

Supplementary Information

A Theoretical Study of the Hydrolysis Mechanism of A-234; The Suspected Novichok Agent in the Skripal Attack

Yadhav A. Imrit¹, Hanusha Bhakhoa¹, Tetiana Sergeieva², Sergi Danés², Nandini Savoo¹, Mohamed I. Elzagheid³, Lydia Rhyman^{1,4}, Diego M. Andrada² and Ponnadurai Ramasami^{1,4} *

¹Computational Chemistry Group, Department of Chemistry, Faculty of Science, University of Mauritius, Réduit 80837, Mauritius

²Faculty of Natural Sciences and Technology, Department of Chemistry, Saarland University, 66123 Saarbrücken, Federal Republic of Germany

³Department of Chemical and Process Engineering, Jubail Industrial College, Jubail Industrial City 31961, Saudi Arabia

⁴Department of Chemical Sciences, University of Johannesburg, Doornfontein, Johannesburg 2028, South Africa

*Corresponding author e-mail: p.ramasami@uom.ac.mu (P.R.)

Table of contents

Page number	Description
S3	Table S1 Relative energies in kcal mol ⁻¹ computed at B3LYP/6-31+G(d,p)
S5	Table S2 Energy barriers in kcal mol ⁻¹ computed at B3LYP/6-31+G(d,p)
S6	Figure S1 Energy profile for Pathway B
S6	Figure S2 Energy profile for Channel 1 up till PC1
S7	Figure S3 Energy profile for Channel 1 from RC3
S7	Figure S4 Energy profile for Channel 2
S8	Figure S5 Energy profile for Channel 3
S8	Figure S6 Energy profile for reaction (I)
S9	Figure S7 Energy profile for reaction (II)
S9	Figure S8 Energy profile for reaction (III)
S10	Figure S9 Energy profile for reaction (V)
S10	Figure S10 Energy profile for reaction (VI)
S11	- Cartesian coordinates of the B3LYP/6-31+G(d,p) optimised geometries in the gas phase
S77	Cartesian coordinates of the CPCM(water)-B3LYP/6-31+G(d,p) optimised geometries
S141	Cartesian coordinates of the B3LYP/6-31++G(d,p) optimised geometries in the gas phase
S156	Cartesian coordinates of the CPCM(water)-B3LYP/6-31++G(d,p) optimised geometries

Table S1. Relative energies^a computed at B3LYP/6-31+G(d,p) and in kcal mol⁻¹ as follows:

- Electronic energies, including ZPE correction, in the gaseous phase, $\Delta E_{(g)}$
- Gibbs free energies, including thermal corrections, in the gaseous phase, $\Delta G_{(g)}$
- Gibbs free energies, including thermal corrections, in the aqueous state using CPCM (water), $\Delta G_{(aq)}$

	$\Delta E_{(g)}$	$\Delta G_{(g)}$	$\Delta G_{(aq)}$
Hydrolysis at the acetoamidine (C₂) moiety			
Pathway A			
RC1	-3.59	4.17	6.96
TS1	37.94	48.02	49.86
IM1	12.76	23.95	30.83
Channel 1			
IM2	13.96	24.06	30.09
TS2	38.56	49.69	54.80
PC1	-2.67	3.46	5.92
PC1 + H₂O	-	-	-
RC3^b	-4.60	2.42	9.60
TS3^b	41.52	52.12	56.89
Pdt1^b	-11.90	-6.04	-0.21
Channel 2			
IM3	11.19	21.41	29.65
TS4	37.70	49.21	58.34
IMA	20.40	32.35	39.97
TS5	35.12	46.77	53.58
PC2	-0.73	7.50	11.25
TS6	34.90	42.10	48.49
Pdt2	-13.32	-6.66	-6.65
Channel 3			
IM4	13.32	24.35	30.98
TS7	40.73	51.39	55.58
PC3	4.93	10.57	35.91
TS8	31.08	37.16	43.53
PC1	-2.67	3.46	5.92
Channel 4			
IM5	11.14	22.17	29.22
TS9	25.99	35.86	34.58
A1...X	-17.64	-10.74	-6.26
TS11	16.93	28.76	36.02
Pathway B			
RC2	-4.05	4.45	5.74
TS10	48.07	58.77	59.55
PC3	4.93	10.57	35.91

^aRelative to the reactants A-234 and H₂O and ^brelative to **PC1** and H₂O.

Table S1. (Continued) Relative energies^a computed at B3LYP/6-31+G(d,p) and in kcal mol⁻¹ as follows:

- Electronic energies, including ZPE correction, in the gaseous phase, $\Delta E_{(g)}$
- Gibbs free energies, including thermal corrections, in the gaseous phase, $\Delta G_{(g)}$
- Gibbs free energies, including thermal corrections, in the aqueous state using CPCM (water), $\Delta G_{(aq)}$

	$\Delta E_{(g)}$	$\Delta G_{(g)}$	$\Delta G_{(aq)}$
Hydrolysis at the phosphinate moiety			
Frontside attack (S_N2)			
TSP1	46.21	56.90	56.62
P1f	-1.25	7.30	8.91
TSP2	43.32	53.87	52.83
P2f	1.25	7.84	12.79
TSP3	44.61	55.29	56.06
P3f	-1.05	5.84	4.01
Backside attack (addition-elimination)			
TSP4	27.07	37.62	41.50
IMB1	13.48	24.46	29.09
TSP5	29.41	40.66	36.95
IMB2	13.04	23.37	29.09
TSP6	17.34	28.22	32.81
P1b	-4.98	3.17	2.46
TSP7	33.61	44.39	51.86
IMB3	24.71	35.31	29.44
TSP8	26.47	36.60	33.94
IMB4	21.41	32.01	28.84
TSP9	31.87	42.82	49.38
P2b	-0.29	6.33	11.25
TSP10	37.14	48.53	51.95
IMB5	25.72	36.87	41.80
TSP11	31.62	42.71	48.60
IMB6	25.39	36.13	43.10
TSP12	36.41	47.48	53.13
P3b	1.25	9.38	11.56

^aRelative to the reactants A-234 and H₂O.

Table S2. Energy barriers computed at B3LYP/6-31+G(d,p) and in kcal mol⁻¹ as follows:

- Activation energy in the gaseous state, $E_{a(g)}$
- Gibbs energy of activation in the gaseous state, $\Delta G^\ddagger_{(g)}$
- Gibbs energy of activation in aqueous solution, $\Delta G^\ddagger_{(aq)}$

	$E_{a(g)}$	$\Delta G^\ddagger_{(g)}$	$\Delta G^\ddagger_{(aq)}$
Hydrolysis at the acetoamidine (C₂) moiety			
Pathway A			
TS1	41.53	43.85	42.90
Channel 1			
TS2	24.59	25.63	24.71
TS3	46.11	49.70	47.29
Channel 2			
TS4	26.50	27.79	28.69
TS5	14.72	14.42	13.61
TS6	36.62	34.59	37.24
Channel 3			
TS7	27.41	27.04	24.60
TS8	26.16	26.59	7.62
Channel 4			
TS9	14.85	13.69	5.36
TS11	4.17	4.81	5.19
Pathway B			
TS10	52.13	54.33	53.81
Hydrolysis at the phosphinate moiety			
Frontside attack (S_N2)			
TSP1	46.21	56.90	56.62
TSP2	43.32	53.87	52.83
TSP3	44.61	55.29	56.06
Backside attack (addition-elimination)			
TSP4	27.07	37.62	41.50
TSP5	15.93	16.20	7.86
TSP6	4.29	4.85	3.72
TSP7	33.61	44.39	51.86
TSP8	1.17	1.29	4.50
TSP9	10.46	10.81	20.54
TSP10	37.14	48.53	51.95
TSP11	5.90	5.84	6.80
TSP12	11.02	11.34	10.03

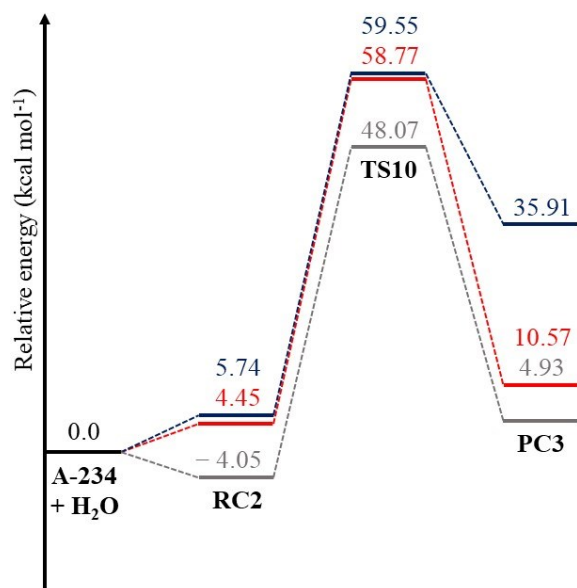


Figure S1. The energy profile of Pathway B. $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

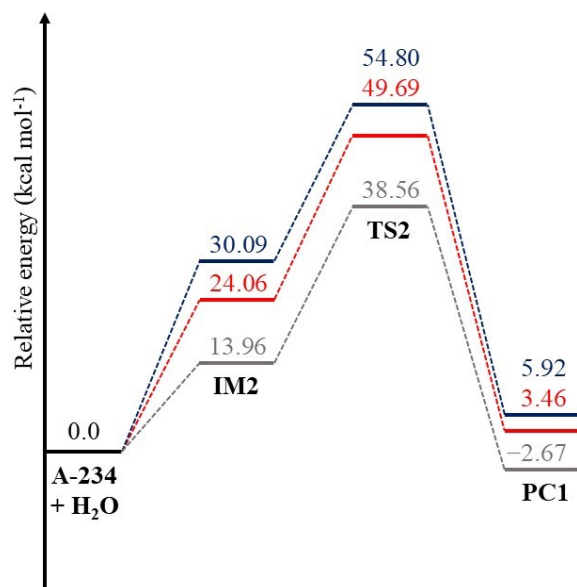


Figure S2. The energy profile of Channel 1 till PC1. $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

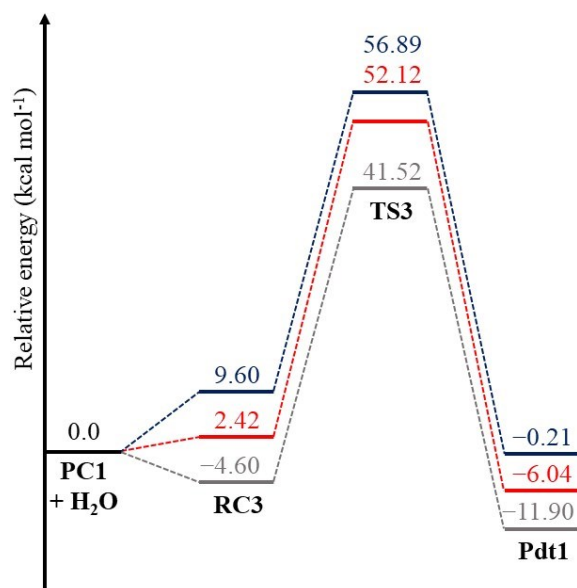


Figure S3. The energy profile of Channel 1 from **RC3**, relative to **PC1** + H₂O. $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

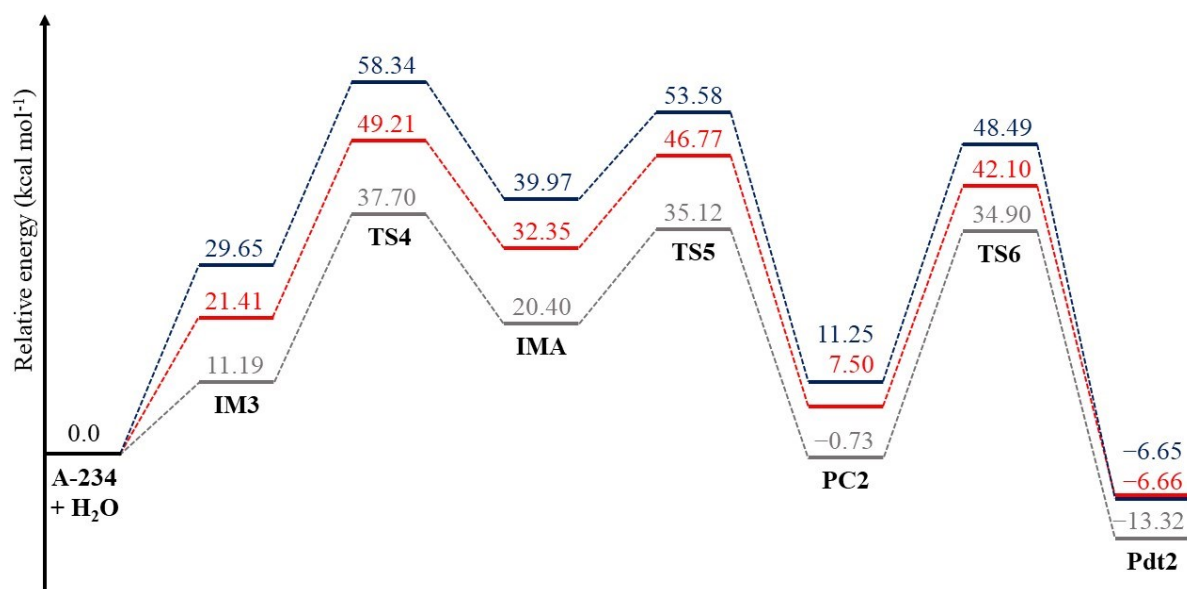


Figure S4. The energy profile of Channel 2. $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

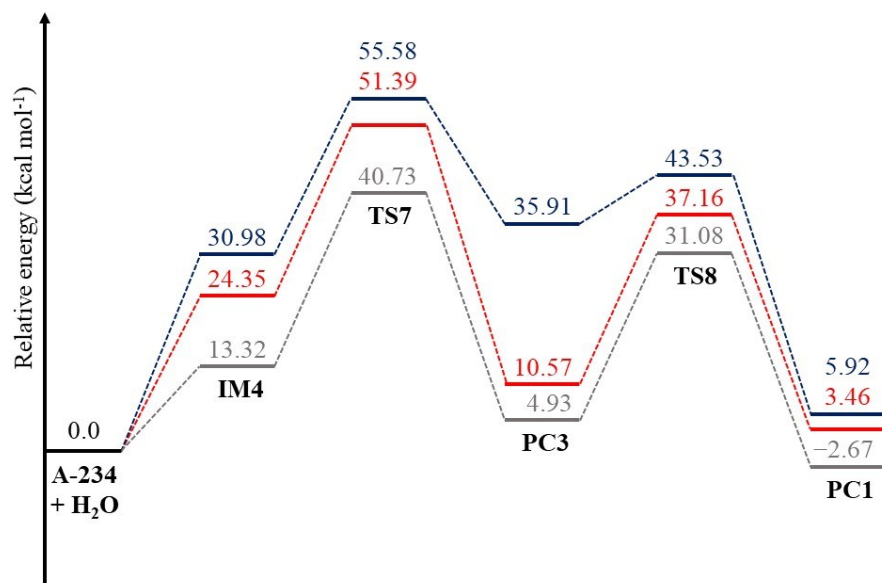


Figure S5. The energy profile of Channel 3. $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

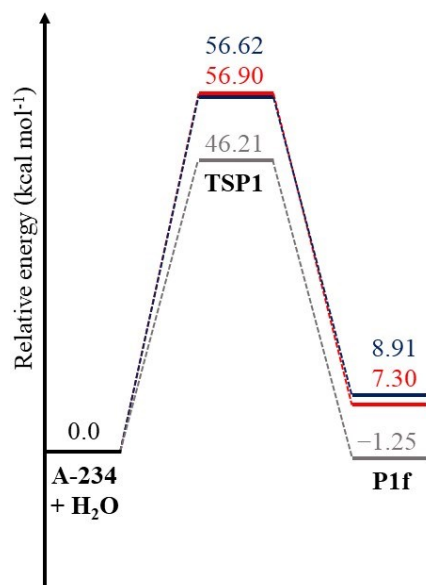


Figure S6. The energy profile of reaction (I). $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

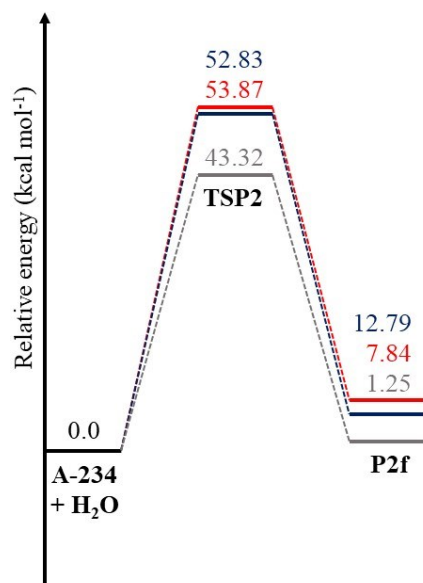


Figure S7. The energy profile of reaction (II). $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

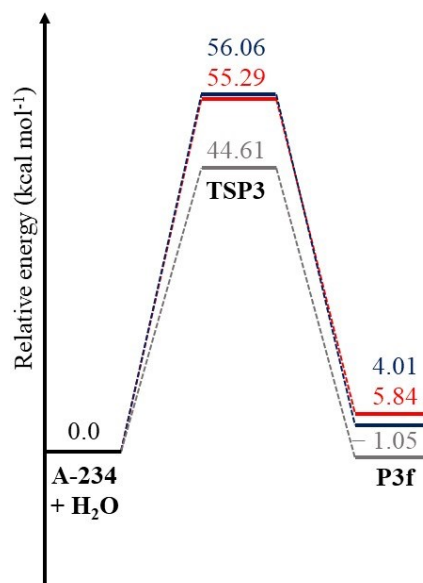


Figure S8. The energy profile of reaction (III). $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

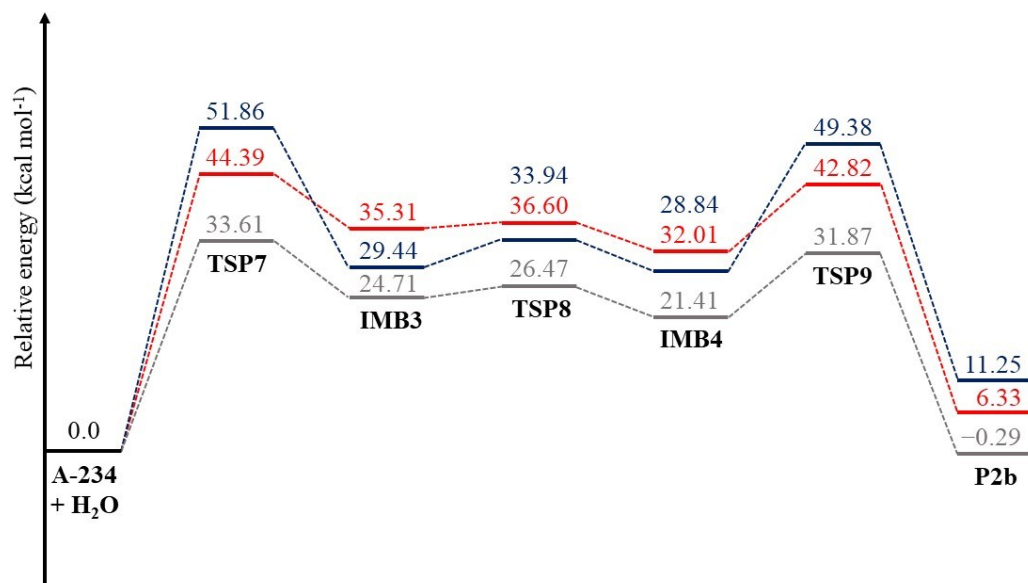


Figure S9. The energy profile of reaction (V). $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

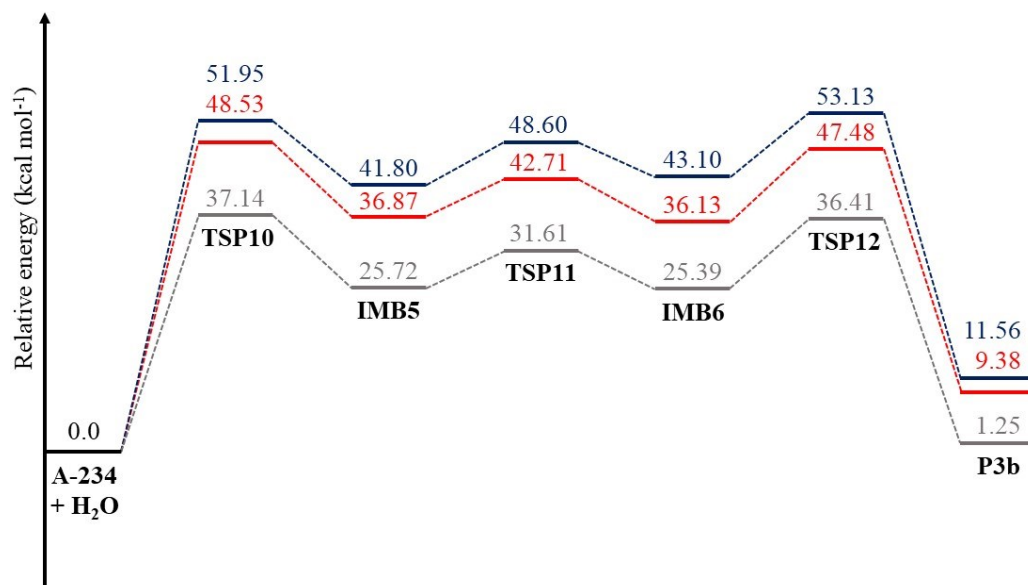


Figure S10. The energy profile of reaction (VI). $\Delta G_{(aq)}$ (in blue) was obtained using the CPCM(water)-B3LYP/6-31+G(d,p) method, and $\Delta E_{(g)}$ (in grey) and $\Delta G_{(g)}$ (in red) were obtained using the B3LYP/6-31+G(d,p) method.

Cartesian coordinates of the B3LYP/6-31G+(d,p) optimised geometries in the gas phase

A-234

7	-2.289100000	0.309809000	-0.086121000
6	-1.165582000	-0.432805000	-0.258541000
7	-0.076002000	-0.022707000	0.337055000
15	1.403442000	-0.705406000	0.356828000
8	1.712533000	-2.014586000	-0.281675000
9	1.714167000	-0.774326000	1.934412000
8	2.353715000	0.513201000	-0.096907000
6	-2.248071000	1.513758000	0.762903000
6	-1.797913000	2.762774000	0.000208000
1	-1.568479000	1.316746000	1.593315000
1	-3.253965000	1.654026000	1.171452000
1	-1.817128000	3.633249000	0.664915000
1	-0.776982000	2.634340000	-0.367684000
1	-2.456093000	2.973851000	-0.850148000
6	-3.577753000	0.001746000	-0.717782000
6	-4.528466000	-0.791719000	0.186785000
1	-3.407866000	-0.534560000	-1.652422000
1	-4.037655000	0.957241000	-0.993281000
1	-5.485995000	-0.950084000	-0.321042000
1	-4.110162000	-1.770395000	0.441255000
1	-4.726550000	-0.257645000	1.121355000
6	-1.262301000	-1.663276000	-1.141073000
1	-2.114893000	-2.289355000	-0.865186000
1	-1.387531000	-1.366053000	-2.188750000
1	-0.346361000	-2.246907000	-1.058712000
6	3.775734000	0.277844000	-0.277278000
6	4.362244000	1.486992000	-0.981263000
1	3.912092000	-0.637198000	-0.861676000

1	4.230924000	0.134783000	0.709539000
1	5.440210000	1.347563000	-1.117609000
1	3.903536000	1.623769000	-1.965229000
1	4.202144000	2.396141000	-0.393854000

H₂O

8	0.000000000	0.000000000	0.116562000
1	0.000000000	0.769394000	-0.466249000
1	0.000000000	-0.769394000	-0.466249000

Acetoamidine hydrolysis

Pathway A

RC1

7	-2.195708000	0.429719000	-0.321513000
6	-1.106633000	-0.318492000	-0.600213000
7	-0.049346000	-0.178266000	0.172822000
15	1.454181000	-0.775177000	-0.056301000
8	1.795234000	-1.788325000	-1.090461000
9	1.782921000	-1.347919000	1.417039000
8	2.361517000	0.553245000	-0.080537000
6	-2.165678000	1.439058000	0.758995000
6	-1.541544000	2.760035000	0.302508000
1	-1.627480000	1.034542000	1.614150000
1	-3.201520000	1.591926000	1.074507000
1	-1.578093000	3.487706000	1.120161000
1	-0.495330000	2.612264000	0.023277000
1	-2.079031000	3.185004000	-0.552735000
6	-3.467527000	0.313033000	-1.050503000
6	-4.474422000	-0.613704000	-0.359753000
1	-3.277973000	-0.022963000	-2.070311000
1	-3.881709000	1.323522000	-1.131770000

1	-5.416888000	-0.625022000	-0.917670000
1	-4.095964000	-1.638878000	-0.303925000
1	-4.686649000	-0.280364000	0.660512000
6	-1.184647000	-1.268838000	-1.780402000
1	-2.043795000	-1.938832000	-1.685720000
1	-1.294697000	-0.710161000	-2.716400000
1	-0.274524000	-1.862904000	-1.840091000
6	3.786604000	0.443170000	-0.351271000
6	4.318197000	1.838272000	-0.619057000
1	3.932706000	-0.219330000	-1.209553000
1	4.269969000	-0.004334000	0.524602000
1	5.395845000	1.791108000	-0.809672000
1	3.830925000	2.278430000	-1.494288000
1	4.147001000	2.493075000	0.240587000
8	-0.911162000	-0.788710000	3.047448000
1	-0.251180000	-1.229145000	3.596314000
1	-0.466067000	-0.631775000	2.196599000

TS1

7	-2.048200000	0.473362000	-0.076179000
6	-1.276852000	-0.591462000	-0.011850000
7	0.058657000	-0.409119000	0.449004000
15	1.386015000	-0.403745000	-0.519851000
8	1.206596000	0.133964000	-1.893736000
9	1.915627000	-1.929927000	-0.606669000
8	2.479541000	0.248872000	0.435129000
6	-1.672362000	1.767997000	0.544698000
6	-1.160585000	2.779758000	-0.481268000
1	-0.919558000	1.572734000	1.305522000
1	-2.569378000	2.144573000	1.043246000
1	-0.935868000	3.721489000	0.028761000

1	-0.249272000	2.419953000	-0.965673000
1	-1.906533000	2.986456000	-1.254697000
6	-3.425025000	0.411671000	-0.622604000
6	-4.462480000	-0.000028000	0.424737000
1	-3.433958000	-0.264714000	-1.477109000
1	-3.646637000	1.409200000	-1.007169000
1	-5.454466000	0.007155000	-0.036296000
1	-4.267309000	-1.003943000	0.810428000
1	-4.476722000	0.695479000	1.268883000
6	-1.631927000	-1.866374000	-0.719615000
1	-2.677752000	-2.141093000	-0.593585000
1	-1.425490000	-1.750249000	-1.792152000
1	-1.011517000	-2.669378000	-0.326909000
6	3.902223000	0.267781000	0.066941000
6	4.631196000	1.108414000	1.093489000
1	3.992028000	0.690129000	-0.937478000
1	4.261704000	-0.764536000	0.059447000
1	5.696945000	1.130912000	0.844717000
1	4.255424000	2.135591000	1.097095000
1	4.519962000	0.685384000	2.096093000
8	-1.364719000	-1.559170000	2.043720000
1	-1.862716000	-0.988239000	2.646817000
1	0.010581000	-0.896959000	1.390002000

IM1

7	-1.751478000	0.215385000	-0.086129000
6	-1.135600000	-1.013361000	0.372788000
7	0.294573000	-0.711099000	0.642939000
15	1.277362000	0.231868000	-0.312907000
8	1.197353000	1.706817000	-0.249420000
9	1.056512000	-0.280698000	-1.822333000
8	2.697287000	-0.420920000	0.066453000
6	-1.828102000	1.284228000	0.931470000
6	-1.925841000	2.688632000	0.331967000
1	-0.911107000	1.238461000	1.522996000
1	-2.674274000	1.119455000	1.620444000
1	-1.867182000	3.427525000	1.138611000
1	-1.093093000	2.861208000	-0.353738000
1	-2.870968000	2.857934000	-0.193463000
6	-2.955238000	0.102171000	-0.926037000
6	-4.255228000	-0.338012000	-0.230391000
1	-2.732721000	-0.571838000	-1.755552000
1	-3.108509000	1.082428000	-1.385864000
1	-5.064737000	-0.391261000	-0.967468000
1	-4.153965000	-1.319895000	0.240946000
1	-4.563578000	0.371723000	0.544041000
6	-1.261222000	-2.178203000	-0.614342000
1	-2.294198000	-2.520720000	-0.694966000
1	-0.883577000	-1.897032000	-1.598340000
1	-0.664102000	-3.009894000	-0.232607000
6	3.930661000	0.333333000	-0.123564000
6	5.008641000	-0.312944000	0.724373000
1	3.752278000	1.373412000	0.162283000
1	4.185727000	0.299140000	-1.188060000

1	5.954602000	0.220255000	0.581235000
1	4.746948000	-0.272361000	1.785936000
1	5.156482000	-1.359138000	0.440355000
8	-1.655282000	-1.540053000	1.603474000
1	-1.550169000	-0.865504000	2.289753000
1	0.782147000	-1.487461000	1.078749000

Channel 1

IM2

7	2.194208000	0.318320000	-0.356267000
6	1.190491000	-0.623850000	0.171066000
7	-0.110615000	-0.043019000	-0.204012000
15	-1.611535000	-0.609370000	0.213408000
8	-1.839852000	-1.051984000	1.603171000
9	-1.964061000	-1.787729000	-0.830260000
8	-2.516354000	0.578657000	-0.376222000
6	3.592409000	-0.131097000	-0.207271000
6	4.428982000	0.132429000	-1.463393000
1	3.585618000	-1.204377000	-0.011316000
1	4.071287000	0.348720000	0.660471000
1	4.466514000	1.196214000	-1.720139000
1	5.459587000	-0.205877000	-1.306859000
1	4.016300000	-0.405896000	-2.322885000
6	2.025988000	1.766230000	-0.118029000
6	2.100809000	2.286940000	1.328414000
1	1.080224000	2.094203000	-0.556094000
1	2.810637000	2.251043000	-0.707775000
1	2.164447000	3.381020000	1.313155000
1	1.211802000	2.018167000	1.903930000
1	2.981536000	1.913058000	1.860535000

6	1.261789000	-0.945314000	1.668986000
1	2.279051000	-1.257838000	1.914044000
1	0.994999000	-0.078610000	2.271365000
1	0.578825000	-1.758581000	1.916559000
6	-3.970111000	0.480388000	-0.312954000
6	-4.543641000	1.829117000	-0.700279000
1	-4.255905000	0.199066000	0.705215000
1	-4.291299000	-0.306629000	-1.003291000
1	-5.637448000	1.783627000	-0.670232000
1	-4.209966000	2.606901000	-0.007377000
1	-4.237561000	2.107942000	-1.713039000
8	1.394988000	-1.876488000	-0.472958000
1	1.450505000	-1.706863000	-1.425811000
1	-0.085276000	0.357189000	-1.138459000

TS2

7	-2.192752000	0.244549000	0.477773000
6	-1.194743000	-1.045640000	0.471779000
7	0.192454000	-0.584899000	0.681859000
15	1.448519000	-0.477514000	-0.382586000
8	1.136798000	-0.049419000	-1.764539000
9	2.178014000	-1.916341000	-0.396097000
8	2.497414000	0.378150000	0.476817000
6	-3.441282000	0.051056000	-0.305065000
6	-4.560863000	1.008307000	0.107024000
1	-3.770727000	-0.971715000	-0.112177000
1	-3.232682000	0.138561000	-1.377601000
1	-4.347957000	2.048206000	-0.156137000
1	-5.484206000	0.721396000	-0.406194000
1	-4.745171000	0.954780000	1.185282000
6	-1.634625000	1.620509000	0.417079000

6	-1.366324000	2.165962000	-0.988084000
1	-0.712351000	1.609652000	0.998931000
1	-2.338417000	2.267120000	0.950703000
1	-0.909884000	3.158052000	-0.901977000
1	-0.674790000	1.528496000	-1.545214000
1	-2.286313000	2.281525000	-1.569851000
6	-1.322716000	-1.942472000	-0.755668000
1	-2.339718000	-2.322511000	-0.844358000
1	-1.030327000	-1.437928000	-1.680136000
1	-0.664997000	-2.802582000	-0.602168000
6	3.854940000	0.586167000	-0.016848000
6	4.528333000	1.595790000	0.891324000
1	3.798354000	0.946957000	-1.048604000
1	4.375043000	-0.376980000	-0.003877000
1	5.555475000	1.765082000	0.551235000
1	3.996012000	2.551193000	0.874441000
1	4.561447000	1.231815000	1.922452000
8	-1.684968000	-1.534152000	1.638206000
1	-2.288595000	-0.383668000	1.559561000
1	0.441707000	-0.709908000	1.658804000

PC1

7	1.108050000	1.726230000	0.170449000
6	0.307545000	2.247963000	-0.867651000
7	-3.176815000	-0.179121000	-0.285050000
1	1.522447000	2.451830000	0.748193000
8	0.174160000	3.456507000	-0.941187000
1	-4.076706000	0.078251000	-0.687696000
6	-2.986277000	-1.630589000	-0.384863000
6	-3.080049000	-2.093492000	-1.838246000
1	-3.711385000	-2.202861000	0.220270000

1	-1.989798000	-1.852355000	0.014224000
1	-2.918848000	-3.174485000	-1.910480000
1	-4.069272000	-1.878171000	-2.261556000
1	-2.331876000	-1.589041000	-2.458181000
6	-3.063264000	0.377443000	1.069091000
6	-4.147501000	-0.041309000	2.075817000
1	-3.067309000	1.470789000	0.974250000
1	-2.074502000	0.096732000	1.450089000
1	-3.987573000	0.458448000	3.038444000
1	-5.146567000	0.237241000	1.717961000
1	-4.142511000	-1.120572000	2.259247000
15	1.519406000	0.142590000	0.522655000
6	-0.351596000	1.267004000	-1.799686000
1	0.328120000	0.463368000	-2.098143000
1	-1.225303000	0.809531000	-1.310326000
1	-0.685796000	1.813077000	-2.682422000
8	0.448587000	-0.868543000	0.629298000
9	2.278393000	0.422007000	1.902542000
8	2.709867000	-0.206972000	-0.483633000
6	3.089174000	-1.592702000	-0.767267000
6	4.114170000	-2.101380000	0.230908000
1	3.499791000	-1.550244000	-1.778108000
1	2.183361000	-2.204756000	-0.772597000
1	4.433693000	-3.108067000	-0.060457000
1	4.994467000	-1.452499000	0.251924000
1	3.696168000	-2.158445000	1.240435000

RC3

6	0.008332000	2.020554000	-0.184916000
8	0.397932000	3.098042000	-0.622593000
7	-0.956409000	1.328654000	-0.927055000
1	-1.248865000	1.826808000	-1.762877000
8	2.193623000	4.436682000	1.149977000
1	2.277713000	5.384241000	0.994781000
1	1.613429000	4.095312000	0.443653000
6	0.522764000	1.388062000	1.075658000
1	1.014179000	2.154638000	1.676309000
1	-0.279992000	0.920262000	1.652639000
1	1.260209000	0.608097000	0.822036000
15	-1.697695000	-0.146242000	-0.617395000
8	-0.855855000	-1.330531000	-0.360915000
9	-2.537787000	-0.235022000	-1.974193000
8	-2.804509000	0.183162000	0.482972000
6	-3.382435000	-0.867321000	1.326515000
6	-4.588644000	-1.506758000	0.662668000
1	-3.658035000	-0.343001000	2.243563000
1	-2.601247000	-1.598431000	1.550163000
1	-5.041347000	-2.226519000	1.353543000
1	-5.339836000	-0.753643000	0.408002000
1	-4.306826000	-2.044220000	-0.247796000
7	2.893910000	-0.990417000	0.250996000
1	3.814342000	-0.722048000	0.595661000
6	2.506919000	-2.286495000	0.818970000
6	2.530390000	-2.240832000	2.346241000
1	3.149733000	-3.116075000	0.475549000
1	1.490599000	-2.501112000	0.468400000
1	2.222890000	-3.204720000	2.765806000

1	3.537724000	-2.022727000	2.722454000
1	1.855331000	-1.466620000	2.724675000
6	2.870535000	-0.913010000	-1.214598000
6	3.894935000	-1.780286000	-1.964898000
1	3.024954000	0.138356000	-1.488680000
1	1.855652000	-1.177676000	-1.534813000
1	3.813356000	-1.617663000	-3.046056000
1	4.919414000	-1.526002000	-1.666271000
1	3.743320000	-2.848415000	-1.779035000

TS3

6	0.038736000	2.449741000	-0.700652000
8	-0.510301000	3.331491000	-0.146336000
7	1.233915000	1.426797000	0.712936000
1	0.932399000	1.870524000	1.578971000
8	1.772833000	2.869700000	-1.121176000
1	1.928112000	2.241436000	-0.230111000
1	1.893965000	3.802798000	-0.882390000
6	-0.331569000	1.425299000	-1.703465000
1	-0.615251000	1.961814000	-2.616267000
1	0.501911000	0.758690000	-1.911421000
1	-1.201454000	0.868607000	-1.319676000
15	1.423172000	-0.195426000	0.897591000
8	0.293022000	-1.068792000	1.310914000
9	2.636548000	-0.350821000	1.954221000
8	2.123816000	-0.592938000	-0.498096000
6	2.203634000	-1.983323000	-0.920145000
6	3.508194000	-2.623435000	-0.472905000
1	2.137277000	-1.945376000	-2.010792000
1	1.333764000	-2.521068000	-0.531634000
1	3.568684000	-3.643011000	-0.870335000
1	4.366858000	-2.056064000	-0.844124000
1	3.571240000	-2.676483000	0.617589000
7	-3.028650000	-0.251391000	-0.425321000
1	-3.904487000	-0.019864000	-0.892976000
6	-2.797768000	-1.700175000	-0.510844000
6	-2.731594000	-2.157478000	-1.967576000
1	-3.571986000	-2.287296000	0.012640000
1	-1.847233000	-1.903449000	-0.005075000
1	-2.548308000	-3.235809000	-2.026014000

1	-3.673506000	-1.954350000	-2.492763000
1	-1.929621000	-1.641263000	-2.505934000
6	-3.044951000	0.292885000	0.942278000
6	-4.212405000	-0.153108000	1.836866000
1	-3.056929000	1.387061000	0.857899000
1	-2.092036000	0.017496000	1.407336000
1	-4.151977000	0.339797000	2.814173000
1	-5.178691000	0.112145000	1.389260000
1	-4.204727000	-1.233501000	2.012693000

Pdt1

6	2.083739000	2.654187000	0.100761000
8	1.087914000	2.977996000	-0.531602000
7	-1.674984000	2.016705000	-0.286780000
1	-0.711351000	2.351980000	-0.372168000
8	3.271071000	3.261243000	-0.126102000
1	-2.377796000	2.552514000	-0.777503000
1	3.128832000	3.914428000	-0.832437000
6	2.164601000	1.583699000	1.141507000
1	2.799390000	1.906575000	1.970429000
1	1.165300000	1.317547000	1.485485000
1	2.618132000	0.684500000	0.694654000
15	-1.905957000	0.423450000	-0.011170000
8	-0.796931000	-0.285450000	0.668393000
9	-2.216850000	-0.273396000	-1.439066000
8	-3.367618000	0.383892000	0.643649000
6	-4.012468000	-0.885958000	0.954900000
6	-5.199834000	-1.109526000	0.035285000
1	-4.324120000	-0.801925000	1.999223000
1	-3.281974000	-1.697537000	0.882109000
1	-5.715042000	-2.034036000	0.319342000

1	-5.911291000	-0.281840000	0.114137000
1	-4.879295000	-1.198751000	-1.006377000
7	2.929625000	-1.526012000	-0.182078000
1	3.870346000	-1.855351000	-0.393551000
6	2.325538000	-2.382089000	0.846581000
6	3.183372000	-2.400977000	2.111028000
1	2.171000000	-3.420423000	0.503753000
1	1.334251000	-1.971317000	1.069532000
1	2.720279000	-3.025731000	2.882240000
1	4.181342000	-2.810182000	1.908966000
1	3.309153000	-1.390778000	2.513825000
6	2.155483000	-1.399355000	-1.424050000
6	2.024627000	-2.668341000	-2.282123000
1	2.626251000	-0.610207000	-2.024616000
1	1.159280000	-1.037006000	-1.146534000
1	1.459643000	-2.453388000	-3.196724000
1	3.010504000	-3.047431000	-2.579474000
1	1.499835000	-3.468957000	-1.751194000

Channel 2

IM3

7	-2.226062000	-0.031389000	-0.370825000
6	-0.890966000	-0.594477000	-0.265718000
7	0.048234000	0.481687000	-0.676640000
15	1.470726000	0.852140000	0.066301000
8	1.422323000	1.122850000	1.523717000
9	1.879516000	2.136052000	-0.803500000
8	2.566957000	-0.222925000	-0.394320000
6	-2.498245000	1.128738000	0.498268000
6	-3.345746000	2.199459000	-0.195871000

1	-1.544280000	1.578138000	0.781705000
1	-2.988419000	0.817336000	1.433276000
1	-3.516048000	3.042254000	0.483426000
1	-2.837062000	2.573968000	-1.089995000
1	-4.326246000	1.819154000	-0.500404000
6	-3.354807000	-0.972932000	-0.459874000
6	-3.645006000	-1.847049000	0.773496000
1	-3.208090000	-1.610811000	-1.335806000
1	-4.240870000	-0.370685000	-0.685306000
1	-4.529014000	-2.466483000	0.581962000
1	-2.806583000	-2.505609000	1.013690000
1	-3.852192000	-1.241963000	1.661787000
6	-0.696253000	-1.817291000	-1.168843000
1	-1.272156000	-2.672782000	-0.811439000
1	-0.989665000	-1.586612000	-2.196503000
1	0.361434000	-2.084337000	-1.151446000
6	3.817556000	-0.377273000	0.343839000
6	4.420823000	-1.714600000	-0.037754000
1	3.598288000	-0.316617000	1.412969000
1	4.476917000	0.453007000	0.068528000
1	5.372985000	-1.848760000	0.486739000
1	3.753573000	-2.535220000	0.241318000
1	4.609516000	-1.766895000	-1.114187000
8	-0.506651000	-1.033609000	1.036356000
1	-0.366086000	-0.274833000	1.626661000
1	-0.132905000	0.881110000	-1.589021000

TS4

7	-2.128424000	0.114832000	0.384091000
6	-0.734636000	0.488665000	0.554652000
7	0.040323000	-0.681050000	1.060401000
15	1.287315000	-0.935246000	0.026418000
8	0.933741000	-1.218734000	-1.468158000
9	1.824119000	-2.325363000	0.593937000
8	2.607019000	-0.080177000	0.254444000
6	-2.398261000	-0.998342000	-0.541812000
6	-3.554041000	-1.889019000	-0.073283000
1	-1.502168000	-1.614371000	-0.615291000
1	-2.600931000	-0.633174000	-1.560412000
1	-3.695163000	-2.718180000	-0.775812000
1	-3.343346000	-2.306769000	0.916873000
1	-4.502914000	-1.346372000	-0.013037000
6	-3.100958000	1.213830000	0.264258000
6	-2.988585000	2.108643000	-0.983267000
1	-3.046671000	1.830357000	1.165496000
1	-4.094996000	0.756130000	0.286768000
1	-3.776827000	2.870496000	-0.962325000
1	-2.019756000	2.612713000	-1.034578000
1	-3.107657000	1.534037000	-1.907199000
6	-0.571725000	1.664783000	1.526342000
1	-0.944681000	2.593922000	1.091391000
1	-1.090082000	1.472154000	2.471019000
1	0.493484000	1.789133000	1.728783000
6	3.052862000	0.968407000	-0.664571000
6	4.327790000	1.556576000	-0.095085000
1	2.249810000	1.703528000	-0.746935000
1	3.219616000	0.509035000	-1.643156000

1	4.692714000	2.341650000	-0.765987000
1	4.149356000	1.999604000	0.889091000
1	5.106056000	0.793973000	0.001002000
8	0.022056000	0.755903000	-0.617725000
1	0.265567000	-0.288007000	-1.440314000
1	-0.258685000	-1.316574000	1.789583000

IMA

7	-2.134116000	0.208258000	0.353815000
6	-0.741792000	0.358596000	0.655674000
7	-0.109184000	-0.892739000	1.064994000
15	1.139622000	-0.877123000	-0.039504000
8	1.077615000	-1.562456000	-1.515634000
9	1.803563000	-2.235331000	0.587614000
8	2.527144000	-0.077425000	0.197225000
6	-2.521514000	-0.915642000	-0.514037000
6	-3.746423000	-1.667499000	0.016485000
1	-1.685220000	-1.611813000	-0.572038000
1	-2.714970000	-0.565803000	-1.539432000
1	-4.009324000	-2.487714000	-0.661343000
1	-3.538962000	-2.088878000	1.005222000
1	-4.623846000	-1.017985000	0.104809000
6	-2.924713000	1.426705000	0.124755000
6	-2.567097000	2.249466000	-1.125345000
1	-2.867428000	2.061325000	1.013758000
1	-3.971185000	1.111974000	0.059670000
1	-3.244406000	3.107070000	-1.211970000
1	-1.540532000	2.624534000	-1.083868000
1	-2.662580000	1.655822000	-2.040017000
6	-0.470508000	1.514402000	1.622816000
1	-0.671297000	2.483149000	1.160896000

1	-1.084474000	1.417102000	2.523687000
1	0.582211000	1.487788000	1.910449000
6	2.861984000	1.159314000	-0.474022000
6	4.292976000	1.503482000	-0.101135000
1	2.162711000	1.940967000	-0.167331000
1	2.761983000	1.018996000	-1.556298000
1	4.586846000	2.438297000	-0.591026000
1	4.391673000	1.633532000	0.980931000
1	4.979747000	0.712996000	-0.417020000
8	0.152841000	0.478962000	-0.513626000
1	0.538174000	-0.999177000	-2.090661000
1	-0.170689000	-1.341581000	1.969091000

TS5

7	2.258964000	-0.184301000	-0.180875000
6	0.992957000	-0.616563000	-0.011716000
7	-0.065776000	0.520750000	1.334802000
15	-1.235500000	0.630740000	0.230407000
8	-1.402777000	1.785019000	-0.918758000
9	-2.357848000	1.424444000	1.160275000
8	-2.210899000	-0.628768000	-0.131644000
6	2.542878000	1.039408000	-0.951409000
6	2.529239000	2.320119000	-0.109371000
1	1.809959000	1.100466000	-1.755398000
1	3.524024000	0.897408000	-1.417962000
1	2.746240000	3.181291000	-0.750932000
1	1.554456000	2.459943000	0.361959000
1	3.288327000	2.294629000	0.680016000
6	3.388429000	-0.732734000	0.582856000
6	4.227328000	-1.739045000	-0.212394000
1	3.017790000	-1.184980000	1.503846000

1	4.014803000	0.111090000	0.890041000
1	5.083302000	-2.069410000	0.386076000
1	3.640142000	-2.620845000	-0.484266000
1	4.613400000	-1.292691000	-1.134444000
6	0.758068000	-1.988182000	0.585933000
1	1.211736000	-2.745160000	-0.066047000
1	1.170089000	-2.090529000	1.590047000
1	-0.315303000	-2.160977000	0.627722000
6	-3.654417000	-0.537158000	-0.094122000
6	-4.207567000	-1.814085000	-0.702774000
1	-3.974923000	0.342839000	-0.661404000
1	-3.983568000	-0.414235000	0.941840000
1	-5.302862000	-1.786974000	-0.686577000
1	-3.877876000	-1.927849000	-1.739946000
1	-3.876396000	-2.690909000	-0.137346000
8	0.080758000	-0.151569000	-0.859699000
1	-0.808047000	1.579590000	-1.653733000
1	-0.332619000	0.753045000	2.289223000

PC2

7	3.148580000	0.009686000	-0.165353000
6	1.891206000	-0.436910000	-0.394382000
7	-1.230673000	-0.457850000	1.667606000
15	-2.086110000	0.124699000	0.515519000
8	-1.435865000	-0.029534000	-0.908826000
9	-2.392783000	1.716801000	0.613341000
8	-3.585480000	-0.427282000	0.346365000
6	3.542845000	1.322193000	-0.709069000
6	3.234010000	2.478199000	0.246183000
1	3.014659000	1.464045000	-1.652970000
1	4.615494000	1.274015000	-0.924601000

1	3.567525000	3.425050000	-0.192125000
1	2.158603000	2.544231000	0.429815000
1	3.744488000	2.354467000	1.207675000
6	4.149280000	-0.699325000	0.644757000
6	5.058843000	-1.618054000	-0.177033000
1	3.647588000	-1.257906000	1.436946000
1	4.748474000	0.065908000	1.148955000
1	5.817307000	-2.075064000	0.467764000
1	4.485103000	-2.419868000	-0.652147000
1	5.575672000	-1.060912000	-0.965088000
6	1.435841000	-1.777976000	0.130056000
1	2.234972000	-2.432281000	0.475800000
1	0.713739000	-1.598541000	0.937965000
1	0.891696000	-2.280223000	-0.674110000
6	-4.472606000	0.048337000	-0.703931000
6	-5.755626000	-0.757044000	-0.626877000
1	-3.971607000	-0.083966000	-1.667898000
1	-4.658922000	1.115593000	-0.545185000
1	-6.449492000	-0.420331000	-1.404910000
1	-5.555261000	-1.821909000	-0.777580000
1	-6.238080000	-0.628839000	0.346731000
8	1.090998000	0.275412000	-1.046225000
1	-0.417903000	0.075584000	-0.963017000
1	-1.582697000	-0.328873000	2.610625000

TS6

7	2.570085000	0.189580000	0.129421000
6	1.633174000	0.927858000	-0.537372000
7	-3.129669000	-2.255102000	-0.656705000
15	-2.295914000	-1.036302000	-0.083787000
8	-1.013730000	-1.415204000	-0.883461000

9	-1.959381000	-1.058558000	1.480701000
8	-2.900237000	0.416617000	-0.249659000
6	2.765565000	0.430292000	1.565432000
6	1.877157000	-0.448603000	2.451804000
1	2.554334000	1.484480000	1.753745000
1	3.823563000	0.252751000	1.789686000
1	2.078326000	-0.241502000	3.509000000
1	0.820875000	-0.247903000	2.255992000
1	2.060490000	-1.514575000	2.277913000
6	3.345006000	-0.896148000	-0.478677000
6	4.741517000	-0.468072000	-0.945973000
1	2.778154000	-1.322837000	-1.308201000
1	3.432337000	-1.694352000	0.267176000
1	5.288032000	-1.328585000	-1.347853000
1	4.680197000	0.294414000	-1.729065000
1	5.327107000	-0.053120000	-0.119145000
6	1.435336000	0.675866000	-2.022548000
1	2.369639000	0.527268000	-2.569856000
1	0.798638000	-0.205527000	-2.156425000
1	0.913262000	1.540729000	-2.433473000
6	-2.337846000	1.625896000	0.386593000
6	-3.071386000	2.816426000	-0.192864000
1	-1.265137000	1.666850000	0.180760000
1	-2.502340000	1.530962000	1.463289000
1	-2.685481000	3.730994000	0.269551000
1	-2.911782000	2.884899000	-1.272660000
1	-4.146565000	2.754670000	0.001355000
8	0.945191000	1.776180000	0.048562000
1	-1.882685000	-2.288330000	-1.238239000
1	-4.121659000	-2.442913000	-0.653966000

Pdt2

7	2.603571000	0.162644000	0.099805000
6	1.735838000	0.871169000	-0.684697000
7	-3.533362000	-2.017803000	-0.417193000
15	-2.263915000	-1.029026000	-0.048598000
8	-0.978664000	-1.415280000	-0.672503000
9	-2.174571000	-1.083760000	1.554226000
8	-2.855793000	0.437632000	-0.261275000
6	2.857974000	0.630524000	1.468112000
6	1.892921000	0.038058000	2.500364000
1	2.776695000	1.719125000	1.464012000
1	3.892492000	0.370267000	1.720053000
1	2.144460000	0.401379000	3.503345000
1	0.864624000	0.331528000	2.274910000
1	1.939605000	-1.056200000	2.517236000
6	3.225787000	-1.101979000	-0.302406000
6	4.652182000	-0.941018000	-0.842469000
1	2.590264000	-1.597479000	-1.038405000
1	3.234192000	-1.757974000	0.575583000
1	5.080452000	-1.920645000	-1.082920000
1	4.664597000	-0.330001000	-1.750740000
1	5.304075000	-0.459798000	-0.105963000
6	1.481184000	0.383244000	-2.100700000
1	2.386393000	0.052510000	-2.616848000
1	0.763427000	-0.444055000	-2.072338000
1	1.034816000	1.209935000	-2.654723000
6	-2.162481000	1.634432000	0.239923000
6	-2.846072000	2.843308000	-0.364419000
1	-1.108083000	1.587850000	-0.044132000
1	-2.246139000	1.627352000	1.331062000

1	-2.355000000	3.751219000	0.000652000
1	-2.769029000	2.828265000	-1.455444000
1	-3.904012000	2.882877000	-0.086285000
8	1.157156000	1.879673000	-0.256832000
1	-3.378901000	-2.702971000	-1.142930000
1	-4.482106000	-1.680464000	-0.330855000

Channel 3

IM4

7	2.207026000	-0.018624000	-0.227800000
6	0.958442000	-0.307520000	0.474882000
7	-0.078792000	-0.371524000	-0.597411000
15	-1.641688000	-0.794223000	-0.243958000
8	-1.872702000	-1.583476000	0.994556000
9	-2.053743000	-1.575966000	-1.579819000
8	-2.497262000	0.552443000	-0.359056000
6	3.451511000	-0.437252000	0.434470000
6	4.591387000	-0.648365000	-0.565910000
1	3.251518000	-1.378007000	0.943237000
1	3.770218000	0.284595000	1.206426000
1	5.473147000	-1.031798000	-0.041167000
1	4.300213000	-1.377249000	-1.329329000
1	4.888821000	0.275692000	-1.072556000
6	2.272508000	1.283697000	-0.918877000
6	2.890163000	2.472702000	-0.159237000
1	1.257305000	1.539151000	-1.231256000
1	2.844812000	1.137344000	-1.843294000
1	2.838597000	3.363999000	-0.794930000
1	2.365256000	2.697215000	0.773294000
1	3.944623000	2.305825000	0.081319000
6	0.533011000	0.720416000	1.541365000

1	1.333191000	0.810340000	2.279756000
1	0.336244000	1.697800000	1.096194000
1	-0.369932000	0.389000000	2.063094000
6	-3.878869000	0.590745000	0.114673000
6	-4.302990000	2.044080000	0.188025000
1	-3.925561000	0.099974000	1.090722000
1	-4.496242000	0.029475000	-0.594852000
1	-5.343935000	2.103967000	0.523106000
1	-3.679325000	2.596883000	0.896592000
1	-4.226937000	2.523558000	-0.792216000
8	1.120708000	-1.576770000	1.082398000
1	0.249994000	-1.851583000	1.418213000
1	0.302436000	-0.836691000	-1.417664000

TS7

7	-1.896522000	0.136700000	0.266083000
6	-1.008051000	-0.857771000	-0.617795000
7	0.022275000	-0.916969000	0.392509000
15	1.630180000	-0.880450000	0.154544000
8	2.239883000	-1.557693000	-1.019089000
9	2.175336000	-1.477351000	1.545068000
8	2.071606000	0.675401000	0.322336000
6	-3.305353000	-0.248916000	0.524499000
6	-3.880321000	0.435663000	1.764738000
1	-3.319070000	-1.329395000	0.657321000
1	-3.918188000	-0.031817000	-0.359142000
1	-4.875845000	0.029943000	1.970089000
1	-3.252209000	0.248717000	2.642181000
1	-3.986319000	1.517868000	1.643084000
6	-1.687163000	1.589854000	0.004250000
6	-2.546081000	2.221834000	-1.093676000

1	-0.622031000	1.719352000	-0.202053000
1	-1.875021000	2.105063000	0.951683000
1	-2.249137000	3.268913000	-1.214386000
1	-2.422549000	1.727277000	-2.059592000
1	-3.610312000	2.213027000	-0.839883000
6	-0.683202000	-0.392752000	-2.029071000
1	-1.584769000	-0.419711000	-2.645886000
1	-0.246101000	0.606157000	-2.052660000
1	0.044673000	-1.092642000	-2.445280000
6	3.468215000	1.036486000	0.154624000
6	3.564104000	2.550579000	0.121129000
1	3.839225000	0.587190000	-0.771817000
1	4.037443000	0.624366000	0.995925000
1	4.611289000	2.852873000	0.011730000
1	2.998804000	2.958419000	-0.722758000
1	3.173883000	2.987458000	1.045622000
8	-1.683231000	-2.084526000	-0.725632000
1	-1.296268000	-2.658667000	-0.047293000
1	-0.917448000	-0.224933000	1.016087000

PC3

7	2.045367000	-0.194260000	0.035326000
6	-1.029447000	-2.212648000	-0.342363000
7	-1.650145000	-1.152180000	-0.726819000
15	-2.026114000	0.145828000	0.222691000
8	-2.087093000	0.048625000	1.701138000
9	-3.446873000	0.558842000	-0.387047000
8	-1.071029000	1.299743000	-0.370176000
6	2.919750000	-0.548264000	-1.090099000
6	3.586819000	0.617363000	-1.839149000
1	2.310600000	-1.125258000	-1.796207000

1	3.689754000	-1.237144000	-0.723784000
1	4.177147000	0.239638000	-2.682146000
1	2.835388000	1.308316000	-2.239557000
1	4.262643000	1.189523000	-1.194962000
6	2.670956000	0.508098000	1.163994000
6	3.613974000	-0.389192000	1.968785000
1	1.855887000	0.840767000	1.816663000
1	3.217200000	1.417599000	0.856219000
1	3.989940000	0.148673000	2.845830000
1	3.092540000	-1.288668000	2.312361000
1	4.483048000	-0.704307000	1.381725000
6	-0.407096000	-2.537271000	0.978474000
1	-0.321686000	-3.617965000	1.101166000
1	0.597510000	-2.090310000	0.971792000
1	-0.974985000	-2.086573000	1.793132000
6	-1.182717000	2.652041000	0.167897000
6	-0.124237000	3.510058000	-0.496766000
1	-1.049995000	2.606987000	1.253040000
1	-2.188715000	3.026157000	-0.049588000
1	-0.199709000	4.536810000	-0.123255000
1	0.880718000	3.138693000	-0.275124000
1	-0.260236000	3.526320000	-1.582106000
8	-0.848143000	-3.185320000	-1.250221000
1	-1.248301000	-2.882308000	-2.084602000
1	1.260360000	0.355630000	-0.307646000

TS8

7	-2.508157000	-0.347285000	0.059284000
6	0.448748000	2.460980000	-0.690326000
7	1.435413000	1.567102000	-0.503875000
15	1.602264000	0.305380000	0.548539000
8	0.397672000	-0.189531000	1.259045000
9	2.708721000	0.812620000	1.593638000
8	2.438276000	-0.736078000	-0.325151000
6	-2.587588000	-1.274273000	-1.075105000
6	-2.654444000	-2.773176000	-0.735066000
1	-1.704021000	-1.089886000	-1.698571000
1	-3.452855000	-0.999598000	-1.690269000
1	-2.653274000	-3.372592000	-1.653260000
1	-1.790475000	-3.076106000	-0.131931000
1	-3.560500000	-3.029742000	-0.176269000
6	-3.640690000	-0.349727000	0.992887000
6	-4.906210000	0.266749000	0.391307000
1	-3.332418000	0.243198000	1.861788000
1	-3.878406000	-1.357149000	1.377563000
1	-5.698875000	0.318960000	1.145888000
1	-4.706990000	1.279915000	0.026120000
1	-5.292158000	-0.323440000	-0.446737000
6	-0.843536000	2.615654000	0.021135000
1	-1.332331000	3.533277000	-0.306376000
1	-1.488256000	1.744847000	-0.183252000
1	-0.679832000	2.633745000	1.102302000
6	2.877622000	-2.001632000	0.255603000
6	3.428832000	-2.857189000	-0.867357000
1	2.021932000	-2.476913000	0.744736000
1	3.642874000	-1.783699000	1.007754000

1	3.779162000	-3.811656000	-0.460486000
1	2.657854000	-3.061268000	-1.615799000
1	4.270326000	-2.360309000	-1.358634000
8	0.836913000	3.200646000	-1.662376000
1	1.817962000	2.342648000	-1.505130000
1	-1.642241000	-0.511847000	0.571253000

Channel 4**TS11**

7	1.648471000	0.100657000	-0.040879000
6	1.104416000	-1.203221000	-0.439783000
7	-0.355292000	-1.121202000	-0.234173000
15	-1.190982000	0.272598000	0.078842000
8	-1.096183000	1.456875000	-0.807005000
9	-0.852309000	0.671281000	1.597878000
8	-2.659139000	-0.372781000	0.233813000
6	2.093071000	1.005496000	-1.115373000
6	2.196374000	2.466138000	-0.670182000
1	1.344550000	0.982135000	-1.910195000
1	3.047188000	0.676120000	-1.556533000
1	2.415767000	3.084872000	-1.546809000
1	1.247732000	2.803705000	-0.244398000
1	2.997524000	2.636874000	0.055446000
6	2.354794000	0.227420000	1.239282000
6	3.868301000	-0.048870000	1.228972000
1	1.859934000	-0.413914000	1.971118000
1	2.186089000	1.246296000	1.601852000
1	4.280764000	0.124200000	2.229927000
1	4.103209000	-1.077686000	0.942433000
1	4.393048000	0.617580000	0.536873000
6	1.640320000	-2.428645000	0.312866000
1	2.700445000	-2.568410000	0.096769000
1	1.486907000	-2.350889000	1.388938000
1	1.105980000	-3.310460000	-0.051071000
6	-3.838111000	0.479739000	0.190541000
6	-5.048517000	-0.407661000	-0.026527000
1	-3.715571000	1.207576000	-0.616589000

1	-3.905094000	1.017697000	1.142547000
1	-5.955197000	0.206617000	-0.041420000
1	-4.976314000	-0.939279000	-0.980134000
1	-5.143693000	-1.143677000	0.777421000
8	1.362592000	-1.514142000	-1.804457000
1	0.833099000	-0.926391000	-2.360614000
1	-0.905152000	-1.961657000	-0.371332000

IM5

7	-1.783724000	-0.113913000	-0.038493000
6	-1.010237000	1.060871000	-0.464981000
7	0.292168000	0.965664000	0.245167000
15	1.277933000	-0.340753000	-0.054973000
8	1.160509000	-1.028965000	-1.366166000
9	1.023379000	-1.368666000	1.144488000
8	2.705337000	0.275177000	0.335900000
6	-2.908209000	-0.506479000	-0.900771000
6	-3.212053000	-2.004346000	-0.805278000
1	-2.639704000	-0.262190000	-1.927634000
1	-3.821354000	0.068885000	-0.671096000
1	-4.003541000	-2.266587000	-1.515946000
1	-2.319974000	-2.591206000	-1.045499000
1	-3.555608000	-2.300177000	0.191497000
6	-2.044938000	-0.249910000	1.408473000
6	-3.366354000	0.322303000	1.954195000
1	-1.206074000	0.207329000	1.935213000
1	-2.004930000	-1.318095000	1.652460000
1	-3.385049000	0.191611000	3.042194000
1	-3.482834000	1.389860000	1.744969000
1	-4.242227000	-0.195265000	1.550747000
6	-1.619868000	2.435655000	-0.157133000

1	-2.602156000	2.505670000	-0.629740000
1	-1.727322000	2.584897000	0.919146000
1	-0.989279000	3.228548000	-0.571219000
6	3.925644000	-0.493473000	0.111892000
6	5.102887000	0.448990000	0.263775000
1	3.881980000	-0.930847000	-0.889844000
1	3.959097000	-1.299696000	0.852163000
1	6.035597000	-0.105980000	0.117492000
1	5.058041000	1.251093000	-0.478653000
1	5.119831000	0.895624000	1.262282000
8	-0.828556000	1.035355000	-1.863805000
1	-0.310645000	0.236739000	-2.082065000
1	0.798083000	1.842604000	0.312561000

TS9

7	2.128433000	0.015443000	-0.149916000
6	1.586945000	-1.171246000	-0.441217000
7	-0.481508000	-1.328398000	-0.052205000
15	-1.372370000	0.014783000	0.053195000
8	-1.071835000	1.111803000	-0.908647000
9	-1.202948000	0.606424000	1.574730000
8	-2.924886000	-0.444179000	0.129061000
6	2.111135000	1.117933000	-1.153945000
6	1.851453000	2.504812000	-0.570888000
1	1.322972000	0.883284000	-1.864113000
1	3.069566000	1.096024000	-1.688243000
1	1.787014000	3.207190000	-1.407992000
1	0.891984000	2.532577000	-0.049552000
1	2.649881000	2.858612000	0.089298000
6	2.729571000	0.293250000	1.163034000
6	4.256266000	0.409477000	1.106317000

1	2.436724000	-0.491587000	1.857891000
1	2.289930000	1.216995000	1.546168000
1	4.646937000	0.630993000	2.104976000
1	4.713908000	-0.522157000	0.758604000
1	4.574502000	1.213948000	0.436629000
6	1.921796000	-2.400649000	0.375620000
1	2.992595000	-2.614251000	0.272090000
1	1.678226000	-2.298026000	1.432364000
1	1.366021000	-3.246038000	-0.029566000
6	-3.967536000	0.560180000	0.210638000
6	-5.301770000	-0.129357000	-0.008120000
1	-3.781928000	1.324776000	-0.550730000
1	-3.922140000	1.031930000	1.199240000
1	-6.113644000	0.603314000	0.059429000
1	-5.338349000	-0.597675000	-0.996319000
1	-5.469779000	-0.902439000	0.748136000
8	1.395874000	-1.383983000	-1.769249000
1	0.502788000	-1.775182000	-1.826891000
1	-0.733987000	-2.016697000	0.654979000

A1 ... X

7	-3.004261000	0.236557000	0.004793000
6	-2.108557000	-0.634237000	0.545748000
7	1.330915000	-0.055493000	1.612244000
15	2.026854000	-0.457780000	0.191250000
8	1.133139000	-0.496784000	-0.990199000
9	2.747804000	-1.892200000	0.402063000
8	3.321665000	0.489919000	0.136859000
6	-3.279637000	1.495792000	0.713147000
6	-2.322221000	2.625474000	0.320961000
1	-3.204441000	1.296613000	1.783612000

1	-4.315691000	1.775860000	0.493269000
1	-2.584488000	3.543655000	0.858383000
1	-1.293021000	2.359058000	0.574652000
1	-2.368786000	2.839153000	-0.752557000
6	-3.653768000	0.044899000	-1.296865000
6	-5.056348000	-0.565771000	-1.197532000
1	-3.012243000	-0.567512000	-1.933083000
1	-3.708937000	1.026710000	-1.780240000
1	-5.508231000	-0.641692000	-2.192691000
1	-5.020879000	-1.568671000	-0.760337000
1	-5.713832000	0.049064000	-0.574344000
6	-1.807496000	-1.928685000	-0.185231000
1	-2.680480000	-2.377001000	-0.664803000
1	-1.034411000	-1.741488000	-0.939601000
1	-1.400230000	-2.630314000	0.543968000
6	4.281938000	0.350379000	-0.947114000
6	5.248664000	1.515793000	-0.864039000
1	3.739069000	0.346996000	-1.897749000
1	4.798701000	-0.608276000	-0.830459000
1	5.991929000	1.434645000	-1.664449000
1	4.720275000	2.467022000	-0.975587000
1	5.773328000	1.519264000	0.096080000
8	-1.530499000	-0.370624000	1.615999000
1	0.320836000	-0.217277000	1.707974000
1	1.872019000	-0.078701000	2.465668000

		Pathway B	
RC2			
7	-1.147314827	-0.440411406	0.113985137
6	0.077905173	-0.259194406	-0.408783863
7	1.060003173	-1.026422406	0.033289137
15	2.597619173	-1.042629406	-0.465868863
8	2.981377173	-1.168067406	-1.906105863
9	3.159197173	-2.337566406	0.323322137
8	3.338123173	0.148488594	0.326891137
6	-1.384392827	-1.482164406	1.131570137
6	-1.146725827	-0.979772406	2.558054137
1	-0.731925827	-2.327189406	0.910470137
1	-2.418859827	-1.815058406	1.012366137
1	-1.363318827	-1.781551406	3.271662137
1	-0.106693827	-0.670368406	2.691927137
1	-1.796758827	-0.131537406	2.796276137
6	-2.317368827	0.379213594	-0.252388863
6	-3.182665827	-0.257905406	-1.344006863
1	-1.984398827	1.372676594	-0.552412863
1	-2.905581827	0.513399594	0.660066137
1	-4.055685827	0.374411594	-1.534910863
1	-2.627935827	-0.367293406	-2.280825863
1	-3.541133827	-1.246669406	-1.041671863
6	0.256208173	0.830923594	-1.443669863
1	-0.527271827	0.800467594	-2.203770863
1	0.224060173	1.814073594	-0.959167863
1	1.217024173	0.717930594	-1.944244863
6	4.758826173	0.419440594	0.117032137
6	5.110406173	1.682604594	0.877104137
1	4.936749173	0.531515594	-0.955959863

1	5.331185173	-0.438465406	0.484318137
1	6.174040173	1.903261594	0.740667137
1	4.531482173	2.534583594	0.508116137
1	4.918179173	1.562304594	1.947508137
8	0.074403774	3.690043457	0.329605042
1	-0.733011226	4.209673457	0.444177042
1	0.791781774	4.338190457	0.345528042

TS10

7	2.325069000	0.532755000	0.168562000
6	1.074801000	-0.268237000	0.566584000
7	0.101515000	-0.166894000	-0.274468000
15	-1.374522000	-0.869062000	-0.159157000
8	-1.726250000	-1.817399000	0.930391000
9	-1.493442000	-1.583639000	-1.596091000
8	-2.367420000	0.379251000	-0.337989000
6	2.100202000	1.499592000	-0.967031000
6	1.321396000	2.747092000	-0.564540000
1	1.578606000	0.959341000	-1.758426000
1	3.098705000	1.773462000	-1.320324000
1	1.234904000	3.392903000	-1.445052000
1	0.323344000	2.491883000	-0.210096000
1	1.831799000	3.304007000	0.226312000
6	3.576525000	-0.272495000	-0.010149000
6	3.570791000	-1.173876000	-1.242961000
1	3.725436000	-0.857426000	0.897983000
1	4.394469000	0.452137000	-0.062707000
1	4.501906000	-1.748262000	-1.268753000
1	2.737887000	-1.882033000	-1.226160000
1	3.507932000	-0.599183000	-2.170661000
6	1.324921000	-1.433091000	1.497970000

1	1.638620000	-2.311567000	0.920093000
1	2.074623000	-1.211039000	2.256856000
1	0.379865000	-1.687687000	1.979856000
6	-3.787399000	0.220503000	-0.067393000
6	-4.393700000	1.605411000	0.055317000
1	-3.908638000	-0.359572000	0.851932000
1	-4.235338000	-0.338109000	-0.897284000
1	-5.469355000	1.520440000	0.244666000
1	-3.937159000	2.155734000	0.883195000
1	-4.248443000	2.178499000	-0.865373000
8	1.084366000	1.187196000	2.008381000
1	2.268403000	1.069990000	1.133231000
1	0.924383000	0.882360000	2.911185000

Phosphinate hydrolysis

Frontside attack (S_N2)

Reaction (I)

TSP1

7	2.245762000	0.271465000	0.094697000
6	1.129334000	-0.394277000	-0.303513000
7	-0.022994000	0.027776000	0.162779000
15	-1.479734000	-0.712112000	-0.107735000
8	-1.936209000	-1.395828000	-1.349307000
9	-0.702164000	-2.337130000	0.694883000
8	-2.432881000	0.640023000	0.114580000
6	2.138034000	1.395702000	1.038190000
6	2.195616000	0.948150000	2.501684000
1	1.197416000	1.911258000	0.840158000
1	2.958622000	2.086316000	0.817347000
1	2.130393000	1.818236000	3.164281000
1	1.361260000	0.278554000	2.725769000

1	3.130553000	0.423200000	2.726418000
6	3.601293000	-0.069053000	-0.354598000
6	4.078295000	0.762677000	-1.551453000
1	3.651864000	-1.133848000	-0.585590000
1	4.271075000	0.090058000	0.497703000
1	5.108648000	0.494663000	-1.809247000
1	3.449993000	0.589969000	-2.430581000
1	4.055018000	1.833716000	-1.326316000
6	1.307023000	-1.547523000	-1.270120000
1	0.342207000	-1.839708000	-1.681287000
1	1.982700000	-1.287357000	-2.088879000
1	1.714862000	-2.414324000	-0.739871000
6	-2.474016000	1.613444000	-0.943549000
6	-3.454751000	2.704060000	-0.546024000
1	-2.787257000	1.119270000	-1.869956000
1	-1.467786000	2.028220000	-1.091043000
1	-3.512750000	3.460666000	-1.336495000
1	-4.454936000	2.287010000	-0.393113000
1	-3.138633000	3.196145000	0.379620000
8	-2.383073000	-1.180155000	1.538241000
1	-1.707683000	-1.891031000	1.768173000
1	-2.437122000	-0.421252000	2.140835000

P1f

7	-2.130771000	-0.573797000	-0.021990000
6	-1.089289000	0.180143000	-0.445005000
7	0.109483000	-0.137973000	-0.012272000
15	1.515755000	0.617898000	-0.366881000
8	1.810659000	1.113156000	-1.744575000
9	-0.664990000	2.803363000	1.745031000
8	2.665541000	-0.334202000	0.246224000

6	-1.896925000	-1.707778000	0.889690000
6	-1.894411000	-1.292823000	2.363600000
1	-0.939857000	-2.158286000	0.624515000
1	-2.684919000	-2.443118000	0.696182000
1	-1.737593000	-2.172263000	2.997660000
1	-1.090704000	-0.578486000	2.556245000
1	-2.844859000	-0.832723000	2.654647000
6	-3.534155000	-0.280552000	-0.342999000
6	-4.065164000	-1.077888000	-1.539624000
1	-3.654678000	0.790838000	-0.508886000
1	-4.121388000	-0.516150000	0.550790000
1	-5.125490000	-0.854583000	-1.699488000
1	-3.521186000	-0.829993000	-2.456328000
1	-3.968740000	-2.155441000	-1.372680000
6	-1.382482000	1.351250000	-1.361320000
1	-0.472717000	1.632107000	-1.892491000
1	-2.157015000	1.122661000	-2.095649000
1	-1.713085000	2.206183000	-0.759738000
6	3.111437000	-1.484265000	-0.514072000
6	4.288959000	-2.100766000	0.217901000
1	3.390786000	-1.156544000	-1.520889000
1	2.279625000	-2.194927000	-0.592394000
1	4.644730000	-2.981038000	-0.328470000
1	5.113250000	-1.385642000	0.296874000
1	4.000666000	-2.410683000	1.226826000
8	1.568508000	1.839073000	0.758050000
1	0.163685000	2.445529000	1.445425000
1	2.251601000	2.488071000	0.529000000

Reaction (II)**TSP2**

7	-2.452840000	0.159574000	-0.244540000
6	-1.285282000	-0.515086000	-0.254092000
7	-0.214043000	0.082130000	0.236292000
15	1.430178000	-0.450694000	0.580818000
8	1.526722000	-1.840563000	0.011264000
9	1.630449000	-0.665818000	2.156109000
8	2.642387000	0.403447000	-0.102749000
6	-2.558268000	1.507820000	0.350113000
6	-2.182658000	2.626724000	-0.626236000
1	-1.935729000	1.549400000	1.246720000
1	-3.594861000	1.625216000	0.678288000
1	-2.311681000	3.598444000	-0.139375000
1	-1.139500000	2.544825000	-0.941879000
1	-2.818411000	2.606325000	-1.517829000
6	-3.690343000	-0.374973000	-0.839137000
6	-4.613270000	-1.046175000	0.183147000
1	-3.435730000	-1.069211000	-1.640272000
1	-4.204007000	0.468282000	-1.312761000
1	-5.531896000	-1.381862000	-0.309228000
1	-4.133671000	-1.915713000	0.642153000
1	-4.894091000	-0.354687000	0.983547000
6	-1.245129000	-1.903765000	-0.836144000
1	-2.077821000	-2.508625000	-0.470682000
1	-1.315709000	-1.846492000	-1.928833000
1	-0.291164000	-2.365443000	-0.577299000
6	3.616802000	-0.293751000	-0.934270000
6	4.494731000	0.767179000	-1.573386000
1	3.092012000	-0.899002000	-1.676419000

1	4.199292000	-0.969001000	-0.301044000
1	5.254966000	0.286352000	-2.199218000
1	3.903573000	1.438650000	-2.204443000
1	5.004131000	1.367012000	-0.812892000
8	1.066080000	1.561761000	1.339555000
1	-0.036039000	1.110030000	0.663997000
1	1.706784000	2.171359000	0.953420000

P2f

7	2.710775000	-0.129389000	-0.079909000
6	1.759006000	-1.004270000	0.407655000
7	1.212593000	-1.981429000	-0.246935000
15	-2.345879000	1.022962000	0.092976000
8	-0.962251000	1.339255000	0.481010000
9	-2.627872000	1.333498000	-1.453661000
8	-2.908048000	-0.456669000	0.244498000
6	3.217828000	-0.262858000	-1.444884000
6	2.342092000	0.419923000	-2.505311000
1	3.344381000	-1.326518000	-1.677290000
1	4.224613000	0.168128000	-1.465428000
1	2.781685000	0.293930000	-3.501353000
1	1.332359000	0.000025000	-2.517844000
1	2.251776000	1.492776000	-2.307071000
6	3.178126000	1.045146000	0.664676000
6	4.522768000	0.832917000	1.372088000
1	2.414169000	1.346034000	1.382207000
1	3.262033000	1.877835000	-0.044326000
1	4.838516000	1.755056000	1.873439000
1	4.452284000	0.040931000	2.124369000
1	5.307727000	0.551041000	0.662060000

6	1.307822000	-0.806451000	1.839175000
1	2.147598000	-0.693166000	2.531369000
1	0.664050000	0.075781000	1.918827000
1	0.730800000	-1.685000000	2.127932000
6	-2.231993000	-1.617112000	-0.365579000
6	-2.830093000	-2.864824000	0.248062000
1	-1.156325000	-1.553732000	-0.177189000
1	-2.418840000	-1.567012000	-1.443133000
1	-2.348003000	-3.743085000	-0.193084000
1	-2.656232000	-2.887598000	1.327647000
1	-3.906898000	-2.925744000	0.061740000
8	-3.461732000	1.892690000	0.840586000
1	1.539692000	-2.033114000	-1.211215000
1	-4.367009000	1.586214000	0.680510000

Reaction (III)

TSP3

7	-2.515965000	0.199068000	0.130004000
6	-1.371536000	-0.401136000	-0.303370000
7	-0.267244000	0.299138000	-0.287760000
15	1.249839000	-0.344614000	-0.560472000
8	1.722557000	-1.259752000	-1.638475000
9	1.156552000	-1.395289000	0.754017000
8	2.573566000	0.473820000	0.438784000
6	-2.470488000	1.567883000	0.664414000
6	-2.676646000	2.637009000	-0.413462000
1	-1.504749000	1.704721000	1.152966000
1	-3.249561000	1.646532000	1.430137000
1	-2.646045000	3.635912000	0.035446000
1	-1.890688000	2.574440000	-1.170764000
1	-3.644833000	2.523800000	-0.913487000

6	-3.836891000	-0.438886000	0.095373000
6	-4.230363000	-1.105746000	1.419591000
1	-3.871603000	-1.165622000	-0.717313000
1	-4.566897000	0.337816000	-0.159180000
1	-5.240198000	-1.523732000	1.344533000
1	-3.541890000	-1.916704000	1.675477000
1	-4.223983000	-0.386716000	2.244887000
6	-1.485525000	-1.821926000	-0.823910000
1	-1.963698000	-2.478790000	-0.092288000
1	-2.083384000	-1.841288000	-1.741894000
1	-0.500929000	-2.219534000	-1.062486000
6	3.777032000	-0.272081000	0.800238000
6	4.784529000	0.688352000	1.404145000
1	4.157298000	-0.764773000	-0.099313000
1	3.449604000	-1.031326000	1.510858000
1	5.679444000	0.131782000	1.702252000
1	5.089985000	1.454240000	0.683658000
1	4.374800000	1.182455000	2.290103000
8	1.708721000	1.299562000	-1.396589000
1	0.968236000	1.915908000	-1.301192000
1	2.555587000	1.230383000	-0.375053000

P3f

7	-2.519344000	0.449972000	0.099306000
6	-1.360659000	0.031186000	-0.463723000
7	-0.567303000	-0.721488000	0.261150000
15	0.859163000	-1.403382000	-0.146278000
8	1.551464000	-1.182370000	-1.437029000
9	0.558885000	-2.955997000	0.119560000
8	3.553721000	1.376659000	1.175302000
6	-2.865110000	0.041913000	1.472346000

6	-2.311438000	0.998516000	2.532094000
1	-2.478127000	-0.965564000	1.630363000
1	-3.957225000	-0.002618000	1.530478000
1	-2.609831000	0.663201000	3.531152000
1	-1.219638000	1.028885000	2.490145000
1	-2.690214000	2.016832000	2.393054000
6	-3.484451000	1.327805000	-0.577630000
6	-4.627354000	0.566666000	-1.259403000
1	-2.961852000	1.957029000	-1.299001000
1	-3.888698000	2.005176000	0.182173000
1	-5.334782000	1.274087000	-1.704889000
1	-4.252874000	-0.087316000	-2.052760000
1	-5.176454000	-0.053025000	-0.543663000
6	-1.059298000	0.481919000	-1.879651000
1	-1.907710000	0.305607000	-2.545704000
1	-0.836651000	1.554958000	-1.891555000
1	-0.185823000	-0.045423000	-2.259727000
6	4.631753000	1.479501000	0.244678000
6	4.158919000	1.647152000	-1.197538000
1	5.293079000	0.603303000	0.326867000
1	5.209527000	2.354076000	0.562105000
1	5.017399000	1.750541000	-1.872918000
1	3.571650000	0.781488000	-1.523496000
1	3.535502000	2.542908000	-1.293556000
8	1.844402000	-1.073163000	1.103582000
1	1.388265000	-1.090206000	1.958457000
1	3.082722000	0.544401000	1.015544000

Backside attack (addition-elimination)**Reaction (IV)****TSP4**

7	2.305105000	0.388436000	0.026546000
6	1.259682000	-0.478741000	0.124867000
7	0.051079000	0.009540000	0.047272000
15	-1.353515000	-0.844665000	-0.022927000
8	-1.677704000	-2.098208000	0.869715000
9	-1.118813000	-1.655340000	-1.411670000
8	-2.535530000	0.037809000	-0.617966000
6	2.051065000	1.817521000	-0.216420000
6	1.855124000	2.618336000	1.074154000
1	1.165539000	1.899531000	-0.848680000
1	2.904850000	2.207483000	-0.779928000
1	1.707318000	3.678118000	0.839577000
1	0.974650000	2.261967000	1.614770000
1	2.726573000	2.538427000	1.733337000
6	3.713242000	-0.013965000	0.123721000
6	4.375719000	-0.267734000	-1.236231000
1	3.798488000	-0.898570000	0.756491000
1	4.242549000	0.788226000	0.650039000
1	5.432301000	-0.521353000	-1.097859000
1	3.892167000	-1.093758000	-1.766528000
1	4.323138000	0.618537000	-1.876277000
6	1.589044000	-1.944004000	0.347215000
1	2.295803000	-2.312534000	-0.400915000
1	2.037928000	-2.088914000	1.336267000
1	0.686545000	-2.549814000	0.301331000
6	-2.996374000	1.323312000	-0.124085000
6	-3.952012000	1.881532000	-1.162257000

1	-2.126070000	1.971910000	0.014408000
1	-3.470014000	1.169359000	0.845070000
1	-4.332979000	2.850422000	-0.820625000
1	-3.453096000	2.023781000	-2.125697000
1	-4.802685000	1.209296000	-1.309189000
1	-1.100632000	0.253470000	2.431159000
8	-1.856633000	-0.117843000	1.958622000
1	-1.837620000	-1.414988000	1.766696000

IMB1

7	-2.387608000	0.341255000	0.000891000
6	-1.303238000	-0.472034000	-0.172822000
7	-0.131948000	0.082098000	-0.298402000
15	1.374598000	-0.643616000	-0.245658000
8	1.802165000	-2.076561000	-0.924516000
9	1.000069000	-1.528939000	1.123160000
8	2.479945000	0.119686000	0.663081000
6	-2.199477000	1.792130000	0.136944000
6	-2.257655000	2.532878000	-1.202988000
1	-1.235540000	1.961008000	0.619282000
1	-2.981349000	2.163448000	0.808193000
1	-2.129902000	3.609521000	-1.045230000
1	-1.461314000	2.185902000	-1.866830000
1	-3.218155000	2.379428000	-1.707283000
6	-3.770002000	-0.142602000	0.074972000
6	-4.269659000	-0.361530000	1.508979000
1	-3.868102000	-1.063289000	-0.502322000
1	-4.402308000	0.598793000	-0.426992000
1	-5.317375000	-0.681696000	1.498128000
1	-3.681659000	-1.128864000	2.021451000
1	-4.204920000	0.559015000	2.097649000

6	-1.569164000	-1.963139000	-0.272191000
1	-2.165195000	-2.323098000	0.570569000
1	-2.116585000	-2.188208000	-1.194794000
1	-0.631833000	-2.513057000	-0.285426000
6	3.348855000	1.185573000	0.229545000
6	4.221519000	1.557574000	1.416780000
1	2.745645000	2.040358000	-0.095761000
1	3.948983000	0.852418000	-0.620546000
1	4.901459000	2.369742000	1.135792000
1	3.610989000	1.890247000	2.261685000
1	4.818759000	0.700446000	1.741939000
1	1.188470000	0.811053000	-1.936670000
8	1.834540000	0.125230000	-1.725228000
1	2.076970000	-1.891869000	-1.835835000

TSP5

7	2.231916000	0.248892000	0.093064000
6	1.125517000	-0.570061000	0.143572000
7	-0.048614000	-0.020365000	0.123104000
15	-1.607382000	-0.797074000	0.101884000
8	-3.068543000	-1.613418000	0.026189000
9	-1.084550000	-1.793115000	-1.138429000
8	-2.426147000	0.534106000	-0.301735000
6	2.053330000	1.700658000	-0.025468000
6	1.943957000	2.404998000	1.331034000
1	1.153365000	1.881924000	-0.615094000
1	2.908150000	2.094788000	-0.585812000
1	1.840787000	3.486979000	1.191003000
1	1.068260000	2.044944000	1.877813000
1	2.833675000	2.229689000	1.946210000
6	3.616658000	-0.230814000	0.085097000

6	4.201400000	-0.414117000	-1.322397000
1	3.690007000	-1.165146000	0.643787000
1	4.217775000	0.498905000	0.640103000
1	5.248505000	-0.730865000	-1.259150000
1	3.648307000	-1.171333000	-1.886651000
1	4.165876000	0.520084000	-1.891930000
6	1.420341000	-2.061303000	0.264513000
1	2.025662000	-2.419184000	-0.573474000
1	1.970306000	-2.271854000	1.188285000
1	0.499586000	-2.636095000	0.278489000
6	-1.928239000	1.878653000	-0.439006000
6	-3.128093000	2.768061000	-0.722134000
1	-1.204871000	1.912916000	-1.258327000
1	-1.415304000	2.177308000	0.479089000
1	-2.796925000	3.805891000	-0.842175000
1	-3.635939000	2.456150000	-1.639566000
1	-3.848361000	2.724774000	0.100230000
1	-0.704813000	-0.824852000	2.086218000
8	-1.502298000	-1.221797000	1.705639000
1	-2.928798000	-2.568138000	-0.006645000

IMB2

7	2.327483000	0.306096000	0.027385000
6	1.242605000	-0.526390000	0.113075000
7	0.081671000	-0.004621000	0.348508000
15	-1.438153000	-0.673145000	0.390954000
8	-1.837928000	-2.252728000	0.559115000
9	-1.320857000	-1.054430000	-1.339870000
8	-2.580530000	0.436805000	0.074708000
6	2.141495000	1.756952000	0.157406000
6	2.217065000	2.243366000	1.608473000

1	1.171447000	2.011903000	-0.273005000
1	2.914752000	2.243300000	-0.447092000
1	2.086098000	3.330452000	1.650178000
1	1.430040000	1.777691000	2.207226000
1	3.185151000	2.003983000	2.062409000
6	3.701438000	-0.159280000	-0.179249000
6	4.147294000	-0.134311000	-1.647347000
1	3.815762000	-1.164014000	0.231156000
1	4.358045000	0.485602000	0.416228000
1	5.193005000	-0.450725000	-1.730563000
1	3.536288000	-0.805280000	-2.259069000
1	4.065015000	0.872084000	-2.070085000
6	1.505062000	-2.013609000	-0.034901000
1	2.064062000	-2.238261000	-0.947271000
1	2.081240000	-2.387582000	0.818653000
1	0.564245000	-2.556950000	-0.061433000
6	-2.848314000	1.039982000	-1.212278000
6	-3.836038000	2.170373000	-0.979412000
1	-3.257660000	0.284033000	-1.886402000
1	-1.911622000	1.408419000	-1.641328000
1	-4.081872000	2.648057000	-1.934454000
1	-4.761109000	1.792847000	-0.533068000
1	-3.416112000	2.928782000	-0.311234000
1	-1.541337000	0.396653000	2.297475000
8	-1.660742000	-0.524692000	2.034475000
1	-1.889564000	-2.641857000	-0.326045000

TSP6

7	2.266515000	0.257973000	0.016666000
6	1.164441000	-0.522005000	0.167599000
7	0.038756000	0.072181000	0.469410000
15	-1.478271000	-0.486714000	0.677252000
8	-1.891441000	-2.013875000	0.860672000
9	-1.307044000	-1.488019000	-1.322733000
8	-2.523652000	0.490778000	-0.033796000
6	2.146137000	1.722512000	0.111436000
6	2.347546000	2.247542000	1.535889000
1	1.158630000	2.002244000	-0.256924000
1	2.892861000	2.153184000	-0.564122000
1	2.264760000	3.339797000	1.549014000
1	1.588178000	1.835017000	2.205237000
1	3.335280000	1.981430000	1.927906000
6	3.622958000	-0.256719000	-0.223310000
6	3.958861000	-0.426416000	-1.708542000
1	3.763776000	-1.195069000	0.316363000
1	4.314743000	0.457419000	0.234671000
1	4.996497000	-0.757742000	-1.825042000
1	3.306130000	-1.166253000	-2.181123000
1	3.842353000	0.518381000	-2.249170000
6	1.276633000	-2.016119000	-0.022237000
1	0.564942000	-2.282307000	-0.810267000
1	2.271455000	-2.361083000	-0.293904000
1	0.963060000	-2.524672000	0.894255000
6	-2.518849000	0.899076000	-1.430910000
6	-3.473232000	2.072492000	-1.553615000
1	-2.818306000	0.044178000	-2.035279000
1	-1.497346000	1.171606000	-1.709997000

1	-3.515414000	2.397459000	-2.599163000
1	-4.482987000	1.788811000	-1.241440000
1	-3.147402000	2.919922000	-0.941804000
1	-1.624036000	0.860389000	2.374698000
8	-1.799666000	-0.077464000	2.221396000
1	-1.805519000	-2.318592000	-0.094665000

P1b

7	2.365581000	-0.092546000	0.118180000
6	1.199477000	0.407844000	-0.367323000
7	0.162148000	-0.391615000	-0.404151000
15	-1.374128000	-0.095573000	-0.909123000
8	-1.838476000	1.324809000	-1.070197000
9	-2.685195000	2.834283000	0.766776000
8	-2.294583000	-0.994213000	0.061792000
6	2.431266000	-1.484071000	0.594115000
6	2.780314000	-2.476231000	-0.518942000
1	1.464506000	-1.735739000	1.031878000
1	3.183893000	-1.520556000	1.388300000
1	2.840505000	-3.491457000	-0.112097000
1	2.012098000	-2.461749000	-1.296409000
1	3.745786000	-2.241176000	-0.980132000
6	3.613615000	0.678424000	0.199762000
6	3.841913000	1.329173000	1.569259000
1	3.628662000	1.433540000	-0.587158000
1	4.433189000	-0.012800000	-0.024980000
1	4.805091000	1.850437000	1.581067000
1	3.057200000	2.055907000	1.800249000
1	3.854022000	0.581363000	2.368449000
6	1.202431000	1.846331000	-0.847399000
1	1.654195000	2.517672000	-0.113038000

1	1.775764000	1.927854000	-1.778227000
1	0.182781000	2.171907000	-1.043130000
6	-2.438088000	-0.659119000	1.469272000
6	-3.441215000	-1.622088000	2.075226000
1	-2.777843000	0.377567000	1.556326000
1	-1.455947000	-0.753287000	1.947574000
1	-3.569939000	-1.396968000	3.139325000
1	-4.413073000	-1.527688000	1.582286000
1	-3.099302000	-2.657210000	1.977849000
1	-1.372254000	-1.824562000	-2.230491000
8	-1.567822000	-0.879657000	-2.308430000
1	-2.395999000	2.292023000	0.020875000

Reaction (V)

TSP7

7	-2.442720000	0.140099000	0.051620000
6	-1.166909000	-0.052462000	-0.394558000
7	-0.258978000	-0.370656000	0.479597000
15	1.337103000	-0.714591000	0.207216000
8	1.292736000	-1.929920000	-0.806709000
9	1.688520000	-1.044531000	1.733550000
8	1.852881000	0.743812000	-0.208229000
6	-2.748995000	-0.050949000	1.477841000
6	-2.516314000	1.211575000	2.313250000
1	-2.123814000	-0.864475000	1.849169000
1	-3.795241000	-0.367598000	1.546005000
1	-2.783908000	1.024544000	3.359088000
1	-1.463313000	1.501159000	2.274208000
1	-3.125266000	2.049364000	1.954860000
6	-3.555912000	0.566140000	-0.801868000
6	-4.415510000	-0.594493000	-1.318977000

1	-3.174520000	1.156764000	-1.636778000
1	-4.175771000	1.248272000	-0.208882000
1	-5.254318000	-0.209971000	-1.909685000
1	-3.831730000	-1.270327000	-1.951632000
1	-4.826428000	-1.182033000	-0.491912000
6	-0.917705000	0.150666000	-1.879486000
1	-1.692993000	-0.313919000	-2.493062000
1	-0.890022000	1.220628000	-2.115059000
1	0.037999000	-0.286716000	-2.159861000
6	3.209403000	1.265445000	-0.317415000
6	3.083770000	2.752532000	-0.594515000
1	3.727472000	0.730294000	-1.112321000
1	3.733710000	1.067621000	0.619186000
1	4.084738000	3.189334000	-0.682000000
1	2.547577000	2.935684000	-1.531024000
1	2.553398000	3.263496000	0.214962000
8	3.375647000	-1.403627000	-0.085895000
1	3.743335000	-1.839322000	0.693882000
1	2.366671000	-2.092118000	-0.746820000

IMB3

7	-2.366943000	0.064600000	0.138726000
6	-1.063586000	0.289303000	-0.238586000
7	-0.205949000	-0.654757000	-0.022051000
15	1.435634000	-0.700808000	-0.436586000
8	1.117498000	-0.524664000	-2.047841000
9	1.560236000	-2.113931000	0.398201000
8	1.842634000	0.613564000	0.442543000
6	-2.731513000	-1.229395000	0.730672000
6	-2.513879000	-1.278734000	2.246571000
1	-2.131022000	-2.001140000	0.246047000

1	-3.784424000	-1.414761000	0.490300000
1	-2.825839000	-2.252295000	2.641627000
1	-1.455237000	-1.136394000	2.477133000
1	-3.094519000	-0.504679000	2.761828000
6	-3.438850000	1.055058000	0.031277000
6	-4.294287000	0.908155000	-1.234915000
1	-3.020128000	2.061654000	0.086351000
1	-4.075893000	0.946686000	0.917306000
1	-5.105059000	1.645660000	-1.234070000
1	-3.694431000	1.058384000	-2.138076000
1	-4.744089000	-0.088116000	-1.294625000
6	-0.770414000	1.650369000	-0.851734000
1	-1.502126000	1.913934000	-1.620043000
1	-0.789702000	2.428308000	-0.080176000
1	0.214873000	1.650709000	-1.308202000
6	3.174349000	1.128520000	0.680683000
6	3.027663000	2.382151000	1.526626000
1	3.662794000	1.338965000	-0.273908000
1	3.766504000	0.371226000	1.203387000
1	4.017414000	2.799889000	1.742158000
1	2.440109000	3.142270000	1.002418000
1	2.532237000	2.157095000	2.475964000
8	3.076027000	-1.019640000	-0.933717000
1	3.457670000	-1.753157000	-0.436076000
1	1.938301000	-0.682274000	-2.542536000

TSP8

7	2.357632000	0.103101000	-0.030009000
6	0.992253000	0.273345000	-0.033733000
7	0.249279000	-0.770470000	0.145753000
15	-1.460349000	-0.851980000	0.237295000

8	-1.564114000	-1.350421000	1.800763000
9	-1.369620000	-1.884939000	-1.052775000
8	-1.748974000	0.728504000	-0.064284000
6	2.918164000	-1.232240000	0.208949000
6	3.015638000	-2.051270000	-1.082744000
1	2.234805000	-1.702062000	0.918726000
1	3.902116000	-1.093066000	0.670631000
1	3.442899000	-3.044038000	-0.900686000
1	2.011580000	-2.178023000	-1.495468000
1	3.590556000	-1.524056000	-1.852701000
6	3.320982000	1.172064000	-0.298914000
6	3.891546000	1.825854000	0.967249000
1	2.864962000	1.928940000	-0.939744000
1	4.138774000	0.736807000	-0.885689000
1	4.638634000	2.582311000	0.701166000
1	3.104069000	2.311947000	1.551772000
1	4.376152000	1.084744000	1.611000000
6	0.495258000	1.690037000	-0.277636000
1	1.349733000	2.334624000	-0.506097000
1	-0.199286000	1.744853000	-1.117483000
1	0.064109000	2.119505000	0.625940000
6	-3.034840000	1.355681000	-0.299060000
6	-2.814280000	2.849296000	-0.468671000
1	-3.743737000	1.151448000	0.506981000
1	-3.484218000	0.935533000	-1.203002000
1	-3.765366000	3.305872000	-0.764788000
1	-2.478060000	3.327265000	0.456646000
1	-2.117894000	3.056061000	-1.287285000
8	-3.156520000	-1.092480000	0.164347000
1	-3.370158000	-1.922979000	-0.279240000

1	-1.527702000	-2.321396000	1.795423000
---	--------------	--------------	-------------

IMB4

7	-2.331014000	0.093772000	-0.036415000
---	--------------	-------------	--------------

6	-1.025307000	0.113831000	0.399064000
---	--------------	-------------	-------------

7	-0.162892000	-0.638509000	-0.204342000
---	--------------	--------------	--------------

15	1.534378000	-0.782959000	0.122201000
----	-------------	--------------	-------------

8	1.647469000	-2.024425000	-0.938455000
---	-------------	--------------	--------------

9	1.211921000	-1.272454000	1.679862000
---	-------------	--------------	-------------

8	1.785492000	0.769034000	-0.332269000
---	-------------	-------------	--------------

6	-2.700216000	-0.744129000	-1.182167000
---	--------------	--------------	--------------

6	-3.052810000	-2.183290000	-0.789353000
---	--------------	--------------	--------------

1	-1.864328000	-0.740299000	-1.884467000
---	--------------	--------------	--------------

1	-3.553963000	-0.268106000	-1.677266000
---	--------------	--------------	--------------

1	-3.329181000	-2.763068000	-1.677521000
---	--------------	--------------	--------------

1	-2.197304000	-2.667158000	-0.310892000
---	--------------	--------------	--------------

1	-3.898925000	-2.212448000	-0.093593000
---	--------------	--------------	--------------

6	-3.422850000	0.827576000	0.606982000
---	--------------	-------------	-------------

6	-3.739391000	2.175495000	-0.055304000
---	--------------	-------------	--------------

1	-3.198610000	0.971711000	1.665426000
---	--------------	-------------	-------------

1	-4.312232000	0.186926000	0.574979000
---	--------------	-------------	-------------

1	-4.593052000	2.651586000	0.440345000
---	--------------	-------------	-------------

1	-2.884781000	2.856827000	0.003629000
---	--------------	-------------	-------------

1	-3.991974000	2.047196000	-1.112805000
---	--------------	-------------	--------------

6	-0.727973000	1.020542000	1.583159000
---	--------------	-------------	-------------

1	-1.105544000	0.572612000	2.509042000
---	--------------	-------------	-------------

1	0.344269000	1.158975000	1.691748000
---	-------------	-------------	-------------

1	-1.186273000	2.005954000	1.467554000
---	--------------	-------------	-------------

6	3.062035000	1.442531000	-0.491451000
---	-------------	-------------	--------------

6	2.771222000	2.822782000	-1.055551000
---	-------------	-------------	--------------

1	3.694109000	0.857629000	-1.163882000
---	-------------	-------------	--------------

1	3.561496000	1.497700000	0.478748000
1	3.711341000	3.368500000	-1.194210000
1	2.266181000	2.752387000	-2.023849000
1	2.135857000	3.400299000	-0.376499000
8	3.171775000	-0.937992000	0.491992000
1	3.360039000	-1.816862000	0.845661000
1	0.751100000	-2.155682000	-1.291031000

TSP9

7	-2.414556000	0.117833000	-0.036446000
6	-1.107357000	0.247287000	0.347380000
7	-0.198401000	-0.524997000	-0.154866000
15	1.605595000	-0.826202000	0.112158000
8	1.235721000	-2.060970000	-0.817858000
9	1.370784000	-0.908520000	1.724365000
8	1.932263000	0.714408000	-0.306128000
6	-2.788768000	-0.885600000	-1.041159000
6	-3.056115000	-2.272244000	-0.444801000
1	-1.992278000	-0.938078000	-1.787448000
1	-3.684239000	-0.516759000	-1.552244000
1	-3.342428000	-2.973845000	-1.235884000
1	-2.164049000	-2.662476000	0.052101000
1	-3.870554000	-2.238915000	0.287186000
6	-3.508578000	0.911376000	0.532659000
6	-3.888690000	2.134301000	-0.311711000
1	-3.248142000	1.218367000	1.547100000
1	-4.375327000	0.247711000	0.632557000
1	-4.737914000	2.657887000	0.141235000
1	-3.053773000	2.837733000	-0.388965000
1	-4.175710000	1.842410000	-1.327022000
6	-0.770325000	1.309582000	1.373005000

1	-1.255285000	2.262376000	1.146520000
1	-1.088210000	0.989909000	2.371616000
1	0.305566000	1.463290000	1.390364000
6	3.260442000	1.275925000	-0.478694000
6	3.082499000	2.715400000	-0.929346000
1	3.804841000	0.687380000	-1.220517000
1	3.803459000	1.212675000	0.467977000
1	4.064724000	3.177285000	-1.079190000
1	2.529890000	2.764325000	-1.872721000
1	2.539502000	3.300035000	-0.179914000
8	3.215800000	-1.249839000	0.281407000
1	3.312797000	-2.169179000	-0.000445000
1	0.087939000	-1.587220000	-0.798152000

P2b

7	-2.940455000	-0.149228000	0.112450000
6	-2.148165000	0.977812000	-0.031131000
7	-0.858061000	0.992336000	-0.104449000
15	2.704738000	-0.831617000	-0.218866000
8	1.315756000	-1.340151000	-0.203876000
9	3.700457000	-1.703532000	0.649791000
8	3.055266000	0.588501000	0.373476000
6	-2.330963000	-1.479973000	0.198919000
6	-1.917288000	-1.871698000	1.623111000
1	-1.466179000	-1.530896000	-0.469594000
1	-3.058919000	-2.201004000	-0.188508000
1	-1.479769000	-2.875747000	1.627873000
1	-1.170376000	-1.177997000	2.018383000
1	-2.780488000	-1.870302000	2.298109000
6	-4.402181000	-0.106060000	0.189272000
6	-5.103665000	-0.353483000	-1.153767000

1	-4.719144000	0.853359000	0.602176000
1	-4.721244000	-0.864459000	0.915005000
1	-6.192044000	-0.349450000	-1.022909000
1	-4.843119000	0.420700000	-1.882559000
1	-4.819332000	-1.322053000	-1.578148000
6	-2.856416000	2.316950000	-0.099182000
1	-3.339453000	2.565352000	0.853021000
1	-2.104204000	3.075862000	-0.311753000
1	-3.622927000	2.346989000	-0.880457000
6	2.450449000	1.826713000	-0.152514000
6	2.861028000	2.950436000	0.775371000
1	1.363658000	1.705301000	-0.185734000
1	2.844451000	1.972846000	-1.163234000
1	2.444677000	3.891845000	0.401423000
1	2.472833000	2.780649000	1.783601000
1	3.949738000	3.046802000	0.826849000
8	3.399997000	-0.846230000	-1.674202000
1	2.910657000	-1.409013000	-2.292462000
1	-0.439333000	0.064350000	-0.035860000

Reaction (VI)

TSP10

7	-2.069327000	-0.288998000	-0.279933000
6	-1.068756000	-0.920333000	0.382979000
7	0.163976000	-0.531924000	0.498689000
15	1.262889000	0.630670000	0.342132000
8	2.094296000	1.096640000	1.594374000
9	1.069172000	1.765874000	-0.760803000
8	2.395691000	-0.133518000	-0.541315000
6	-1.879350000	0.999483000	-0.978361000
6	-1.426982000	0.821770000	-2.430466000

1	-1.186939000	1.615101000	-0.406103000
1	-2.844597000	1.514618000	-0.946614000
1	-1.319016000	1.803142000	-2.903133000
1	-0.458631000	0.318203000	-2.486285000
1	-2.153250000	0.243063000	-3.012415000
6	-3.418424000	-0.867873000	-0.408550000
6	-4.405857000	-0.343615000	0.639965000
1	-3.361253000	-1.956114000	-0.368123000
1	-3.776513000	-0.618824000	-1.412807000
1	-5.401240000	-0.764351000	0.461419000
1	-4.095950000	-0.618874000	1.652892000
1	-4.487715000	0.746808000	0.598481000
6	-1.392072000	-2.252403000	1.043117000
1	-2.294601000	-2.205245000	1.658581000
1	-1.535688000	-3.037420000	0.292026000
1	-0.546444000	-2.529898000	1.670162000
6	3.172454000	-1.207572000	0.026658000
6	4.160669000	-1.678269000	-1.025885000
1	2.496415000	-2.018424000	0.324440000
1	3.689224000	-0.838041000	0.918933000
1	4.770578000	-2.494877000	-0.623897000
1	3.638291000	-2.040836000	-1.916676000
1	4.825829000	-0.862286000	-1.323755000
8	-0.017764000	1.985572000	1.507702000
1	-0.684566000	1.541206000	2.048759000
1	1.269780000	1.699897000	1.975229000
IMB5			
7	-1.917744000	0.124635000	0.098102000
6	-1.078921000	-0.125426000	-0.952027000
7	0.105904000	-0.633532000	-0.888625000

15	1.452436000	-0.851159000	0.031175000
8	2.913033000	-0.964460000	-0.696337000
9	1.502509000	-1.024862000	1.638981000
8	1.696331000	0.796578000	0.314256000
6	-1.577699000	-0.223191000	1.488190000
6	-1.051825000	0.958320000	2.308170000
1	-0.851692000	-1.035557000	1.481366000
1	-2.487909000	-0.625226000	1.947648000
1	-0.868345000	0.635582000	3.338451000
1	-0.111220000	1.326354000	1.893290000
1	-1.778037000	1.778649000	2.337972000
6	-3.273086000	0.666531000	-0.086340000
6	-4.362877000	-0.407114000	-0.203796000
1	-3.291288000	1.321465000	-0.958430000
1	-3.480772000	1.307909000	0.776394000
1	-5.346896000	0.066285000	-0.291418000
1	-4.210152000	-1.039458000	-1.083773000
1	-4.380975000	-1.056387000	0.676983000
6	-1.599674000	0.193002000	-2.346949000
1	-2.571699000	-0.264867000	-2.551017000
1	-1.702848000	1.274899000	-2.487394000
1	-0.873011000	-0.177933000	-3.068067000
6	2.014152000	1.711399000	-0.736289000
6	2.197647000	3.092773000	-0.124348000
1	1.205028000	1.727116000	-1.481108000
1	2.931053000	1.388820000	-1.242194000
1	2.451564000	3.819687000	-0.904493000
1	1.281574000	3.426725000	0.374057000
1	3.004399000	3.080761000	0.614871000
8	1.290611000	-2.571385000	-0.060000000

1	0.588326000	-2.787690000	-0.686137000
1	3.060565000	-1.897327000	-0.914813000

TSP11

7	-1.950824000	0.237745000	0.143531000
6	-1.118234000	0.221535000	-0.944096000
7	0.083223000	-0.238146000	-0.992400000
15	1.298776000	-0.912972000	-0.114381000
8	2.554796000	-1.197768000	-1.145174000
9	1.575727000	-1.374846000	1.426166000
8	1.904872000	0.582335000	0.436355000
6	-1.574539000	-0.350936000	1.440185000
6	-0.950788000	0.655421000	2.412788000
1	-0.911328000	-1.199310000	1.269481000
1	-2.488443000	-0.772335000	1.872752000
1	-0.752366000	0.165119000	3.371765000
1	-0.002014000	1.036803000	2.027610000
1	-1.625414000	1.498973000	2.598349000
6	-3.302219000	0.815127000	0.095486000
6	-4.404317000	-0.211305000	-0.196643000
1	-3.333203000	1.621426000	-0.638579000
1	-3.486020000	1.285785000	1.067453000
1	-5.386648000	0.273098000	-0.168665000
1	-4.275779000	-0.665267000	-1.184113000
1	-4.405317000	-1.016682000	0.544430000
6	-1.656407000	0.809831000	-2.240781000
1	-2.625619000	0.387139000	-2.520763000
1	-1.773157000	1.896615000	-2.163334000
1	-0.934619000	0.599105000	-3.028578000
6	2.152089000	1.670250000	-0.456917000
6	3.040218000	2.679439000	0.257949000
1	1.201790000	2.138598000	-0.747772000
1	2.637460000	1.305071000	-1.370232000

1	3.227923000	3.543475000	-0.390227000
1	2.562819000	3.033639000	1.177354000
1	4.001906000	2.230439000	0.525645000
8	0.657473000	-2.491352000	-0.263172000
1	0.401448000	-2.635371000	-1.184403000
1	3.324663000	-1.537209000	-0.667753000

IMB6

7	-2.059892000	0.287921000	0.220583000
6	-1.105509000	0.670548000	-0.673419000
7	0.131335000	0.305866000	-0.662353000
15	1.211717000	-0.856230000	-0.327616000
8	2.372272000	-1.330946000	-1.400717000
9	1.329943000	-1.706237000	1.061994000
8	2.314662000	0.231350000	0.416220000
6	-1.765068000	-0.658453000	1.310711000
6	-1.170132000	0.022832000	2.547395000
1	-1.110434000	-1.443327000	0.935129000
1	-2.710621000	-1.145304000	1.569362000
1	-1.000744000	-0.719670000	3.334070000
1	-0.208758000	0.488832000	2.317162000
1	-1.844929000	0.790396000	2.943144000
6	-3.431324000	0.816602000	0.198575000
6	-4.424598000	-0.097165000	-0.529226000
1	-3.436322000	1.811565000	-0.248309000
1	-3.743860000	0.950250000	1.240406000
1	-5.434605000	0.323861000	-0.474435000
1	-4.156792000	-0.212785000	-1.583949000
1	-4.448883000	-1.094813000	-0.079924000
6	-1.507259000	1.673189000	-1.744611000
1	-2.401646000	1.354936000	-2.287985000

1	-1.706240000	2.662008000	-1.315957000
1	-0.679426000	1.761504000	-2.446389000
6	2.526825000	1.566282000	-0.042521000
6	3.717570000	2.142940000	0.711490000
1	1.629463000	2.170603000	0.137193000
1	2.714441000	1.583281000	-1.127471000
1	3.894512000	3.179765000	0.402817000
1	3.531348000	2.127517000	1.789902000
1	4.626458000	1.564096000	0.516613000
8	0.179166000	-2.043271000	-0.963261000
1	0.659509000	-2.868673000	-1.118152000
1	3.210366000	-0.918662000	-1.142843000

TSP12

7	-1.922981000	0.090862000	0.132704000
6	-1.057794000	0.005522000	-0.910816000
7	0.106306000	-0.552244000	-0.882229000
15	1.398117000	-1.131813000	-0.167821000
8	2.871377000	-0.942046000	-0.694646000
9	1.390437000	-1.290833000	1.432443000
8	2.006640000	0.886073000	0.341789000
6	-1.609060000	-0.466950000	1.459571000
6	-0.946066000	0.543000000	2.400893000
1	-0.978100000	-1.345914000	1.329248000
1	-2.554300000	-0.819790000	1.884975000
1	-0.782077000	0.077836000	3.378544000
1	0.024627000	0.863528000	2.015175000
1	-1.581976000	1.422979000	2.549541000
6	-3.243634000	0.730825000	0.018173000
6	-4.377786000	-0.255025000	-0.286169000
1	-3.206322000	1.514339000	-0.739524000

1	-3.436220000	1.237167000	0.969701000
1	-5.336267000	0.274355000	-0.313517000
1	-4.231340000	-0.746713000	-1.252692000
1	-4.445637000	-1.033819000	0.479682000
6	-1.495689000	0.587372000	-2.244926000
1	-2.479560000	0.223802000	-2.553591000
1	-1.536646000	1.681169000	-2.199555000
1	-0.759274000	0.301043000	-2.993662000
6	1.558578000	2.038296000	-0.332822000
6	2.389143000	3.255960000	0.073368000
1	0.499508000	2.227815000	-0.087115000
1	1.609065000	1.909340000	-1.429371000
1	2.030043000	4.160606000	-0.433500000
1	2.331053000	3.414026000	1.155203000
1	3.441978000	3.108717000	-0.190214000
8	1.171584000	-2.716602000	-0.516309000
1	2.013481000	-3.193993000	-0.498178000
1	2.906033000	0.094483000	-0.309462000

P3b

7	1.812730000	-0.250080000	0.117311000
6	1.093077000	0.165351000	-0.942482000
7	0.293148000	1.202475000	-0.941874000
15	-0.967013000	1.752532000	-0.153889000
8	-1.941320000	0.790766000	0.451667000
9	-0.461147000	2.772496000	0.999892000
8	-1.389638000	-1.893547000	-0.306791000
6	1.819382000	0.481690000	1.397896000
6	0.873890000	-0.101961000	2.452590000
1	1.574524000	1.523756000	1.192338000
1	2.851328000	0.459155000	1.765172000

1	0.966088000	0.477445000	3.377238000
1	-0.166818000	-0.060087000	2.124477000
1	1.120374000	-1.143661000	2.682431000
6	2.649835000	-1.463161000	0.080606000
6	4.115157000	-1.184312000	-0.270761000
1	2.208455000	-2.181197000	-0.610711000
1	2.584166000	-1.919851000	1.072351000
1	4.688983000	-2.116439000	-0.236776000
1	4.214257000	-0.759454000	-1.274175000
1	4.570567000	-0.484653000	0.437027000
6	1.218918000	-0.590817000	-2.247010000
1	2.230348000	-0.936824000	-2.468158000
1	0.544622000	-1.454693000	-2.197100000
1	0.874343000	0.063305000	-3.046905000
6	-2.553518000	-2.686373000	-0.522368000
6	-3.313913000	-2.987505000	0.767638000
1	-2.203833000	-3.618321000	-0.981125000
1	-3.222121000	-2.196364000	-1.247218000
1	-4.182959000	-3.625341000	0.564135000
1	-2.666262000	-3.502418000	1.485154000
1	-3.672735000	-2.062817000	1.233040000
8	-1.627853000	2.815459000	-1.175309000
1	-2.477841000	3.137893000	-0.841421000
1	-1.667611000	-1.005538000	-0.001714000

Cartesian coordinates of the CPCM(water)-B3LYP/6-31G+(d,p) optimised geometries

A-234

7	-2.273245000	0.067631000	-0.190840000
6	-1.034188000	-0.421718000	-0.013899000
7	-0.111994000	0.384816000	0.481967000
15	1.421323000	0.018599000	0.844460000
8	1.787670000	-1.131188000	1.727853000
9	1.897183000	1.385675000	1.563916000
8	2.240855000	0.093343000	-0.540022000
6	-2.591411000	1.458140000	0.187497000
6	-2.330813000	2.453665000	-0.945899000
1	-1.997861000	1.714334000	1.065416000
1	-3.645631000	1.476561000	0.476149000
1	-2.609345000	3.461579000	-0.621144000
1	-1.272751000	2.460056000	-1.221158000
1	-2.921497000	2.210674000	-1.835169000
6	-3.379832000	-0.706785000	-0.783541000
6	-4.283382000	-1.365374000	0.263346000
1	-2.976083000	-1.450790000	-1.470167000
1	-3.960838000	-0.008855000	-1.393292000
1	-5.107344000	-1.883131000	-0.237941000
1	-3.733643000	-2.097027000	0.863239000
1	-4.713911000	-0.622192000	0.941434000
6	-0.767197000	-1.856004000	-0.422308000
1	-1.559840000	-2.531297000	-0.095797000
1	-0.690686000	-1.925661000	-1.512868000
1	0.171401000	-2.200123000	0.010092000
6	3.674648000	-0.188668000	-0.579392000
6	4.107052000	-0.209042000	-2.031738000

1	3.853121000	-1.150797000	-0.091635000
1	4.194739000	0.595534000	-0.019980000
1	5.181560000	-0.411641000	-2.086604000
1	3.579932000	-0.991719000	-2.585592000
1	3.913396000	0.754788000	-2.512054000

H₂O

8	0.000000000	0.000000000	0.116562000
1	0.000000000	0.769394000	-0.466249000
1	0.000000000	-0.769394000	-0.466249000

Acetoamidine hydrolysis

Pathway A

RC1

7	-2.310450000	0.206955000	-0.264557000
6	-1.245285000	-0.596201000	-0.140772000
7	-0.044163000	-0.038095000	-0.019271000
15	1.377366000	-0.805588000	-0.195586000
8	1.622180000	-1.752702000	-1.323880000
9	1.658328000	-1.596283000	1.200183000
8	2.410819000	0.412466000	-0.068626000
6	-2.155696000	1.673282000	-0.374767000
6	-1.938085000	2.124418000	-1.821074000
1	-1.324520000	1.987737000	0.253829000
1	-3.065668000	2.119564000	0.033651000
1	-1.861796000	3.215912000	-1.856604000
1	-1.014336000	1.700990000	-2.224844000
1	-2.771112000	1.822240000	-2.463778000
6	-3.699183000	-0.289872000	-0.343416000
6	-4.410990000	-0.284674000	1.012363000
1	-3.707063000	-1.287148000	-0.781586000
1	-4.224569000	0.361081000	-1.047454000

1	-5.445233000	-0.618522000	0.882748000
1	-3.920661000	-0.956327000	1.723484000
1	-4.431170000	0.719188000	1.447296000
6	-1.479132000	-2.092986000	-0.135729000
1	-2.255604000	-2.372190000	0.579661000
1	-1.793723000	-2.433166000	-1.127686000
1	-0.567751000	-2.624616000	0.129369000
6	3.847638000	0.179494000	-0.205627000
6	4.538878000	1.527866000	-0.202677000
1	4.024933000	-0.361492000	-1.139149000
1	4.177507000	-0.440138000	0.634099000
1	5.619208000	1.379227000	-0.298510000
1	4.199357000	2.142901000	-1.041400000
1	4.346498000	2.065249000	0.730670000
8	0.266172000	1.700421000	2.428751000
1	-0.403400000	1.366419000	3.040262000
1	0.173711000	1.151987000	1.625133000

TS1

7	-2.048200000	0.473362000	-0.076179000
6	-1.276852000	-0.591462000	-0.011850000
7	0.058657000	-0.409119000	0.449004000
15	1.386015000	-0.403745000	-0.519851000
8	1.206596000	0.133964000	-1.893736000
9	1.915627000	-1.929927000	-0.606669000
8	2.479541000	0.248872000	0.435129000
6	-1.672362000	1.767997000	0.544698000
6	-1.160585000	2.779758000	-0.481268000
1	-0.919558000	1.572734000	1.305522000
1	-2.569378000	2.144573000	1.043246000
1	-0.935868000	3.721489000	0.028761000

1	-0.249272000	2.419953000	-0.965673000
1	-1.906533000	2.986456000	-1.254697000
6	-3.425025000	0.411671000	-0.622604000
6	-4.462480000	-0.000028000	0.424737000
1	-3.433958000	-0.264714000	-1.477109000
1	-3.646637000	1.409200000	-1.007169000
1	-5.454466000	0.007155000	-0.036296000
1	-4.267309000	-1.003943000	0.810428000
1	-4.476722000	0.695479000	1.268883000
6	-1.631927000	-1.866374000	-0.719615000
1	-2.677752000	-2.141093000	-0.593585000
1	-1.425490000	-1.750249000	-1.792152000
1	-1.011517000	-2.669378000	-0.326909000
6	3.902223000	0.267781000	0.066941000
6	4.631196000	1.108414000	1.093489000
1	3.992028000	0.690129000	-0.937478000
1	4.261704000	-0.764536000	0.059447000
1	5.696945000	1.130912000	0.844717000
1	4.255424000	2.135591000	1.097095000
1	4.519962000	0.685384000	2.096093000
8	-1.364719000	-1.559170000	2.043720000
1	-1.862716000	-0.988239000	2.646817000
1	0.010581000	-0.896959000	1.390002000

IM1

7	-1.813858000	0.434491000	-0.187870000
6	-1.328472000	-0.742689000	0.485852000
7	0.138988000	-0.573842000	0.740303000
15	1.356688000	-0.569247000	-0.366989000
8	1.034160000	-0.244825000	-1.778440000
9	2.022831000	-2.046532000	-0.298221000

8	2.477511000	0.293447000	0.375085000
6	-1.617775000	1.715631000	0.518439000
6	-1.239322000	2.866915000	-0.419027000
1	-0.807800000	1.585628000	1.239888000
1	-2.516323000	1.994811000	1.090354000
1	-1.106590000	3.786461000	0.161678000
1	-0.302752000	2.649918000	-0.941548000
1	-2.012731000	3.060914000	-1.168739000
6	-3.097336000	0.339855000	-0.905087000
6	-4.366601000	0.149307000	-0.056279000
1	-3.025579000	-0.460641000	-1.645816000
1	-3.195300000	1.263836000	-1.482424000
1	-5.246021000	0.166507000	-0.709939000
1	-4.360134000	-0.803439000	0.480336000
1	-4.486584000	0.949925000	0.680855000
6	-1.603422000	-2.042690000	-0.272846000
1	-2.671869000	-2.255185000	-0.327007000
1	-1.193558000	-1.992073000	-1.283795000
1	-1.119927000	-2.860542000	0.265569000
6	3.846726000	0.375032000	-0.146970000
6	4.603454000	1.377601000	0.698869000
1	3.798443000	0.686741000	-1.193928000
1	4.292275000	-0.621690000	-0.087223000
1	5.632296000	1.451706000	0.332452000
1	4.143027000	2.367967000	0.638131000
1	4.632284000	1.063078000	1.746229000
8	-1.881847000	-0.960978000	1.800311000
1	-1.909786000	-0.116768000	2.274854000
1	0.402819000	-0.919118000	1.658507000

Channel 1**IM2**

7	-0.029599000	0.239649000	-0.416561000
6	0.965430000	0.011176000	0.659682000
7	2.324205000	0.162702000	0.150049000
1	0.093480000	1.146507000	-0.859296000
8	0.722756000	1.041704000	1.622313000
1	1.453268000	1.015120000	2.259796000
6	2.799972000	-0.936023000	-0.724034000
6	3.811635000	-1.869286000	-0.052826000
1	3.267195000	-0.486627000	-1.606831000
1	1.947645000	-1.509953000	-1.107098000
1	4.154096000	-2.626644000	-0.767703000
1	4.684316000	-1.308001000	0.296028000
1	3.378359000	-2.388351000	0.806739000
6	2.637357000	1.499387000	-0.398162000
6	4.119623000	1.849405000	-0.253953000
1	2.046608000	2.238254000	0.146472000
1	2.351179000	1.565478000	-1.462503000
1	4.308461000	2.846052000	-0.667389000
1	4.415255000	1.848890000	0.800301000
1	4.761406000	1.141468000	-0.788307000
15	-1.586122000	-0.308392000	-0.505469000
6	0.756524000	-1.349731000	1.328917000
1	-0.223969000	-1.372229000	1.808666000
1	0.818924000	-2.182915000	0.628590000
1	1.517659000	-1.473213000	2.102001000
8	-1.818514000	-1.774949000	-0.517973000
9	-1.998034000	0.367472000	-1.906150000
8	-2.464732000	0.513775000	0.546840000

6	-3.810837000	0.092866000	0.956028000
6	-4.874987000	0.679590000	0.046931000
1	-3.904549000	0.467183000	1.976670000
1	-3.840794000	-0.998984000	0.973916000
1	-5.863063000	0.407807000	0.433520000
1	-4.806148000	1.770993000	0.017580000
1	-4.791820000	0.292798000	-0.973130000

TS2

7	-0.223590000	0.131579000	0.905339000
6	0.978571000	-0.699289000	0.785837000
7	2.194103000	0.067500000	0.086263000
1	-0.327513000	0.529157000	1.832870000
8	1.609474000	-0.782797000	2.007719000
1	2.518561000	-0.262899000	1.275619000
6	2.834787000	-0.548505000	-1.114872000
6	4.052034000	-1.401427000	-0.760677000
1	3.136925000	0.257610000	-1.787083000
1	2.090082000	-1.134690000	-1.657808000
1	4.485866000	-1.823306000	-1.672913000
1	4.818158000	-0.797320000	-0.264369000
1	3.791196000	-2.230669000	-0.096220000
6	2.036781000	1.543383000	-0.035179000
6	3.381395000	2.269342000	0.003457000
1	1.428883000	1.880055000	0.804138000
1	1.488373000	1.774664000	-0.956325000
1	3.205857000	3.348067000	-0.055505000
1	3.909273000	2.060196000	0.939491000
1	4.036043000	1.996089000	-0.829114000
15	-1.457586000	0.327018000	-0.165318000
6	0.663675000	-2.048378000	0.147448000

1	-0.030199000	-2.561682000	0.818263000
1	0.197207000	-1.960420000	-0.837483000
1	1.565091000	-2.656566000	0.065952000
8	-1.118016000	0.249430000	-1.609079000
9	-1.993581000	1.784211000	0.253236000
8	-2.649080000	-0.614989000	0.328376000
6	-3.865678000	-0.833279000	-0.467394000
6	-4.991259000	0.069867000	0.001185000
1	-4.103474000	-1.886471000	-0.308937000
1	-3.625990000	-0.682546000	-1.522811000
1	-5.898933000	-0.171619000	-0.562258000
1	-5.197070000	-0.082862000	1.064670000
1	-4.756773000	1.125056000	-0.165715000

PC1

7	1.360232000	0.666656000	1.121493000
6	0.817190000	1.936516000	0.906791000
7	-4.372599000	-0.088691000	0.158752000
1	1.327814000	0.369942000	2.094015000
8	0.327951000	2.536430000	1.855883000
1	-4.877952000	0.301034000	0.953413000
6	-5.179750000	0.084122000	-1.055361000
6	-5.441709000	1.563301000	-1.334787000
1	-6.144437000	-0.449112000	-1.009201000
1	-4.617716000	-0.356965000	-1.888786000
1	-6.035906000	1.684107000	-2.246869000
1	-5.998721000	2.026197000	-0.511212000
1	-4.501506000	2.111253000	-1.458253000
6	-3.989990000	-1.474310000	0.464786000
6	-5.134374000	-2.450090000	0.783078000
1	-3.301769000	-1.441034000	1.318010000

1	-3.411908000	-1.851829000	-0.388612000
1	-4.730655000	-3.436076000	1.041236000
1	-5.724171000	-2.094535000	1.636630000
1	-5.811766000	-2.580711000	-0.066976000
15	2.127178000	-0.363658000	0.039074000
6	0.864964000	2.492531000	-0.493327000
1	1.899676000	2.576484000	-0.841643000
1	0.332851000	1.836420000	-1.187642000
1	0.405367000	3.480090000	-0.491464000
8	1.463747000	-0.613574000	-1.260413000
9	2.181189000	-1.661796000	0.968070000
8	3.631748000	0.135506000	-0.003754000
6	4.572678000	-0.237064000	-1.077884000
6	5.383904000	-1.456295000	-0.686654000
1	5.198644000	0.648534000	-1.191686000
1	4.001536000	-0.392186000	-1.995530000
1	6.122360000	-1.654862000	-1.470630000
1	5.917647000	-1.286234000	0.252663000
1	4.753765000	-2.344397000	-0.581503000

RC3

6	0.258931000	-1.705046000	0.774634000
8	0.125810000	-2.877454000	1.103187000
7	1.066549000	-1.411748000	-0.332650000
1	1.495237000	-2.233728000	-0.751989000
8	4.417441000	-1.308775000	1.476477000
1	3.836167000	-0.742994000	0.943282000
1	4.220535000	-2.211702000	1.193899000
6	-0.425931000	-0.563808000	1.474179000
1	-0.727204000	-0.901044000	2.466363000
1	0.214210000	0.317109000	1.565879000
1	-1.325040000	-0.279167000	0.906825000
15	1.458566000	0.071617000	-1.006083000
8	0.367556000	1.034776000	-1.268483000
9	2.161398000	-0.453695000	-2.338550000
8	2.679786000	0.603504000	-0.127102000
6	3.151126000	2.004863000	-0.232564000
6	3.933954000	2.330215000	1.020159000
1	2.273074000	2.643194000	-0.344550000
1	3.768872000	2.067002000	-1.131356000
1	4.289655000	3.363179000	0.951624000
1	3.305594000	2.240471000	1.910695000
1	4.804221000	1.676812000	1.127597000
7	-3.501218000	0.369226000	-0.063561000
1	-3.395661000	0.719206000	-1.014966000
6	-4.536885000	-0.671082000	-0.044769000
6	-4.171101000	-1.828220000	-0.973183000
1	-5.533478000	-0.288876000	-0.323285000
1	-4.618499000	-1.034652000	0.987901000
1	-4.944992000	-2.602667000	-0.945861000

1	-4.080300000	-1.485542000	-2.011063000
1	-3.217932000	-2.280957000	-0.680712000
6	-3.734162000	1.501313000	0.843692000
6	-4.962540000	2.377352000	0.550188000
1	-2.834706000	2.128537000	0.819677000
1	-3.805841000	1.096960000	1.861761000
1	-5.009747000	3.212678000	1.258515000
1	-4.909427000	2.797285000	-0.461504000
1	-5.898203000	1.815622000	0.636279000

TS3

6	0.147334000	2.110745000	-1.007288000
8	-0.179841000	3.142162000	-0.580056000
7	1.770030000	1.391149000	0.407632000
1	1.672432000	2.084774000	1.147505000
8	1.831314000	2.250367000	-1.948640000
1	2.204940000	1.930957000	-1.042080000
1	2.049488000	3.191499000	-2.052946000
6	-0.404911000	0.868716000	-1.559756000
1	-0.814881000	1.121514000	-2.544544000
1	0.358469000	0.101308000	-1.653426000
1	-1.218811000	0.541537000	-0.889176000
15	2.100054000	-0.073125000	1.006138000
8	1.458044000	-0.599776000	2.253536000
9	3.719005000	-0.142337000	1.255717000
8	1.974233000	-1.023035000	-0.290950000
6	2.191185000	-2.460271000	-0.178163000
6	1.900516000	-3.086945000	-1.527540000
1	1.528540000	-2.853784000	0.598057000
1	3.229751000	-2.631727000	0.122884000
1	2.063492000	-4.167860000	-1.467195000

1	0.862507000	-2.911465000	-1.825608000
1	2.562382000	-2.681697000	-2.298897000
7	-2.979585000	-0.349720000	0.240090000
1	-2.636105000	-0.800076000	1.087594000
6	-4.032894000	0.609790000	0.597426000
6	-3.509319000	1.664674000	1.570802000
1	-4.920059000	0.124185000	1.036665000
1	-4.366337000	1.091967000	-0.330684000
1	-4.300024000	2.378587000	1.824498000
1	-3.166876000	1.202185000	2.504373000
1	-2.669665000	2.218164000	1.138001000
6	-3.375553000	-1.382548000	-0.728570000
6	-4.457313000	-2.374011000	-0.272627000
1	-2.470373000	-1.940515000	-0.997535000
1	-3.707904000	-0.867809000	-1.639341000
1	-4.637243000	-3.121956000	-1.053457000
1	-4.143301000	-2.904063000	0.634533000
1	-5.409676000	-1.876452000	-0.063625000

Pdt1

6	-0.819042000	1.782235000	-0.163553000
8	-1.489003000	2.582985000	-0.788617000
7	2.680550000	0.373710000	1.543511000
1	2.759330000	0.636349000	2.518798000
8	0.507155000	1.985746000	0.055405000
1	1.977401000	0.900070000	1.027422000
1	0.763017000	2.829756000	-0.357957000
6	-1.307077000	0.500279000	0.445799000
1	-0.735673000	-0.341684000	0.043333000
1	-1.141166000	0.521283000	1.527453000
1	-2.368206000	0.367165000	0.233984000

15	4.070141000	-0.066811000	0.796626000
8	5.078479000	-0.748150000	1.649842000
9	4.728545000	1.263426000	0.149786000
8	3.536189000	-0.806548000	-0.510711000
6	4.446162000	-1.211381000	-1.588044000
6	3.646140000	-2.018647000	-2.588514000
1	5.256588000	-1.801162000	-1.151058000
1	4.860824000	-0.305724000	-2.038933000
1	4.303756000	-2.326701000	-3.407580000
1	3.229463000	-2.916702000	-2.123412000
1	2.829277000	-1.423794000	-3.007483000
7	-5.073227000	-0.369434000	0.111329000
1	-5.078146000	0.155601000	0.984907000
6	-6.297864000	-0.063988000	-0.638881000
6	-6.383518000	1.425656000	-0.967819000
1	-7.214755000	-0.367300000	-0.105611000
1	-6.268229000	-0.648058000	-1.567864000
1	-7.295533000	1.643445000	-1.533784000
1	-6.408121000	2.029252000	-0.052440000
1	-5.521620000	1.746420000	-1.562429000
6	-4.859305000	-1.792957000	0.406492000
6	-5.885456000	-2.465839000	1.332268000
1	-3.861619000	-1.887374000	0.852160000
1	-4.824374000	-2.325501000	-0.552805000
1	-5.601648000	-3.508262000	1.518344000
1	-5.932633000	-1.952609000	2.300366000
1	-6.891015000	-2.467495000	0.899393000

Channel 2**IM3**

7	-2.233576000	-0.056667000	-0.351762000
6	-0.878276000	-0.529192000	-0.193582000
7	0.009265000	0.611151000	-0.549685000
15	1.494254000	0.900089000	0.107349000
8	1.587845000	1.299212000	1.536211000
9	1.950474000	2.105749000	-0.857353000
8	2.470075000	-0.287410000	-0.334355000
6	-2.624072000	1.107559000	0.468071000
6	-3.428132000	2.142299000	-0.325216000
1	-1.717520000	1.590819000	0.839284000
1	-3.199899000	0.789661000	1.349573000
1	-3.707890000	2.978623000	0.325145000
1	-2.835480000	2.534539000	-1.158122000
1	-4.350849000	1.717879000	-0.733851000
6	-3.305284000	-1.057402000	-0.502496000
6	-3.605946000	-1.951315000	0.712839000
1	-3.084636000	-1.680550000	-1.372989000
1	-4.209478000	-0.498854000	-0.763025000
1	-4.469105000	-2.588758000	0.490001000
1	-2.760477000	-2.598037000	0.962779000
1	-3.850906000	-1.359856000	1.601037000
6	-0.564434000	-1.741575000	-1.074363000
1	-1.125294000	-2.622081000	-0.756932000
1	-0.798020000	-1.522317000	-2.118991000
1	0.500674000	-1.961802000	-0.990101000
6	3.777926000	-0.486347000	0.301775000
6	4.329308000	-1.811966000	-0.180461000
1	3.636813000	-0.472666000	1.384904000

1	4.425541000	0.346953000	0.013764000
1	5.310560000	-1.979371000	0.275141000
1	3.670743000	-2.637223000	0.105837000
1	4.449773000	-1.815516000	-1.267772000
8	-0.508599000	-0.930514000	1.136897000
1	-0.734743000	-0.223817000	1.760508000
1	-0.148827000	0.985254000	-1.479552000

TS4

7	-2.143942000	0.125861000	0.372562000
6	-0.747837000	0.435226000	0.566940000
7	-0.007701000	-0.768373000	1.012788000
15	1.275700000	-0.921386000	-0.000887000
8	0.937317000	-1.242617000	-1.496519000
9	1.865348000	-2.306860000	0.558892000
8	2.599493000	-0.073099000	0.247827000
6	-2.455690000	-0.984804000	-0.545111000
6	-3.615149000	-1.854100000	-0.047720000
1	-1.571588000	-1.615351000	-0.636113000
1	-2.680315000	-0.611383000	-1.555575000
1	-3.803426000	-2.666165000	-0.759109000
1	-3.375801000	-2.296723000	0.925020000
1	-4.545613000	-1.286807000	0.056680000
6	-3.081750000	1.257457000	0.260050000
6	-2.934010000	2.162536000	-0.975219000
1	-3.017221000	1.861785000	1.168537000
1	-4.087963000	0.828079000	0.265512000
1	-3.721618000	2.924659000	-0.966156000
1	-1.966470000	2.672297000	-0.992207000
1	-3.030810000	1.595832000	-1.906894000
6	-0.537457000	1.593991000	1.546152000

1	-0.888390000	2.539590000	1.129239000
1	-1.055521000	1.403571000	2.490830000
1	0.531489000	1.687411000	1.746032000
6	2.988060000	1.109865000	-0.528239000
6	4.408710000	1.460736000	-0.138329000
1	2.284190000	1.909351000	-0.294984000
1	2.908373000	0.861778000	-1.589635000
1	4.720624000	2.349048000	-0.697122000
1	4.478301000	1.685203000	0.930144000
1	5.097474000	0.644587000	-0.374978000
8	0.038857000	0.695759000	-0.619055000
1	0.233944000	-0.298273000	-1.447322000
1	-0.126377000	-1.234166000	1.904751000

IMA

7	-2.131606000	0.208254000	0.341291000
6	-0.747406000	0.358422000	0.646277000
7	-0.111964000	-0.894888000	1.062069000
15	1.132653000	-0.864061000	-0.043651000
8	1.086111000	-1.616735000	-1.490459000
9	1.824149000	-2.226754000	0.616938000
8	2.536887000	-0.083681000	0.170199000
6	-2.524416000	-0.913439000	-0.529783000
6	-3.713268000	-1.700501000	0.030260000
1	-1.676012000	-1.588838000	-0.634237000
1	-2.762828000	-0.548499000	-1.538824000
1	-3.989198000	-2.506861000	-0.658857000
1	-3.459732000	-2.145367000	0.998279000
1	-4.595586000	-1.066715000	0.168608000
6	-2.940290000	1.422624000	0.138109000
6	-2.607369000	2.263434000	-1.105576000

1	-2.879619000	2.046452000	1.033707000
1	-3.982302000	1.094061000	0.078358000
1	-3.312331000	3.098716000	-1.184520000
1	-1.595798000	2.677349000	-1.056961000
1	-2.684973000	1.673250000	-2.024375000
6	-0.465347000	1.521794000	1.596860000
1	-0.671582000	2.486044000	1.128971000
1	-1.070469000	1.430822000	2.503677000
1	0.588704000	1.499752000	1.878985000
6	2.845690000	1.202329000	-0.438752000
6	4.296301000	1.515980000	-0.124480000
1	2.173371000	1.960597000	-0.033357000
1	2.681241000	1.133996000	-1.518358000
1	4.560589000	2.482935000	-0.565055000
1	4.458391000	1.574945000	0.956270000
1	4.963717000	0.754146000	-0.538539000
8	0.157865000	0.461551000	-0.539576000
1	0.566329000	-1.084469000	-2.113480000
1	-0.124337000	-1.277113000	1.999728000

TS5

7	-2.242873000	0.183928000	-0.144533000
6	-0.980436000	0.608925000	0.024229000
7	0.088835000	-0.481884000	1.339544000
15	1.209307000	-0.628844000	0.185519000
8	1.338208000	-1.870295000	-0.883399000
9	2.357894000	-1.419366000	1.138384000
8	2.229943000	0.569136000	-0.255693000
6	-2.554136000	-1.038750000	-0.910575000
6	-2.588819000	-2.313542000	-0.061222000
1	-1.823582000	-1.130840000	-1.713164000

1	-3.528594000	-0.871744000	-1.379179000
1	-2.859752000	-3.163112000	-0.696922000
1	-1.613737000	-2.506760000	0.390824000
1	-3.332211000	-2.245590000	0.739826000
6	-3.379080000	0.780271000	0.583413000
6	-4.179772000	1.777638000	-0.259281000
1	-3.017080000	1.252368000	1.497181000
1	-4.026820000	-0.042652000	0.899038000
1	-5.038446000	2.137671000	0.316777000
1	-3.572174000	2.641690000	-0.542581000
1	-4.559159000	1.310348000	-1.173422000
6	-0.738389000	2.001269000	0.564930000
1	-1.183538000	2.734803000	-0.117311000
1	-1.161945000	2.145854000	1.558785000
1	0.334632000	2.174518000	0.614186000
6	3.662198000	0.562753000	-0.022452000
6	4.237947000	1.800132000	-0.687496000
1	4.093034000	-0.348810000	-0.447099000
1	3.853679000	0.567646000	1.053914000
1	5.320749000	1.829570000	-0.526042000
1	4.050625000	1.790701000	-1.765796000
1	3.802684000	2.711131000	-0.264851000
8	-0.067477000	0.123183000	-0.850863000
1	0.715020000	-1.736216000	-1.613227000
1	0.381757000	-0.606295000	2.306116000

PC2

7	-3.280816000	0.093320000	-0.064011000
6	-2.012986000	0.470689000	0.153066000
7	1.994887000	-1.483252000	1.577351000
15	2.382395000	-0.653600000	0.322354000

8	1.322490000	0.412862000	-0.115050000
9	2.597628000	-1.538642000	-1.030793000
8	3.785503000	0.121237000	0.376891000
6	-3.556118000	-1.121219000	-0.856871000
6	-3.598226000	-2.388032000	0.001314000
1	-2.786740000	-1.205043000	-1.625485000
1	-4.515020000	-0.966303000	-1.358070000
1	-3.836466000	-3.251742000	-0.627958000
1	-2.630988000	-2.566992000	0.479170000
1	-4.363650000	-2.316627000	0.780817000
6	-4.450437000	0.819210000	0.465444000
6	-5.061373000	1.794290000	-0.544853000
1	-4.165744000	1.339656000	1.380173000
1	-5.187482000	0.064401000	0.755006000
1	-5.945964000	2.268191000	-0.107665000
1	-4.351731000	2.580934000	-0.818894000
1	-5.371387000	1.279389000	-1.459262000
6	-1.727133000	1.710312000	0.971297000
1	-2.318344000	2.567225000	0.641528000
1	-1.954370000	1.528840000	2.027177000
1	-0.669293000	1.956359000	0.885378000
6	4.299682000	0.909900000	-0.745095000
6	5.590434000	1.566027000	-0.299226000
1	3.543832000	1.651348000	-1.017770000
1	4.462618000	0.235646000	-1.590611000
1	5.997502000	2.159183000	-1.124525000
1	5.417891000	2.231918000	0.551527000
1	6.333939000	0.815241000	-0.015388000
8	-1.061713000	-0.218801000	-0.317423000
1	0.302312000	0.136053000	-0.165477000

1	2.652722000	-2.215819000	1.832961000
---	-------------	--------------	-------------

TS6

7	3.567554000	-0.027359000	-0.057751000
6	2.330468000	-0.588044000	-0.107608000
7	-1.402403000	0.160438000	1.200967000
15	-2.587038000	0.406597000	0.181160000
8	-1.729895000	0.109978000	-1.081566000
9	-3.174001000	1.898556000	0.084482000
8	-3.912938000	-0.440467000	0.367291000
6	3.775753000	1.308689000	-0.637523000
6	3.565755000	2.438713000	0.375140000
1	3.088472000	1.421900000	-1.477564000
1	4.795273000	1.340082000	-1.033609000
1	3.756286000	3.407050000	-0.100124000
1	2.538506000	2.436752000	0.751413000
1	4.246443000	2.342497000	1.227692000
6	4.739918000	-0.675255000	0.550364000
6	5.617761000	-1.420884000	-0.460604000
1	4.409286000	-1.351803000	1.339628000
1	5.323590000	0.108694000	1.043660000
1	6.492763000	-1.841794000	0.045850000
1	5.068900000	-2.241245000	-0.933746000
1	5.974251000	-0.749897000	-1.248557000
6	2.139035000	-1.968815000	0.498300000
1	2.884565000	-2.688081000	0.149456000
1	2.200885000	-1.925739000	1.591283000
1	1.145887000	-2.322603000	0.221985000
6	-5.072803000	-0.330564000	-0.537009000
6	-6.103158000	-1.340320000	-0.081698000
1	-4.725317000	-0.532605000	-1.553731000

1	-5.449584000	0.692885000	-0.475691000
1	-6.977287000	-1.275860000	-0.737397000
1	-5.705879000	-2.357847000	-0.134544000
1	-6.425068000	-1.135418000	0.943326000
8	1.365312000	0.006817000	-0.626070000
1	-0.871821000	0.063279000	-0.105859000
1	-1.290813000	0.540500000	2.132884000

Pdt2

7	-3.545691000	-0.029940000	-0.025410000
6	-2.319141000	-0.430077000	-0.432223000
7	1.414068000	-0.122528000	-0.949932000
15	2.492854000	0.296003000	0.200371000
8	2.056387000	0.101047000	1.609057000
9	2.885246000	1.855356000	-0.018429000
8	3.837007000	-0.416824000	-0.287274000
6	-3.720252000	1.328093000	0.517427000
6	-4.066198000	2.358966000	-0.560997000
1	-2.797736000	1.608212000	1.028177000
1	-4.515880000	1.280279000	1.266531000
1	-4.211525000	3.342970000	-0.102658000
1	-3.259983000	2.437871000	-1.296137000
1	-4.989262000	2.092351000	-1.086411000
6	-4.750228000	-0.873307000	-0.100170000
6	-5.060690000	-1.605267000	1.209432000
1	-4.641573000	-1.584852000	-0.919540000
1	-5.584834000	-0.218828000	-0.370387000
1	-5.986809000	-2.179467000	1.102050000
1	-4.257174000	-2.298575000	1.477130000
1	-5.194014000	-0.901308000	2.036829000
6	-2.156324000	-1.829531000	-0.996339000

1	-2.611205000	-2.593860000	-0.361651000
1	-2.615830000	-1.899224000	-1.988437000
1	-1.091041000	-2.037640000	-1.094711000
6	5.120365000	-0.158801000	0.371564000
6	6.143350000	-1.104780000	-0.222041000
1	4.997079000	-0.323139000	1.445707000
1	5.388445000	0.886697000	0.195746000
1	7.114507000	-0.925727000	0.250269000
1	5.860891000	-2.146965000	-0.046941000
1	6.248432000	-0.941872000	-1.298724000
8	-1.332565000	0.338208000	-0.360363000
1	0.411412000	0.013098000	-0.739910000
1	1.665514000	0.027766000	-1.920536000

Channel 3

IM4

7	2.145803000	0.233720000	-0.376882000
6	1.115924000	-0.657518000	0.186068000
7	-0.171452000	-0.008080000	-0.157706000
15	-1.683334000	-0.569189000	0.188613000
8	-1.909228000	-1.199744000	1.513154000
9	-2.080158000	-1.624219000	-0.972837000
8	-2.570212000	0.690599000	-0.223999000
6	3.501976000	-0.345498000	-0.442989000
6	4.358395000	0.310583000	-1.528796000
1	3.401956000	-1.407283000	-0.666699000
1	4.022169000	-0.275573000	0.525046000
1	5.328170000	-0.195209000	-1.584427000
1	3.871812000	0.231580000	-2.506803000
1	4.550820000	1.369199000	-1.328300000
6	2.126256000	1.649354000	0.069997000

6	2.962052000	2.031986000	1.304382000
1	1.086491000	1.927344000	0.246979000
1	2.465624000	2.258160000	-0.775723000
1	2.794952000	3.093341000	1.518762000
1	2.683423000	1.464297000	2.196189000
1	4.035364000	1.898740000	1.139137000
6	1.220204000	-0.945534000	1.686771000
1	2.222661000	-1.318697000	1.908146000
1	1.041284000	-0.036638000	2.262568000
1	0.488326000	-1.696039000	1.987883000
6	-4.034280000	0.603181000	-0.298454000
6	-4.568073000	2.001919000	-0.524257000
1	-4.402320000	0.178240000	0.639308000
1	-4.290352000	-0.066135000	-1.124062000
1	-5.659864000	1.961310000	-0.592044000
1	-4.297551000	2.662886000	0.304187000
1	-4.180317000	2.423279000	-1.456317000
8	1.206002000	-1.926318000	-0.449324000
1	1.194144000	-1.780079000	-1.408939000
1	-0.113033000	0.476453000	-1.051420000

TS7

7	1.945472000	0.154782000	-0.280679000
6	1.024923000	-0.731793000	0.651004000
7	-0.050194000	-0.725786000	-0.330864000
15	-1.647484000	-0.816315000	-0.103472000
8	-2.213852000	-1.585375000	1.045759000
9	-2.154829000	-1.464778000	-1.499037000
8	-2.232406000	0.678586000	-0.262830000
6	3.270049000	-0.409826000	-0.647495000
6	3.874377000	0.272272000	-1.874791000

1	3.125622000	-1.466923000	-0.865645000
1	3.952331000	-0.348540000	0.208475000
1	4.777325000	-0.270620000	-2.169946000
1	3.175257000	0.252691000	-2.717354000
1	4.161030000	1.310492000	-1.686862000
6	1.959274000	1.618621000	0.008349000
6	2.956445000	2.105302000	1.062217000
1	0.938671000	1.900210000	0.276800000
1	2.167155000	2.113605000	-0.944154000
1	2.832977000	3.186179000	1.184442000
1	2.801115000	1.638834000	2.037287000
1	3.991816000	1.926222000	0.758958000
6	0.755331000	-0.196672000	2.049893000
1	1.661355000	-0.260262000	2.655943000
1	0.392727000	0.830841000	2.042591000
1	-0.008291000	-0.829471000	2.507563000
6	-3.668360000	0.930128000	-0.167498000
6	-3.886517000	2.428948000	-0.226026000
1	-4.034166000	0.507359000	0.772490000
1	-4.164406000	0.423419000	-1.001672000
1	-4.958519000	2.641977000	-0.161720000
1	-3.384978000	2.929883000	0.607518000
1	-3.508799000	2.843633000	-1.165511000
8	1.575270000	-2.013374000	0.816525000
1	1.323156000	-2.542157000	0.044056000
1	0.852176000	-0.103189000	-0.988609000
PC3			
7	2.036727000	0.105681000	-0.380340000
6	1.010933000	-1.038949000	0.284313000
7	-0.099897000	-1.025772000	-0.536365000

15	-1.632188000	-0.909827000	-0.132946000
8	-2.251957000	-1.614614000	1.039235000
9	-2.370262000	-1.443958000	-1.482667000
8	-2.051408000	0.660743000	-0.203344000
6	3.440710000	0.081007000	0.158097000
6	4.445702000	0.721764000	-0.795590000
1	3.683060000	-0.969105000	0.316901000
1	3.435107000	0.583666000	1.125445000
1	5.447893000	0.615802000	-0.370565000
1	4.441838000	0.223084000	-1.770665000
1	4.259711000	1.788007000	-0.949451000
6	1.438549000	1.489020000	-0.535272000
6	1.664271000	2.451067000	0.626325000
1	0.375921000	1.322167000	-0.714051000
1	1.864135000	1.908050000	-1.450094000
1	1.114489000	3.369574000	0.400176000
1	1.288221000	2.070663000	1.577930000
1	2.715307000	2.723691000	0.751222000
6	0.889421000	-0.767299000	1.778602000
1	1.867124000	-0.764298000	2.264691000
1	0.383597000	0.178632000	1.974588000
1	0.292495000	-1.571948000	2.212189000
6	-3.408582000	1.079883000	0.111100000
6	-3.460690000	2.595051000	0.061214000
1	-3.671648000	0.702914000	1.103754000
1	-4.091280000	0.638223000	-0.623319000
1	-4.476204000	2.933554000	0.291823000
1	-2.777064000	3.033821000	0.794644000
1	-3.192625000	2.964592000	-0.933427000
8	1.766202000	-2.221564000	0.116330000

1	1.396380000	-2.658940000	-0.667262000
1	2.076333000	-0.274282000	-1.329920000
TS8			
7	-3.230983000	-0.074878000	-0.437715000
6	1.829124000	-2.451369000	-0.544315000
7	1.706227000	-1.132806000	-0.732633000
15	1.523109000	0.137069000	0.311132000
8	1.554182000	-0.129861000	1.771652000
9	0.095846000	0.742992000	-0.118665000
8	2.530197000	1.211405000	-0.285410000
6	-3.758552000	-0.806293000	0.725063000
6	-3.743179000	-0.061214000	2.069651000
1	-3.166150000	-1.724266000	0.819091000
1	-4.781427000	-1.125950000	0.495078000
1	-4.107472000	-0.717377000	2.868758000
1	-2.725998000	0.254461000	2.330564000
1	-4.381312000	0.828332000	2.056238000
6	-3.950350000	1.151128000	-0.819596000
6	-5.306445000	0.863239000	-1.467504000
1	-3.315247000	1.677389000	-1.541060000
1	-4.096100000	1.841524000	0.028584000
1	-5.775445000	1.799201000	-1.790413000
1	-5.189607000	0.216068000	-2.343731000
1	-5.997037000	0.373410000	-0.772882000
6	1.847277000	-3.251176000	0.707253000
1	0.957189000	-3.888551000	0.723655000
1	2.721832000	-3.907114000	0.695839000
1	1.858750000	-2.613810000	1.589954000
6	2.656470000	2.554676000	0.302343000
6	3.826612000	3.239864000	-0.370069000

1	2.813662000	2.444034000	1.378071000
1	1.718246000	3.087178000	0.124553000
1	3.936057000	4.247086000	0.044225000
1	4.755897000	2.690746000	-0.193541000
1	3.663271000	3.326397000	-1.448119000
8	1.930286000	-2.958895000	-1.722101000
1	-2.256897000	0.159139000	-0.260497000
1	1.808782000	-1.671404000	-1.940993000

Channel 4

TS11

7	1.654345000	-0.104736000	0.040002000
6	1.095365000	1.187657000	0.465149000
7	-0.369750000	1.080136000	0.316275000
15	-1.207482000	-0.295389000	-0.036067000
8	-1.110111000	-1.518235000	0.804710000
9	-0.865264000	-0.676084000	-1.565779000
8	-2.670588000	0.344806000	-0.182452000
6	2.226993000	-0.967888000	1.088047000
6	2.366343000	-2.429545000	0.655097000
1	1.556038000	-0.952190000	1.948255000
1	3.201445000	-0.593638000	1.439825000
1	2.676390000	-3.024636000	1.520617000
1	1.409811000	-2.819343000	0.294935000
1	3.119716000	-2.573495000	-0.124786000
6	2.296892000	-0.202393000	-1.280195000
6	3.795256000	0.135936000	-1.357518000
1	1.736315000	0.417190000	-1.982270000
1	2.153931000	-1.229033000	-1.632134000
1	4.149603000	-0.022942000	-2.382445000
1	4.003956000	1.174510000	-1.087734000

1	4.388338000	-0.508154000	-0.700378000
6	1.580204000	2.429922000	-0.293820000
1	2.640542000	2.597805000	-0.099108000
1	1.412997000	2.350705000	-1.367480000
1	1.026394000	3.295951000	0.077910000
6	-3.870552000	-0.492359000	-0.159345000
6	-5.073044000	0.424217000	-0.064703000
1	-3.806473000	-1.166893000	0.698074000
1	-3.890718000	-1.085019000	-1.078881000
1	-5.985735000	-0.180266000	-0.056186000
1	-5.042405000	1.015971000	0.854981000
1	-5.117849000	1.103204000	-0.921330000
8	1.390030000	1.485205000	1.828494000
1	0.814573000	0.952963000	2.396054000
1	-0.918819000	1.927602000	0.418868000

IM5

7	-1.867547000	-0.139871000	-0.057915000
6	-1.035994000	1.050310000	-0.315948000
7	0.300995000	0.825535000	0.284740000
15	1.347731000	-0.330047000	-0.220595000
8	1.109932000	-0.842105000	-1.600066000
9	1.276102000	-1.565512000	0.813869000
8	2.761756000	0.300391000	0.147562000
6	-3.132269000	-0.194593000	-0.814319000
6	-3.644608000	-1.626401000	-0.992069000
1	-2.946671000	0.238291000	-1.796940000
1	-3.918657000	0.416371000	-0.341951000
1	-4.541480000	-1.618942000	-1.620746000
1	-2.888434000	-2.251620000	-1.478940000
1	-3.914119000	-2.096502000	-0.041038000

6	-1.992803000	-0.579769000	1.349010000
6	-3.143980000	-0.001162000	2.192077000
1	-1.044581000	-0.371340000	1.846048000
1	-2.093084000	-1.671446000	1.339952000
1	-3.066466000	-0.402101000	3.208855000
1	-3.111714000	1.089648000	2.261521000
1	-4.126887000	-0.285512000	1.804034000
6	-1.565274000	2.387003000	0.217370000
1	-2.571767000	2.558511000	-0.170066000
1	-1.606424000	2.386304000	1.308614000
1	-0.918626000	3.203935000	-0.113724000
6	3.998199000	-0.494738000	0.147953000
6	5.152472000	0.452469000	0.396856000
1	4.086492000	-0.992073000	-0.821631000
1	3.913243000	-1.247434000	0.935677000
1	6.086219000	-0.118639000	0.409151000
1	5.218691000	1.206044000	-0.393063000
1	5.043833000	0.956536000	1.361559000
8	-0.907739000	1.217477000	-1.715565000
1	-0.460690000	0.423459000	-2.063677000
1	0.600061000	1.452357000	1.021665000

TS9

7	2.452902000	0.217037000	0.162751000
6	1.254676000	0.466630000	0.748232000
7	-0.124647000	-0.247183000	-0.438716000
15	-1.588399000	-0.552587000	0.120915000
8	-1.640956000	-0.637378000	1.627701000
9	-2.113672000	-1.978974000	-0.464491000
8	-2.679213000	0.428410000	-0.544416000
6	3.010119000	-1.152581000	0.184595000

6	2.894511000	-1.903292000	-1.147120000
1	2.491475000	-1.700444000	0.967901000
1	4.059934000	-1.081591000	0.485406000
1	3.286671000	-2.917248000	-1.015651000
1	1.851329000	-1.975290000	-1.466100000
1	3.472243000	-1.429194000	-1.946418000
6	3.031763000	1.143170000	-0.827000000
6	4.541455000	1.331987000	-0.657649000
1	2.547796000	2.111022000	-0.721081000
1	2.810332000	0.785646000	-1.840836000
1	4.883835000	2.094481000	-1.364082000
1	4.782504000	1.669126000	0.355576000
1	5.104786000	0.417366000	-0.861998000
6	0.768827000	1.900072000	0.864431000
1	1.498777000	2.477903000	1.442610000
1	0.609014000	2.378183000	-0.100812000
1	-0.176961000	1.903569000	1.407261000
6	-4.108429000	0.278908000	-0.273622000
6	-4.828812000	1.456212000	-0.899390000
1	-4.256067000	0.249303000	0.809974000
1	-4.441511000	-0.669730000	-0.705086000
1	-5.904155000	1.361323000	-0.716937000
1	-4.487237000	2.400361000	-0.464682000
1	-4.664431000	1.485420000	-1.980767000
8	1.030284000	-0.296569000	1.849730000
1	0.053086000	-0.366500000	2.005705000
1	-0.035738000	0.034547000	-1.410517000

Pdt4

7	-3.539597000	0.123702000	0.071993000
6	-2.310638000	-0.437906000	0.139784000
7	1.414453000	-0.461033000	0.933907000
15	2.470674000	0.014451000	-0.214315000
8	2.107952000	1.244767000	-0.967816000
9	2.661208000	-1.208633000	-1.263534000
8	3.876090000	-0.028780000	0.544475000
6	-3.738354000	1.492451000	0.578196000
6	-3.517872000	2.561706000	-0.495802000
1	-3.052723000	1.645996000	1.412858000
1	-4.758550000	1.550599000	0.968376000
1	-3.704796000	3.555620000	-0.075515000
1	-2.489336000	2.533486000	-0.867098000
1	-4.196376000	2.421595000	-1.343857000
6	-4.719240000	-0.549233000	-0.496568000
6	-5.597090000	-1.229904000	0.558507000
1	-4.395341000	-1.270275000	-1.248041000
1	-5.297369000	0.211788000	-1.030033000
1	-6.476417000	-1.672320000	0.078955000
1	-5.052199000	-2.026081000	1.075310000
1	-5.946342000	-0.512871000	1.308098000
6	-2.121620000	-1.847622000	-0.389734000
1	-2.869862000	-2.543756000	-0.002894000
1	-2.184377000	-1.860475000	-1.483272000
1	-1.130522000	-2.194038000	-0.097510000
6	5.138052000	0.153327000	-0.178040000
6	6.249012000	0.247173000	0.846958000
1	5.066123000	1.065853000	-0.776487000
1	5.274553000	-0.703693000	-0.843366000

1	7.205017000	0.375642000	0.329441000
1	6.097774000	1.103178000	1.511004000
1	6.303304000	-0.664158000	1.449767000
8	-1.339448000	0.190231000	0.619974000
1	0.411227000	-0.271818000	0.777760000
1	1.610987000	-1.311723000	1.448859000

Pathway B

RC2

7	-2.191352000	-0.361332000	0.123693000
6	-0.966132000	-0.180115000	-0.399076000
7	0.015966000	-0.947343000	0.042997000
15	1.553582000	-0.963550000	-0.456161000
8	1.937340000	-1.088988000	-1.896398000
9	2.115160000	-2.258487000	0.333030000
8	2.294086000	0.227568000	0.336599000
6	-2.428430000	-1.403085000	1.141278000
6	-2.190763000	-0.900693000	2.567762000
1	-1.775963000	-2.248110000	0.920178000
1	-3.462897000	-1.735979000	1.022074000
1	-2.407356000	-1.702472000	3.281370000
1	-1.150731000	-0.591289000	2.701635000
1	-2.840796000	-0.052458000	2.805984000
6	-3.361406000	0.458293000	-0.242681000
6	-4.226703000	-0.178826000	-1.334299000
1	-3.028436000	1.451756000	-0.542705000
1	-3.949619000	0.592479000	0.669774000
1	-5.099723000	0.453491000	-1.525203000
1	-3.671973000	-0.288214000	-2.271118000
1	-4.585171000	-1.167590000	-1.031964000
6	-0.787829000	0.910003000	-1.433962000

1	-1.571309000	0.879547000	-2.194063000
1	-0.819977000	1.893153000	-0.949460000
1	0.172987000	0.797010000	-1.934537000
6	3.714789000	0.498520000	0.126740000
6	4.066369000	1.761684000	0.886812000
1	3.892712000	0.610595000	-0.946252000
1	4.287148000	-0.359386000	0.494026000
1	5.130003000	1.982341000	0.750375000
1	3.487445000	2.613663000	0.517824000
1	3.874142000	1.641384000	1.957216000
8	-1.027371000	3.909934000	0.342561000
1	-1.834786000	4.429564000	0.457133000
1	-0.309993000	4.558081000	0.358484000

TS10

7	2.321308000	0.523399000	0.158553000
6	1.097835000	-0.297256000	0.546574000
7	0.087858000	-0.150287000	-0.240274000
15	-1.381013000	-0.863916000	-0.147523000
8	-1.732422000	-1.898247000	0.867266000
9	-1.519070000	-1.492986000	-1.626412000
8	-2.369115000	0.391708000	-0.229063000
6	2.095211000	1.509021000	-0.967758000
6	1.342369000	2.764008000	-0.545653000
1	1.567983000	0.981643000	-1.762003000
1	3.092190000	1.774108000	-1.323981000
1	1.260728000	3.418165000	-1.419454000
1	0.339831000	2.531430000	-0.187115000
1	1.878418000	3.307745000	0.237271000
6	3.588692000	-0.276705000	-0.048650000
6	3.570725000	-1.148996000	-1.298788000

1	3.750738000	-0.874160000	0.847179000
1	4.390948000	0.462520000	-0.094573000
1	4.512472000	-1.703033000	-1.344471000
1	2.755712000	-1.878073000	-1.281856000
1	3.487643000	-0.557154000	-2.213549000
6	1.361500000	-1.466643000	1.460264000
1	1.660332000	-2.336169000	0.862100000
1	2.135619000	-1.258658000	2.196348000
1	0.434663000	-1.722733000	1.972517000
6	-3.814052000	0.219942000	-0.057457000
6	-4.438226000	1.598375000	0.011893000
1	-3.988663000	-0.350610000	0.858119000
1	-4.193566000	-0.349053000	-0.911657000
1	-5.521587000	1.496604000	0.131901000
1	-4.047999000	2.161731000	0.864654000
1	-4.244786000	2.163653000	-0.904545000
8	1.098259000	1.171666000	2.137166000
1	2.327810000	1.052827000	1.091812000
1	1.126069000	0.731547000	2.998401000

Phosphinate hydrolysis

Frontside attack (S_N2)

Reaction (I)

TSP1

7	2.228100000	0.229251000	0.115663000
6	1.125030000	-0.357096000	-0.388277000
7	-0.044280000	-0.002107000	0.114420000
15	-1.496848000	-0.699841000	-0.149688000
8	-2.042030000	-1.340648000	-1.393603000
9	-0.709049000	-2.433733000	0.468576000
8	-2.448835000	0.639752000	0.136629000

6	2.126872000	1.189897000	1.230917000
6	2.179706000	0.507759000	2.600345000
1	1.196245000	1.746281000	1.117352000
1	2.956548000	1.893730000	1.124234000
1	2.132616000	1.262996000	3.391901000
1	1.335259000	-0.175651000	2.724982000
1	3.108147000	-0.058467000	2.728336000
6	3.588184000	-0.017955000	-0.395770000
6	4.042657000	1.017158000	-1.429928000
1	3.643946000	-1.024597000	-0.809253000
1	4.257730000	-0.001823000	0.469280000
1	5.072117000	0.803558000	-1.734957000
1	3.409630000	0.994227000	-2.322208000
1	4.015782000	2.030551000	-1.017752000
6	1.302276000	-1.341774000	-1.524574000
1	0.331030000	-1.626594000	-1.922457000
1	1.904814000	-0.914274000	-2.329948000
1	1.804869000	-2.246166000	-1.168221000
6	-2.395578000	1.738688000	-0.796722000
6	-3.334285000	2.827556000	-0.306565000
1	-2.695510000	1.381837000	-1.789049000
1	-1.364977000	2.107903000	-0.856324000
1	-3.312706000	3.673174000	-1.002152000
1	-4.363198000	2.458986000	-0.245132000
1	-3.032646000	3.187557000	0.682254000
8	-2.324620000	-1.243933000	1.456611000
1	-1.712875000	-1.975629000	1.727722000
1	-2.424684000	-0.533163000	2.115304000
P1f			
7	-2.436031000	0.167058000	0.169294000

6	-1.279883000	0.355626000	-0.493974000
7	-0.154657000	0.062448000	0.131152000
15	1.392564000	0.218182000	-0.335849000
8	1.798174000	0.583855000	-1.730929000
9	4.154177000	2.743116000	0.320598000
8	2.144936000	-1.090903000	0.247078000
6	-2.433927000	-0.350805000	1.550707000
6	-2.310732000	0.760314000	2.596621000
1	-1.609521000	-1.057706000	1.646650000
1	-3.368391000	-0.901385000	1.687777000
1	-2.343729000	0.326609000	3.601592000
1	-1.364086000	1.295850000	2.483148000
1	-3.131106000	1.480562000	2.512452000
6	-3.761921000	0.463780000	-0.403339000
6	-4.438850000	-0.762215000	-1.024225000
1	-3.671071000	1.265554000	-1.135721000
1	-4.376492000	0.858264000	0.411214000
1	-5.433149000	-0.486276000	-1.389861000
1	-3.860663000	-1.153443000	-1.866866000
1	-4.559469000	-1.564992000	-0.290356000
6	-1.351016000	0.896660000	-1.906530000
1	-0.369680000	0.838416000	-2.372243000
1	-2.070524000	0.342519000	-2.513283000
1	-1.663659000	1.946523000	-1.889791000
6	1.828963000	-2.407793000	-0.287671000
6	2.648282000	-3.432819000	0.471913000
1	2.069465000	-2.420145000	-1.355879000
1	0.755467000	-2.585777000	-0.163538000
1	2.428733000	-4.433182000	0.085062000
1	3.719400000	-3.244225000	0.351664000

1	2.404824000	-3.414334000	1.538592000
8	2.033504000	1.347256000	0.688413000
1	3.365030000	2.210680000	0.447317000
1	1.718974000	1.271032000	1.603790000

Reaction (II)

TSP2

7	-2.416249000	0.136029000	-0.239634000
6	-1.272511000	-0.541345000	-0.207845000
7	-0.189202000	0.061808000	0.315211000
15	1.431646000	-0.441525000	0.637250000
8	1.541430000	-1.898704000	0.275020000
9	1.698206000	-0.446244000	2.226706000
8	2.582376000	0.361515000	-0.166433000
6	-2.549303000	1.503176000	0.315729000
6	-2.167060000	2.591651000	-0.690834000
1	-1.956447000	1.576154000	1.229879000
1	-3.593644000	1.613817000	0.613298000
1	-2.324444000	3.573708000	-0.235145000
1	-1.117723000	2.518689000	-0.989159000
1	-2.787613000	2.530156000	-1.589680000
6	-3.647611000	-0.409519000	-0.859925000
6	-4.584355000	-1.062847000	0.158235000
1	-3.373705000	-1.108953000	-1.648191000
1	-4.143246000	0.433497000	-1.347932000
1	-5.490688000	-1.400660000	-0.353228000
1	-4.117290000	-1.928765000	0.636171000
1	-4.880573000	-0.357529000	0.940227000
6	-1.213755000	-1.929701000	-0.775612000
1	-2.069189000	-2.521951000	-0.448868000
1	-1.234638000	-1.872132000	-1.869740000

1	-0.287763000	-2.409942000	-0.470577000
6	3.463732000	-0.362761000	-1.092500000
6	4.404714000	0.660795000	-1.696801000
1	2.850502000	-0.848636000	-1.854575000
1	4.004856000	-1.130511000	-0.535705000
1	5.081779000	0.157760000	-2.395267000
1	3.852119000	1.428782000	-2.246502000
1	5.007719000	1.146577000	-0.923642000
8	1.117148000	1.760755000	1.282696000
1	-0.141994000	1.070981000	0.626192000
1	1.670852000	2.297951000	0.701361000

P2f

7	3.036033000	-0.006100000	0.123628000
6	2.108764000	0.750886000	-0.551591000
7	1.339054000	1.661593000	-0.026853000
15	-2.847913000	-0.918942000	-0.152633000
8	-1.482045000	-1.472501000	-0.265861000
9	-3.495401000	-1.255760000	1.272875000
8	-3.073890000	0.641959000	-0.286405000
6	3.266098000	0.190245000	1.559311000
6	2.306263000	-0.608835000	2.449922000
1	3.210696000	1.259048000	1.793976000
1	4.296819000	-0.108936000	1.769104000
1	2.541016000	-0.435866000	3.505724000
1	1.265270000	-0.318161000	2.279521000
1	2.396488000	-1.682190000	2.253178000
6	3.872774000	-1.028505000	-0.523111000
6	5.259014000	-0.520366000	-0.937468000
1	3.346954000	-1.434398000	-1.387870000
1	3.979538000	-1.858841000	0.183566000

1	5.841972000	-1.338665000	-1.374184000
1	5.181972000	0.279447000	-1.680894000
1	5.815046000	-0.132799000	-0.077564000
6	1.953995000	0.500289000	-2.037814000
1	2.905381000	0.569974000	-2.572991000
1	1.534563000	-0.492920000	-2.231936000
1	1.268642000	1.246477000	-2.438963000
6	-2.275008000	1.622892000	0.478735000
6	-2.691033000	3.001750000	0.015329000
1	-1.217404000	1.428908000	0.280938000
1	-2.492483000	1.469321000	1.539119000
1	-2.117576000	3.750200000	0.571532000
1	-2.486270000	3.134346000	-1.050957000
1	-3.755085000	3.176686000	0.198934000
8	-3.879037000	-1.550293000	-1.188194000
1	1.483448000	1.751148000	0.978594000
1	-4.772725000	-1.168715000	-1.178821000

Reaction (III)

TSP3

7	-2.515965000	0.199068000	0.130004000
6	-1.371536000	-0.401136000	-0.303370000
7	-0.267244000	0.299138000	-0.287760000
15	1.249839000	-0.344614000	-0.560472000
8	1.722557000	-1.259752000	-1.638475000
9	1.156552000	-1.395289000	0.754017000
8	2.573566000	0.473820000	0.438784000
6	-2.470488000	1.567883000	0.664414000
6	-2.676646000	2.637009000	-0.413462000
1	-1.504749000	1.704721000	1.152966000
1	-3.249561000	1.646532000	1.430137000

1	-2.646045000	3.635912000	0.035446000
1	-1.890688000	2.574440000	-1.170764000
1	-3.644833000	2.523800000	-0.913487000
6	-3.836891000	-0.438886000	0.095373000
6	-4.230363000	-1.105746000	1.419591000
1	-3.871603000	-1.165622000	-0.717313000
1	-4.566897000	0.337816000	-0.159180000
1	-5.240198000	-1.523732000	1.344533000
1	-3.541890000	-1.916704000	1.675477000
1	-4.223983000	-0.386716000	2.244887000
6	-1.485525000	-1.821926000	-0.823910000
1	-1.963698000	-2.478790000	-0.092288000
1	-2.083384000	-1.841288000	-1.741894000
1	-0.500929000	-2.219534000	-1.062486000
6	3.777032000	-0.272081000	0.800238000
6	4.784529000	0.688352000	1.404145000
1	4.157298000	-0.764773000	-0.099313000
1	3.449604000	-1.031326000	1.510858000
1	5.679444000	0.131782000	1.702252000
1	5.089985000	1.454240000	0.683658000
1	4.374800000	1.182455000	2.290103000
8	1.708721000	1.299562000	-1.396589000
1	0.968236000	1.915908000	-1.301192000
1	2.555587000	1.230383000	-0.375053000

P3f

7	-2.257231000	-0.784853000	0.090509000
6	-1.637202000	0.400186000	-0.055761000
7	-0.364876000	0.483692000	0.289924000
15	0.583327000	1.803488000	0.249593000
8	0.172413000	3.082622000	0.903972000

9	0.842139000	2.093188000	-1.335694000
8	2.949901000	-1.002923000	-0.039088000
6	-1.527044000	-1.951941000	0.621030000
6	-1.573709000	-2.032021000	2.149098000
1	-0.495546000	-1.893693000	0.272695000
1	-1.982920000	-2.841960000	0.179371000
1	-1.046105000	-2.929879000	2.487497000
1	-1.092180000	-1.159165000	2.598163000
1	-2.604470000	-2.088483000	2.514024000
6	-3.675247000	-1.012266000	-0.243662000
6	-3.878530000	-1.591167000	-1.647429000
1	-4.231503000	-0.082473000	-0.126214000
1	-4.068970000	-1.703768000	0.506988000
1	-4.943725000	-1.779945000	-1.814942000
1	-3.527997000	-0.899794000	-2.419752000
1	-3.344184000	-2.538391000	-1.768798000
6	-2.448730000	1.560379000	-0.597087000
1	-2.986503000	1.287009000	-1.507386000
1	-3.184990000	1.885890000	0.145373000
1	-1.803996000	2.408551000	-0.818126000
6	4.393029000	-1.091329000	-0.150780000
6	4.825885000	-2.324070000	-0.927835000
1	4.834305000	-1.078351000	0.852427000
1	4.690017000	-0.175774000	-0.667573000
1	5.917405000	-2.339843000	-1.018291000
1	4.518107000	-3.242872000	-0.416368000
1	4.395241000	-2.322625000	-1.933915000
8	2.023559000	1.333088000	0.729679000
1	2.323301000	0.420227000	0.433309000
1	2.622599000	-1.756462000	0.473879000

Backside attack (addition-elimination)**Reaction (IV)****TSP4**

7	2.281552000	0.388865000	0.015676000
6	1.269790000	-0.495074000	0.111371000
7	0.039856000	-0.048934000	-0.045053000
15	-1.358573000	-0.860338000	-0.087013000
8	-1.727953000	-2.181830000	0.707958000
9	-1.238963000	-1.611463000	-1.542805000
8	-2.570588000	0.067644000	-0.542463000
6	2.010610000	1.809298000	-0.275018000
6	1.770679000	2.636212000	0.990903000
1	1.144615000	1.862292000	-0.935678000
1	2.874798000	2.194366000	-0.822760000
1	1.603484000	3.684066000	0.720551000
1	0.890665000	2.274716000	1.529651000
1	2.633301000	2.594872000	1.663928000
6	3.699544000	0.026734000	0.192781000
6	4.419279000	-0.261019000	-1.128682000
1	3.776817000	-0.826253000	0.866723000
1	4.177850000	0.867226000	0.704094000
1	5.474019000	-0.478215000	-0.931855000
1	3.982518000	-1.122859000	-1.642378000
1	4.371633000	0.599121000	-1.803498000
6	1.614209000	-1.938470000	0.416107000
1	2.394785000	-2.314246000	-0.248751000
1	1.974764000	-2.032229000	1.445996000
1	0.734616000	-2.570285000	0.311018000
6	-2.782928000	1.447144000	-0.109007000
6	-3.954013000	1.995681000	-0.899301000

1	-1.864790000	2.007215000	-0.305331000
1	-2.970590000	1.433015000	0.964271000
1	-4.138244000	3.030100000	-0.590866000
1	-3.747795000	1.988611000	-1.973868000
1	-4.862254000	1.415070000	-0.710715000
1	-0.978863000	-0.013419000	2.449215000
8	-1.783332000	-0.295455000	1.992081000
1	-1.819961000	-1.610359000	1.650797000

IMB1

7	-2.373097000	0.352538000	0.003454000
6	-1.313193000	-0.476568000	-0.162192000
7	-0.117744000	0.049766000	-0.259155000
15	1.371118000	-0.669867000	-0.224731000
8	1.819429000	-2.147033000	-0.797267000
9	1.026837000	-1.510822000	1.225953000
8	2.492339000	0.123055000	0.647962000
6	-2.168452000	1.803848000	0.141683000
6	-2.180956000	2.540280000	-1.201346000
1	-1.219184000	1.965424000	0.654116000
1	-2.965790000	2.183216000	0.787413000
1	-2.048082000	3.614920000	-1.036814000
1	-1.370476000	2.187707000	-1.845161000
1	-3.130379000	2.395197000	-1.727349000
6	-3.771930000	-0.105085000	0.029681000
6	-4.314100000	-0.322972000	1.446619000
1	-3.870394000	-1.016312000	-0.560575000
1	-4.367894000	0.656938000	-0.482284000
1	-5.367657000	-0.617372000	1.397617000
1	-3.762370000	-1.111300000	1.967941000
1	-4.246884000	0.592095000	2.043378000

6	-1.600608000	-1.959673000	-0.290667000
1	-2.246486000	-2.318998000	0.513916000
1	-2.104446000	-2.163412000	-1.241717000
1	-0.672849000	-2.525808000	-0.269064000
6	3.326904000	1.206025000	0.162036000
6	4.166771000	1.684813000	1.332891000
1	2.691791000	2.010783000	-0.219649000
1	3.953038000	0.842509000	-0.655440000
1	4.814721000	2.504149000	1.004014000
1	3.534616000	2.051212000	2.147749000
1	4.799843000	0.878744000	1.716960000
1	1.198473000	0.699463000	-1.981984000
8	1.822372000	0.001338000	-1.739246000
1	2.068255000	-2.042758000	-1.729597000

TSP5

7	-2.385179000	0.332960000	0.023920000
6	-1.339316000	-0.503907000	-0.176564000
7	-0.148807000	0.016434000	-0.345218000
15	1.376513000	-0.618773000	-0.298981000
8	2.035556000	-2.007269000	-0.909948000
9	0.977001000	-1.532789000	1.131271000
8	2.477286000	0.104997000	0.651350000
6	-2.165721000	1.784406000	0.142975000
6	-2.224234000	2.511431000	-1.203995000
1	-1.197128000	1.943042000	0.618472000
1	-2.935859000	2.172895000	0.815682000
1	-2.075833000	3.585741000	-1.051523000
1	-1.442509000	2.147533000	-1.876298000
1	-3.194561000	2.371912000	-1.691853000
6	-3.788488000	-0.110727000	0.079588000

6	-4.302173000	-0.323317000	1.507541000
1	-3.909073000	-1.019011000	-0.511384000
1	-4.386275000	0.658759000	-0.418598000
1	-5.359865000	-0.605244000	1.480919000
1	-3.748633000	-1.117925000	2.017307000
1	-4.211353000	0.590820000	2.102519000
6	-1.640040000	-1.985689000	-0.279189000
1	-2.343304000	-2.317816000	0.486739000
1	-2.074833000	-2.211884000	-1.258996000
1	-0.724969000	-2.560493000	-0.162668000
6	3.370045000	1.174613000	0.240733000
6	4.209071000	1.544979000	1.450766000
1	2.779435000	2.028423000	-0.102881000
1	3.992851000	0.829324000	-0.587002000
1	4.897976000	2.352376000	1.180996000
1	3.579192000	1.891079000	2.276178000
1	4.799327000	0.690275000	1.795790000
1	1.204793000	0.939674000	-1.860258000
8	1.804878000	0.190883000	-1.734892000
1	1.391208000	-2.598158000	-1.323993000

IMB2

7	-2.370993000	0.351942000	0.005451000
6	-1.317853000	-0.480582000	-0.183278000
7	-0.120558000	0.039648000	-0.277001000
15	1.378560000	-0.651738000	-0.274474000
8	1.871258000	-2.102021000	-0.871697000
9	1.021797000	-1.534796000	1.209943000
8	2.473792000	0.133895000	0.636810000
6	-2.155582000	1.799417000	0.166476000
6	-2.172248000	2.557551000	-1.164380000

1	-1.201861000	1.946181000	0.675062000
1	-2.945969000	2.173304000	0.823740000
1	-2.030476000	3.628384000	-0.983438000
1	-1.369013000	2.209789000	-1.819788000
1	-3.126432000	2.427637000	-1.685689000
6	-3.772576000	-0.097161000	0.036467000
6	-4.303448000	-0.333989000	1.454619000
1	-3.882287000	-0.998288000	-0.567069000
1	-4.367844000	0.676629000	-0.458296000
1	-5.359034000	-0.621706000	1.410237000
1	-3.751665000	-1.133407000	1.958723000
1	-4.225841000	0.571287000	2.064866000
6	-1.617621000	-1.958028000	-0.340541000
1	-2.251189000	-2.332466000	0.466856000
1	-2.137765000	-2.137705000	-1.287426000
1	-0.694908000	-2.531661000	-0.348176000
6	3.317494000	1.218571000	0.167997000
6	4.158968000	1.674597000	1.346506000
1	2.687868000	2.033575000	-0.201526000
1	3.941774000	0.862942000	-0.654385000
1	4.811942000	2.494922000	1.030338000
1	3.528209000	2.032608000	2.166121000
1	4.786867000	0.859051000	1.718790000
1	1.212297000	0.749194000	-1.963538000
8	1.814609000	0.020523000	-1.759712000
1	1.841535000	-2.763581000	-0.163338000
TSP6			
7	-2.272017000	0.348584000	-0.027918000
6	-1.254597000	-0.508468000	-0.232285000
7	-0.043160000	-0.012485000	-0.362102000

15	1.435032000	-0.652160000	-0.422232000
8	1.877194000	-2.178582000	-0.657801000
9	0.950249000	-1.712650000	1.441565000
8	2.480177000	0.090811000	0.542280000
6	-2.019845000	1.795822000	0.103033000
6	-2.048705000	2.526844000	-1.241952000
1	-1.052538000	1.928259000	0.588972000
1	-2.788530000	2.195829000	0.769650000
1	-1.882739000	3.597350000	-1.082598000
1	-1.264952000	2.151925000	-1.905794000
1	-3.015428000	2.406234000	-1.741513000
6	-3.683918000	-0.068870000	0.052745000
6	-4.169185000	-0.275242000	1.491038000
1	-3.830600000	-0.974050000	-0.536233000
1	-4.273857000	0.714024000	-0.432681000
1	-5.231610000	-0.539063000	1.484644000
1	-3.619186000	-1.081084000	1.986410000
1	-4.050925000	0.635558000	2.086015000
6	-1.577899000	-1.979412000	-0.368286000
1	-2.215649000	-2.331280000	0.445109000
1	-2.103607000	-2.157339000	-1.312705000
1	-0.663514000	-2.564836000	-0.366677000
6	2.864840000	1.483030000	0.321348000
6	3.791298000	1.885295000	1.451465000
1	1.959247000	2.097495000	0.311779000
1	3.358360000	1.558887000	-0.650606000
1	4.103442000	2.924845000	1.307771000
1	3.288595000	1.806230000	2.419853000
1	4.686302000	1.255991000	1.465860000
1	1.331245000	0.521057000	-2.268842000

8	1.930793000	-0.146699000	-1.905568000
1	1.677197000	-2.580716000	0.227203000

P1b

7	2.433925000	-0.133248000	-0.100279000
6	1.146800000	-0.171037000	-0.482542000
7	0.229088000	-0.401684000	0.441781000
15	-1.381364000	-0.492009000	0.256618000
8	-1.942847000	-1.401207000	-0.816504000
9	-4.240217000	-1.881142000	-1.484459000
8	-2.056298000	0.957305000	0.035254000
6	2.803213000	-0.333275000	1.314723000
6	3.010086000	-1.808652000	1.666770000
1	2.019217000	0.102061000	1.934926000
1	3.722670000	0.232046000	1.487245000
1	3.309183000	-1.897756000	2.716280000
1	2.086537000	-2.375601000	1.521987000
1	3.796468000	-2.258976000	1.052341000
6	3.555754000	0.087434000	-1.032328000
6	4.006023000	1.550128000	-1.095819000
1	3.283095000	-0.276076000	-2.022804000
1	4.379820000	-0.543972000	-0.687989000
1	4.865368000	1.639292000	-1.767935000
1	3.208481000	2.198144000	-1.471710000
1	4.308390000	1.916925000	-0.110193000
6	0.832835000	0.035492000	-1.950184000
1	1.350832000	0.906443000	-2.356476000
1	1.140860000	-0.842312000	-2.528387000
1	-0.237134000	0.170014000	-2.096042000
6	-1.815319000	2.066199000	0.952129000
6	-2.573371000	3.273627000	0.437057000

1	-0.738715000	2.258344000	0.992874000
1	-2.160833000	1.771599000	1.947855000
1	-2.408871000	4.119527000	1.112331000
1	-2.226417000	3.556889000	-0.561218000
1	-3.647808000	3.071653000	0.393025000
1	-1.156482000	-1.061164000	2.346779000
8	-1.892754000	-0.951691000	1.725058000
1	-3.314268000	-1.666891000	-1.191840000

Reaction (V)

TSP7

7	-2.434282000	0.085002000	0.102837000
6	-1.158190000	0.176222000	-0.340826000
7	-0.256440000	-0.606119000	0.204011000
15	1.340328000	-0.720622000	-0.177734000
8	1.326794000	-1.245473000	-1.683483000
9	1.688861000	-1.816810000	0.944224000
8	1.850121000	0.732976000	0.233399000
6	-2.788922000	-0.886032000	1.152353000
6	-2.605665000	-0.327384000	2.566437000
1	-2.174493000	-1.776410000	1.013508000
1	-3.832533000	-1.169563000	0.989502000
1	-2.908321000	-1.078105000	3.304291000
1	-1.558794000	-0.068670000	2.746695000
1	-3.218174000	0.566583000	2.724335000
6	-3.534116000	0.934483000	-0.384230000
6	-4.365601000	0.278836000	-1.492082000
1	-3.136176000	1.892380000	-0.719625000
1	-4.171725000	1.154338000	0.477693000
1	-5.190538000	0.940893000	-1.775056000
1	-3.761193000	0.085016000	-2.383614000

1	-4.794384000	-0.671130000	-1.158063000
6	-0.873337000	1.199376000	-1.424889000
1	-1.610987000	1.154813000	-2.228725000
1	-0.891880000	2.210820000	-1.005148000
1	0.109821000	1.032333000	-1.858962000
6	3.192025000	1.308426000	0.329431000
6	3.030910000	2.695966000	0.919783000
1	3.626288000	1.331505000	-0.669640000
1	3.800232000	0.659894000	0.959161000
1	4.018313000	3.161866000	1.005313000
1	2.407246000	3.329264000	0.281592000
1	2.583962000	2.652549000	1.917694000
8	3.418030000	-1.174531000	-0.743913000
1	3.728553000	-1.960101000	-0.273606000
1	2.362969000	-1.422972000	-1.731171000

IMB3

7	-2.408937000	0.205791000	0.089424000
6	-1.061802000	0.379915000	0.165667000
7	-0.286710000	-0.638027000	-0.075202000
15	1.340881000	-0.771826000	-0.247490000
8	1.344939000	-0.017552000	-1.763182000
9	1.404907000	-1.637562000	1.267169000
8	2.446871000	0.210775000	0.456027000
6	-2.965852000	-1.100112000	-0.296044000
6	-3.190091000	-2.031787000	0.899396000
1	-2.286635000	-1.562470000	-1.014045000
1	-3.913333000	-0.910864000	-0.809195000
1	-3.626382000	-2.976969000	0.558535000
1	-2.244634000	-2.250786000	1.403296000
1	-3.876927000	-1.586903000	1.627249000

6	-3.387392000	1.262220000	0.389875000
6	-3.876336000	2.013427000	-0.853840000
1	-2.964871000	1.959763000	1.113511000
1	-4.234876000	0.782190000	0.889616000
1	-4.634049000	2.750514000	-0.567652000
1	-3.055431000	2.541477000	-1.348988000
1	-4.327902000	1.329311000	-1.579242000
6	-0.562153000	1.754391000	0.567635000
1	-1.002139000	2.541073000	-0.049894000
1	-0.816997000	1.964635000	1.611668000
1	0.519677000	1.802950000	0.473585000
6	3.232399000	1.225220000	-0.224257000
6	4.060667000	1.937832000	0.829862000
1	2.568554000	1.917853000	-0.746572000
1	3.879153000	0.742149000	-0.963791000
1	4.673459000	2.707915000	0.349689000
1	3.417951000	2.422120000	1.571528000
1	4.726546000	1.239628000	1.346077000
8	1.913533000	-2.145808000	-0.938035000
1	2.070880000	-2.818145000	-0.256704000
1	2.100726000	-0.280309000	-2.308629000

TSP8

7	6.310418714	-0.714587532	-0.046379422
6	4.945039714	-0.544343532	-0.050103422
7	4.202065714	-1.588158532	0.129382578
15	2.492437714	-1.669668532	0.220924578
8	2.388672714	-2.168109532	1.784392578
9	2.583166714	-2.702627532	-1.069145422
8	2.203812714	-0.089184532	-0.080654422
6	6.870950714	-2.049928532	0.192578578

6	6.968424714	-2.868958532	-1.099114422
1	6.187591714	-2.519750532	0.902355578
1	7.854902714	-1.910754532	0.654260578
1	7.395685714	-3.861726532	-0.917056422
1	5.964366714	-2.995711532	-1.511838422
1	7.543342714	-2.341744532	-1.869071422
6	7.273768714	0.354375468	-0.315284422
6	7.844332714	1.008165468	0.950878578
1	6.817748714	1.111251468	-0.956114422
1	8.091560714	-0.080881532	-0.902059422
1	8.591420714	1.764622468	0.684795578
1	7.056855714	1.494258468	1.535401578
1	8.328938714	0.267055468	1.594629578
6	4.448044714	0.872348468	-0.294006422
1	5.302519714	1.516935468	-0.522467422
1	3.753500714	0.927164468	-1.133853422
1	4.016895714	1.301816468	0.609569578
6	0.917946714	0.537992468	-0.315430422
6	1.138506714	2.031607468	-0.485041422
1	0.209049714	0.333759468	0.490610578
1	0.468568714	0.117844468	-1.219372422
1	0.187420714	2.488183468	-0.781158422
1	1.474726714	2.509576468	0.440275578
1	1.834892714	2.238372468	-1.303655422
8	0.796266714	-1.910168532	0.147976578
1	0.582628714	-2.740667532	-0.295610422
1	2.425084714	-3.139084532	1.779052578

IMB4

7	-2.306093000	0.129523000	-0.024581000
6	-1.043794000	0.091114000	0.470829000

7	-0.179008000	-0.711598000	-0.094516000
15	1.448323000	-0.804121000	0.109813000
8	2.254171000	-1.441126000	-1.168102000
9	1.294384000	-2.457326000	0.624946000
8	1.732839000	0.800509000	-0.366911000
6	-2.665498000	-0.672953000	-1.205364000
6	-3.138453000	-2.084856000	-0.845957000
1	-1.796006000	-0.719978000	-1.862396000
1	-3.455307000	-0.132883000	-1.735596000
1	-3.412527000	-2.628359000	-1.756549000
1	-2.345633000	-2.640405000	-0.337833000
1	-4.017337000	-2.056784000	-0.193226000
6	-3.395395000	0.916858000	0.575250000
6	-3.596416000	2.282906000	-0.090094000
1	-3.216292000	1.035511000	1.644059000
1	-4.309344000	0.321568000	0.483292000
1	-4.447478000	2.796481000	0.369248000
1	-2.711451000	2.916400000	0.025074000
1	-3.803148000	2.177382000	-1.159760000
6	-0.746574000	0.945864000	1.687451000
1	-1.241818000	0.528368000	2.571001000
1	0.323710000	0.969833000	1.877650000
1	-1.099453000	1.971555000	1.558777000
6	3.009941000	1.455019000	-0.225494000
6	3.003976000	2.712786000	-1.079416000
1	3.821949000	0.784941000	-0.538524000
1	3.172449000	1.700333000	0.829297000
1	3.956194000	3.242711000	-0.967638000
1	2.867166000	2.469591000	-2.138172000
1	2.198309000	3.387219000	-0.771464000

8	2.285966000	-0.562511000	1.502254000
1	2.330047000	-1.389846000	2.006263000
1	2.456846000	-0.736760000	-1.802693000

TSP9

7	-2.396164000	0.120815000	-0.027782000
6	-1.100109000	0.240118000	0.356796000
7	-0.192171000	-0.545731000	-0.155352000
15	1.578750000	-0.821724000	0.100293000
8	1.235870000	-2.071244000	-0.846382000
9	1.367701000	-0.939808000	1.727237000
8	1.928566000	0.706349000	-0.324617000
6	-2.787051000	-0.875799000	-1.036946000
6	-3.081508000	-2.255438000	-0.438860000
1	-1.993221000	-0.941943000	-1.784248000
1	-3.675833000	-0.490171000	-1.544029000
1	-3.384293000	-2.947690000	-1.231629000
1	-2.197738000	-2.666571000	0.057170000
1	-3.894567000	-2.202655000	0.292648000
6	-3.487189000	0.933979000	0.534394000
6	-3.841135000	2.154819000	-0.321564000
1	-3.228647000	1.239951000	1.548434000
1	-4.359293000	0.278811000	0.626848000
1	-4.685276000	2.689127000	0.126851000
1	-2.997175000	2.847774000	-0.395067000
1	-4.128938000	1.859675000	-1.335570000
6	-0.757272000	1.294243000	1.387541000
1	-1.112673000	0.986528000	2.376715000
1	0.320161000	1.428295000	1.434538000
1	-1.216051000	2.255912000	1.147849000
6	3.258444000	1.289878000	-0.456877000

6	3.075846000	2.722854000	-0.921746000
1	3.833333000	0.703740000	-1.176266000
1	3.763373000	1.243941000	0.510999000
1	4.058011000	3.194236000	-1.033833000
1	2.564363000	2.760389000	-1.888638000
1	2.497301000	3.303288000	-0.196512000
8	3.196631000	-1.259488000	0.278897000
1	3.293287000	-2.191282000	0.038106000
1	0.102970000	-1.625673000	-0.821558000

P2b

7	3.031048000	-0.135635000	-0.116558000
6	2.299636000	1.026366000	-0.032648000
7	1.001274000	1.110345000	-0.000880000
15	-2.771518000	-0.842421000	0.224626000
8	-1.347274000	-1.244552000	0.288492000
9	-3.615858000	-1.747236000	-0.772950000
8	-3.163513000	0.572373000	-0.360306000
6	2.364969000	-1.441368000	-0.183388000
6	1.993060000	-1.860844000	-1.611180000
1	1.476074000	-1.432080000	0.454726000
1	3.044708000	-2.179103000	0.253046000
1	1.517682000	-2.847640000	-1.603014000
1	1.295789000	-1.150003000	-2.064928000
1	2.883812000	-1.918419000	-2.245584000
6	4.500726000	-0.168165000	-0.138716000
6	5.131736000	-0.402620000	1.239327000
1	4.880047000	0.757512000	-0.572840000
1	4.801103000	-0.968795000	-0.823682000
1	6.222043000	-0.459233000	1.148030000
1	4.888022000	0.411421000	1.929597000

1	4.781622000	-1.340541000	1.682795000
6	3.073406000	2.328910000	0.019233000
1	3.599289000	2.518563000	-0.922973000
1	2.363896000	3.139065000	0.186162000
1	3.816873000	2.339438000	0.821753000
6	-2.609252000	1.820147000	0.204706000
6	-3.092475000	2.961693000	-0.662767000
1	-1.519246000	1.739308000	0.204675000
1	-2.976623000	1.906968000	1.230759000
1	-2.704186000	3.902072000	-0.258679000
1	-2.731870000	2.853013000	-1.689699000
1	-4.184939000	3.015572000	-0.672027000
8	-3.597737000	-0.948953000	1.591873000
1	-3.210551000	-1.564454000	2.235676000
1	0.543054000	0.200150000	-0.052459000

Reaction (VI)

TSP10

7	-2.072896000	0.361893000	0.250453000
6	-1.084058000	0.809599000	-0.537981000
7	0.162206000	0.407354000	-0.492794000
15	1.259286000	-0.697944000	-0.238432000
8	2.047944000	-1.356926000	-1.452773000
9	1.161255000	-1.706224000	1.006765000
8	2.461867000	0.143508000	0.467126000
6	-1.854502000	-0.672803000	1.282327000
6	-1.368885000	-0.081388000	2.608668000
1	-1.162915000	-1.417233000	0.893212000
1	-2.812525000	-1.178711000	1.424410000
1	-1.248115000	-0.883647000	3.343530000
1	-0.404984000	0.421741000	2.492004000

1	-2.087978000	0.639926000	3.009702000
6	-3.443567000	0.915724000	0.199366000
6	-4.390853000	0.081029000	-0.666487000
1	-3.407908000	1.946648000	-0.150119000
1	-3.806427000	0.949558000	1.230438000
1	-5.396188000	0.512103000	-0.627199000
1	-4.065799000	0.064355000	-1.711096000
1	-4.451689000	-0.951765000	-0.310035000
6	-1.388470000	1.915093000	-1.529136000
1	-2.267976000	1.687900000	-2.136301000
1	-1.570795000	2.862389000	-1.010576000
1	-0.526425000	2.039660000	-2.182170000
6	3.070428000	1.276956000	-0.202156000
6	4.158451000	1.828722000	0.700066000
1	2.297093000	2.026832000	-0.396345000
1	3.484238000	0.942305000	-1.159620000
1	4.633090000	2.688169000	0.215262000
1	3.742204000	2.159587000	1.656682000
1	4.927477000	1.074635000	0.894091000
8	-0.070812000	-2.253179000	-1.139028000
1	-0.794182000	-1.867825000	-1.652887000
1	1.250794000	-1.981001000	-1.741599000

IMB5

7	-1.948156000	0.183095000	0.106083000
6	-1.108356000	-0.040821000	-0.937224000
7	0.084128000	-0.547411000	-0.866231000
15	1.408111000	-0.879144000	0.016371000
8	2.827337000	-1.098388000	-0.778089000
9	1.569553000	-1.096630000	1.630617000
8	1.824970000	0.730464000	0.341604000

6	-1.602313000	-0.163659000	1.493856000
6	-1.061722000	1.021152000	2.299907000
1	-0.886336000	-0.985530000	1.485255000
1	-2.511682000	-0.551557000	1.962825000
1	-0.867887000	0.705547000	3.330654000
1	-0.127621000	1.389626000	1.869234000
1	-1.785761000	1.841902000	2.331676000
6	-3.314151000	0.712763000	-0.077128000
6	-4.381659000	-0.379268000	-0.206653000
1	-3.335691000	1.374240000	-0.942806000
1	-3.529685000	1.340818000	0.792082000
1	-5.370192000	0.082846000	-0.297012000
1	-4.213854000	-1.001545000	-1.090890000
1	-4.394933000	-1.032011000	0.671675000
6	-1.609502000	0.301236000	-2.330169000
1	-2.574791000	-0.161597000	-2.549752000
1	-1.722020000	1.384268000	-2.446791000
1	-0.875572000	-0.049066000	-3.054168000
6	1.969605000	1.696867000	-0.708774000
6	2.578812000	2.959755000	-0.118680000
1	0.988647000	1.917611000	-1.147465000
1	2.612154000	1.294478000	-1.500905000
1	2.681237000	3.722819000	-0.898135000
1	1.943711000	3.364837000	0.676021000
1	3.570792000	2.758716000	0.298862000
8	1.105548000	-2.588358000	-0.041078000
1	0.425121000	-2.760731000	-0.706666000
1	2.887806000	-2.026534000	-1.054085000

TSP11

7	-1.865202000	0.216378000	0.101676000
6	-1.111883000	-0.197010000	-0.959774000
7	0.111280000	-0.632616000	-0.954192000
15	1.392900000	-0.901048000	0.079666000
8	2.531171000	-1.437057000	-0.962643000
9	2.239885000	-1.024783000	1.523470000
8	1.822926000	0.724369000	0.239903000
6	-1.405034000	0.194178000	1.500289000
6	-0.967632000	1.563076000	2.029585000
1	-0.605199000	-0.537822000	1.610449000
1	-2.234146000	-0.188297000	2.104649000
1	-0.711518000	1.477384000	3.091034000
1	-0.088671000	1.928409000	1.494670000
1	-1.769263000	2.302627000	1.938465000
6	-3.275738000	0.629998000	-0.055173000
6	-4.275173000	-0.518776000	0.120692000
1	-3.411230000	1.111467000	-1.022991000
1	-3.466100000	1.401510000	0.695884000
1	-5.296494000	-0.132692000	0.037210000
1	-4.139524000	-1.291021000	-0.642542000
1	-4.173798000	-0.990133000	1.103219000
6	-1.767270000	-0.135398000	-2.331922000
1	-2.724985000	-0.660775000	-2.360930000
1	-1.943744000	0.902681000	-2.633285000
1	-1.091121000	-0.593274000	-3.051996000
6	1.653822000	1.682068000	-0.823944000
6	2.497613000	2.902148000	-0.488299000
1	0.598398000	1.960225000	-0.913812000
1	1.969408000	1.238888000	-1.774742000

1	2.377186000	3.659567000	-1.270556000
1	2.187802000	3.341923000	0.465311000
1	3.558226000	2.639955000	-0.421640000
8	0.729579000	-2.370159000	0.625089000
1	0.009547000	-2.620134000	0.027095000
1	3.418565000	-1.356981000	-0.581631000

IMB6

7	-1.977817000	0.264294000	0.126631000
6	-1.121959000	0.182777000	-0.925613000
7	0.097585000	-0.254144000	-0.892641000
15	1.306340000	-0.950116000	-0.057168000
8	2.596427000	-1.447082000	-0.945480000
9	1.488011000	-1.299595000	1.531839000
8	2.080479000	0.528229000	0.359646000
6	-1.607264000	-0.170871000	1.482822000
6	-0.991578000	0.948768000	2.328183000
1	-0.935184000	-1.025817000	1.414676000
1	-2.520327000	-0.538815000	1.959203000
1	-0.783512000	0.577142000	3.337127000
1	-0.052358000	1.300556000	1.893265000
1	-1.676362000	1.798456000	2.416307000
6	-3.347321000	0.799566000	-0.001987000
6	-4.405810000	-0.286954000	-0.218527000
1	-3.380624000	1.531804000	-0.808243000
1	-3.562186000	1.349782000	0.919091000
1	-5.400127000	0.169832000	-0.259913000
1	-4.238099000	-0.826345000	-1.155818000
1	-4.403120000	-1.014874000	0.598892000
6	-1.621823000	0.662665000	-2.277629000
1	-2.574293000	0.201671000	-2.551184000

1	-1.760457000	1.748949000	-2.280521000
1	-0.876097000	0.408461000	-3.029292000
6	2.106781000	1.668132000	-0.513046000
6	3.110034000	2.669849000	0.039184000
1	1.108119000	2.116189000	-0.567275000
1	2.387282000	1.370298000	-1.533217000
1	3.135059000	3.560743000	-0.597898000
1	2.831680000	2.979923000	1.051728000
1	4.116978000	2.241169000	0.072447000
8	0.638551000	-2.520399000	-0.159331000
1	0.222409000	-2.636817000	-1.024928000
1	3.285604000	-0.764843000	-0.940421000

TSP12

7	-1.901165000	0.012514000	0.125039000
6	-1.033307000	-0.087236000	-0.895271000
7	0.124413000	-0.693646000	-0.828040000
15	1.491586000	-1.086653000	-0.159359000
8	2.930607000	-0.718710000	-0.715221000
9	1.545679000	-1.257795000	1.444301000
8	1.897080000	1.004567000	0.389217000
6	-1.620828000	-0.542409000	1.462279000
6	-1.031248000	0.487679000	2.428856000
1	-0.953196000	-1.396358000	1.350897000
1	-2.568698000	-0.926354000	1.848946000
1	-0.884443000	0.020821000	3.408311000
1	-0.065241000	0.850685000	2.070264000
1	-1.706140000	1.339395000	2.560984000
6	-3.231460000	0.641330000	-0.023811000
6	-4.341004000	-0.364115000	-0.346577000
1	-3.180382000	1.419258000	-0.784715000

1	-3.446251000	1.146630000	0.921510000
1	-5.300313000	0.160081000	-0.401244000
1	-4.167704000	-0.860175000	-1.306095000
1	-4.421515000	-1.133890000	0.426765000
6	-1.433387000	0.475453000	-2.244670000
1	-2.404695000	0.099460000	-2.574789000
1	-1.490837000	1.567969000	-2.205808000
1	-0.676291000	0.194068000	-2.974262000
6	1.310914000	2.098129000	-0.285051000
6	2.065172000	3.394347000	0.014658000
1	0.260741000	2.215906000	0.027016000
1	1.299451000	1.934386000	-1.377270000
1	1.599463000	4.242104000	-0.502576000
1	2.062094000	3.603793000	1.090187000
1	3.107390000	3.321222000	-0.316285000
8	1.594158000	-2.686823000	-0.512843000
1	0.723437000	-3.107592000	-0.558099000
1	2.881618000	0.285129000	-0.342749000

P3b

7	2.360658000	-0.616264000	-0.108470000
6	1.854428000	0.381797000	-0.849627000
7	0.785672000	1.106510000	-0.587346000
15	-0.459602000	1.268057000	0.394800000
8	-1.413880000	0.162319000	0.716073000
9	0.122726000	1.865138000	1.785942000
8	-3.534877000	-1.109486000	-0.586023000
6	1.762810000	-1.086688000	1.156302000
6	0.855798000	-2.305282000	0.968846000
1	1.224738000	-0.267268000	1.628679000
1	2.593116000	-1.331804000	1.824162000

1	0.486243000	-2.633400000	1.945607000
1	-0.005194000	-2.059132000	0.343714000
1	1.398532000	-3.141086000	0.516905000
6	3.597569000	-1.335287000	-0.495872000
6	4.858866000	-0.734616000	0.130774000
1	3.677293000	-1.363901000	-1.581500000
1	3.473139000	-2.370244000	-0.168430000
1	5.727267000	-1.336361000	-0.155074000
1	5.027723000	0.291483000	-0.208721000
1	4.798008000	-0.727928000	1.223179000
6	2.565398000	0.741289000	-2.139817000
1	3.636916000	0.895870000	-1.996171000
1	2.434920000	-0.054254000	-2.881583000
1	2.122839000	1.654820000	-2.531815000
6	-4.762336000	-0.588983000	-0.066239000
6	-5.925863000	-1.303674000	-0.734677000
1	-4.826723000	0.492609000	-0.256155000
1	-4.806138000	-0.736817000	1.022982000
1	-6.878019000	-0.921017000	-0.351849000
1	-5.905470000	-1.149809000	-1.819068000
1	-5.885298000	-2.380625000	-0.538394000
8	-1.282829000	2.542840000	-0.150948000
1	-0.726260000	3.169367000	-0.639903000
1	-2.789779000	-0.646050000	-0.152295000

Cartesian coordinates of the B3LYP/6-31++G(d,p) optimised geometries in the gas phase

TSP1

7	2.245804000	0.271170000	0.094623000
6	1.129077000	-0.394015000	-0.303602000
7	-0.022876000	0.027154000	0.164491000
15	-1.479750000	-0.711912000	-0.107306000
8	-1.936508000	-1.393802000	-1.349862000
9	-0.703917000	-2.339587000	0.691851000
8	-2.432959000	0.639961000	0.115638000
6	2.138753000	1.394791000	1.038883000
6	2.197769000	0.946545000	2.502153000
1	1.197985000	1.910495000	0.841981000
1	2.959171000	2.085573000	0.817923000
1	2.132486000	1.816332000	3.165126000
1	1.364028000	0.276322000	2.726549000
1	3.133142000	0.422027000	2.725998000
6	3.600997000	-0.068879000	-0.355992000
6	4.077076000	0.763995000	-1.552450000
1	3.651531000	-1.133442000	-0.588043000
1	4.271437000	0.089687000	0.495886000
1	5.107070000	0.495844000	-1.811533000
1	3.447770000	0.592557000	-2.431085000
1	4.054398000	1.834773000	-1.326086000
6	1.305761000	-1.545666000	-1.272192000
1	0.340731000	-1.835059000	-1.684907000
1	1.982955000	-1.285556000	-2.089678000
1	1.710956000	-2.414321000	-0.742926000
6	-2.475547000	1.612348000	-0.943249000
6	-3.456011000	2.703197000	-0.545644000

1	-2.789820000	1.117203000	-1.868794000
1	-1.469609000	2.027290000	-1.092501000
1	-3.514498000	3.459420000	-1.336444000
1	-4.456095000	2.286241000	-0.391934000
1	-3.139360000	3.195842000	0.379512000
8	-2.379053000	-1.178452000	1.541574000
1	-1.704301000	-1.890604000	1.769323000
1	-2.428045000	-0.419471000	2.144520000

P1f

7	-2.129843000	-0.573034000	-0.021758000
6	-1.088430000	0.181111000	-0.444499000
7	0.110434000	-0.137326000	-0.012134000
15	1.516432000	0.619158000	-0.366396000
8	1.811033000	1.116022000	-1.743599000
9	-0.664661000	2.804156000	1.745276000
8	2.666425000	-0.333703000	0.245183000
6	-1.896211000	-1.707595000	0.889180000
6	-1.896193000	-1.294029000	2.363518000
1	-0.938504000	-2.157229000	0.624926000
1	-2.683427000	-2.443387000	0.694240000
1	-1.739055000	-2.173942000	2.996828000
1	-1.093723000	-0.578797000	2.557927000
1	-2.847603000	-0.835483000	2.653849000
6	-3.533077000	-0.280632000	-0.344054000
6	-4.062293000	-1.078550000	-1.541121000
1	-3.654107000	0.790610000	-0.510363000
1	-4.121077000	-0.516581000	0.549131000
1	-5.122475000	-0.855648000	-1.702483000
1	-3.517079000	-0.830877000	-2.457131000
1	-3.965687000	-2.155983000	-1.373592000

6	-1.381741000	1.352267000	-1.360628000
1	-0.471384000	1.634845000	-1.889843000
1	-2.154456000	1.122768000	-2.096625000
1	-1.714852000	2.206378000	-0.759305000
6	3.110790000	-1.483117000	-0.516842000
6	4.280792000	-2.108547000	0.219642000
1	3.397850000	-1.152898000	-1.520694000
1	2.275973000	-2.189350000	-0.603070000
1	4.635726000	-2.988039000	-0.328534000
1	5.108035000	-1.397817000	0.306824000
1	3.984897000	-2.421592000	1.225377000
8	1.569375000	1.839030000	0.759676000
1	0.164065000	2.445777000	1.446479000
1	2.251741000	2.488749000	0.530508000

TSP2

7	-2.452964000	0.157599000	-0.244937000
6	-1.284997000	-0.516183000	-0.252753000
7	-0.214017000	0.083373000	0.235596000
15	1.429980000	-0.447133000	0.582965000
8	1.526237000	-1.840926000	0.023127000
9	1.631371000	-0.651118000	2.159519000
8	2.640941000	0.402691000	-0.107633000
6	-2.559435000	1.507085000	0.346611000
6	-2.185402000	2.624127000	-0.632541000
1	-1.936497000	1.551352000	1.242797000
1	-3.596010000	1.624438000	0.674845000
1	-2.314210000	3.596776000	-0.147490000
1	-1.142591000	2.541868000	-0.949182000
1	-2.822134000	2.601706000	-1.523369000
6	-3.689953000	-0.379223000	-0.838502000

6	-4.613100000	-1.047563000	0.185480000
1	-3.434692000	-1.076039000	-1.637166000
1	-4.203814000	0.462313000	-1.314965000
1	-5.531138000	-1.385503000	-0.306451000
1	-4.133158000	-1.915183000	0.647714000
1	-4.894882000	-0.353586000	0.983366000
6	-1.243505000	-1.906450000	-0.830646000
1	-2.075551000	-2.511204000	-0.463530000
1	-1.313790000	-1.852334000	-1.923536000
1	-0.289049000	-2.366305000	-0.570175000
6	3.613135000	-0.299745000	-0.937306000
6	4.500764000	0.756396000	-1.570935000
1	3.086474000	-0.899030000	-1.683061000
1	4.188640000	-0.981027000	-0.304264000
1	5.260247000	0.271514000	-2.194557000
1	3.916950000	1.433100000	-2.203203000
1	5.011178000	1.351223000	-0.807238000
8	1.066127000	1.571285000	1.328920000
1	-0.037066000	1.113535000	0.656044000
1	1.706450000	2.177576000	0.936905000

P2f

7	2.696634000	0.130225000	0.091513000
6	1.750163000	1.035484000	-0.348204000
7	1.196169000	1.967991000	0.362869000
15	-2.326245000	-1.020144000	-0.141022000
8	-0.953683000	-1.299896000	-0.591394000
9	-2.544850000	-1.390197000	1.402834000
8	-2.916126000	0.454358000	-0.218147000
6	3.187798000	0.173350000	1.468078000
6	2.301655000	-0.580043000	2.470503000

1	3.308826000	1.219398000	1.772100000
1	4.195385000	-0.256300000	1.471618000
1	2.728590000	-0.518268000	3.478028000
1	1.290288000	-0.164843000	2.497759000
1	2.217781000	-1.637911000	2.201558000
6	3.169777000	-0.995343000	-0.721835000
6	4.522074000	-0.741342000	-1.400257000
1	2.412788000	-1.248041000	-1.464907000
1	3.244964000	-1.871837000	-0.066703000
1	4.841446000	-1.630165000	-1.956476000
1	4.460798000	0.097464000	-2.100798000
1	5.299993000	-0.507406000	-0.665520000
6	1.314761000	0.932208000	-1.794497000
1	2.161971000	0.861367000	-2.483242000
1	0.669888000	0.058949000	-1.938176000
1	0.743147000	1.829410000	-2.032109000
6	-2.244901000	1.600180000	0.424100000
6	-2.839949000	2.862453000	-0.162129000
1	-1.167676000	1.543129000	0.242576000
1	-2.439076000	1.522481000	1.498646000
1	-2.362361000	3.729685000	0.305018000
1	-2.658288000	2.913039000	-1.239475000
1	-3.918188000	2.917420000	0.017603000
8	-3.455677000	-1.881084000	-0.878202000
1	1.512055000	1.956591000	1.332232000
1	-4.359020000	-1.596448000	-0.673185000

TSP3

7	-2.515642000	0.199541000	0.128739000
6	-1.371505000	-0.401444000	-0.304175000
7	-0.267102000	0.298712000	-0.289919000
15	1.249643000	-0.346444000	-0.559877000
8	1.722723000	-1.266215000	-1.633858000
9	1.155431000	-1.392009000	0.758721000
8	2.572752000	0.475720000	0.436502000
6	-2.469447000	1.568503000	0.662648000
6	-2.674119000	2.637432000	-0.415738000
1	-1.504034000	1.704867000	1.151992000
1	-3.249119000	1.648130000	1.427640000
1	-2.642333000	3.636437000	0.032853000
1	-1.888103000	2.573512000	-1.172811000
1	-3.642360000	2.525253000	-0.915873000
6	-3.836549000	-0.438436000	0.096120000
6	-4.229491000	-1.102256000	1.422066000
1	-3.871514000	-1.167222000	-0.714682000
1	-4.566715000	0.337658000	-0.159872000
1	-5.238595000	-1.522120000	1.347650000
1	-3.539695000	-1.911281000	1.680438000
1	-4.224637000	-0.380992000	2.245394000
6	-1.485790000	-1.822857000	-0.822852000
1	-1.963396000	-2.478845000	-0.090057000
1	-2.084180000	-1.843370000	-1.740477000
1	-0.501243000	-2.220541000	-1.061713000
6	3.776575000	-0.269149000	0.799070000
6	4.781221000	0.691421000	1.407498000
1	4.159384000	-0.759309000	-0.100804000
1	3.448599000	-1.030439000	1.507230000

1	5.676175000	0.135420000	1.706580000
1	5.087379000	1.459401000	0.689564000
1	4.368530000	1.182875000	2.293539000
8	1.709641000	1.294001000	-1.403324000
1	0.969602000	1.911344000	-1.311081000
1	2.555648000	1.228831000	-0.379956000

P3f

7	-2.519295000	0.447828000	0.103338000
6	-1.359335000	0.035953000	-0.462103000
7	-0.564371000	-0.719984000	0.257718000
15	0.861754000	-1.398583000	-0.156597000
8	1.556347000	-1.161429000	-1.443265000
9	0.559156000	-2.954316000	0.087781000
8	3.567121000	1.357667000	1.191837000
6	-2.865250000	0.028546000	1.472893000
6	-2.314355000	0.978089000	2.540459000
1	-2.476431000	-0.979345000	1.623549000
1	-3.957303000	-0.018583000	1.530031000
1	-2.612874000	0.634370000	3.536616000
1	-1.222613000	1.010904000	2.499505000
1	-2.695084000	1.996687000	2.409110000
6	-3.485744000	1.328887000	-0.567442000
6	-4.627369000	0.570682000	-1.254669000
1	-2.964212000	1.963819000	-1.284526000
1	-3.891249000	2.000244000	0.197015000
1	-5.335431000	1.280124000	-1.695906000
1	-4.251610000	-0.077727000	-2.051968000
1	-5.176010000	-0.054306000	-0.543217000
6	-1.058502000	0.497632000	-1.874549000
1	-1.906316000	0.324665000	-2.542223000

1	-0.837637000	1.571126000	-1.878276000
1	-0.183702000	-0.024983000	-2.258125000
6	4.631681000	1.471290000	0.246942000
6	4.138170000	1.666446000	-1.184852000
1	5.289363000	0.590322000	0.303466000
1	5.218946000	2.337152000	0.570804000
1	4.987060000	1.778701000	-1.870859000
1	3.542692000	0.808943000	-1.517320000
1	3.517251000	2.566328000	-1.255585000
8	1.845118000	-1.086229000	1.099022000
1	1.386871000	-1.110650000	1.952599000
1	3.090767000	0.529649000	1.026017000

TSP4

7	2.304771000	0.388665000	0.026623000
6	1.259551000	-0.478739000	0.124786000
7	0.050881000	0.008832000	0.044128000
15	-1.353473000	-0.845226000	-0.026127000
8	-1.677125000	-2.100697000	0.864050000
9	-1.120987000	-1.652880000	-1.416683000
8	-2.536532000	0.038883000	-0.616254000
6	2.050764000	1.817086000	-0.219945000
6	1.853243000	2.620887000	1.068596000
1	1.166075000	1.897536000	-0.853539000
1	2.905140000	2.206063000	-0.783236000
1	1.704546000	3.679916000	0.831221000
1	0.972818000	2.264935000	1.609536000
1	2.724357000	2.543573000	1.728505000
6	3.712831000	-0.013080000	0.127109000
6	4.378051000	-0.268064000	-1.231305000
1	3.797132000	-0.897085000	0.760797000

1	4.240912000	0.789854000	0.653527000
1	5.434368000	-0.521483000	-1.090533000
1	3.895497000	-1.094555000	-1.761758000
1	4.326653000	0.617570000	-1.872294000
6	1.588978000	-1.943454000	0.350295000
1	2.298516000	-2.312700000	-0.394834000
1	2.034317000	-2.086764000	1.341199000
1	0.686859000	-2.549704000	0.302231000
6	-2.992702000	1.325508000	-0.120914000
6	-3.955715000	1.882919000	-1.152681000
1	-2.120802000	1.973608000	0.009937000
1	-3.459112000	1.173245000	0.852012000
1	-4.332926000	2.852831000	-0.809773000
1	-3.464238000	2.023154000	-2.120218000
1	-4.808260000	1.211440000	-1.291820000
1	-1.097005000	0.245910000	2.433330000
8	-1.853629000	-0.123499000	1.960212000
1	-1.835141000	-1.421378000	1.762770000

P1b

7	2.365193000	-0.090808000	0.117076000
6	1.198679000	0.408313000	-0.368793000
7	0.162532000	-0.392650000	-0.407180000
15	-1.374616000	-0.097069000	-0.909815000
8	-1.839495000	1.323071000	-1.071647000
9	-2.691582000	2.829882000	0.764785000
8	-2.293289000	-0.994891000	0.063597000
6	2.432608000	-1.482405000	0.592479000
6	2.785574000	-2.473513000	-0.520343000
1	1.465588000	-1.736160000	1.028431000
1	3.183994000	-1.518070000	1.387876000

1	2.847322000	-3.488660000	-0.113544000
1	2.018641000	-2.460511000	-1.299061000
1	3.751252000	-2.236330000	-0.979982000
6	3.611895000	0.682053000	0.200529000
6	3.837931000	1.331648000	1.570993000
1	3.626396000	1.438244000	-0.585336000
1	4.432862000	-0.007551000	-0.024079000
1	4.800112000	1.854721000	1.584071000
1	3.051630000	2.056554000	1.802258000
1	3.850856000	0.582930000	2.369304000
6	1.199985000	1.847171000	-0.847556000
1	1.649064000	2.518719000	-0.111713000
1	1.774926000	1.930476000	-1.777229000
1	0.180126000	2.171019000	-1.045030000
6	-2.433343000	-0.658576000	1.471032000
6	-3.433580000	-1.622242000	2.080680000
1	-2.774345000	0.377730000	1.557923000
1	-1.449865000	-0.750917000	1.946961000
1	-3.559351000	-1.396517000	3.145008000
1	-4.407025000	-1.529259000	1.590652000
1	-3.090877000	-2.657077000	1.983096000
1	-1.374344000	-1.827221000	-2.229605000
8	-1.570461000	-0.882449000	-2.307977000
1	-2.400105000	2.288633000	0.018975000

TSP7

7	-2.442465000	0.134808000	0.058775000
6	-1.165934000	-0.029087000	-0.396481000
7	-0.259324000	-0.401071000	0.457667000
15	1.337473000	-0.725673000	0.166850000
8	1.296076000	-1.879998000	-0.916028000
9	1.688628000	-1.142921000	1.671568000
8	1.851069000	0.755057000	-0.163354000
6	-2.750915000	-0.145662000	1.469670000
6	-2.517930000	1.061151000	2.383700000
1	-2.127293000	-0.981907000	1.789587000
1	-3.797686000	-0.464483000	1.516299000
1	-2.786446000	0.808157000	3.415318000
1	-1.464692000	1.351715000	2.363789000
1	-3.125960000	1.920539000	2.078949000
6	-3.553910000	0.615636000	-0.767401000
6	-4.414998000	-0.508739000	-1.357057000
1	-3.170561000	1.256639000	-1.563315000
1	-4.173321000	1.260321000	-0.133455000
1	-5.252304000	-0.086364000	-1.923549000
1	-3.831663000	-1.144904000	-2.029953000
1	-4.828061000	-1.146034000	-0.568832000
6	-0.913936000	0.266079000	-1.865371000
1	-1.690757000	-0.154257000	-2.508155000
1	-0.879625000	1.348639000	-2.032666000
1	0.039910000	-0.157987000	-2.171532000
6	3.206519000	1.284066000	-0.247135000
6	3.078028000	2.784404000	-0.438232000
1	3.722388000	0.796277000	-1.073364000
1	3.734506000	1.033593000	0.674654000

1	4.078168000	3.226985000	-0.503349000
1	2.539002000	3.020240000	-1.361223000
1	2.549431000	3.247427000	0.400685000
8	3.378018000	-1.393634000	-0.163927000
1	3.744900000	-1.874060000	0.589519000
1	2.369986000	-2.043798000	-0.865038000

P2b

7	2.938558000	-0.149483000	-0.109475000
6	2.149065000	0.980058000	0.029251000
7	0.859267000	0.997573000	0.107632000
15	-2.702416000	-0.832051000	0.216921000
8	-1.312861000	-1.339156000	0.225727000
9	-3.682115000	-1.703673000	-0.670043000
8	-3.044048000	0.588387000	-0.380005000
6	2.325770000	-1.479214000	-0.187319000
6	1.909356000	-1.878155000	-1.608743000
1	1.461808000	-1.524017000	0.482566000
1	3.052355000	-2.199775000	0.203552000
1	1.466873000	-2.880042000	-1.606485000
1	1.165418000	-1.183458000	-2.007869000
1	2.771892000	-1.885250000	-2.284499000
6	4.399961000	-0.110044000	-0.193648000
6	5.107125000	-0.352350000	1.147359000
1	4.717314000	0.846545000	-0.612708000
1	4.713916000	-0.872998000	-0.916844000
1	6.194904000	-0.350820000	1.011507000
1	4.851144000	0.425698000	1.873633000
1	4.823027000	-1.318370000	1.577616000
6	2.859994000	2.318331000	0.085138000
1	3.339812000	2.559304000	-0.870589000

1	2.109965000	3.080054000	0.295274000
1	3.629541000	2.352411000	0.863263000
6	-2.448818000	1.826126000	0.157717000
6	-2.865027000	2.954506000	-0.761986000
1	-1.361397000	1.711110000	0.191826000
1	-2.845634000	1.961920000	1.168806000
1	-2.454798000	3.895464000	-0.380197000
1	-2.474484000	2.794949000	-1.770971000
1	-3.954200000	3.044795000	-0.814251000
8	-3.422803000	-0.848699000	1.659854000
1	-2.942523000	-1.409896000	2.286670000
1	0.438707000	0.069774000	0.047959000

TSP10

7	-2.069356000	0.289590000	0.279568000
6	-1.069494000	0.918876000	-0.386245000
7	0.163243000	0.530226000	-0.501479000
15	1.262636000	-0.631221000	-0.341307000
8	2.094958000	-1.099612000	-1.591858000
9	1.069230000	-1.764357000	0.763800000
8	2.394621000	0.135347000	0.541185000
6	-1.877853000	-0.996180000	0.982319000
6	-1.423534000	-0.813110000	2.433208000
1	-1.185856000	-1.613207000	0.411124000
1	-2.842774000	-1.512124000	0.953887000
1	-1.311815000	-1.792930000	2.908216000
1	-0.456634000	-0.306457000	2.485967000
1	-2.150461000	-0.234955000	3.014842000
6	-3.418555000	0.868289000	0.407315000
6	-4.406736000	0.339541000	-0.638276000

1	-3.362140000	1.956386000	0.362525000
1	-3.775669000	0.622730000	1.412789000
1	-5.402097000	0.760633000	-0.460426000
1	-4.097774000	0.610964000	-1.652514000
1	-4.488096000	-0.750733000	-0.592514000
6	-1.393485000	2.248705000	-1.050413000
1	-2.296497000	2.199523000	-1.665014000
1	-1.536455000	3.036151000	-0.301751000
1	-0.548432000	2.524217000	-1.679102000
6	3.170181000	1.209486000	-0.027997000
6	4.160614000	1.679788000	1.022702000
1	2.493642000	2.020525000	-0.324142000
1	3.685281000	0.840318000	-0.921421000
1	4.769890000	2.496326000	0.619591000
1	3.640262000	2.042482000	1.914609000
1	4.826233000	0.863650000	1.319028000
8	-0.016618000	-1.990155000	-1.504630000
1	-0.682231000	-1.547246000	-2.048372000
1	1.271304000	-1.704451000	-1.971812000

P3b

7	-1.814317000	0.250993000	0.117114000
6	-1.093566000	-0.160566000	-0.943369000
7	-0.292525000	-1.196934000	-0.946312000
15	0.965268000	-1.750049000	-0.156255000
8	1.937876000	-0.790793000	0.455925000
9	0.455993000	-2.774708000	0.991927000
8	1.386188000	1.898535000	-0.289568000
6	-1.821616000	-0.484390000	1.395553000
6	-0.878438000	0.097479000	2.453375000

1	-1.575223000	-1.525535000	1.187318000
1	-2.854093000	-0.464399000	1.761540000
1	-0.969608000	-0.486335000	3.375356000
1	0.162549000	0.059827000	2.125680000
1	-1.127991000	1.137448000	2.687543000
6	-2.651683000	1.464028000	0.083701000
6	-4.116404000	1.186085000	-0.270885000
1	-2.209423000	2.184931000	-0.604075000
1	-2.587827000	1.916769000	1.077356000
1	-4.690481000	2.117965000	-0.234603000
1	-4.213932000	0.764517000	-1.275820000
1	-4.572581000	0.483942000	0.433933000
6	-1.218672000	0.599795000	-2.245514000
1	-2.229167000	0.949133000	-2.465504000
1	-0.542250000	1.461871000	-2.193280000
1	-0.875916000	-0.052670000	-3.047538000
6	2.553106000	2.683333000	-0.517725000
6	3.338283000	2.965016000	0.761820000
1	2.203769000	3.622710000	-0.961309000
1	3.205023000	2.194639000	-1.258585000
1	4.209533000	3.596875000	0.549377000
1	2.707890000	3.478794000	1.495330000
1	3.696396000	2.032543000	1.211905000
8	1.628833000	-2.808626000	-1.180312000
1	2.476880000	-3.134226000	-0.844588000
1	1.662157000	1.008298000	0.010737000

Cartesian coordinates of the CPCM(water)-B3LYP/6-31++G(d,p) optimised geometries

TSP1

7	2.228055000	0.230035000	0.114917000
6	1.124958000	-0.357826000	-0.387173000
7	-0.044284000	-0.001883000	0.115109000
15	-1.496742000	-0.700032000	-0.148359000
8	-2.041553000	-1.342062000	-1.391816000
9	-0.709624000	-2.433779000	0.471808000
8	-2.449026000	0.639635000	0.136205000
6	2.126999000	1.194040000	1.227229000
6	2.180544000	0.516294000	2.598851000
1	1.196263000	1.749941000	1.112302000
1	2.956546000	1.897692000	1.118220000
1	2.133384000	1.274126000	3.387912000
1	1.336393000	-0.167008000	2.725900000
1	3.109173000	-0.049236000	2.728428000
6	3.588194000	-0.019573000	-0.395114000
6	4.044047000	1.012362000	-1.431862000
1	3.643490000	-1.027342000	-0.805888000
1	4.257351000	-0.001409000	0.470208000
1	5.073478000	0.797013000	-1.735752000
1	3.411411000	0.987602000	-2.324357000
1	4.017805000	2.026859000	-1.022410000
6	1.302064000	-1.345008000	-1.521249000
1	0.330787000	-1.628806000	-1.919821000
1	1.906559000	-0.920301000	-2.326597000
1	1.802268000	-2.249678000	-1.162245000
6	-2.395233000	1.737281000	-0.798445000
6	-3.337588000	2.824990000	-0.312683000

1	-2.691587000	1.378499000	-1.791162000
1	-1.365197000	2.108488000	-0.855574000
1	-3.315087000	3.669967000	-1.009016000
1	-4.366036000	2.454645000	-0.254454000
1	-3.040072000	3.186609000	0.676793000
8	-2.323874000	-1.241643000	1.459467000
1	-1.712109000	-1.973206000	1.730889000
1	-2.421755000	-0.529847000	2.117389000

P1f

7	-2.258109000	-0.353460000	0.037171000
6	-1.228419000	0.437680000	-0.312043000
7	-0.001623000	-0.025950000	-0.142730000
15	1.393176000	0.693722000	-0.564380000
8	1.576193000	1.294125000	-1.926960000
9	1.317485000	1.536404000	3.149553000
8	2.543883000	-0.365655000	-0.163877000
6	-2.017111000	-1.712836000	0.558121000
6	-1.840157000	-1.740763000	2.078555000
1	-1.131937000	-2.112417000	0.063165000
1	-2.874274000	-2.324214000	0.263226000
1	-1.692313000	-2.772939000	2.412828000
1	-0.968563000	-1.152707000	2.377981000
1	-2.722249000	-1.343566000	2.591292000
6	-3.670471000	0.064444000	-0.037625000
6	-4.361310000	-0.373343000	-1.332775000
1	-3.738158000	1.144700000	0.091149000
1	-4.176179000	-0.380262000	0.824312000
1	-5.414170000	-0.074911000	-1.305662000
1	-3.896733000	0.088403000	-2.209308000
1	-4.320822000	-1.459778000	-1.457301000

6	-1.542003000	1.821738000	-0.842536000
1	-0.666137000	2.237329000	-1.338220000
1	-2.366738000	1.811561000	-1.557058000
1	-1.818659000	2.484202000	-0.014889000
6	2.724539000	-1.575097000	-0.955907000
6	3.866768000	-2.367085000	-0.350398000
1	2.943381000	-1.287248000	-1.989122000
1	1.790204000	-2.145589000	-0.936021000
1	4.022152000	-3.282208000	-0.930985000
1	4.795096000	-1.787976000	-0.364925000
1	3.642969000	-2.648207000	0.683137000
8	1.662830000	1.823260000	0.621111000
1	1.445732000	1.627024000	2.202009000
1	2.356272000	2.458940000	0.378485000

TSP2

7	-2.415904000	0.135339000	-0.239678000
6	-1.271886000	-0.541512000	-0.207611000
7	-0.188778000	0.062286000	0.315185000
15	1.431898000	-0.440473000	0.638221000
8	1.541578000	-1.898096000	0.277857000
9	1.698879000	-0.443235000	2.227601000
8	2.582280000	0.361542000	-0.166809000
6	-2.549731000	1.502357000	0.315610000
6	-2.169617000	2.591016000	-0.691593000
1	-1.955914000	1.576149000	1.229046000
1	-3.593882000	1.612210000	0.614180000
1	-2.326214000	3.572991000	-0.235454000
1	-1.120852000	2.518001000	-0.991902000
1	-2.791821000	2.529571000	-1.589284000
6	-3.646857000	-0.410835000	-0.860112000

6	-4.583761000	-1.063733000	0.158187000
1	-3.372545000	-1.110849000	-1.647709000
1	-4.142646000	0.431704000	-1.348805000
1	-5.489633000	-1.402497000	-0.353458000
1	-4.116378000	-1.928902000	0.637150000
1	-4.880684000	-0.357839000	0.939383000
6	-1.212414000	-1.930054000	-0.774648000
1	-2.067633000	-2.522611000	-0.447890000
1	-1.232787000	-1.872909000	-1.868816000
1	-0.286199000	-2.409546000	-0.469052000
6	3.463053000	-0.363838000	-1.092399000
6	4.402974000	0.659033000	-1.699535000
1	2.849498000	-0.851500000	-1.853073000
1	4.005262000	-1.130232000	-0.534761000
1	5.080302000	0.154772000	-2.396876000
1	3.849751000	1.425201000	-2.251112000
1	5.005864000	1.147241000	-0.927838000
8	1.117506000	1.762458000	1.280934000
1	-0.141912000	1.071833000	0.624382000
1	1.671327000	2.298205000	0.698363000

P2f

7	3.073266000	0.026450000	0.105749000
6	2.114332000	0.516817000	-0.747838000
7	1.359489000	1.556497000	-0.532300000
15	-2.900900000	-0.919227000	0.071946000
8	-1.548058000	-1.514726000	0.072880000
9	-3.536808000	-0.917585000	1.541563000
8	-3.095590000	0.579039000	-0.401675000
6	3.359449000	0.694793000	1.380042000
6	2.442113000	0.250107000	2.526278000

1	3.305280000	1.780220000	1.241321000
1	4.400117000	0.477538000	1.636751000
1	2.715861000	0.770195000	3.450554000
1	1.392798000	0.470581000	2.308245000
1	2.534030000	-0.826668000	2.702457000
6	3.886592000	-1.163213000	-0.188146000
6	5.252616000	-0.839792000	-0.805235000
1	3.327591000	-1.832845000	-0.842489000
1	4.025411000	-1.705899000	0.753390000
1	5.820569000	-1.763541000	-0.960998000
1	5.141648000	-0.339068000	-1.772307000
1	5.841662000	-0.188827000	-0.150974000
6	1.904254000	-0.219885000	-2.054864000
1	2.834484000	-0.341594000	-2.617291000
1	1.483369000	-1.217049000	-1.886394000
1	1.199576000	0.351780000	-2.658118000
6	-2.258535000	1.681703000	0.116677000
6	-2.650748000	2.935565000	-0.633699000
1	-1.210073000	1.420703000	-0.049108000
1	-2.457365000	1.772130000	1.187980000
1	-2.050033000	3.772393000	-0.263248000
1	-2.462559000	2.825206000	-1.705560000
1	-3.706895000	3.174866000	-0.479554000
8	-3.958421000	-1.739532000	-0.789642000
1	1.542054000	1.979595000	0.377356000
1	-4.845931000	-1.348487000	-0.851217000

TSP3

7	-2.460906000	0.234185000	0.119434000
6	-1.369612000	-0.455158000	-0.275534000
7	-0.227989000	0.194831000	-0.381796000
15	1.263817000	-0.474159000	-0.574920000
8	1.768827000	-1.517442000	-1.533210000
9	1.187460000	-1.422296000	0.834987000
8	2.495264000	0.493445000	0.324580000
6	-2.354289000	1.655942000	0.493119000
6	-2.560480000	2.600351000	-0.694548000
1	-1.373366000	1.816070000	0.941464000
1	-3.109588000	1.843394000	1.261441000
1	-2.493610000	3.639589000	-0.355873000
1	-1.795607000	2.436767000	-1.458572000
1	-3.544848000	2.458124000	-1.152453000
6	-3.813262000	-0.347018000	0.188046000
6	-4.187654000	-0.841924000	1.589088000
1	-3.902042000	-1.153957000	-0.539221000
1	-4.511556000	0.432800000	-0.130479000
1	-5.215459000	-1.219022000	1.582924000
1	-3.527894000	-1.651433000	1.915958000
1	-4.128438000	-0.034515000	2.325454000
6	-1.552423000	-1.916257000	-0.634321000
1	-2.074712000	-2.463765000	0.153537000
1	-2.140475000	-2.006023000	-1.553967000
1	-0.587533000	-2.387970000	-0.807012000
6	3.702977000	-0.086104000	0.936863000
6	4.508142000	1.034102000	1.562648000
1	4.257511000	-0.610916000	0.155072000
1	3.343394000	-0.801680000	1.674549000

1	5.398006000	0.604645000	2.033966000
1	4.838178000	1.758470000	0.812161000
1	3.927966000	1.554059000	2.330106000
8	1.741320000	1.028085000	-1.665049000
1	1.008735000	1.663783000	-1.662910000
1	2.525530000	1.135213000	-0.583444000

P3f

7	-2.258820000	-0.782790000	0.089783000
6	-1.637057000	0.401274000	-0.057233000
7	-0.365044000	0.483393000	0.289821000
15	0.585091000	1.801728000	0.249936000
8	0.174165000	3.082321000	0.901454000
9	0.848591000	2.088608000	-1.334998000
8	2.949785000	-1.005581000	-0.036866000
6	-1.530745000	-1.950269000	0.622125000
6	-1.580049000	-2.029333000	2.150251000
1	-0.498653000	-1.893479000	0.275410000
1	-1.986982000	-2.840163000	0.180555000
1	-1.053124000	-2.927039000	2.490066000
1	-1.099275000	-1.156175000	2.599494000
1	-2.611424000	-2.085443000	2.513473000
6	-3.676910000	-1.008518000	-0.244884000
6	-3.879909000	-1.589783000	-1.647756000
1	-4.231810000	-0.077637000	-0.129843000
1	-4.072418000	-1.697955000	0.506736000
1	-4.945291000	-1.776676000	-1.816157000
1	-3.526899000	-0.900572000	-2.420880000
1	-3.347316000	-2.538287000	-1.766723000
6	-2.446326000	1.562052000	-0.600566000
1	-2.986755000	1.287725000	-1.508960000

1	-3.179858000	1.892033000	0.142643000
1	-1.799317000	2.407486000	-0.825549000
6	4.392737000	-1.092012000	-0.150500000
6	4.826443000	-2.323087000	-0.929805000
1	4.835424000	-1.079826000	0.852094000
1	4.688117000	-0.175500000	-0.666581000
1	5.917858000	-2.336588000	-1.021962000
1	4.521161000	-3.243091000	-0.419033000
1	4.394317000	-2.321253000	-1.935243000
8	2.023409000	1.330117000	0.734712000
1	2.323406000	0.417442000	0.438222000
1	2.624217000	-1.759415000	0.476766000

TSP4

7	2.281088000	0.389361000	0.016046000
6	1.269972000	-0.495306000	0.111640000
7	0.040310000	-0.051462000	-0.052781000
15	-1.358550000	-0.861382000	-0.093496000
8	-1.726874000	-2.186207000	0.696520000
9	-1.244972000	-1.605693000	-1.552808000
8	-2.571378000	0.069898000	-0.539536000
6	2.009932000	1.807988000	-0.282878000
6	1.764754000	2.641078000	0.978041000
1	1.146385000	1.856973000	-0.947008000
1	2.875807000	2.191217000	-0.829243000
1	1.597694000	3.687392000	0.701716000
1	0.883059000	2.281575000	1.515363000
1	2.624970000	2.603860000	1.654356000
6	3.698773000	0.029494000	0.199651000
6	4.423523000	-0.261951000	-1.118279000
1	3.774611000	-0.821211000	0.876588000

1	4.174364000	0.872291000	0.709723000
1	5.477566000	-0.478289000	-0.916834000
1	3.988756000	-1.125370000	-1.630996000
1	4.378135000	0.596161000	-1.795805000
6	1.614547000	-1.936781000	0.424915000
1	2.398599000	-2.314841000	-0.234535000
1	1.970293000	-2.025197000	1.456945000
1	0.736041000	-2.569948000	0.318671000
6	-2.779624000	1.447961000	-0.099630000
6	-3.956202000	1.999955000	-0.879316000
1	-1.862579000	2.008168000	-0.300697000
1	-2.959472000	1.430046000	0.974928000
1	-4.137471000	3.033420000	-0.565950000
1	-3.758092000	1.996634000	-1.955419000
1	-4.863369000	1.419261000	-0.685989000
1	-0.970678000	-0.028015000	2.448905000
8	-1.776714000	-0.306257000	1.992189000
1	-1.815741000	-1.621538000	1.641891000

P1b

7	-2.230039000	-0.440425000	-0.008900000
6	-1.186883000	0.289735000	0.421084000
7	0.026662000	-0.222414000	0.297807000
15	1.444000000	0.476928000	0.673305000
8	1.758829000	1.843845000	0.094146000
9	1.023484000	2.940156000	-1.959077000
8	2.559837000	-0.624664000	0.311909000
6	-2.017105000	-1.762623000	-0.628823000
6	-2.009178000	-2.900075000	0.395795000
1	-1.073859000	-1.732605000	-1.174133000
1	-2.822152000	-1.908728000	-1.353983000

1	-1.876049000	-3.857450000	-0.118572000
1	-1.189651000	-2.774273000	1.108436000
1	-2.951389000	-2.944138000	0.951665000
6	-3.635274000	-0.011413000	0.121128000
6	-4.172848000	0.680397000	-1.135400000
1	-3.740046000	0.633632000	0.993453000
1	-4.220383000	-0.911151000	0.331787000
1	-5.229059000	0.929854000	-0.992502000
1	-3.628173000	1.605473000	-1.347019000
1	-4.094377000	0.029830000	-2.011767000
6	-1.474078000	1.637087000	1.052271000
1	-2.200528000	2.213281000	0.476623000
1	-1.875704000	1.498543000	2.062012000
1	-0.558805000	2.221829000	1.126731000
6	2.729717000	-1.099096000	-1.056472000
6	3.828998000	-2.142736000	-1.057292000
1	2.991428000	-0.245335000	-1.689912000
1	1.777781000	-1.517227000	-1.396623000
1	3.977368000	-2.511973000	-2.077183000
1	4.773138000	-1.717517000	-0.703831000
1	3.563062000	-2.990756000	-0.419008000
1	1.465275000	-0.215030000	2.756160000
8	1.653702000	0.605881000	2.274485000
1	1.305361000	2.470153000	-1.130650000

TSP7

7	-2.433950000	0.082995000	0.102724000
6	-1.157621000	0.179816000	-0.338952000
7	-0.256437000	-0.610108000	0.195873000
15	1.340739000	-0.719135000	-0.185146000
8	1.329794000	-1.227059000	-1.696655000
9	1.688638000	-1.827609000	0.924699000
8	1.849108000	0.730163000	0.242213000
6	-2.789395000	-0.901736000	1.139090000
6	-2.607737000	-0.361316000	2.560466000
1	-2.174535000	-1.790013000	0.989374000
1	-3.832787000	-1.183397000	0.971572000
1	-2.910383000	-1.121821000	3.288215000
1	-1.561174000	-0.104229000	2.744755000
1	-3.220980000	0.530090000	2.729547000
6	-3.533157000	0.939679000	-0.372923000
6	-4.365253000	0.299137000	-1.489123000
1	-3.134643000	1.901568000	-0.695954000
1	-4.170567000	1.148627000	0.491869000
1	-5.189798000	0.965388000	-1.763258000
1	-3.761041000	0.116537000	-2.383141000
1	-4.794501000	-0.654851000	-1.167465000
6	-0.871617000	1.217174000	-1.409052000
1	-1.610385000	1.186115000	-2.212459000
1	-0.886453000	2.222661000	-0.975055000
1	0.110547000	1.053374000	-1.846645000
6	3.189976000	1.307134000	0.342798000
6	3.026900000	2.688032000	0.948031000
1	3.622923000	1.341989000	-0.656531000
1	3.800156000	0.652998000	0.964738000

1	4.013525000	3.154895000	1.037294000
1	2.401334000	3.326892000	0.317306000
1	2.581277000	2.633316000	1.945956000
8	3.420351000	-1.165835000	-0.753065000
1	3.729088000	-1.957411000	-0.291738000
1	2.365677000	-1.403116000	-1.745613000

P2b

7	3.025967000	-0.141450000	-0.106359000
6	2.298970000	1.023539000	-0.025360000
7	1.002361000	1.110523000	0.045014000
15	-2.769572000	-0.837267000	0.218169000
8	-1.352598000	-1.223319000	0.411349000
9	-3.505797000	-1.736933000	-0.865934000
8	-3.122878000	0.581227000	-0.382462000
6	2.356129000	-1.446790000	-0.122957000
6	1.938646000	-1.897778000	-1.528380000
1	1.487823000	-1.420774000	0.542453000
1	3.047842000	-2.176139000	0.308752000
1	1.461520000	-2.882691000	-1.482339000
1	1.228863000	-1.195604000	-1.976081000
1	2.808774000	-1.972341000	-2.189012000
6	4.493922000	-0.177502000	-0.179176000
6	5.173044000	-0.381328000	1.180723000
1	4.859174000	0.737024000	-0.647689000
1	4.769113000	-0.994613000	-0.855254000
1	6.259366000	-0.441873000	1.051993000
1	4.954822000	0.448747000	1.860290000
1	4.838110000	-1.308186000	1.657840000
6	3.075404000	2.325532000	-0.026396000
1	3.570855000	2.494140000	-0.988890000

1	2.372468000	3.140342000	0.145677000
1	3.844360000	2.351903000	0.751338000
6	-2.609825000	1.824650000	0.228912000
6	-3.077413000	2.976562000	-0.633442000
1	-1.519681000	1.758103000	0.266772000
1	-3.015745000	1.886863000	1.242217000
1	-2.715950000	3.913829000	-0.198389000
1	-2.679410000	2.892226000	-1.648790000
1	-4.169451000	3.016922000	-0.680511000
8	-3.719685000	-0.974938000	1.499366000
1	-3.379014000	-1.585307000	2.173615000
1	0.541638000	0.200248000	0.026715000

TSP10

7	-2.194466000	0.369122000	-0.001775000
6	-1.041020000	-0.182011000	-0.418966000
7	0.019369000	-0.060636000	0.351857000
15	1.491993000	-0.704533000	0.344779000
8	2.151715000	-1.669186000	-0.737852000
9	1.984112000	-0.960629000	1.837028000
8	2.465455000	0.594189000	0.184077000
6	-2.273483000	1.039738000	1.310229000
6	-1.906220000	2.524310000	1.239088000
1	-1.611376000	0.514566000	1.999345000
1	-3.298461000	0.917437000	1.669829000
1	-2.010294000	2.976052000	2.230985000
1	-0.872319000	2.653203000	0.908133000
1	-2.563449000	3.065853000	0.551070000
6	-3.430393000	0.377545000	-0.806558000
6	-4.385872000	-0.766300000	-0.452572000

1	-3.175489000	0.352457000	-1.865865000
1	-3.916967000	1.340884000	-0.628527000
1	-5.298671000	-0.678044000	-1.050226000
1	-3.935097000	-1.741939000	-0.657976000
1	-4.669347000	-0.736091000	0.603859000
6	-1.020093000	-0.860860000	-1.772022000
1	-1.843233000	-1.569910000	-1.883733000
1	-1.109123000	-0.112718000	-2.566848000
1	-0.080450000	-1.389786000	-1.915753000
6	2.430967000	1.388914000	-1.027668000
6	3.415952000	2.532314000	-0.870347000
1	1.412562000	1.765838000	-1.174952000
1	2.698268000	0.753658000	-1.879046000
1	3.407821000	3.148784000	-1.775104000
1	3.146588000	3.165296000	-0.019275000
1	4.431956000	2.154754000	-0.719702000
8	0.662421000	-2.738441000	0.654538000
1	-0.279513000	-2.826427000	0.455932000
1	1.579607000	-2.514007000	-0.450867000

P3b

7	-2.331356000	0.497460000	-0.073385000
6	-1.747097000	-0.447502000	-0.827632000
7	-0.645072000	-1.111710000	-0.553615000
15	0.625918000	-1.183709000	0.393754000
8	1.514576000	-0.008592000	0.668170000
9	0.135887000	-1.787258000	1.819070000
8	3.230229000	1.664391000	-0.787630000
6	-1.796393000	0.959762000	1.221889000
6	-0.970433000	2.243254000	1.104038000

1	-1.215424000	0.159805000	1.676629000
1	-2.656537000	1.122837000	1.877051000
1	-0.646241000	2.555702000	2.101903000
1	-0.081029000	2.080657000	0.491577000
1	-1.558276000	3.058595000	0.671640000
6	-3.599279000	1.152041000	-0.472823000
6	-4.837417000	0.466219000	0.111580000
1	-3.657234000	1.200407000	-1.559119000
1	-3.542608000	2.184943000	-0.120832000
1	-5.732845000	1.020958000	-0.185803000
1	-4.936587000	-0.561624000	-0.249562000
1	-4.803192000	0.442752000	1.204901000
6	-2.406112000	-0.816694000	-2.142649000
1	-3.469872000	-1.036956000	-2.030180000
1	-2.304844000	0.002986000	-2.862417000
1	-1.900777000	-1.692859000	-2.544026000
6	4.449656000	0.978644000	-1.087964000
6	5.327577000	0.758939000	0.141393000
1	4.974863000	1.602145000	-1.819339000
1	4.232879000	0.016280000	-1.574263000
1	6.263090000	0.261896000	-0.141628000
1	5.576216000	1.714135000	0.616463000
1	4.819311000	0.128944000	0.879802000
8	1.427206000	-2.457469000	-0.194219000
1	2.317086000	-2.536790000	0.185193000
1	2.646162000	1.061269000	-0.284499000