1.53451200
H	0.08512300	-1.94439300	-0.93115600
C	1.75568100	-0.11688600	-0.12201500
C	-0.31061000	1.28252200	0.32636700
O	-0.15489600	2.03530600	-0.80049100
O	2.22888100	0.79614200	-0.79013500
C	-1.83640200	-0.96076400	-0.99452200
C	-3.00601000	-0.88077000	-0.36124900
H	-3.09556300	-1.03475600	0.71034400
C	-1.02072800	1.75667400	1.35254100
C	2.61986700	-1.27991900	0.29032500
H	2.16468600	-2.24038600	0.03277400
H	3.59060000	-1.19299000	-0.19662800
H	2.75287600	-1.26323200	1.37712800
H	-1.44865000	2.75124400	1.29921500
H	-1.79986500	-0.80169900	-2.07039900
H	-3.91896300	-0.65502400	-0.90249500
H	-1.19354200	1.16880600	2.24393900
H	0.71534500	1.81238800	-1.17509600

### Tau-2

E(RwB97XD) = -500.440880502

C	-0.48645400	-1.06960600	1.21130500
C	-0.81707800	-1.18753900	-0.23254800
C	0.27702900	-0.20146300	0.22313900
H	-1.18321200	-0.55662000	1.86507000
H	0.07680300	-1.87807300	1.66439100
H	-0.39168000	-2.05086300	-0.73887700
C	1.68991800	-0.64424700	-0.06089000
C	-0.02040400	1.25816100	0.15444200
O	0.03120400	1.70173800	-1.13723800
O	1.96448500	-1.83297100	-0.09952800
C	-2.08290700	-0.67771900	-0.82111200
C	-3.19689300	-0.39533800	-0.14602700
H	-3.26724100	-0.52814700	0.93019800
C	-0.28971800	2.04060100	1.20281600
C	2.74351000	0.41186700	-0.26873400
H	2.74599500	1.11617900	0.56897800
H	3.72012100	-0.06143200	-0.36817400
H	2.51241300	0.98735300	-1.17027700
H	-0.30273800	1.62503100	2.20211800
H	-0.50100300	3.09957600	1.08814400
H	-2.06419500	-0.53854100	-1.90046600
H	-4.08071200	-0.02375100	-0.65468300
H	-0.13207400	2.65084900	-1.16663500

## 2.2 Route 1

### CM1

E(RwB97XD) = -1315.27960305

C	-4.54211500	-2.33354100	0.37940300
C	-4.02311900	-1.62091700	-0.84136800
H	-4.99441500	-1.62241500	1.07741000
H	-5.27085800	-3.08571600	0.07723500
H	-3.71293800	-2.82522800	0.89956500
C	-3.11332300	-0.42860300	-0.67739700
C	-3.40533900	0.79503000	-1.51470600
C	-4.76565800	0.94120100	-2.14494500
H	-5.55489100	0.72096300	-1.41889700
H	-4.87715700	1.95653900	-2.52531800
H	-4.87167500	0.22132900	-2.96055900
O	-4.32042800	-1.99157800	-1.96452800
O	-2.56378800	1.67067000	-1.62354000
C	-2.43469800	-0.13857600	0.65952200
C	-1.61944600	-0.72123000	-0.43276100
H	-2.71608100	-0.76411000	1.50045000

H	-2.28188700	0.91022200	0.89157900
C	-1.11200600	-2.11933000	-0.43425500
H	-0.98409200	-0.01799400	-0.96814200
C	-0.92052900	-2.87984100	0.64342000
H	-0.86573700	-2.51524100	-1.41769100
H	-0.53134300	-3.88892800	0.55481200
H	-1.13160900	-2.51854700	1.64716600
P	2.08119100	0.47140600	-0.39262900
C	3.84951900	0.65742400	-0.93724600
C	4.54449500	-0.67581000	-1.22370500
H	4.41415600	1.21985600	-0.18035100
H	3.83687700	1.26920700	-1.84857100
C	5.93396800	-0.50414200	-1.84121900
H	4.63857000	-1.24955400	-0.29245000
H	3.92311100	-1.28065800	-1.89835500
C	6.64263200	-1.83722800	-2.07684600
H	5.83934800	0.03621800	-2.79179700
H	6.54610100	0.12785600	-1.18472200
H	7.62486800	-1.69250600	-2.53698300
H	6.78940000	-2.37402600	-1.13301500
H	6.05326300	-2.48176700	-2.73839700
C	2.34728800	-0.40733600	1.22814600
C	1.16376300	-0.32374500	2.19609400
H	3.25485300	-0.02321500	1.71490800
H	2.53662200	-1.45985000	0.98242900
C	1.24483800	-1.35039100	3.32602900
H	1.11493100	0.68284400	2.63061200
H	0.22281700	-0.47184600	1.65259800
C	0.08965400	-1.22428900	4.31761200
H	1.24970900	-2.35777800	2.88931500
H	2.20033800	-1.23729000	3.85427000
H	0.14937400	-1.98358400	5.10314200
H	0.09105400	-0.24034500	4.79910500
H	-0.87641300	-1.34126900	3.81225400
C	1.75871800	2.21703500	0.17016300
C	0.27474200	2.52083000	0.39457200
H	2.14640700	2.87632100	-0.61756700
H	2.34182500	2.43141200	1.07710700
C	0.00446300	3.96812100	0.80515700
H	-0.28984300	2.29606300	-0.51828600
H	-0.12789200	1.85552300	1.16751100
C	-1.48211600	4.23155300	1.04409700
H	0.57284700	4.20365100	1.71495400
H	0.37778600	4.64217100	0.02326900

H	-1.66836000	5.27741600	1.30709300
H	-2.06602500	3.99565000	0.14795200
H	-1.86156500	3.60749400	1.86174800

### TS-1

E(RwB97XD) = -1315.24088607

C	-4.62693800	2.34117800	-0.83937000
C	-3.48202300	1.37739000	-1.05469500
H	-4.38310100	3.07384600	-0.06602900
H	-4.83635200	2.83908200	-1.78799500
H	-5.51670400	1.81449200	-0.48497900
C	-2.91365300	0.62999900	0.05172800
C	-3.51934400	0.55154800	1.36800700
C	-2.96689800	-0.47138600	2.36157000
H	-1.88887500	-0.38187500	2.52817900
H	-3.48142800	-0.33602100	3.31324800
H	-3.15553200	-1.48800000	1.99795700
O	-3.02934400	1.24556900	-2.20598600
O	-4.49364100	1.22585200	1.72767800
C	-1.69259400	-0.20070900	-0.25853000
C	-0.80532200	0.85956500	0.27040700
H	-1.59458400	-0.36585600	-1.33012700
H	-1.62252700	-1.14494900	0.27849900
C	-0.37054100	2.02550200	-0.49917900
H	-0.81793500	0.99247200	1.34451900
C	-0.29487500	2.08305900	-1.83519700
H	-0.08286900	2.89347200	0.08819700
H	0.03213300	2.99255600	-2.32836500
H	-0.57298200	1.24805200	-2.46779300
P	1.48498600	-0.24190300	0.50578000
C	2.83594200	0.71683200	1.32469300
C	2.99081100	2.15517600	0.82398300
H	3.77678500	0.16543900	1.19081900
H	2.61845200	0.72113200	2.39969400
C	4.15050800	2.88551800	1.50372100
H	3.14841400	2.16365000	-0.26205800
H	2.06216000	2.70849900	1.00649100
C	4.28814100	4.33258700	1.03375100
H	4.00123200	2.86328900	2.59081800
H	5.08404500	2.34292800	1.30740700
H	5.12598400	4.83286800	1.52821500
H	4.45968800	4.38052000	-0.04715300
H	3.37907800	4.90332300	1.25255700

C	2.12571000	-0.44994900	-1.21005900
C	1.39189100	-1.51770100	-2.02529200
H	3.19949900	-0.67400700	-1.16238800
H	2.02017500	0.52438300	-1.70273500
C	1.82835000	-1.54057600	-3.49075000
H	1.56708200	-2.50737600	-1.58435800
H	0.30956400	-1.34552700	-1.97950100
C	1.09799900	-2.61165700	-4.29886900
H	1.64546300	-0.55387000	-3.93488700
H	2.91148800	-1.70977500	-3.54345900
H	1.42687500	-2.61677600	-5.34217400
H	1.28078100	-3.60881100	-3.88348300
H	0.01638100	-2.43896600	-4.28860200
C	1.69622600	-1.91025500	1.28533200
C	0.44782800	-2.79624000	1.24330500
H	1.97973100	-1.73360100	2.32980200
H	2.54642000	-2.41475700	0.80736700
C	0.68051300	-4.17340100	1.86524000
H	-0.36854800	-2.29606500	1.78023200
H	0.10475600	-2.92297300	0.20886000
C	-0.57505700	-5.04331700	1.83981800
H	1.49366600	-4.67987800	1.32937200
H	1.02285100	-4.04730200	2.90045200
H	-0.39392900	-6.01876700	2.30045600
H	-1.39584200	-4.56239800	2.38325500
H	-0.91245500	-5.21426000	0.81177300

### TS-1'

E(RwB97XD) = -1315.24064195

C	-3.07321800	-1.95242200	2.44637500
C	-3.40112500	-1.94513300	0.96145400
H	-3.17345800	-0.95781100	2.89179700
H	-3.75303800	-2.64519400	2.94387500
H	-2.04610200	-2.29245400	2.61407200
C	-2.80149800	-0.92569900	0.11362800
C	-3.34663800	-0.54316700	-1.18004700
C	-4.59048400	-1.19816800	-1.73550600
H	-5.39451300	-1.22576900	-0.99641100
H	-4.90096500	-0.64342000	-2.62273200
H	-4.38485500	-2.23934400	-1.99697600
O	-4.19101000	-2.79679100	0.53620500
O	-2.80040100	0.35522800	-1.84711200
C	-1.65985500	-0.05634400	0.59254000

C	-0.76544700	-0.92191100	-0.19810600
H	-1.48543200	-0.09008000	1.66615800
H	-1.72817900	0.96860100	0.23145100
C	-0.14462200	-2.15120900	0.32905400
H	-0.88454000	-0.84307200	-1.26923000
C	0.27148100	-2.32389500	1.58721500
H	-0.00095400	-2.94935500	-0.39525500
H	0.72868400	-3.25575200	1.90194700
H	0.18370800	-1.54031000	2.33585100
P	1.41086800	0.37922200	-0.53000800
C	2.80112100	-0.40923400	-1.45935500
C	3.30892700	-1.72870000	-0.87213600
H	3.62361600	0.31642200	-1.52530000
H	2.43879700	-0.57336100	-2.48165500
C	4.43009500	-2.34356700	-1.71242300
H	3.67688500	-1.56825800	0.14933300
H	2.48259700	-2.44486900	-0.79417400
C	4.95133600	-3.65600700	-1.12985600
H	4.06199100	-2.51312400	-2.73227700
H	5.25398200	-1.62322700	-1.79561700
H	5.74697400	-4.07749600	-1.75122300
H	5.35664700	-3.50567100	-0.12317800
H	4.15086400	-4.40063300	-1.06007500
C	2.18886600	0.76083200	1.09877200
C	1.35570900	1.68782100	1.98685900
H	3.18440000	1.19106900	0.92497700
H	2.33869200	-0.19979600	1.60745000
C	1.97851500	1.89326000	3.36864100
H	1.23928500	2.66389000	1.49968400
H	0.34418100	1.27991500	2.10651800
C	1.13166100	2.79777900	4.26228000
H	2.11238800	0.91683500	3.85188100
H	2.98176000	2.32233000	3.25107600
H	1.59874800	2.94071100	5.24110100
H	0.99765900	3.78477800	3.80625600
H	0.13725700	2.36736500	4.42359300
C	1.27529700	2.01186200	-1.38998800
C	-0.08971700	2.69036700	-1.23730700
H	1.46421900	1.81591100	-2.45275100
H	2.08332500	2.66857600	-1.04008000
C	-0.17861200	4.01241300	-2.00025600
H	-0.87548800	2.01189300	-1.59180100
H	-0.29809000	2.87941500	-0.17609700
C	-1.54619200	4.67633200	-1.84599600

H	0.60674200	4.69396600	-1.64737300
H	0.02341800	3.82845200	-3.06340700
H	-1.59860000	5.61795600	-2.40075300
H	-2.34066900	4.01943300	-2.21520400
H	-1.75725900	4.89438800	-0.79313400

### Int-1

E(RwB97XD) = -1315.28873086

C	-1.42521400	0.65617500	0.10616600
C	-0.14275500	0.38963300	-0.75784700
C	-2.75833900	0.53171700	-0.58431400
H	-1.46045100	-0.05052800	0.93726300
H	-1.29266100	1.65199700	0.54731600
H	0.15550400	1.33372500	-1.23028900
C	-3.18267400	1.49913200	-1.54490500
C	-3.53273100	-0.60941200	-0.20945100
O	-3.08919200	-1.48220100	0.58719300
O	-4.26155000	1.48280000	-2.17617300
C	-0.22308300	-0.65487700	-1.84877900
C	-0.87313200	-1.81444700	-1.75985200
H	-1.44078500	-2.08978600	-0.87325700
C	1.26955200	1.16095800	1.74612200
H	0.31667500	1.03590000	2.27033900
C	1.20989800	-1.69924000	0.99085900
H	1.18760900	-2.35803400	0.11596200
C	2.85484900	0.21081100	-0.52336200
H	2.78802000	1.15702500	-1.07255800
C	-4.92506700	-0.82879800	-0.76468500
C	-2.22562900	2.64903900	-1.87939800
H	-1.69704800	3.05013000	-1.00841300
H	-1.47460800	2.30419600	-2.60092700
H	-2.79798200	3.45020900	-2.35027600
H	-4.88600700	-0.97172500	-1.84850100
H	-5.35167400	-1.71254800	-0.28450700
H	0.29415200	-0.40397100	-2.77316900
H	-0.88364500	-2.50167000	-2.60039300
H	3.61592400	0.34866900	0.25475200
H	2.17818200	-1.85240400	1.48540600
H	2.06010200	0.83263100	2.43127600
C	0.05565900	-2.04030500	1.94145000
H	0.05647000	-1.35390100	2.79755200
H	-0.90869200	-1.91989700	1.43546100
C	0.17093600	-3.47806800	2.45149000

H	0.18043400	-4.16140700	1.59284300
H	1.12995000	-3.61164200	2.96923400
C	-0.98107400	-3.84715800	3.38408600
H	-1.94350400	-3.73578900	2.87515400
H	-0.89372600	-4.88179400	3.72828100
H	-0.99348500	-3.19906900	4.26731300
P	1.26661900	-0.00106700	0.34808500
C	1.47208000	2.62653200	1.34240800
H	2.44652700	2.75165600	0.85488700
H	0.71084000	2.92400500	0.61052500
C	1.39162300	3.55911600	2.55256200
H	0.41338700	3.43685400	3.03315800
H	2.14386100	3.25556500	3.29113200
C	1.60104400	5.02328200	2.17275000
H	1.54092800	5.67070000	3.05195700
H	2.58313600	5.17357000	1.71143300
H	0.84072100	5.35584500	1.45827000
C	3.26395200	-0.92868600	-1.46433000
H	3.36763000	-1.86160300	-0.89831900
H	2.48290000	-1.10086900	-2.21197300
C	4.58572700	-0.62247100	-2.17159200
H	4.48591700	0.31619900	-2.73056500
H	5.36757300	-0.45636500	-1.41962900
C	5.01002000	-1.74303800	-3.11845100
H	5.95712700	-1.50593300	-3.61098600
H	5.13985700	-2.68722400	-2.57891200
H	4.25717700	-1.90394400	-3.89739300
H	-5.56354300	0.04307700	-0.60444800

### Int-1'

E(RwB97XD) = -1315.29174248

C	-1.48539100	-0.56287500	0.18202800
C	-0.26229000	-0.03798300	-0.62365800
C	-2.76884300	-0.37058600	-0.59512500
H	-1.32567200	-1.61059700	0.44129900
H	-1.54632900	-0.00164900	1.12200300
H	-0.53909500	0.97822700	-0.93028800
C	-3.16596400	0.98750300	-0.76203400
C	-3.53075500	-1.48466500	-1.07021500
O	-4.56324100	-1.40031800	-1.76923300
O	-2.46118400	1.93170200	-0.30284800
C	0.07111400	-0.85492400	-1.85391400
C	0.30785800	-2.16639700	-1.86945500

H	0.28254000	-2.77261000	-0.96665900
C	0.77342200	1.13659900	1.92716300
H	0.11340200	0.47115300	2.49329000
C	2.13255000	-1.24363900	0.84807400
H	2.36723500	-1.76465900	-0.08608800
C	2.38089000	1.35654600	-0.50190000
H	1.79610500	2.22253300	-0.83238900
C	-3.07877900	-2.90153600	-0.69896400
C	-4.44183300	1.36760500	-1.48509400
H	-4.39675500	1.06789200	-2.53581600
H	-5.30767000	0.84894000	-1.06643600
H	-4.56853700	2.45024100	-1.40807400
H	-2.97134200	-3.03237400	0.38346000
H	-3.82928500	-3.60291200	-1.06657700
H	0.08891400	-0.31035100	-2.79510200
H	0.51103800	-2.68590100	-2.79999700
H	3.09702800	1.72219000	0.24451500
H	3.08514300	-0.91347800	1.28044700
H	1.69513800	1.24588300	2.51208900
C	1.39792500	-2.17843500	1.81581600
H	1.21518800	-1.66600500	2.76743000
H	0.41513200	-2.44542300	1.41169900
C	2.19353100	-3.45853500	2.07646300
H	2.37171600	-3.96924000	1.12190600
H	3.17940500	-3.19674600	2.48056000
C	1.47348000	-4.40072700	3.03888200
H	0.49504100	-4.69204800	2.64254600
H	2.05236900	-5.31329100	3.20575500
H	1.31244800	-3.92215500	4.01070600
P	1.22933600	0.26880900	0.39762400
C	0.09269200	2.49213800	1.69240500
H	0.81409000	3.19532800	1.25724600
H	-0.73507800	2.37844300	0.98080000
C	-0.45594900	3.07322300	2.99680600
H	-1.19728500	2.37617400	3.40751700
H	0.34908200	3.15123900	3.73952900
C	-1.10393200	4.44005000	2.78549700
H	-1.52171400	4.82925300	3.71857700
H	-0.37330800	5.16784100	2.41544900
H	-1.91336900	4.37432300	2.05166700
C	3.12335100	0.72561300	-1.68547900
H	3.68705900	-0.15354700	-1.35114300
H	2.40600300	0.37274900	-2.43302200
C	4.08698000	1.72005000	-2.33626100

H	3.52672100	2.60605500	-2.65945500
H	4.81201800	2.06424100	-1.58809200
C	4.82412700	1.11424000	-3.52904900
H	5.51101800	1.83785400	-3.97684500
H	5.40890100	0.23861100	-3.22690300
H	4.11931800	0.79508900	-4.30397500
H	-2.11634900	-3.14408300	-1.16124900

### Int-2

E(RwB97XD) = -1315.26344434

C	3.20474300	-2.91311300	-2.11235900
C	2.78643900	-2.11521200	-1.08052200
H	3.35894400	-3.97705700	-1.95476400
H	3.38611000	-2.50474500	-3.10199400
C	2.55875900	-0.60736400	-1.39298100
C	3.31188400	0.20786800	-0.35704100
C	4.78775800	-0.05895100	-0.22725400
H	5.26486300	0.73201000	0.35287700
H	4.90883600	-1.01906000	0.28488300
H	5.25909300	-0.15790400	-1.20888200
O	2.54633600	-2.44599400	0.13584200
O	2.75415200	1.03680900	0.35004600
C	1.07608800	-0.21368500	-1.46179000
H	1.01885000	0.87867800	-1.48561100
H	0.65887100	-0.56264300	-2.40928800
C	0.24872200	-0.78182000	-0.28787700
H	0.93049700	-0.90329800	0.56313600
C	-0.38144600	-2.14111200	-0.51193400
C	-0.72214200	-2.68360000	-1.67842600
H	-0.53390900	-2.72434000	0.39328600
H	-1.14421300	-3.68230700	-1.71625300
H	-0.56629100	-2.18727400	-2.63151200
P	-0.99600300	0.41087200	0.32637900
C	-2.07567000	-0.43968500	1.51529300
C	-1.33395200	-0.94587300	2.76033800
H	-2.55011800	-1.27226200	0.98466200
H	-2.86887700	0.26439300	1.79262100
C	-2.24716300	-1.77499900	3.66472100
H	-0.47201300	-1.55782000	2.46787900
H	-0.93443200	-0.09623900	3.32642100
C	-1.52717400	-2.26761300	4.91829900
H	-3.11993000	-1.17340800	3.94903200
H	-2.62897500	-2.63248700	3.09701400

H	-2.19233300	-2.86917000	5.54416900
H	-0.66252600	-2.88596300	4.65536100
H	-1.16689000	-1.42717900	5.52107800
C	-0.19122200	1.78335200	1.21712500
C	0.24108400	2.98949700	0.37651900
H	0.68172100	1.35223400	1.71742300
H	-0.90349800	2.09945600	1.98927200
C	0.93969700	4.03903100	1.24229400
H	0.93568700	2.66619300	-0.40344400
H	-0.62774200	3.44489800	-0.11384000
C	1.38304400	5.25456100	0.43065500
H	0.26413500	4.35712500	2.04695800
H	1.81044900	3.57623600	1.72051500
H	1.87893100	5.99348600	1.06655600
H	2.08763600	4.96206900	-0.35495300
H	0.52748400	5.74323500	-0.04861100
C	-2.01941700	1.11384000	-1.00361300
C	-3.04943400	0.16748600	-1.63148400
H	-1.32573000	1.48976000	-1.76470000
H	-2.52044700	1.99006200	-0.57420300
C	-3.81722400	0.85470900	-2.76237700
H	-2.55255900	-0.72742100	-2.01719400
H	-3.75983300	-0.17028200	-0.86746800
C	-4.86077600	-0.06359400	-3.39527900
H	-4.30467100	1.75768400	-2.37333100
H	-3.10565600	1.18878300	-3.52754900
H	-5.39343900	0.44352400	-4.20482700
H	-4.39191500	-0.96090800	-3.81266200
H	-5.60140300	-0.38597500	-2.65567100
H	3.01582600	-0.37403100	-2.36302500

## TS-2

E(RwB97XD) = -1315.22962644

C	2.00957100	-3.46735900	0.69013300
C	2.55230200	-2.18574500	0.98047500
H	2.06426400	-4.18647000	1.50467300
H	2.21145400	-3.88257800	-0.29651800
C	2.67312300	-1.19449400	-0.20246000
C	3.56438800	-0.02226200	0.18659200
C	4.96466900	-0.34547600	0.64004100
H	5.62051200	0.50896000	0.46579000
H	4.92128700	-0.55704100	1.71277500
H	5.35571600	-1.23853200	0.14537500
O	2.66087300	-1.71910100	2.12780900

O	3.17506000	1.13285200	0.12130400
C	1.28839400	-0.73312200	-0.70373800
H	1.45381000	0.16211500	-1.30818600
H	0.88374500	-1.49447300	-1.37677700
C	0.27348700	-0.45540600	0.42796000
H	0.75234600	0.22458800	1.14731100
C	-0.26121500	-1.69479300	1.11768000
C	0.08804500	-2.97502200	0.63766100
H	-0.36539500	-1.58576300	2.19552400
H	-0.28367900	-3.80662000	1.23288400
H	-0.00949500	-3.17808200	-0.42896400
P	-1.12079500	0.58639800	-0.22247300
C	-2.51935400	0.47052300	0.92644900
C	-2.24839300	1.09334400	2.30050300
H	-2.69932100	-0.60499400	1.03522700
H	-3.39301700	0.92687300	0.44698000
C	-3.39257800	0.82416400	3.27906300
H	-1.31941700	0.68268800	2.71477600
H	-2.10551900	2.17648800	2.20483800
C	-3.14675100	1.45280600	4.64922600
H	-4.32782700	1.21230000	2.85549900
H	-3.52295700	-0.25943600	3.38707300
H	-3.97482000	1.24742600	5.33371900
H	-2.23141200	1.05684000	5.10172400
H	-3.03726700	2.53984600	4.56895600
C	-0.69703000	2.35721700	-0.36955700
C	0.43815900	2.70111500	-1.34041500
H	-0.43395100	2.69713900	0.63850700
H	-1.62236000	2.87670500	-0.65042500
C	0.62237300	4.21330700	-1.48158100
H	1.37137300	2.25896500	-0.97616200
H	0.23791200	2.27307500	-2.33113400
C	1.79739700	4.56707600	-2.39139800
H	-0.30048400	4.65964000	-1.87415600
H	0.78299400	4.64992800	-0.48780900
H	1.91427500	5.65032800	-2.48802200
H	2.73258700	4.15987500	-1.99315800
H	1.65359900	4.15374000	-3.39584400
C	-1.68321400	0.03491400	-1.86476100
C	-2.30103000	-1.36690100	-1.91417800
H	-0.81426200	0.08776300	-2.53093700
H	-2.39983600	0.78580900	-2.22010500
C	-2.68761300	-1.75792400	-3.34125500
H	-1.59591200	-2.09837400	-1.50776000

H	-3.18886900	-1.40628700	-1.27188700
C	-3.30355800	-3.15365000	-3.41755800
H	-3.39424100	-1.01923100	-3.74132500
H	-1.79602500	-1.71423500	-3.97985300
H	-3.56278200	-3.41432800	-4.44780400
H	-2.60519400	-3.91011200	-3.04408900
H	-4.21620300	-3.21430900	-2.81500600
H	3.18181100	-1.70007500	-1.03482200

### TS-3

E(RwB97XD) = -1315.24112246

C	-1.38488800	2.08830800	-0.08032900
H	-1.34698400	2.51100400	-1.09155700
C	-2.60559800	-0.24347200	-1.34021900
H	-2.44325800	0.25217400	-2.30571900
C	-1.59914400	-0.40354300	1.40763400
H	-0.77630400	-0.10655600	2.06921900
H	-2.50718400	0.07466800	1.79581900
H	-2.47855600	-1.31718700	-1.52760000
H	-2.37712700	2.31248700	0.33085300
C	-4.02260800	0.03493000	-0.83136200
H	-4.17142800	-0.44911500	0.14231700
H	-4.15959100	1.11116500	-0.66962600
C	-5.09359800	-0.46584500	-1.80302600
H	-4.95123600	0.01886900	-2.77716400
H	-4.95267200	-1.54152100	-1.96826300
C	-6.51211000	-0.20444700	-1.30009400
H	-6.68514700	0.86714000	-1.15250400
H	-7.25881600	-0.56954200	-2.01123700
H	-6.68718400	-0.70556800	-0.34178100
P	-1.20287500	0.26622200	-0.26152500
C	-0.29509700	2.72705700	0.78728900
H	-0.27159800	2.25447000	1.77773800
H	0.68531000	2.54942200	0.33016700
C	-0.49583000	4.23312900	0.96058300
H	-0.55059800	4.70436100	-0.02898000
H	-1.46367100	4.41412300	1.44534200
C	0.62113600	4.88092400	1.77676600
H	0.45171100	5.95419500	1.90243400
H	0.68942200	4.43263100	2.77404500
H	1.59149600	4.74880500	1.28598000
C	-1.74313100	-1.92840400	1.41664800
H	-2.59528200	-2.22586900	0.79164500

H	-0.85384200	-2.38959200	0.96641800
C	-1.93794900	-2.49072100	2.82551700
H	-1.08118200	-2.20275700	3.44779100
H	-2.82248600	-2.02564000	3.27911100
C	-2.09287500	-4.01023700	2.83412500
H	-2.22696000	-4.39044200	3.85097500
H	-2.96198200	-4.31980400	2.24324600
H	-1.20875100	-4.49628400	2.40786500
C	1.71213900	1.53884100	-2.14907200
C	4.76024200	-1.89359500	-1.81880700
C	3.41371900	-1.44552000	-1.32245100
C	0.99289600	0.41641400	-2.22743000
C	3.19285900	-0.74364500	-0.14104100
C	0.92314800	-0.61196700	-1.16802600
C	1.71681000	-0.49985900	0.12022400
H	0.43590000	0.18944000	-3.13315600
H	1.30888600	-1.22102800	0.84206800
H	1.56339800	0.49181400	0.55397700
O	2.39289200	-1.71907400	-2.04945300
C	4.20650900	-0.31873500	0.77924300
C	3.74570500	0.42154800	2.03136600
H	4.60494600	0.58908500	2.68209800
H	3.30738000	1.39197500	1.76792300
H	2.98085700	-0.14278400	2.57631800
O	5.42547200	-0.50456300	0.61823200
H	0.33796500	-1.49552200	-1.36497700
H	1.74670300	2.23591000	-2.97948300
H	2.30544600	1.78125900	-1.27199300
H	5.29468400	-2.45057900	-1.04625600
H	4.62943500	-2.50355100	-2.71465400
H	5.38051200	-1.02286500	-2.05099600

### Pr-1

E(RwB97XD) = -500.493181630

C	0.36043300	-0.77312300	1.49926700
C	0.03783400	-1.96513100	0.62821000
C	0.44437300	0.58529500	0.77440800
H	-0.36576700	-0.68882200	2.31764100
H	1.32237200	-0.95498800	1.98812100
H	0.51566600	-2.89483500	0.93091600
C	1.37771100	0.54784300	-0.43920500
C	-0.91249800	1.16369200	0.38657100
O	-1.13118400	2.34937500	0.54831600

O	1.03034000	0.99173400	-1.51677500
C	-0.73806700	-2.00176800	-0.45961200
C	-1.55074100	-0.88999700	-1.07148000
H	-2.46025000	-1.33729000	-1.48593300
C	-1.99006600	0.23409500	-0.12602300
C	2.75119200	-0.03684000	-0.22552100
H	2.67063200	-1.12656600	-0.15277400
H	3.39200600	0.21771000	-1.06993000
H	3.19253900	0.32554300	0.70752800
H	-2.46349100	-0.20908500	0.76182600
H	-2.74439900	0.86182500	-0.60607900
H	-0.81099200	-2.95559100	-0.97923700
H	-1.01278300	-0.46550000	-1.92774500
H	0.89020200	1.31433600	1.46365000

### Pr-3

$$E(RwB97XD) = -500.472553671$$

C	-2.97642300	-1.28759500	0.97039400
C	0.88313000	2.45999600	0.32579400
C	0.20309300	1.21329900	-0.10666600
C	-2.69626000	-0.14471600	0.34822000
C	0.63319200	-0.06944200	-0.19436000
C	-1.67115000	0.06977800	-0.73538200
C	-0.48321800	-0.90621600	-0.78547200
H	-3.26403300	0.75169100	0.59183800
H	-0.26331400	-1.20801900	-1.81585400
H	-0.67955700	-1.81827200	-0.21660800
O	-1.07376200	1.38146900	-0.50474200
C	1.96304900	-0.56779900	0.14327100
C	2.22469700	-2.03118200	-0.14595100
H	3.26795200	-2.26415900	0.06813100
H	1.57734100	-2.65971800	0.47572800
H	1.99928000	-2.26774600	-1.19122100
O	2.84430100	0.13302800	0.63973400
H	-2.18101300	0.14952000	-1.69941200
H	-3.76101200	-1.32909400	1.71878600
H	-2.45611900	-2.21782800	0.76164000
H	1.93847200	2.26985200	0.51047500
H	0.76214200	3.22740900	-0.44457600
H	0.41489400	2.83365400	1.24206600

### 2.3 Channel 2 in route 3

**TS-4**

E(RwB97XD) = -1315.21758266

C	3.70499900	0.53611400	1.13926000
C	2.98108400	0.15360600	-0.07229800
C	3.55191100	0.39010100	-1.35857500
C	2.92750300	-0.22282500	-2.60379900
H	1.85350200	-0.04237400	-2.70022000
H	3.43213200	0.18809500	-3.47863900
H	3.07449300	-1.30898000	-2.59164600
O	4.61582800	1.04656700	-1.52783400
C	1.64256100	-0.52708800	0.02663800
C	0.88085300	0.72950100	-0.21126200
H	1.45630100	-0.97803500	1.00000200
H	1.46153000	-1.28515100	-0.73619000
C	0.69969400	1.75169300	0.81333700
H	0.91363800	1.10054800	-1.22821100
C	0.64481800	1.51559000	2.13321100
H	0.61638300	2.77428700	0.45514600
H	0.54447200	2.33123900	2.84120900
H	0.67560800	0.51387600	2.54558700
P	-1.49169000	0.01990900	-0.53862700
C	-2.58369900	1.31639000	-1.26881700
C	-2.41645600	2.70473100	-0.64502900
H	-3.62496000	0.97931900	-1.17377300
H	-2.35883500	1.36153300	-2.34127800
C	-3.39574600	3.72670500	-1.22547500
H	-2.55998400	2.65016400	0.44158000
H	-1.39123300	3.05916600	-0.80511700
C	-3.23052500	5.11223900	-0.60356500
H	-3.25070200	3.78938300	-2.31147800
H	-4.42198900	3.37113300	-1.06825200
H	-3.94456900	5.82560100	-1.02548000
H	-3.39251000	5.07645900	0.47929100
H	-2.22247200	5.50400600	-0.77725200
C	-2.19720500	-0.20259100	1.14770600
C	-1.69171200	-1.45236900	1.87339500
H	-3.29213400	-0.22090300	1.07226100
H	-1.92653200	0.69104000	1.72203200
C	-2.09293600	-1.47031000	3.34890900
H	-2.08306300	-2.35150400	1.38051500
H	-0.59805000	-1.51528900	1.80218800
C	-1.63175900	-2.73604400	4.06832000
H	-1.66659500	-0.58770100	3.84262100

H	-3.18317400	-1.37351400	3.42896400
H	-1.90887900	-2.71526600	5.12627100
H	-2.08188200	-3.62848400	3.62012800
H	-0.54338700	-2.84604300	4.00888200
C	-2.02951800	-1.50205600	-1.44893800
C	-0.98039900	-2.61766400	-1.49312500
H	-2.28161200	-1.19585900	-2.47088000
H	-2.95807200	-1.86462700	-0.98814800
C	-1.53122800	-3.91557200	-2.08441100
H	-0.12341400	-2.28164400	-2.09098500
H	-0.59249500	-2.81927800	-0.48657500
C	-0.46446100	-5.00205500	-2.20825600
H	-2.35490100	-4.27445800	-1.45394100
H	-1.96429400	-3.70912200	-3.07163700
H	-0.88411400	-5.92632600	-2.61588300
H	0.34612800	-4.68041200	-2.87105300
H	-0.02458800	-5.23351200	-1.23214300
C	3.42309900	0.10484000	2.39377300
H	2.66459000	-0.63792900	2.59589600
H	4.02584200	0.45444800	3.22420300
O	4.73158500	1.41200300	0.98698700
H	4.90058800	1.48131200	0.01218400

#### TS-4'

E(RwB97XD) = -1315.21546530

C	3.15797900	2.06054700	1.09636700
C	2.70362500	0.95485200	0.27460900
C	3.38672700	0.45369000	-0.86661200
C	4.72611300	1.01652000	-1.31666800
H	5.36804700	1.30568400	-0.48186900
H	5.22175000	0.25408600	-1.92169600
H	4.57433600	1.90801800	-1.93258200
O	2.91237800	-0.49975600	-1.54534300
C	1.47876700	0.18756200	0.67655400
C	0.60734200	0.85476500	-0.32332000
H	1.16170300	0.35391500	1.70605700
H	1.58624400	-0.88179900	0.48669100
C	0.04466400	2.20061500	-0.07461900
H	0.92442800	0.65994100	-1.34339900
C	-0.16028800	2.75160800	1.12613500
H	-0.23357500	2.75921200	-0.96610900
H	-0.57997000	3.74878100	1.21255200
H	0.10436800	2.24833000	2.04991100
P	-1.35175800	-0.39046600	-0.55109300

C	-2.69387500	0.44093700	-1.49626900
C	-3.40142200	1.58819600	-0.76770900
H	-3.42151500	-0.33198000	-1.77771400
H	-2.24133700	0.80509800	-2.42665200
C	-4.45708400	2.26225500	-1.64641100
H	-3.88395700	1.20984300	0.14189400
H	-2.66889700	2.33443700	-0.44418300
C	-5.17430700	3.40088000	-0.92298800
H	-3.97711500	2.64765500	-2.55480200
H	-5.18893300	1.51335000	-1.97493700
H	-5.91957300	3.87426600	-1.56865200
H	-5.68842100	3.03455900	-0.02774400
H	-4.46375000	4.17242400	-0.60747200
C	-2.07675500	-0.75570800	1.09388400
C	-1.36953800	-1.86226900	1.88190600
H	-3.13412400	-1.01293900	0.95091400
H	-2.04865200	0.18747600	1.65434600
C	-1.95705600	-2.02883300	3.28452800
H	-1.45944500	-2.81355900	1.34331400
H	-0.29734500	-1.64916100	1.96271400
C	-1.28189300	-3.15132300	4.07012400
H	-1.85668000	-1.08208500	3.82990200
H	-3.03300800	-2.22903400	3.20224000
H	-1.72144200	-3.25726700	5.06621900
H	-1.38876700	-4.11123800	3.55330600
H	-0.21143700	-2.95584600	4.19378500
C	-1.11076400	-1.97897000	-1.44216500
C	0.24619700	-2.65085300	-1.20326400
H	-1.22186500	-1.74431700	-2.50791500
H	-1.94008900	-2.64869400	-1.17714800
C	0.39253400	-3.94893000	-1.99820600
H	1.05566900	-1.96045100	-1.47173100
H	0.37172100	-2.87409000	-0.13670300
C	1.76022300	-4.59735500	-1.78987500
H	-0.40015700	-4.65090700	-1.70671700
H	0.24492800	-3.73786500	-3.06532500
H	1.85102700	-5.52809400	-2.35786800
H	2.56106600	-3.92250700	-2.10818500
H	1.92435700	-4.83119900	-0.73216600
C	2.96383300	2.20564100	2.42874400
H	2.53503000	1.40841200	3.02270100
H	3.23579000	3.12264200	2.94414300
O	3.79053700	3.05519500	0.38565900
H	4.20251500	3.66541900	1.00629700

**Int-3**

E(RwB97XD) = -1315.26126425

C	-1.08465000	2.16138800	0.06008300
H	-1.02915000	2.59379500	-0.94485800
C	-2.44444200	-0.03246000	-1.34647500
H	-2.19800500	0.49035700	-2.27721800
C	-1.52593500	-0.42253500	1.43290800
H	-0.70517200	-0.19410700	2.12100200
H	-2.41808300	0.07793600	1.82585200
H	-2.36948200	-1.10572600	-1.55639100
H	-2.05927100	2.43540300	0.48142900
C	-3.85989600	0.32845900	-0.88133800
H	-4.08427900	-0.17732200	0.06597500
H	-3.93194400	1.40601100	-0.69141500
C	-4.91168200	-0.07073000	-1.91859700
H	-4.69065400	0.43110200	-2.86847700
H	-4.83458000	-1.14825000	-2.10886800
C	-6.33052200	0.27397600	-1.47110000
H	-6.44220000	1.35119800	-1.30846100
H	-7.06401900	-0.02895900	-2.22311800
H	-6.58132500	-0.23456400	-0.53404200
P	-1.12397400	0.35822700	-0.15748700
C	0.05143800	2.70517000	0.93365400
H	0.07534900	2.18937500	1.90143200
H	1.01042600	2.51360600	0.44278900
C	-0.09089900	4.20945100	1.16987800
H	-0.13454200	4.72153600	0.20068300
H	-1.04434100	4.40997200	1.67490400
C	1.06431200	4.77036600	1.99676300
H	0.94615600	5.84536800	2.15854700
H	1.11761200	4.28606100	2.97756500
H	2.02229900	4.60725700	1.49244700
C	-1.74659000	-1.93712700	1.33389200
H	-2.62786100	-2.14580700	0.71476500
H	-0.89246700	-2.41243200	0.83566200
C	-1.93473200	-2.57480400	2.71129700
H	-1.04953000	-2.36628400	3.32420400
H	-2.78604900	-2.10051600	3.21526600
C	-2.15759700	-4.08298300	2.62364000
H	-2.28436700	-4.52064000	3.61760100
H	-3.05354400	-4.31593300	2.03807300
H	-1.30522100	-4.57723300	2.14583700

C	1.75880800	1.43980000	-2.12756100
C	3.93237900	1.29870600	0.70204600
C	3.99932200	0.09181300	0.06991300
C	0.80997400	0.50945200	-2.04104300
C	2.90119400	-0.86116500	-0.13080300
C	0.45923100	-0.30260000	-0.81422400
C	1.51764300	-0.46486400	0.31873400
H	0.21650000	0.28105100	-2.92606100
H	1.11111700	-1.20506100	1.02080100
H	1.58278600	0.46178400	0.88891700
O	5.19985200	-0.27856000	-0.43218900
C	3.14896900	-2.10750300	-0.70128100
C	2.04387800	-3.14469400	-0.84947400
H	2.49627000	-4.13543100	-0.76674800
H	1.25039900	-3.06150700	-0.09952700
H	1.58878100	-3.07391300	-1.84493000
O	4.29442600	-2.48251300	-1.15187500
H	5.06918700	-1.20220900	-0.81931300
H	0.18430500	-1.30622400	-1.16346600
H	1.92569500	1.95463200	-3.06889400
H	2.42411000	1.67970900	-1.30081600
H	4.83382400	1.89492500	0.79078300
H	3.03544400	1.67351400	1.17742100

### Int-3'

E(RwB97XD) = -1315.25483704

C	-1.46911600	2.14163800	0.15409000
H	-1.52918800	2.60753400	-0.83603900
C	-2.35808400	-0.23711600	-1.33572000
H	-2.19374200	0.32247100	-2.26302500
C	-1.41303600	-0.52467800	1.43782600
H	-0.69584000	-0.13040200	2.16551400
H	-2.41230100	-0.25805000	1.80213300
H	-2.08898200	-1.27941100	-1.54226200
H	-2.46275700	2.21927500	0.61092300
C	-3.82297700	-0.13241300	-0.89831300
H	-3.97412000	-0.67557300	0.04249300
H	-4.08196000	0.91585600	-0.70521100
C	-4.77385400	-0.69678500	-1.95583800
H	-4.61237200	-0.17083700	-2.90485400
H	-4.52562100	-1.74978600	-2.13628100
C	-6.23895600	-0.57582200	-1.54172800
H	-6.51660700	0.47213600	-1.38533900

H	-6.90161400	-0.98737800	-2.30806600
H	-6.42921000	-1.11535800	-0.60773200
P	-1.14971600	0.37258100	-0.11815800
C	-0.42229500	2.85791700	1.01477000
H	-0.28554900	2.33316400	1.96826500
H	0.54323200	2.84000800	0.49916900
C	-0.81412000	4.31052800	1.29024100
H	-0.96424100	4.82747300	0.33414700
H	-1.77792500	4.33472400	1.81425500
C	0.24147500	5.04627800	2.11303300
H	-0.05099300	6.08434800	2.29455400
H	0.38877500	4.56331800	3.08494200
H	1.20599500	5.05443800	1.59466100
C	-1.25302800	-2.04346000	1.28437300
H	-2.04005000	-2.42890500	0.62273800
H	-0.28774100	-2.27285700	0.81198200
C	-1.33960800	-2.75900400	2.63285800
H	-0.55216400	-2.37292300	3.29231400
H	-2.29755400	-2.52692500	3.11701100
C	-1.18455600	-4.27158000	2.48578000
H	-1.23614300	-4.77116100	3.45757500
H	-1.97552300	-4.68685300	1.85150600
H	-0.22271400	-4.51769300	2.02523000
C	1.66497600	1.92425700	-2.07495400
C	4.40541800	1.30441500	0.33733500
C	4.09862100	0.14272400	-0.30235600
C	0.74290700	0.96784200	-1.97009900
C	2.88326600	-0.62984000	-0.16959600
C	0.53068600	0.06449700	-0.77948700
C	1.63266900	0.06700700	0.31128200
H	0.08332300	0.79036300	-2.81976200
H	1.24278000	-0.46174600	1.18882700
H	1.84174200	1.09126600	0.62446600
O	4.99281400	-0.36226400	-1.22125200
C	2.75907200	-2.01387100	-0.37185700
C	3.93723900	-2.90602300	-0.74032300
H	3.69347300	-3.92468900	-0.42796400
H	4.09234800	-2.90599300	-1.82416400
H	4.87467200	-2.58884600	-0.27996700
O	1.63624000	-2.60584400	-0.23068200
H	5.83268500	0.09576000	-1.11120900
H	0.46797400	-0.97994000	-1.12076400
H	1.74447300	2.50706800	-2.98758900
H	2.39561300	2.11818500	-1.29358900

H	5.29372200	1.87242700	0.07395800
H	3.78720100	1.69260200	1.13709300

### TS-5

E(RwB97XD) = -1315.23102732

C	-2.19875900	-0.14980500	-1.46300700
H	-1.83959000	0.38950100	-2.34663300
C	-1.57942100	-0.55689700	1.40023900
H	-0.85470500	-0.28593400	2.17639900
C	-1.22805900	2.09305900	0.16701900
H	-0.94945300	2.57403700	-0.77727200
H	-2.29479900	2.28641100	0.32955400
H	-2.54940600	-0.15470000	1.71545500
H	-2.03327900	-1.21586100	-1.65902500
C	-1.64091800	-2.08056200	1.24179500
H	-2.42362900	-2.34851700	0.52116000
H	-0.69482800	-2.454444000	0.82944900
C	-1.91456500	-2.78630100	2.57050600
H	-1.12365500	-2.52366200	3.28384400
H	-2.85410600	-2.40851900	2.99311100
C	-1.98772100	-4.30404100	2.41790900
H	-1.04952400	-4.70342100	2.01778300
H	-2.17506400	-4.78897500	3.37997400
H	-2.792444000	-4.59251300	1.73315400
P	-1.06168900	0.30596000	-0.12037300
C	-3.68149700	0.12387100	-1.19886900
H	-4.00720900	-0.39855800	-0.29003100
H	-3.84285200	1.19410200	-1.02319900
C	-4.55726200	-0.32335800	-2.37156000
H	-4.23006700	0.19434600	-3.28133500
H	-4.40023000	-1.39447600	-2.54888100
C	-6.04029000	-0.05246000	-2.12757600
H	-6.64620700	-0.37828800	-2.97773300
H	-6.39663100	-0.58376400	-1.23836800
H	-6.22411600	1.01644700	-1.97461700
C	-0.40937400	2.65668000	1.33348000
H	-0.68829300	2.15760900	2.26961200
H	0.65546800	2.45622700	1.17492400
C	-0.60963800	4.16517000	1.48675900
H	-0.34676400	4.65829500	0.54268500
H	-1.67263400	4.37268300	1.66287900
C	0.22882200	4.74738900	2.62263100
H	0.06484500	5.82381200	2.72405300

H	-0.02413500	4.27747100	3.57919300
H	1.29682800	4.58518200	2.44278800
C	1.76022300	1.83074200	-1.60301700
C	3.45718800	1.72768800	-0.41202800
C	3.82695500	0.36736600	-0.49483900
C	1.09690000	0.61677600	-1.82176600
C	2.99443100	-0.69317500	-0.05012600
C	0.62106300	-0.21442400	-0.65053900
C	1.63075200	-0.35425600	0.51810900
H	4.19509500	2.43490800	-0.78491200
H	1.40509200	0.02410400	-2.67947600
H	1.29242900	-1.12516300	1.22050300
H	1.68315200	0.56910600	1.10209300
O	4.93054900	0.07347500	-1.18463500
C	3.37260200	-2.03308200	-0.29425800
C	2.47663400	-3.17414500	0.15568800
H	1.49508200	-3.12760600	-0.32887600
H	2.95163400	-4.11940900	-0.10937000
H	2.31169900	-3.14903400	1.23838000
O	4.45289300	-2.35173400	-0.88370100
H	2.96864600	2.04261700	0.50498100
H	4.97174000	-0.93515700	-1.22120600
H	0.42289300	-1.22853100	-1.02461400
H	1.34180000	2.55583800	-0.90873500
H	2.20660600	2.30308700	-2.47470700

### TS-5'

E(RwB97XD) = -1315.21823592

C	-2.18298900	-0.28621800	-1.44856400
H	-1.86205600	0.27185700	-2.33573000
C	-1.54248700	-0.62243100	1.41945400
H	-0.88310500	-0.24465000	2.20918300
C	-1.39872800	2.05005500	0.14407800
H	-1.09977800	2.52415600	-0.79835300
H	-2.48085400	2.18559500	0.25074300
H	-2.56814100	-0.35678400	1.70195800
H	-1.92990800	-1.33734400	-1.63106200
C	-1.37999600	-2.14243600	1.28008800
H	-2.10024800	-2.52506500	0.54542500
H	-0.37799900	-2.38123800	0.90140200
C	-1.59052200	-2.86282500	2.61258500
H	-0.86387300	-2.48212900	3.34125900
H	-2.58638400	-2.62214400	3.00651400

C	-1.43583400	-4.37673000	2.47987400
H	-0.43867800	-4.63348500	2.10778800
H	-1.57669800	-4.87474100	3.44355400
H	-2.17114300	-4.78615700	1.77845300
P	-1.09706700	0.27453500	-0.10282800
C	-3.68524900	-0.13161500	-1.19941100
H	-3.97553000	-0.68128800	-0.29466500
H	-3.93165300	0.92215700	-1.02152600
C	-4.51363500	-0.64230600	-2.38025500
H	-4.21528000	-0.10352900	-3.28793000
H	-4.27858700	-1.69964900	-2.55409600
C	-6.01521700	-0.47895200	-2.15354300
H	-6.58636300	-0.84912700	-3.00961100
H	-6.34183600	-1.03324200	-1.26689600
H	-6.27677100	0.57430900	-2.00488900
C	-0.66831800	2.68866300	1.32992300
H	-0.97351300	2.20692200	2.26679500
H	0.41118200	2.53126200	1.23247500
C	-0.94386700	4.19032500	1.42005700
H	-0.64940100	4.66474100	0.47562600
H	-2.02330700	4.35463300	1.52929000
C	-0.20050300	4.84910200	2.58027900
H	-0.41150900	5.92115000	2.62898000
H	-0.49322600	4.40478700	3.53769500
H	0.88203100	4.72405300	2.47082400
C	1.72078100	1.95345000	-1.58049900
C	3.46463200	1.82980600	-0.52498300
C	3.80245500	0.44514200	-0.54637000
C	1.05126100	0.73883700	-1.80016400
C	2.97439200	-0.54581300	-0.03459300
C	0.62724400	-0.10714300	-0.61942600
C	1.63658900	-0.12629600	0.54543900
H	4.18826600	2.50082800	-0.99231000
H	1.30454200	0.17157400	-2.69257300
H	1.33286100	-0.84937500	1.30905700
H	1.70383500	0.85026300	1.03077000
O	4.86441200	0.06477700	-1.31381900
C	3.16512600	-1.97250800	-0.14450000
C	4.45527400	-2.58071900	-0.66222200
H	5.33432700	-2.12750200	-0.19822300
H	4.43057000	-3.65284200	-0.45802800
H	4.54843600	-2.41936700	-1.73973500
O	2.25384800	-2.75334900	0.20256600
H	3.09637000	2.21709700	0.42088400

H	5.38971500	0.84501600	-1.51659300
H	0.52805600	-1.15115000	-0.94547600
H	1.31809200	2.65083300	-0.84633100
H	2.09503000	2.46379000	-2.46568500

### Pr-2

E(RwB97XD) = -500.495916882

C	0.18171300	-1.40276000	0.71604800
C	1.37921700	-1.80517500	-0.12361900
C	2.34211500	-1.01915300	-0.61470900
C	-0.52025900	-0.12525500	0.29646100
C	2.51790200	0.46763300	-0.44559400
C	0.18515300	1.05662000	0.28345600
C	1.64107200	1.12715600	0.62911900
H	-0.53029700	-2.22898400	0.69387400
H	1.45699800	-2.87030400	-0.33418700
H	3.11613900	-1.49665800	-1.21376200
H	3.56737800	0.65953900	-0.19349400
H	1.81300100	0.63302600	1.59199200
H	1.91601600	2.17850100	0.73814000
C	-1.91020600	-0.09706300	-0.10076100
C	-2.73344600	-1.36113000	-0.11965000
H	-3.74443200	-1.11941000	-0.44766900
H	-2.29818700	-2.09823800	-0.80183200
H	-2.77558500	-1.81536000	0.87519000
O	-2.46718500	0.97347100	-0.44098800
O	-0.35148700	2.21083600	-0.07064500
H	-1.31125500	2.00225700	-0.29940700
H	2.35034600	0.96568000	-1.40985300
H	0.48967600	-1.32974400	1.76956000

### Pr-2'

E(RwB97XD) = -500.472222126

C	0.11905300	-1.29717400	0.85162500
C	1.21047400	-1.85257700	-0.04350600
C	2.20464400	-1.16968900	-0.61852500
C	-0.54374400	-0.01924300	0.35744300
C	2.50537000	0.30203100	-0.49802400
C	0.22707700	1.09502900	0.26068100
C	1.70233300	1.05723900	0.57257700
H	-0.63610600	-2.07151900	0.98458300
H	1.16971700	-2.92465900	-0.22694200

H	2.89544700	-1.72207400	-1.25341700
H	3.57164700	0.41764700	-0.26974200
H	1.86219900	0.58631500	1.54790900
H	2.08979300	2.07850800	0.65971100
C	-1.95854700	-0.03376000	-0.07120400
C	-2.62369600	-1.38266300	-0.29350000
H	-3.57431800	-1.21713600	-0.80118600
H	-1.99671700	-2.05159200	-0.89102200
H	-2.82190700	-1.87724900	0.66367900
O	-2.60791600	0.98797600	-0.26619700
O	-0.26089700	2.26561100	-0.19039600
H	0.44952500	2.91228300	-0.25095700
H	2.35864600	0.78181000	-1.47535400
H	0.52479100	-1.13619100	1.86009000

#### 2.4 Channel 1 in route 3

##### TS-6

$$E(RwB97XD) = -500.413326234$$

C	-0.13817800	-1.33791100	0.94207200
C	-0.47076700	-1.50340200	-0.49561000
C	0.38831700	-0.01319300	0.44728300
H	-0.97303500	-1.28110700	1.63500500
H	0.61732400	-2.01657700	1.32936000
H	0.29212200	-1.94257600	-1.13096700
C	1.77245700	0.07388400	-0.03556300
C	-0.45977000	1.14089500	0.39924000
O	-0.11265300	2.18043900	-0.39230600
O	2.18991300	1.08303200	-0.62274000
C	-1.67663200	-1.09201900	-1.08433500
C	-2.72519500	-0.59255900	-0.34117700
H	-2.91387200	-0.95146100	0.66134700
C	-1.72671800	1.15883200	0.93695700
C	2.73283700	-1.06532800	0.21572200
H	2.37578200	-2.00713800	-0.21087300
H	3.69466700	-0.81493400	-0.23067300
H	2.86021900	-1.21974700	1.29200300
H	-1.95975800	0.55839400	1.80353800
H	-2.33835900	2.03886900	0.77021500
H	-1.68341500	-0.96633700	-2.16387500
H	-3.57532600	-0.13830400	-0.84006700
H	0.80746800	2.01796300	-0.70218400

**TS-7**

E(RwB97XD) = -500.406266708

C	-0.31944100	-1.35199600	0.94941200
C	-0.71105500	-1.47715500	-0.47329800
C	0.39284400	-0.12647400	0.42289400
H	-1.11506300	-1.17152000	1.66784500
H	0.37488600	-2.11197700	1.29762400
H	-0.01607100	-2.00785600	-1.11552300
C	1.81317000	-0.34043100	0.04586700
C	-0.27921000	1.11388500	0.33099900
O	0.20905200	1.97630800	-0.61561100
O	2.26642200	-1.48070300	-0.01006100
C	-1.87044500	-0.91226700	-1.02025800
C	-2.78777100	-0.23246200	-0.23752300
H	-2.99403500	-0.56113100	0.77279600
C	-1.53048700	1.33492800	0.87374400
C	2.73047100	0.83333400	-0.20884100
H	2.53035800	1.66573800	0.46859400
H	3.75995200	0.48911200	-0.10091200
H	2.57685700	1.20213700	-1.22650500
H	-1.78408300	0.87057800	1.81664600
H	-2.04844000	2.26455700	0.65274100
H	-1.91712700	-0.81204200	-2.10161400
H	-3.59154000	0.32221200	-0.71255500
H	-0.20793500	2.83718900	-0.51174400

**2.5 Route 2****TS-8**

E(RwB97XD) = -1315.23391960

C	5.99709000	0.57867100	0.19212900
C	4.66792100	0.03025400	-0.27082200
H	6.63802200	0.69971600	-0.68314100
H	5.85843100	1.53784900	0.69741400
H	6.46671200	-0.08224600	0.92437200
C	3.62187600	-0.34340200	0.67827800
C	3.76435000	-0.21064100	2.11909900
C	2.69903400	-0.80790600	3.01927500
H	3.03663200	-0.72675400	4.05307600
H	1.76388700	-0.24706800	2.90928200
O	4.46955600	-0.10295800	-1.48939100
O	4.71257800	0.37774700	2.65422000

C	2.41297900	-1.00483900	0.04182500
C	1.92666400	0.37677100	-0.06849500
H	1.84375400	-1.65595100	0.70173900
H	2.66042300	-1.49104100	-0.90040300
C	0.88032400	0.98416900	0.65197700
H	2.41416300	0.95811100	-0.84537800
C	-0.13474900	0.29430400	1.31990700
H	0.79800200	2.06509700	0.57907700
H	-0.76410000	0.82780200	2.02447300
H	-0.02039200	-0.76134000	1.54756900
P	-1.95618100	-0.02460100	-0.19683400
C	-1.85957600	-1.49835800	-1.30009400
C	-0.42288800	-1.86448500	-1.68245500
H	-2.46039100	-1.29489300	-2.19680700
H	-2.32982300	-2.34111100	-0.78106200
C	-0.34658700	-3.01495200	-2.68595600
H	0.09510900	-0.99251800	-2.10152900
H	0.12761000	-2.14258100	-0.77750900
C	1.09587600	-3.38728900	-3.02607600
H	-0.86857200	-3.88910000	-2.27587800
H	-0.88224700	-2.73255300	-3.60118000
H	1.13512000	-4.19554100	-3.76198100
H	1.63513100	-2.52845900	-3.43990500
H	1.63621400	-3.71883100	-2.13277900
C	-1.64179100	1.37682100	-1.33710200
C	-1.91483400	2.75076700	-0.71726200
H	-2.22395500	1.23897400	-2.25583800
H	-0.58109800	1.30701100	-1.61065200
C	-1.39447200	3.89334700	-1.59112000
H	-2.99215600	2.88301900	-0.55817200
H	-1.44429700	2.81642500	0.27266200
C	-1.65449700	5.26840900	-0.97943400
H	-0.31726900	3.75744900	-1.74991100
H	-1.86506500	3.83174000	-2.58047000
H	-1.27849700	6.06670300	-1.62582500
H	-2.72659800	5.43589900	-0.82849400
H	-1.16113900	5.36460600	-0.00612800
C	-3.74786300	0.11581600	0.22278000
C	-4.24758400	-0.98528600	1.16281200
H	-4.32918600	0.12226300	-0.70909300
H	-3.88895100	1.09421800	0.69632400
C	-5.72436100	-0.81295000	1.52388500
H	-4.10980500	-1.96952600	0.69761800
H	-3.64643000	-0.98738100	2.08150900

C	-6.23429600	-1.90790700	2.45916100
H	-5.86787300	0.16897500	1.99246300
H	-6.32020100	-0.80745600	0.60225200
H	-7.29318800	-1.76582400	2.69372400
H	-6.12143800	-2.89735300	2.00268900
H	-5.67828300	-1.90966700	3.40291700
H	2.49169300	-1.85583800	2.78297400

#### Int-4

E(RwB97XD) = -1315.28974553

C	5.99992200	-1.10690300	0.25895100
C	4.48389400	-1.15328300	0.26743600
H	6.37794000	-2.05200500	0.65616400
H	6.37782700	-0.94458100	-0.75445000
H	6.37257900	-0.26647500	0.85023800
C	3.71120300	-0.02238300	-0.14367300
C	4.25746300	1.18934400	-0.65567700
C	3.27095500	2.28171800	-1.09267400
O	3.93588400	-2.21931100	0.65020600
O	5.47466700	1.45419700	-0.78288600
C	2.21066800	-0.20867000	-0.05114100
C	1.61259500	-0.70743300	-1.33469400
H	1.70705500	0.70321400	0.28928100
H	2.03715700	-0.97875300	0.71225700
C	0.53745200	-0.23666200	-1.97947600
H	2.14216900	-1.54773500	-1.78054200
C	-0.30199100	0.92362300	-1.50550200
H	0.22565800	-0.69816700	-2.91303100
P	-1.69503200	0.41275900	-0.45063000
C	-2.72072700	-0.77016800	-1.36563700
C	-4.01143800	-1.17237100	-0.64058300
H	-2.08583900	-1.64454600	-1.55012900
H	-2.94049800	-0.32462500	-2.34219100
C	-4.69980500	-2.35330600	-1.32760200
H	-3.79689600	-1.44245600	0.40130700
H	-4.69937400	-0.31926300	-0.60884200
C	-6.00458600	-2.74586700	-0.63828100
H	-4.89470400	-2.09881200	-2.37660600
H	-4.01302800	-3.20853900	-1.33607000
H	-6.46717200	-3.60477900	-1.13198500
H	-5.82959100	-3.01531800	0.40877300
H	-6.72454400	-1.92080400	-0.65646200
C	-2.68805700	1.87654500	-0.03435300

C	-1.90632900	2.96525200	0.71354700
H	-3.53362900	1.52854900	0.57014100
H	-3.10023700	2.26765900	-0.97208600
C	-2.80529600	4.14130700	1.10067300
H	-1.45233200	2.54626400	1.61979300
H	-1.08469900	3.33271700	0.08792500
C	-2.03835400	5.24147100	1.83166700
H	-3.26977200	4.55264600	0.19598200
H	-3.62263300	3.77563100	1.73448200
H	-2.70156800	6.06657900	2.10526900
H	-1.58202900	4.85812300	2.75034400
H	-1.23810600	5.64644200	1.20359500
C	-1.11806000	-0.34602500	1.10092200
C	-0.76984100	-1.83958200	1.02313900
H	-1.90548800	-0.17503200	1.84478500
H	-0.24415900	0.23012900	1.42463600
C	-0.18300700	-2.34345000	2.34259800
H	-1.66928400	-2.41979100	0.78299600
H	-0.05165100	-2.01745100	0.21764300
C	0.22775800	-3.81185300	2.26202200
H	0.69286400	-1.73607000	2.60151500
H	-0.91739300	-2.20008500	3.14578800
H	0.63198300	-4.15913300	3.21667800
H	-0.62639000	-4.44847900	2.00521400
H	1.00174400	-3.95450700	1.50124100
H	0.28770200	1.64076300	-0.92512700
H	-0.74172000	1.46971200	-2.34753100
H	3.83658700	3.10022400	-1.54102600
H	2.54596500	1.90594800	-1.82371000
H	2.71006600	2.67450600	-0.23534300

### Int-5

E(RwB97XD) = -1315.27224337

C	-5.38064100	-0.07836700	0.71768400
C	-4.23798200	-1.05393500	0.83385700
H	-6.18491600	-0.35853800	1.39921600
H	-4.99561600	0.91487700	0.96765700
H	-5.74880400	-0.02945400	-0.31189800
C	-3.19219400	-1.01681400	-0.26451000
C	-2.73734500	0.42452100	-0.61765800
C	-2.43228000	0.66825100	-1.93186700
O	-4.18341700	-1.86337100	1.74672600
O	-2.63312100	1.25942800	0.35799400

C	-2.04253800	-2.02958600	-0.04096700
C	-1.33483400	-2.14481600	1.29425000
H	-1.30827300	-1.83497000	-0.82869500
H	-2.44677700	-3.02385200	-0.25196300
C	-0.51746700	-1.30469700	1.94060900
H	-1.46649000	-3.11125700	1.77587500
C	-0.21790200	0.13202600	1.60649300
H	-0.06936100	-1.66895300	2.86311600
P	1.21698600	0.46616300	0.55771000
C	2.71989600	-0.16528300	1.36106100
C	4.02162500	0.09609400	0.59540700
H	2.56309900	-1.24112100	1.50466100
H	2.75857100	0.28462200	2.35990600
C	5.22720100	-0.54283000	1.28743600
H	3.94322100	-0.29889200	-0.42498500
H	4.19183600	1.17510100	0.50144300
C	6.52800700	-0.30864800	0.52212800
H	5.31614900	-0.13626100	2.30244700
H	5.05056500	-1.61995800	1.39667900
H	7.37798100	-0.76264800	1.03905800
H	6.47492900	-0.74375300	-0.48166800
H	6.73319600	0.76162700	0.41282600
C	1.32844900	2.26979500	0.37321200
C	0.20974000	2.84483400	-0.50882900
H	2.31555700	2.51073700	-0.03635900
H	1.28290900	2.68967700	1.38537600
C	0.15966000	4.37135600	-0.44311600
H	0.37084900	2.53156700	-1.54742400
H	-0.76558400	2.43970900	-0.20764100
C	-0.92249400	4.94076200	-1.35894000
H	-0.03711500	4.67679800	0.59232700
H	1.13754400	4.79147900	-0.71390000
H	-0.98435800	6.02954400	-1.27139600
H	-0.71756900	4.69772400	-2.40726600
H	-1.90191100	4.52231500	-1.10596400
C	1.06137500	-0.26268600	-1.09667500
C	1.38180500	-1.76000700	-1.18407100
H	1.72373000	0.31041600	-1.75700900
H	0.02979900	-0.05066300	-1.41941100
C	1.04730600	-2.32061300	-2.56725000
H	2.44518500	-1.93082000	-0.97478000
H	0.82326600	-2.31304800	-0.42151000
C	1.33367600	-3.81675100	-2.67014600
H	-0.01111800	-2.12967500	-2.78418400

H	1.62214400	-1.77621500	-3.32704200
H	1.09538100	-4.19765200	-3.66725000
H	2.39014900	-4.02973600	-2.47333100
H	0.73672600	-4.37941200	-1.94433400
H	-1.08705900	0.62206500	1.12459400
H	-0.01824600	0.69115900	2.52882400
H	-2.07504000	1.64714000	-2.24002900
H	-2.57782300	-0.08914500	-2.69682600
H	-3.72759500	-1.38707900	-1.15120500

### TS-9

E(RwB97XD) = -1315.21201385

C	4.26374600	0.75745900	0.49402900
C	2.96357100	1.06490700	-0.19367400
H	4.17266300	0.91579600	1.56966700
H	4.52943200	-0.27926300	0.26701400
H	5.05272700	1.40097700	0.08892700
C	2.89032500	0.83049200	-1.70294400
C	2.62659000	-0.68327200	-1.97039000
C	1.67763600	-1.03475200	-2.93935900
H	1.57357600	-2.09414500	-3.15913000
O	2.00252300	1.50042800	0.42151600
O	3.18774900	-1.49823200	-1.19531600
C	1.95833700	1.84437500	-2.38618800
C	0.45706500	1.74116400	-2.29833700
H	2.19848900	1.85646600	-3.45842100
H	2.23590900	2.84366400	-2.02845500
C	-0.34104200	0.73837100	-1.91958000
H	-0.04455200	2.62192800	-2.69819400
C	0.06446800	-0.56351300	-1.34497400
H	-1.41141300	0.87262300	-2.06293900
P	-1.28740000	-0.51175500	0.62045800
C	-2.54577700	0.79228900	0.95493800
C	-1.96335000	2.20909500	0.99930800
H	-3.05244900	0.55467800	1.90050200
H	-3.30103800	0.72786100	0.16189000
C	-3.04446800	3.27436700	1.18823400
H	-1.23666200	2.28842100	1.81660800
H	-1.40938400	2.40912400	0.07463500
C	-2.47089800	4.69031600	1.20408000
H	-3.78461200	3.18607600	0.38235700
H	-3.58192300	3.08248300	2.12587300
H	-3.25697100	5.43788300	1.34664300

H	-1.74169900	4.80936600	2.01274800
H	-1.96026600	4.91438100	0.26120800
C	-0.10561600	-0.36677100	2.01956700
C	0.94192700	-1.48459700	2.07544800
H	-0.67056200	-0.31817900	2.96024500
H	0.40807900	0.59117100	1.88497800
C	1.99785300	-1.21897600	3.14941900
H	0.45835200	-2.45046300	2.27070200
H	1.45252800	-1.58094200	1.10932200
C	3.08814300	-2.28796200	3.17344500
H	2.44895900	-0.23696900	2.96079400
H	1.51158000	-1.15595900	4.13168800
H	3.83579400	-2.07653600	3.94386400
H	2.66445800	-3.27752500	3.37780700
H	3.60175800	-2.33830400	2.20737700
C	-2.18013600	-2.09513700	0.94228600
C	-3.47343600	-2.26727700	0.13606200
H	-2.39087500	-2.16016900	2.01694900
H	-1.48004000	-2.90466200	0.70324100
C	-3.29134100	-2.17863000	-1.38052800
H	-3.90236500	-3.24536800	0.38601000
H	-4.21237100	-1.52241100	0.45749200
C	-4.58797500	-2.44786300	-2.14117400
H	-2.91407600	-1.18403000	-1.65322000
H	-2.52270400	-2.89642500	-1.69488000
H	-4.43785700	-2.36690300	-3.22150900
H	-4.96699800	-3.45300300	-1.92767500
H	-5.36460500	-1.73016400	-1.85513200
H	1.36817500	-0.33775500	-3.70778400
H	-0.41305700	-1.47305300	-1.68100100
H	0.87814400	-0.66526600	-0.65089100
H	3.90094100	1.00883800	-2.09378100

## 2.6 Channel 3 in route 3

### TS-10

E(RwB97XD) = -1315.21318200

C	-5.13912400	0.21419600	-1.27431800
C	-4.83352200	-0.06133000	0.18705200
H	-6.08250300	-0.27155000	-1.52471400
H	-5.23735200	1.29159400	-1.44620900
H	-4.36247200	-0.15399900	-1.95203100
C	-3.61389200	0.41357500	0.76858000

C	-3.38696500	0.29820700	2.20965000
C	-2.42575300	0.95359600	2.90318000
H	-1.80763900	1.71662200	2.45181200
H	-2.32560000	0.78372500	3.96909800
O	-5.70624100	-0.68188800	0.84789800
O	-4.18273100	-0.56778400	2.88891900
H	-4.91941000	-0.81409000	2.27496800
C	-2.54693500	1.01555200	-0.11413700
C	-2.04225100	-0.36370800	-0.30550900
H	-1.87545400	1.69761800	0.40330300
H	-2.92124200	1.49724000	-1.01672600
C	-0.99740700	-0.98903500	0.37205000
H	-2.58031900	-0.95931300	-1.03649800
C	-0.04620600	-0.33893600	1.16845300
H	-0.90466600	-2.06499200	0.25059400
H	0.52715000	-0.91183700	1.88829600
H	-0.16039000	0.70524800	1.42504600
P	1.91706800	0.01454000	-0.20639900
C	1.89769900	1.52369100	-1.26653500
C	0.53931600	1.78354100	-1.92406800
H	2.68337300	1.42670300	-2.02838200
H	2.16728100	2.37534500	-0.63126400
C	0.53128800	3.04730600	-2.78494300
H	0.24883100	0.92660200	-2.54488600
H	-0.22863900	1.87583100	-1.14900300
C	-0.83379000	3.30553400	-3.42050300
H	0.81939100	3.90679600	-2.16623000
H	1.29481600	2.95785000	-3.56817900
H	-0.82519500	4.21539800	-4.02780000
H	-1.12981600	2.47249800	-4.06750000
H	-1.60653800	3.42234500	-2.65263100
C	1.71448300	-1.35445500	-1.41128200
C	1.95335500	-2.74123900	-0.80530400
H	2.36811700	-1.18684600	-2.27591200
H	0.67885300	-1.28837700	-1.76798900
C	1.47779900	-3.86624700	-1.72624600
H	3.02104400	-2.87651300	-0.59226300
H	1.43209000	-2.82602300	0.15779400
C	1.72600600	-5.25423300	-1.13935100
H	0.40589000	-3.73437800	-1.92137800
H	1.98376300	-3.77666100	-2.69594000
H	1.36971100	-6.03860200	-1.81343300
H	2.79437200	-5.42199600	-0.96455600
H	1.20818800	-5.37366100	-0.18148100

C	3.67190000	-0.12047600	0.35069500
C	4.09152400	1.00346700	1.30285500
H	4.32917800	-0.14903700	-0.52892300
H	3.76975300	-1.08782900	0.85725900
C	5.49956200	0.80079100	1.86577000
H	4.05184900	1.96889300	0.78287600
H	3.37654500	1.06765500	2.13383600
C	5.92202300	1.92737100	2.80702200
H	5.53930200	-0.15878500	2.39657300
H	6.21357500	0.72604400	1.03564900
H	6.92536700	1.75620200	3.20771300
H	5.92781600	2.89193200	2.28788700
H	5.23206900	2.00860200	3.65401600

### Int-6

E(RwB97XD) = -1315.26375720

C	4.42959000	1.47963800	-0.97384500
C	4.63645800	0.40027200	0.08724200
H	5.39203300	1.95511200	-1.16983900
H	4.05824000	1.05423300	-1.91462200
H	3.71738200	2.24868500	-0.65462300
C	3.54588400	-0.26868100	0.63543700
C	3.72843100	-1.28974100	1.66600500
C	2.73060700	-1.98147800	2.28534500
O	5.85950300	0.17102700	0.41485800
O	5.00853900	-1.56184100	2.01695900
H	5.58192200	-0.94800800	1.46066100
C	2.13835000	0.02783800	0.18620900
C	1.37053500	0.91667500	1.12932300
H	1.59427600	-0.91188900	0.01457600
H	2.16511800	0.53110500	-0.78671200
C	0.11370900	0.76900600	1.56229100
H	1.92890900	1.77612500	1.49825100
C	-0.79513500	-0.37667800	1.19563200
H	-0.30227300	1.50184300	2.24965300
P	-1.83595600	-0.02364600	-0.25698500
C	-0.83428900	0.05627000	-1.77495100
C	-0.19415200	1.41983700	-2.07241000
H	-1.48885600	-0.24785300	-2.60016700
H	-0.06257700	-0.71578500	-1.67756700
C	0.79984500	1.32859900	-3.23173800
H	-0.97533700	2.14854900	-2.31872200
H	0.32113400	1.79687100	-1.18352900

C	1.49687600	2.66093600	-3.49625100
H	1.55077100	0.56270000	-3.00102200
H	0.27791100	0.99043100	-4.13564700
H	2.21264300	2.57385900	-4.31810700
H	0.77361200	3.44031700	-3.75901900
H	2.04716500	2.99418100	-2.60990600
C	-2.69304600	1.55606600	-0.00834800
C	-3.60083200	1.59286600	1.22687600
H	-3.26319600	1.76374000	-0.92128000
H	-1.91255900	2.32169700	0.06616100
C	-4.25572200	2.96462300	1.40394500
H	-4.38396200	0.82999900	1.14268100
H	-3.02040400	1.35527300	2.12678200
C	-5.17043500	3.01446100	2.62585600
H	-3.47318200	3.72768100	1.49445800
H	-4.82865200	3.20910900	0.50087900
H	-5.63313900	3.99948300	2.73117600
H	-5.97284400	2.27325500	2.54655800
H	-4.61194600	2.80676000	3.54463900
C	-3.05480300	-1.35839800	-0.43867100
C	-2.43080800	-2.73014200	-0.73063800
H	-3.74039400	-1.06281900	-1.24167300
H	-3.63784800	-1.39325800	0.48853900
C	-3.49881400	-3.81821700	-0.86127000
H	-1.84547900	-2.68629600	-1.65689200
H	-1.73559200	-3.00589400	0.07076700
C	-2.89422500	-5.19014300	-1.15216600
H	-4.08189100	-3.86048000	0.06705500
H	-4.19924400	-3.54307000	-1.65942000
H	-3.67278800	-5.95419500	-1.22680000
H	-2.33889400	-5.18328600	-2.09593200
H	-2.20248200	-5.49154300	-0.35882800
H	-0.23425100	-1.28882600	0.96612400
H	-1.47891400	-0.61943500	2.01609300
H	1.68546300	-1.78235400	2.08830000
H	2.97699600	-2.72646800	3.03396900

### TS-11

E(RwB97XD) = -1315.21376397

C	-4.08109500	-1.80331000	-0.06645600
C	-3.75639000	-0.33408300	-0.26700900
H	-4.59815500	-1.91647700	0.88746500
H	-4.73174700	-2.17591300	-0.86507800

H	-3.17956300	-2.42389800	-0.05697700
C	-2.96436000	0.09434000	-1.34772800
C	-2.63317400	1.48257400	-1.46785700
C	-1.71076200	1.99610300	-2.38289400
H	-1.55665300	3.07117900	-2.37512400
O	-4.23230600	0.47017000	0.60622000
O	-3.07113600	2.32366800	-0.52429700
C	-2.39840400	-0.87655000	-2.35499600
C	-0.90244900	-0.98743100	-2.52251200
H	-2.77697200	-0.63571200	-3.36332500
H	-2.78312700	-1.88249900	-2.16650500
C	0.08225900	-0.19291000	-2.08356600
H	-0.60039200	-1.78394100	-3.20211300
C	-0.01056300	0.98469700	-1.18809100
H	1.08533600	-0.39202200	-2.45481500
P	1.41613800	0.13614000	0.52056500
C	3.03726700	-0.72457600	0.31867600
C	2.94029800	-2.07166700	-0.40461400
H	3.47766100	-0.86257000	1.31583900
H	3.70039700	-0.04931400	-0.23491700
C	4.30900900	-2.72407100	-0.60782100
H	2.30246700	-2.75454400	0.16976300
H	2.45474600	-1.94102400	-1.37917900
C	4.20837600	-4.08027900	-1.30397900
H	4.94603200	-2.05221600	-1.19690400
H	4.79971600	-2.84455500	0.36643900
H	5.19515500	-4.53175700	-1.44203700
H	3.59940500	-4.77646200	-0.71708100
H	3.74322100	-3.98030600	-2.29072800
C	0.36696800	-1.10034600	1.39275800
C	-0.87293300	-0.52252600	2.08492700
H	0.99326800	-1.63043200	2.12279300
H	0.05556500	-1.83466700	0.63947400
C	-1.69216300	-1.60979200	2.78444400
H	-0.57532300	0.22766800	2.82762000
H	-1.51676400	-0.01186000	1.35907000
C	-2.92301600	-1.04616300	3.49208900
H	-2.00350000	-2.35522200	2.04218600
H	-1.05161000	-2.13685100	3.50391900
H	-3.50434100	-1.84305300	3.96644900
H	-2.63064700	-0.33470100	4.27278700
H	-3.56987000	-0.52170100	2.78106300
C	1.75302700	1.42318100	1.79924800
C	2.92619000	2.35515300	1.47098900

H	1.92824600	0.91933300	2.75783900
H	0.83183400	2.00793200	1.90790100
C	2.79824600	3.09569300	0.13807700
H	3.00434700	3.09178900	2.27986000
H	3.86683000	1.78999100	1.48406400
C	3.90825700	4.12501700	-0.06514900
H	2.82069500	2.37547000	-0.69054100
H	1.82048300	3.59213000	0.09118000
H	3.80941100	4.62915400	-1.03064300
H	3.88067400	4.88950000	0.71843100
H	4.89432600	3.64883100	-0.03291700
H	-1.51972700	1.47901400	-3.31378300
H	0.62840000	1.83678800	-1.37252500
H	-0.72468400	1.06556300	-0.38781300
H	-3.63719100	1.75622200	0.10378200