

Mechanism and Theory of D-Glucopyranose Homogeneous Acid Catalysis in the Aqueous Solution Phase

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Supporting Information

		Bond Lengths (Å)																							
Anomers	Rotamers	C1 – O1		C1 – O6		C2 – O2		C3 – O3		C4 – O4		C5 – O6		C6 – O5		C1 – C2		C2 – C3		C3 – C4		C4 – C5		C5 – C6	
		R1	R2	R1	R2	R1	R2	R1	R2	R1	R2	R1	R2	R1	R2	R1	R2	R1	R2	R1	R2	R1	R2	R1	R2
α-D-glucopyranose	R1/R2	1.40	1.40	1.42	1.42	1.41	1.41	1.42	1.42	1.43	1.42	1.44	1.43	1.41	1.43	1.53	1.53	1.53	1.52	1.53	1.53	1.54	1.54	1.52	1.53
	$R1G_1^+ / R2G_1^+$	1.88	1.85	1.28	1.29	1.41	1.42	1.40	1.40	1.41	1.40	1.50	1.48	1.40	1.42	1.51	1.51	1.52	1.52	1.53	1.53	1.54	1.54	1.52	1.53
	$R1G_2^+ / R2G_2^+$	1.39	1.43	1.41	1.38	1.53	1.52	1.43	1.41	1.41	1.40	1.45	1.45	1.40	1.42	1.53	1.53	1.51	1.51	1.52	1.53	1.55	1.55	1.53	1.53
	$R1G_3^+ / R2G_3^+$	1.40	1.39	1.41	1.42	1.41	1.41	1.54	1.54	1.41	1.41	1.44	1.43	1.40	1.43	1.54	1.56	1.51	1.50	1.50	1.50	1.55	1.54	1.53	1.53
	$R1G_4^+ / R2G_4^+$	1.39	1.39	1.44	1.44	1.40	1.41	1.42	1.40	1.56	1.50	1.43	1.42	1.40	1.46	1.55	1.55	1.53	1.54	1.51	1.51	1.52	1.54	1.53	1.53
	$R1G_5^+ / R2G_5^+$	1.39		1.44		1.42		1.41		1.40		1.44		1.51		1.55		1.54		1.53		1.52		1.53	
	$R1G_6^+ / R2G_6^+$	1.34	1.33	1.57	1.66	1.41	1.41	1.41	1.40	1.40	1.40	1.50	1.50	1.43	1.41	1.54	1.53	1.54	1.54	1.54	1.53	1.52	1.53	1.52	1.53
	R1/R2	1.39	1.39	1.43	1.43	1.41	1.41	1.42	1.42	1.43	1.42	1.43	1.42	1.41	1.43	1.53	1.53	1.53	1.53	1.52	1.52	1.54	1.54	1.53	1.53
	$R1G_1^+ / R2G_1^+$	1.55	1.54	1.35	1.35	1.42	1.42	1.40	1.40	1.41	1.40	1.48	1.47	1.40	1.42	1.51	1.51	1.52	1.52	1.54	1.54	1.55	1.55	1.52	1.53
	$R1G_2^+ / R2G_2^+$	1.38	1.38	1.41	1.41	1.53	1.53	1.42	1.42	1.41	1.40	1.45	1.44	1.40	1.42	1.52	1.52	1.51	1.51	1.53	1.53	1.55	1.55	1.53	1.53

$R1G_3^+ /$ $R2G_3^+$	1.38	1.38	1.42	1.42	1.41	1.40	1.54	1.54	1.41	1.41	1.43	1.42	1.40	1.43	1.54	1.55	1.50	1.50	1.50	1.50	1.56	1.55	1.53	1.53
$R1G_4^+ /$ $R2G_4^+$	1.37	1.37	1.44	1.45	1.40	1.41	1.42	1.40	1.55	1.50	1.42	1.40	1.40	1.46	1.54	1.54	1.52	1.54	1.51	1.51	1.52	1.54	1.53	1.53
$R1G_5^+ /$ $R2G_5^+$	1.37		1.49		1.41		1.41		1.40		1.44		1.50		1.53		1.53		1.53		1.52		1.54	
$R1G_6^+ /$ $R2G_6^+$	1.34	1.32	1.57	1.67	1.41	1.40	1.40	1.40	1.40	1.40	1.49	1.50	1.43	1.41	1.53	1.52	1.54	1.53	1.53	1.53	1.52	1.54	1.52	1.53

Table S1: Selected bond lengths of neutral and protonated species of different anomers of α - and β -D-glucopyranose computed with B3LYP/6-31G(2df,p).

Table S2. Geometries and vibrational frequencies of the all species calculated at B3LYP/6-31G(2df,p).

Species	Geometries				Frequencies		
α-D-Glucopyranose Rotamer -1	6	1.092454	-1.302364	-0.506046	71.0297	108.1206	124.2801
	6	1.578119	0.124001	-0.642167	143.8044	196.1246	231.3157
	6	0.716472	1.087868	0.161106	247.0186	254.1310	276.0820
	6	-0.758946	0.846065	-0.154915	310.5558	321.1682	360.9734
	6	-1.125812	-0.611513	0.172733	377.4188	398.2372	403.8396
	8	-0.163881	-1.573327	-0.416622	414.4430	438.0031	455.0469
	8	1.855235	-1.631905	1.149811	539.6715	555.9795	602.3338
	8	2.940754	0.146374	-0.258700	637.1669	772.9618	840.2455
	8	1.157454	2.371838	-0.194884	914.0291	1004.2851	1027.4387
	8	-1.472886	1.735870	0.660831	1041.9462	1053.6912	1084.3321
	6	-2.479294	-1.049250	-0.386183	1090.3536	1100.5107	1118.4223
	8	-3.423841	-0.126499	0.123679	1128.7509	1137.9798	1161.4991
	1	1.648685	-2.068552	-1.044068	1194.0658	1229.3822	1241.3386
	1	1.476898	0.366534	-1.712852	1260.3230	1268.3764	1280.7796
	1	0.863102	0.899813	1.236897	1341.5088	1359.2111	1366.0605
	1	-0.936629	1.037297	-1.226362	1378.3778	1388.9822	1400.9466
	1	-1.083911	-0.761908	1.255222	1417.7871	1425.6099	1445.5640
	1	2.131024	-2.554975	1.254792	1448.2802	1468.1167	1502.6039
	1	3.218968	1.072833	-0.221574	2959.6255	2969.9088	2994.0198
	1	0.591480	3.017879	0.247094	3019.3358	3038.8441	3043.1876
	1	-2.417992	1.564303	0.535113	3075.2854	3792.0949	3794.3476
	1	-2.434114	-1.028453	-1.484851	3806.5503	3815.9541	3838.7634
	1	-2.693858	-2.077947	-0.069463			
	1	-4.302563	-0.348572	-0.200617			
	1	2.658271	-1.065898	1.050585			
α-D-Glucopyranose Rotamer -2	6	1.126726	-1.461133	-0.185934	64.4698	106.3837	121.2908
	6	1.690058	-0.078923	-0.530870	179.7257	205.7812	235.4104
	6	0.876162	0.989872	0.187976	245.6283	259.1504	281.5695
	6	-0.598671	0.866581	-0.178230	324.9406	334.9366	347.7423
	6	-1.082761	-0.569946	0.092963	374.9947	390.3081	401.3039
	8	-0.242304	-1.524756	-0.557692	426.7691	480.8560	507.1458
	8	1.316427	-1.697128	1.180714	532.7880	546.8755	574.8077
	8	3.056961	-0.021317	-0.193966	634.5365	765.2630	914.0911
	8	1.410699	2.249476	-0.195670	915.7621	986.4724	1012.3920
	8	-1.291234	1.832441	0.593055	1036.3247	1063.7332	1073.7382
	6	-2.478013	-0.839834	-0.462172	1094.4331	1117.4859	1119.0697
	8	-3.386135	0.070567	0.159148	1137.3330	1145.4871	1161.3576
	1	1.610622	-2.233176	-0.796395	1196.7912	1228.4145	1252.8284
	1	1.548846	0.053724	-1.615974	1263.1927	1269.1315	1284.5716
	1	0.978189	0.845192	1.272466	1317.5633	1335.5682	1361.4027
	1	-0.705158	1.074888	-1.257190	1369.0288	1384.3093	1413.8221
	1	-1.083447	-0.732797	1.178971			
	1	1.073365	-2.611835	1.358713			
	1	3.291490	0.914476	-0.204438			

	1	0.855130	2.920244	0.217456	1418.4521	1429.0219	1453.0106
	1	-2.234256	1.633977	0.508652	1468.4408	1470.9363	1522.4333
	1	-2.457973	-0.702947	-1.552566	2951.0302	2972.3879	2999.4028
	1	-2.755910	-1.881689	-0.254069	3019.7231	3026.1298	3039.0111
	1	-4.237226	0.005981	-0.282739	3047.0954	3735.3707	3792.9275
					3807.4014	3816.2283	3842.2062
β-D-Glucopyranose Rotamer – 1	6	0.550582	-1.467170	0.248984	67.3707	103.7669	120.6940
	6	1.582108	-0.440344	-0.219592	143.0036	180.0647	238.2044
	6	1.140348	0.958521	0.204046	250.5590	265.1890	284.2409
	6	-0.279557	1.267035	-0.255175	287.2168	318.7466	336.1516
	6	-1.214354	0.160389	0.253025	391.9082	392.4418	417.0739
	8	-0.746098	-1.099339	-0.224107	423.6292	432.7533	451.7068
	8	0.873279	-2.697029	-0.294532	499.7147	550.1213	600.4219
	8	2.833645	-0.758170	0.349071	632.5269	644.0707	891.5030
	8	2.084723	1.873307	-0.325746	1001.5601	1011.5478	1025.1079
	8	-0.600379	2.549692	0.280322	1046.5320	1073.8826	1085.5877
	6	-2.650448	0.283356	-0.244060	1101.1727	1106.0317	1120.2406
	8	-3.449529	-0.785730	0.211326	1124.5515	1137.0228	1176.1850
	1	0.533560	-1.494183	1.353879	1196.2998	1231.4463	1242.3471
	1	1.616026	-0.490162	-1.319320	1255.7574	1261.8152	1303.5505
	1	1.150937	1.001384	1.306528	1329.3607	1347.1138	1365.3931
	1	-0.302462	1.284433	-1.354489	1373.1174	1384.7066	1400.8427
	1	-1.217401	0.172547	1.355468	1410.7132	1424.4501	1440.4358
	1	0.307559	-3.364338	0.107813	1444.1840	1491.8030	1502.9262
	1	3.400840	0.005868	0.190493	2938.8624	2959.8285	2963.9719
	1	1.774043	2.754213	-0.086065	2980.0256	2992.6586	3012.3792
	1	-1.307003	2.937784	-0.243352	3076.8951	3791.0526	3795.6381
	1	-3.095163	1.205216	0.144583	3801.2511	3818.7631	3839.3020
	1	-2.641084	0.341662	-1.345786			
	1	-2.957062	-1.586998	-0.003804			
β-D-Glucopyranose Rotamer – 2	6	1.250487	-1.221244	0.295470	64.8871	100.5649	111.9618
	6	1.688670	0.142494	-0.237385	171.0862	203.1564	242.9860
	6	0.662549	1.191527	0.177544	253.8739	263.5612	274.6913
	6	-0.748469	0.808809	-0.249403	302.5404	326.3040	344.5518
	6	-1.065446	-0.600343	0.284065	386.8928	403.6928	414.9586
	8	-0.073937	-1.519099	-0.146723	424.1222	436.2765	475.3376
	8	2.093570	-2.191511	-0.215895	529.1074	543.2573	589.9430
	8	2.960362	0.455573	0.290052	619.3146	673.0178	913.9679
	8	1.073228	2.427677	-0.384597	1002.7460	1009.9261	1024.5693
	8	-1.607865	1.808174	0.269765	1038.9537	1072.5640	1093.1127
	6	-2.383835	-1.157373	-0.246435	1096.4424	1112.6405	1122.8057
	8	-3.431742	-0.268703	0.142171	1139.8810	1148.8299	1175.2083
	1	1.262574	-1.204455	1.401393	1199.8399	1228.4661	1254.3938
	1	1.716473	0.072145	-1.335986	1260.4059	1268.5206	1301.9023
	1	0.668677	1.259726	1.278646	1308.4398	1333.7504	1349.9072
	1	-0.791359	0.781190	-1.351415	1366.4636	1382.7783	1404.1786
	1	-1.110533	-0.550952	1.385386	1406.6250	1427.2144	1449.9320
	1	1.849796	-3.035614	0.178880	1469.2137	1492.8661	1522.2995
	1	3.093584	1.395438	0.117602	2929.4609	2958.3255	2961.0089
	1	0.388059	3.069449	-0.164101			
	1	-2.511203	1.472107	0.186052			
	1	-2.313400	-1.240939	-1.339846			

	1	-2.543698	-2.163258	0.163833	2975.3788	2997.3516	3003.0594
	1	-4.241635	-0.534943	-0.301759	3046.5302	3733.7474	3792.9284
					3802.6244	3815.0120	3842.1150
$\alpha - R1G_1^+$	6	0.531813	-1.410358	-0.559530	55.4066	91.8139	113.0022
	6	1.540911	-0.286883	-0.628447	123.2111	156.4649	178.3276
	6	1.097776	0.925354	0.181372	219.3329	231.1543	256.4078
	6	-0.354067	1.272039	-0.159307	277.8621	297.7404	306.3953
	6	-1.254127	0.067730	0.155918	350.7277	373.3569	381.1386
	8	-0.728260	-1.170693	-0.494959	411.6717	426.7774	431.7271
	8	1.058870	-2.064039	1.119415	445.9337	521.0071	528.0539
	8	2.791025	-0.805409	-0.220876	589.8436	599.3868	684.9871
	8	2.004217	1.944979	-0.147150	761.1592	802.9931	855.5501
	8	-0.704560	2.360105	0.670116	923.0820	976.4366	1013.7496
	6	-2.697775	0.191270	-0.315296	1054.4581	1079.4166	1097.7881
	8	-3.495065	-0.867410	0.145894	1112.4743	1116.4735	1133.7415
	1	0.766423	-2.320426	-1.110062	1138.3175	1157.6300	1212.2503
	1	1.574226	0.000754	-1.693247	1223.7093	1244.7394	1248.4920
	1	1.140371	0.682204	1.255010	1257.3944	1320.3044	1336.3963
	1	-0.423749	1.534238	-1.224563	1360.7838	1368.1238	1379.1643
	1	-1.237735	-0.146017	1.228143	1405.0556	1416.2074	1420.4261
	1	0.926990	-3.019492	1.210459	1434.2000	1444.0755	1486.3838
	1	3.415860	-0.067959	-0.175349	1524.0762	1588.8939	2979.2005
	1	1.759260	2.736482	0.348617	2992.5198	3007.4125	3020.0044
	1	-1.316145	2.946229	0.213080	3084.7495	3100.3373	3157.3388
	1	-3.097468	1.112028	0.122672	3488.0264	3772.2373	3786.9418
	1	-2.721997	0.300111	-1.409392	3796.3868	3833.9139	3834.5839
	1	-3.406529	-1.615169	-0.452959			
	1	2.023487	-1.878154	1.059827			
$\alpha - R1G_2^+$	6	0.415309	-1.633589	-0.167628	69.2336	103.3410	127.2970
	6	1.409813	-0.544137	-0.566625	143.1704	193.2183	216.7476
	6	1.139114	0.743881	0.180394	226.8952	251.8648	273.7598
	6	-0.247321	1.262691	-0.182054	308.2160	340.4241	357.7377
	6	-1.245037	0.121254	0.125699	367.3265	388.9043	410.0829
	8	-0.829945	-1.095192	-0.546609	419.1869	450.5531	490.7715
	8	0.579352	-1.872915	1.187746	529.7727	568.5764	591.0511
	8	2.865233	-0.801496	-0.164589	612.7970	752.8760	814.3441
	8	2.247176	1.572771	-0.183042	823.9800	901.2933	966.1480
	8	-0.442362	2.397340	0.632257	989.5774	1016.2493	1032.6632
	6	-2.663898	0.400652	-0.362047	1065.1475	1076.5070	1094.3856
	8	-3.561705	-0.601881	0.037658	1103.2675	1110.4323	1126.7799
	1	0.528192	-2.539836	-0.774885	1146.8607	1187.2692	1204.5787
	1	1.426620	-0.401530	-1.647683	1222.9234	1243.8955	1261.1960
	1	1.157023	0.550732	1.259847	1276.9561	1335.9888	1346.8275
	1	-0.278451	1.514305	-1.252612	1354.7819	1369.4629	1386.3556
	1	-1.265397	-0.049201	1.207465	1392.5459	1407.0106	1420.6176
	1	0.028909	-2.619004	1.456215	1430.2283	1444.4356	1453.4778
	1	3.193834	0.158443	-0.109716	1491.6515	1595.1163	2987.3635
	1	2.245170	2.370545	0.361915	2997.5204	3006.4822	3047.4749
	1	-1.111740	2.971453	0.246317	3055.5102	3068.2210	3084.4760
	1	-3.010861	1.332818	0.095793			
	1	-2.649746	0.540611	-1.454455			
	1	-3.350940	-1.403373	-0.452901			

	1	3.377521	-1.319491	-0.809097	3131.4544 3802.2270	3723.5026 3820.8532	3796.5522 3833.6942
$\alpha - R1G_3^+$	6	0.400671	-1.627962	-0.264565	66.1735	90.1350	104.7891
	6	1.495598	-0.589128	-0.579351	132.3184	155.6538	192.8849
	6	1.112922	0.668444	0.169328	232.7324	244.4158	293.5393
	6	-0.220410	1.248446	-0.195715	315.8813	348.6065	366.5733
	6	-1.233234	0.118512	0.137438	377.7464	388.1192	410.0862
	8	-0.859058	-1.079234	-0.562781	425.4858	441.4686	530.4896
	8	0.592115	-1.950137	1.086555	533.9907	559.4026	581.0317
	8	2.810684	-0.943069	-0.200715	634.0034	719.1058	828.7492
	8	2.231742	1.662525	-0.183611	837.8496	846.9253	903.0199
	8	-0.346709	2.413068	0.596699	989.9454	1021.4192	1044.2305
	6	-2.659555	0.442068	-0.306699	1066.0946	1080.8941	1087.8725
	8	-3.561533	-0.549033	0.103977	1101.2272	1108.9923	1116.3271
	1	0.495534	-2.503464	-0.914441	1147.0037	1159.7355	1216.9227
	1	1.503160	-0.401812	-1.656976	1223.0296	1245.3550	1266.9056
	1	1.198249	0.539369	1.250030	1282.9918	1313.9407	1343.8379
	1	-0.263527	1.473259	-1.270849	1358.6337	1373.8460	1378.4374
	1	-1.227002	-0.058564	1.219397	1395.0416	1406.4266	1420.6429
	1	0.093220	-2.743963	1.313620	1428.0974	1431.9547	1448.1491
	1	2.746923	-1.504849	0.587018	1491.3374	1553.3620	2988.1082
	1	2.167393	2.471024	0.359445	3019.4416	3055.6236	3076.2778
	1	-1.089549	2.946852	0.294260	3077.7897	3089.2053	3120.4704
	1	-2.979411	1.373581	0.172799	3487.3879	3688.3803	3734.8216
	1	-2.668406	0.595604	-1.397290	3807.8616	3816.8554	3824.3758
	1	-3.366728	-1.352443	-0.390848			
	1	3.076267	1.170165	-0.049774			
$\alpha - R1G_4^+$	6	0.460147	-1.640499	-0.190260	72.9956	91.4777	126.6401
	6	1.570890	-0.621610	-0.560868	140.5748	195.9359	210.2039
	6	1.216098	0.679211	0.157495	232.5310	240.7552	254.1142
	6	-0.175091	1.104126	-0.245083	293.9087	343.3343	362.3180
	6	-1.231180	0.074549	0.124105	372.2969	390.2924	401.2752
	8	-0.810210	-1.093260	-0.581739	419.9451	430.2319	438.2735
	8	0.539099	-1.883873	1.171519	492.3507	542.2788	599.9634
	8	2.855784	-0.958860	-0.111837	639.9539	743.5577	774.3477
	8	2.021229	1.808606	-0.156545	835.8324	911.5842	930.2084
	8	-0.333852	2.490666	0.441559	993.6882	999.2415	1033.4823
	6	-2.650795	0.396913	-0.346354	1052.4123	1059.9683	1091.2988
	8	-3.552861	-0.580937	0.089889	1106.8801	1125.9438	1137.2634
	1	0.544909	-2.552106	-0.791403	1167.8348	1187.7734	1209.9402
	1	1.535889	-0.464534	-1.647681	1218.3895	1234.9614	1242.5278
	1	1.253389	0.471491	1.236383	1306.9878	1335.4106	1342.2402
	1	-0.231134	1.397632	-1.294190	1344.4378	1361.6135	1375.0277
	1	-1.233781	-0.113418	1.206493	1396.1366	1408.2641	1425.0118
	1	0.049001	-2.684255	1.392428	1431.5110	1435.7527	1458.2401
	1	3.252453	-1.614861	-0.695031	1489.4245	1627.2919	2998.3846
	1	2.935206	1.637550	0.106038	3015.9967	3027.1662	3030.4035
	1	-0.615469	2.418797	1.372488	3065.1369	3067.8375	3133.4192
	1	-2.976572	1.347844	0.091762	3193.8409	3689.3258	3793.8933
	1	-2.644774	0.516714	-1.440289			
	1	-3.378435	-1.392224	-0.400166			
	1	0.615379	2.816493	0.406188			

					3810.8731	3815.0696	3823.6780
$\alpha - R1G_5^+$	6	0.355040	-1.587972	-0.259733	76.4709	97.8849	119.8229
	6	1.512415	-0.598758	-0.538622	152.7217	187.5319	223.2144
	6	1.284961	0.763028	0.140577	237.2896	268.8789	317.7575
	6	-0.105037	1.321954	-0.169403	324.5322	359.2117	377.6405
	6	-1.125924	0.272189	0.239614	389.3201	406.8414	425.4716
	8	-0.904223	-0.934241	-0.518240	452.3040	481.5943	499.4668
	8	0.353886	-2.023574	1.055542	545.3868	573.3128	592.1843
	8	2.704116	-1.124271	0.029529	661.9914	787.4919	829.4097
	8	2.204367	1.731258	-0.304572	839.7230	910.7084	958.9917
	8	-0.400969	2.481735	0.564203	992.9560	1018.0004	1052.4694
	6	-2.573014	0.618658	-0.107042	1060.6684	1077.0976	1098.3063
	8	-3.233435	-0.732598	-0.253947	1120.7440	1129.3311	1151.3923
	1	0.353734	-2.423824	-0.971023	1165.0619	1181.8752	1216.7173
	1	1.609338	-0.443113	-1.619328	1239.7800	1251.6467	1265.1747
	1	1.358162	0.619193	1.229347	1316.4333	1331.7165	1340.7396
	1	-0.180663	1.495717	-1.255746	1349.8232	1356.9344	1377.3294
	1	-1.030503	0.051739	1.308337	1382.9053	1400.3160	1408.0070
	1	1.276111	-2.021217	1.356079	1439.8581	1445.7925	1460.1477
	1	3.147985	-1.702648	-0.600970	1487.5025	1576.6561	2525.5190
	1	3.085581	1.481431	-0.003349	2975.1238	3000.4393	3034.5329
	1	0.338388	3.093870	0.454606	3056.8310	3068.9633	3128.8916
	1	-3.103254	1.180681	0.657611	3210.5651	3723.6896	3724.5847
	1	-2.691234	1.073252	-1.089659	3786.3498	3811.4169	3813.7335
	1	-2.368205	-1.297078	-0.438077			
	1	-3.676023	-1.029072	0.559715			
$\alpha - R1G_6^+$	6	0.512505	-1.644061	-0.144330	81.8388	104.2653	137.8333
	6	1.536734	-0.562320	-0.530019	142.2852	186.6179	202.2516
	6	1.240554	0.773111	0.181027	222.5302	252.6668	267.0833
	6	-0.158494	1.305332	-0.158179	322.0835	326.7026	346.9228
	6	-1.201357	0.261410	0.202461	367.7190	384.0981	401.7847
	8	-0.842146	-0.970349	-0.564839	409.0872	432.5390	461.0394
	8	0.510922	-1.899509	1.174893	530.7532	531.8994	577.5198
	8	2.817287	-0.987472	-0.131133	621.1028	701.1814	728.4965
	8	2.138130	1.768029	-0.242939	801.8008	894.2516	927.5217
	8	-0.487801	2.444292	0.589549	987.5729	1004.2499	1037.9116
	6	-2.643285	0.518214	-0.206004	1053.3656	1072.5545	1099.3394
	8	-3.244683	-0.778441	-0.101374	1115.9854	1135.0353	1155.2950
	1	0.521624	-2.523635	-0.792829	1194.8663	1215.0635	1220.3360
	1	1.470050	-0.404652	-1.613091	1231.5988	1237.1817	1254.4658
	1	1.303672	0.611740	1.266872	1268.7606	1295.0336	1327.9304
	1	-0.198857	1.502749	-1.242307	1341.9267	1349.6961	1359.0956
	1	-1.145566	-0.003648	1.260868	1367.8091	1398.9663	1425.6212
	1	0.210313	-2.794348	1.377588	1440.8302	1444.3751	1470.1732
	1	3.296830	-1.351426	-0.882379	1480.0871	1513.8265	2976.5186
	1	3.023698	1.524579	0.052020	3016.2372	3044.3107	3050.3308
	1	0.244608	3.068810	0.506474	3101.7931	3103.3759	3117.5325
	1	-3.092421	1.240472	0.481398	3291.8805	3787.4118	3794.1079
	1	-2.698826	0.904497	-1.230405	3806.9247	3829.3156	3830.3214
	1	-4.109696	-0.787045	-0.525091			
	1	-1.679033	-1.510609	-0.522107			

$\alpha - R2G_1^+$	6	1.092454	-1.302364	-0.506046	53.2204	95.6527	109.2634
	6	1.578119	0.124001	-0.642167	151.2879	161.9629	204.2229
	6	0.716472	1.087868	0.161106	217.8982	255.6651	272.5135
	6	-0.758946	0.846065	-0.154915	292.9597	329.3084	347.9125
	6	-1.125812	-0.611513	0.172733	391.0323	395.0388	411.2934
	8	-0.163881	-1.573327	-0.416622	426.9458	444.4354	469.6002
	8	1.855235	-1.631905	1.149811	494.9010	522.8940	542.0574
	8	2.940754	0.146374	-0.258700	551.6480	606.7951	694.4082
	8	1.157454	2.371838	-0.194884	808.4103	879.4632	892.1851
	8	-1.472886	1.735870	0.660831	923.6283	940.7307	1013.7662
	6	-2.479294	-1.049250	-0.386183	1061.1844	1093.9058	1111.6837
	8	-3.423841	-0.126499	0.123679	1122.4993	1132.9073	1141.0142
	1	1.648685	-2.068552	-1.044068	1149.3842	1165.1623	1219.5959
	1	1.476898	0.366534	-1.712852	1238.8597	1251.3084	1256.5091
	1	0.863102	0.899813	1.236897	1266.9998	1294.0384	1327.4247
	1	-0.936629	1.037297	-1.226362	1342.7253	1362.2715	1372.5353
	1	-1.083911	-0.761908	1.255222	1399.3177	1414.4316	1428.0461
	1	2.131024	-2.554975	1.254792	1452.4129	1474.5702	1514.1487
	1	3.218968	1.072833	-0.221574	1526.5989	1592.7404	2972.2512
	1	0.591480	3.017879	0.247094	2984.3006	3000.0782	3001.7803
	1	-2.417992	1.564303	0.535113	3051.0547	3094.0177	3158.6016
	1	-2.434114	-1.028453	-1.484851	3430.8767	3732.5113	3766.5705
	1	-2.693858	-2.077947	-0.069463	3781.1546	3791.9083	3833.1776
	1	-4.302563	-0.348572	-0.200617			
	1	2.658271	-1.065898	1.050585			
$\alpha - R2G_2^+$	6	1.103371	-1.449759	-0.305538	63.1600	105.4724	116.2674
	6	1.563923	-0.024767	-0.624779	157.5092	195.6211	206.5585
	6	0.758451	1.008410	0.122227	240.1341	264.0920	276.2454
	6	-0.714716	0.857854	-0.243242	332.5993	351.3385	375.4745
	6	-1.126663	-0.581829	0.142503	412.1399	422.1402	427.0883
	8	-0.261006	-1.557270	-0.483911	471.6683	505.8848	541.1291
	8	1.573797	-1.640641	1.027815	543.6491	564.2697	575.1480
	8	2.984239	0.097830	-0.097584	610.0296	773.4975	843.7419
	8	1.370388	2.240514	-0.194598	884.8313	912.5229	967.6518
	8	-1.380040	1.838745	0.504303	977.7434	1017.0648	1034.1147
	6	-2.532166	-0.941517	-0.335984	1060.3377	1085.3809	1107.5157
	8	-3.406371	0.032602	0.215603	1117.4737	1143.4026	1151.2306
	1	1.549935	-2.188553	-0.978334	1165.2255	1171.2178	1189.1983
	1	1.648323	0.180802	-1.690167	1230.6659	1253.1341	1267.5103
	1	0.828946	0.813253	1.203797	1277.0156	1312.2738	1326.4864
	1	-0.851307	0.998736	-1.328904	1346.6389	1366.2316	1378.1877
	1	-1.069914	-0.678062	1.233405	1406.2843	1412.7668	1416.2956
	1	1.560338	-2.577091	1.261896	1431.0798	1456.1134	1475.9302
	1	3.112900	1.051012	0.120881	1526.2100	1569.2151	2968.7779
	1	0.858390	2.952051	0.212936	2994.9876	3009.2745	3046.2796
	1	-2.329368	1.641565	0.462062	3064.0522	3078.1578	3162.1019
	1	-2.548360	-0.931640	-1.434759	3300.9022	3506.6229	3696.1340
	1	-2.784030	-1.954198	0.002472	3784.9380	3803.4432	3836.4252
	1	-4.305360	-0.132570	-0.085222			
	1	2.968249	-0.479883	0.715789			

$\alpha - R2G_3^+$	6	1.124761	-1.511925	-0.196622	68.2074	92.7489	124.4504
	6	1.699154	-0.106180	-0.568620	137.4848	180.5289	215.8727
	6	0.815301	0.855378	0.169938	229.2213	261.0189	266.9308
	6	-0.637461	0.775949	-0.206659	278.6360	320.4080	339.4317
	6	-1.103436	-0.659247	0.120445	365.6226	392.7277	422.7835
	8	-0.245226	-1.573676	-0.558950	427.5788	470.3278	495.7781
	8	1.347154	-1.688841	1.163834	542.6193	551.8675	566.8661
	8	3.007365	0.159915	-0.129838	632.3523	714.1989	829.4963
	8	1.190865	2.308861	-0.171312	855.4895	912.7467	921.0178
	8	-1.240844	1.823995	0.524716	978.3193	1005.6011	1043.3701
	6	-2.519918	-0.911351	-0.388334	1066.9976	1073.6910	1083.8028
	8	-3.322541	0.142893	0.136628	1107.6612	1124.6305	1137.6089
	1	1.601972	-2.286900	-0.807468	1161.7650	1178.6151	1215.5567
	1	1.587474	0.019848	-1.653551	1237.5291	1240.7458	1252.8947
	1	0.963149	0.783276	1.248044	1292.3941	1319.7901	1337.0730
	1	-0.749242	0.931366	-1.291117	1342.4434	1352.4401	1362.3402
	1	-1.061281	-0.807227	1.205975	1374.2179	1412.7822	1419.7432
	1	1.189341	-2.610519	1.400001	1431.0190	1467.0206	1472.2226
	1	3.641480	-0.391214	-0.601678	1525.7533	1558.5680	2993.2593
	1	0.433372	2.839072	0.183934	3016.5039	3032.7736	3051.1319
	1	-2.204081	1.702368	0.465045	3055.1423	3074.5174	3135.0365
	1	-2.513138	-0.908779	-1.486759	3425.7720	3664.2241	3704.2203
	1	-2.864722	-1.893858	-0.046223	3807.9748	3820.3550	3838.1589
	1	-4.237444	0.020342	-0.134855			
	1	2.048530	2.561306	0.217145			
$\alpha - R2G_4^+$	6	1.229164	-1.443437	-0.213797	59.5103	104.3175	124.3847
	6	1.743240	-0.011454	-0.490645	201.1624	207.1637	240.1962
	6	0.818549	1.018657	0.188209	249.3407	263.1782	318.6066
	6	-0.579067	0.763075	-0.322727	334.0062	353.9027	372.5819
	6	-1.004906	-0.672902	0.013448	392.2912	403.4295	426.4475
	8	-0.136393	-1.543452	-0.671678	441.4611	460.1658	496.8227
	8	1.342424	-1.695493	1.143834	513.4706	525.3808	568.9268
	8	3.022919	0.247752	0.030214	631.3018	753.0125	860.0312
	8	1.160226	2.345873	-0.109811	909.0213	917.3780	958.5119
	8	-1.562900	1.722671	0.286005	982.6373	998.4788	1017.6244
	6	-2.441231	-0.965127	-0.408288	1040.0323	1085.1286	1107.3148
	8	-3.241873	-0.000447	0.338652	1133.2819	1145.6564	1159.2462
	1	1.758656	-2.179524	-0.827274	1174.4004	1202.6358	1218.0364
	1	1.704254	0.152212	-1.576535	1227.0554	1243.8205	1272.5102
	1	0.858001	0.827149	1.273479	1297.0979	1332.7646	1342.4675
	1	-0.653307	0.971427	-1.391788	1348.7383	1357.7602	1371.6154
	1	-0.927111	-0.819513	1.099950	1396.2363	1412.1267	1426.2288
	1	1.309130	-2.645340	1.304247	1437.4478	1453.6946	1460.9962
	1	3.698971	-0.093437	-0.564511	1505.5386	1545.4615	2140.3694
	1	2.105901	2.443196	0.066170	2978.6098	3019.8622	3021.2842
	1	-2.457759	1.146222	0.442100	3065.1790	3069.5381	3117.1992
	1	-2.580249	-0.824237	-1.484681	3134.5949	3738.5117	3776.9676
	1	-2.734378	-1.978357	-0.126518	3807.4993	3813.2140	3826.5148
	1	-4.149054	0.034648	0.010751			
	1	-1.202768	2.217440	1.039679			

$\alpha - R2G_6^+$	6	1.416777	-1.413746	-0.240137	45.9283	58.6138	103.1126
	6	1.721479	0.048941	-0.557944	136.9912	155.1865	214.8521
	6	0.771192	1.023297	0.150788	224.2089	262.2177	266.2339
	6	-0.701986	0.833608	-0.213936	291.2912	314.0474	335.6749
	6	-1.175069	-0.569985	0.182308	390.4445	409.8614	425.8480
	8	-0.224728	-1.534533	-0.453166	432.1014	464.5717	489.1892
	8	1.726267	-1.837499	0.976296	500.7835	509.3803	522.0898
	8	3.033252	0.223249	-0.077958	579.2801	659.3549	698.7654
	8	1.236880	2.294615	-0.218657	752.1480	873.4800	915.8924
	8	-1.389048	1.804953	0.530418	925.1953	1014.2157	1044.8336
	6	-2.560270	-0.943350	-0.355485	1087.1325	1097.0304	1108.2119
	8	-3.449019	0.011476	0.184332	1131.5256	1136.5916	1147.6156
	1	1.669631	-2.142515	-1.010317	1207.4732	1212.0171	1239.9490
	1	1.650520	0.201680	-1.643237	1245.7156	1257.6304	1262.8860
	1	0.856911	0.878525	1.242303	1271.1306	1325.6456	1339.9251
	1	-0.832666	0.970551	-1.299466	1350.4820	1355.0506	1369.8257
	1	-1.116785	-0.698061	1.266627	1389.5690	1419.9899	1422.8334
	1	2.095704	-1.106722	1.500212	1432.6689	1449.2552	1474.1118
	1	3.224138	1.171547	-0.114184	1477.2631	1524.9445	2951.1355
	1	0.658211	2.956541	0.181671	2980.3150	2988.7375	3030.9592
	1	-2.340262	1.689224	0.392065	3032.5302	3098.9524	3138.5234
	1	-2.534951	-0.917125	-1.454236	3700.1486	3703.8491	3741.4438
	1	-2.822956	-1.965402	-0.039636	3763.4063	3789.7661	3823.1964
	1	-4.343619	-0.162187	-0.128461			
	1	-0.465448	-2.446736	-0.217025			
$\beta - R1G_1^+$	6	-0.643349	-1.245079	-0.315138	68.3267	99.5643	110.7755
	6	-1.562348	-0.178871	0.235187	137.6641	169.3397	208.8520
	6	-1.013675	1.161429	-0.232784	211.9473	244.0176	279.6500
	6	0.458565	1.262942	0.219968	293.4147	300.6859	318.7974
	6	1.282430	0.036311	-0.236986	373.5813	380.3982	396.6982
	8	0.606160	-1.210265	0.183656	408.9133	429.8685	450.0936
	8	-1.331277	-2.531105	0.204068	466.8006	536.0080	578.2011
	8	-2.846946	-0.554816	-0.237538	603.3684	624.9271	795.0719
	8	-1.827024	2.150089	0.338234	846.0099	880.3196	978.8278
	8	0.958228	2.443080	-0.375468	998.1545	1012.2135	1022.8957
	6	2.685954	-0.031117	0.353379	1069.2588	1090.1028	1102.2075
	8	3.441135	-1.081650	-0.190930	1107.1215	1115.4681	1140.4159
	1	-0.702257	-1.334676	-1.409760	1153.7138	1210.4582	1216.1859
	1	-1.523914	-0.211686	1.333280	1230.7495	1239.9037	1253.7311
	1	-1.037029	1.206854	-1.334010	1267.2601	1333.4352	1338.0283
	1	0.472065	1.325105	1.317242	1352.4195	1363.1239	1378.6272
	1	1.353663	0.026031	-1.332296	1395.4597	1410.0324	1414.4798
	1	-1.111924	-3.333505	-0.303026	1428.9790	1444.9856	1466.0260
	1	-3.508735	0.078396	0.069589	1488.4314	1596.4935	2981.6565
	1	-1.494488	3.010787	0.054260	3003.7447	3014.4292	3019.5674
	1	1.611962	2.854304	0.198719	3032.1742	3046.7843	3090.5054
	1	3.197250	0.899862	0.088372	3260.8103	3707.8224	3796.2779
	1	2.615833	-0.082614	1.449954	3797.3042	3832.6211	3834.5544
	1	3.178457	-1.903810	0.234268			
	1	-2.298550	-2.291400	0.115477			
$\beta - R1G_2^+$	6	-0.517865	-1.466616	-0.305589	69.1654	102.3246	123.3656

	6	-1.441426	-0.396404	0.244428	145.8056	166.8627	186.3486
	6	-1.059660	0.986521	-0.209567	214.6970	262.9101	276.8874
	6	0.364995	1.289224	0.260678	294.7004	311.4302	346.9804
	6	1.274074	0.130780	-0.221435	356.5904	381.9321	407.0286
	8	0.736690	-1.127659	0.241719	426.2976	444.2407	457.5344
	8	-0.970455	-2.672200	0.188494	488.3077	537.6564	578.3734
	8	-2.877391	-0.533930	-0.270925	618.7407	633.1503	801.9761
	8	-2.089926	1.816131	0.308358	872.3547	879.6179	972.6328
	8	0.687433	2.528212	-0.330434	1013.9073	1046.3788	1052.8259
	6	2.701280	0.211931	0.313837	1057.7015	1074.1861	1101.0403
	8	3.521510	-0.787722	-0.231282	1108.1990	1110.8277	1124.1075
	1	-0.478722	-1.442511	-1.407937	1154.0839	1187.2486	1221.4535
	1	-1.512881	-0.486581	1.329565	1229.6195	1243.9973	1258.3237
	1	-1.055796	1.030207	-1.309388	1281.3006	1323.1533	1336.2565
	1	0.381132	1.339447	1.358938	1347.8808	1358.8815	1373.3726
	1	1.308637	0.135654	-1.320692	1385.9248	1409.4648	1422.2153
	1	-0.466103	-3.400074	-0.195435	1432.7557	1445.6552	1474.4214
	1	-3.271093	0.361864	-0.086569	1491.9596	1566.6850	2972.5703
	1	-1.955170	2.721957	0.001080	2989.3715	3002.4387	3010.7780
	1	1.378501	2.967466	0.175659	3025.7624	3085.8502	3129.1089
	1	3.131758	1.171832	0.010946	3337.6224	3704.3593	3796.2957
	1	2.673905	0.180286	1.414291	3803.8132	3821.8496	3833.5256
	1	3.241300	-1.635011	0.130579			
	1	-3.366732	-1.259801	0.157409			
$\beta - R1G_3^+$	6	-0.457047	-1.517460	-0.275958	54.2695	78.9777	101.9421
	6	-1.518232	-0.514398	0.220752	134.7193	148.8310	185.2864
	6	-1.066975	0.845948	-0.224843	218.4104	267.7761	278.4862
	6	0.286724	1.265889	0.268481	313.2252	329.0132	352.8664
	6	1.257518	0.156630	-0.230578	368.8408	383.9939	405.3680
	8	0.797906	-1.106930	0.247283	408.8850	415.5938	434.3773
	8	-0.817118	-2.736572	0.250173	494.0085	529.1758	590.3663
	8	-2.813835	-0.657803	-0.323659	607.9772	633.8178	780.6557
	8	-2.132615	1.817077	0.322290	841.8585	889.0347	966.0421
	8	0.490853	2.548245	-0.292462	1021.2808	1028.9570	1052.3958
	6	2.683465	0.334998	0.292883	1054.6934	1078.8138	1091.5503
	8	3.550136	-0.621627	-0.251141	1098.3154	1109.2092	1140.1878
	1	-0.417931	-1.524420	-1.379416	1153.2022	1189.0398	1227.1907
	1	-1.523374	-0.586327	1.316967	1229.5594	1244.9230	1262.6508
	1	-1.143589	0.962258	-1.309042	1278.1626	1324.9076	1340.3771
	1	0.304628	1.287023	1.366924	1345.5492	1359.0781	1372.8287
	1	1.281299	0.170262	-1.331128	1381.1439	1406.7237	1426.1345
	1	-0.306166	-3.441957	-0.164128	1438.5915	1450.8491	1466.9550
	1	-3.181286	-1.508861	-0.053360	1491.8701	1552.5199	2960.5408
	1	-1.989533	2.716858	-0.029614	2985.9840	3003.3622	3026.1303
	1	1.250847	2.976754	0.116196	3034.3406	3076.9781	3103.7761
	1	3.061403	1.314245	-0.020317	3529.7202	3683.6028	3800.0318
	1	2.662296	0.309117	1.393838	3809.6745	3815.1043	3825.2512
1	3.294080	-1.484612	0.092745				
1	-3.008008	1.440905	0.076042				
$\beta - R1G_4^+$	6	0.587631	-1.495104	0.243918	71.1144	89.2623	125.8087

	6	1.622968	-0.452437	-0.225277	140.7494	183.5602	215.1281
	6	1.120483	0.915875	0.214499	219.6444	255.7295	285.9824
	6	-0.284826	1.120927	-0.303267	328.2067	352.0256	362.7154
	6	-1.255610	0.077908	0.237657	366.7514	397.6623	405.9226
	8	-0.718572	-1.140508	-0.255289	411.1871	425.2587	437.6454
	8	0.959855	-2.697108	-0.303866	479.6983	546.1928	564.5871
	8	2.877733	-0.617009	0.378566	619.9449	636.1113	769.9592
	8	1.833293	2.044494	-0.274391	889.3418	919.5252	990.0765
	8	-0.591693	2.590864	0.081098	1001.6580	1018.6481	1040.2217
	6	-2.692288	0.189037	-0.279670	1057.2367	1076.5119	1090.4632
	8	-3.509020	-0.777806	0.316936	1110.2133	1130.9825	1143.1681
	1	0.548441	-1.519816	1.346432	1175.4706	1201.8344	1207.8697
	1	1.672941	-0.504640	-1.322844	1227.4298	1244.1342	1247.1658
	1	1.116700	0.926071	1.316915	1300.8499	1323.9266	1330.9519
	1	-0.322491	1.185253	-1.390982	1342.2606	1367.8863	1381.8741
	1	-1.266302	0.087682	1.340739	1393.9647	1407.5740	1425.4489
	1	0.492847	-3.422754	0.126595	1428.7349	1449.2494	1468.4476
	1	3.252653	-1.456925	0.086761	1488.4735	1625.1849	2966.3692
	1	2.747778	2.019953	0.036625	2971.4874	2982.6656	3003.3335
	1	-0.927962	2.687578	0.991105	3019.1706	3067.4301	3140.0947
	1	-3.108331	1.167176	-0.010338	3166.1715	3692.9699	3794.1079
	1	-2.677455	0.121190	-1.377730	3804.6558	3809.5457	3815.0091
	1	-3.261394	-1.641079	-0.032801			
	1	0.329664	2.989655	0.017923			
	6	0.475922	-1.480615	0.317700	73.9564	100.1949	117.8157
	6	1.522233	-0.506820	-0.240492	144.6882	158.9445	223.1886
	6	1.229196	0.935145	0.191358	245.9442	270.9975	296.8930
	6	-0.183629	1.353225	-0.218931	333.4599	351.3608	371.1588
	6	-1.171271	0.350250	0.362734	390.2883	401.7729	417.2121
	8	-0.856585	-0.975649	-0.098782	433.8363	440.5217	477.6409
	8	0.646493	-2.713741	-0.243091	525.5561	547.7915	607.3105
	8	2.795578	-0.824577	0.267820	644.2269	675.7342	824.7170
	8	2.099037	1.855293	-0.418229	874.0528	915.6166	990.3185
	8	-0.552159	2.611657	0.280756	1021.7090	1030.4783	1046.8301
	6	-2.615682	0.543233	-0.119226	1064.9601	1084.8391	1108.3894
	8	-3.156282	-0.852840	-0.024704	1125.6114	1136.1287	1157.5091
	1	0.486328	-1.492124	1.415739	1178.0945	1202.2856	1215.6855
	1	1.486233	-0.573763	-1.337332	1238.0082	1244.1697	1251.4495
	1	1.305763	0.988477	1.290620	1271.3320	1314.7075	1341.5104
	1	-0.244225	1.318065	-1.319483	1351.3258	1355.4691	1366.4662
	1	-1.134336	0.383136	1.459519	1381.5613	1408.3553	1425.6848
	1	0.360672	-3.410880	0.358071	1441.0562	1449.2230	1465.0587
	1	3.119710	-1.621539	-0.166685	1487.4493	1504.3687	2241.9300
	1	3.003587	1.620513	-0.177560	2966.3640	2978.7332	3017.6915
	1	0.164098	3.227724	0.078244	3035.6851	3039.7134	3111.1206
	1	-3.219089	1.176021	0.526264	3204.1422	3749.6660	3785.1265
	1	-2.672520	0.854745	-1.162873	3801.6435	3812.0259	3815.4875
	1	-2.212618	-1.369869	-0.108792			
	1	-3.792878	-1.068149	-0.724754			
$\beta - R1G_5^+$	6	0.632845	-1.502985	0.289443	74.6413	101.2795	134.3121
$\beta - R1G_6^+$	6	0.632845	-1.502985	0.289443			

	6	1.581751	-0.418727	-0.227475	144.0363	167.6432	230.1084
	6	1.144714	0.990347	0.205342	241.8303	266.5740	298.3181
	6	-0.279242	1.333241	-0.252205	326.2302	329.7048	344.6924
	6	-1.247810	0.293091	0.284981	378.0644	382.6695	395.3380
	8	-0.769130	-1.020047	-0.224040	408.5338	432.5593	467.3496
	8	0.871466	-2.696088	-0.281186	481.8758	558.1700	590.5198
	8	2.850245	-0.637663	0.341495	616.0412	634.0672	702.0858
	8	1.973500	1.970749	-0.362591	823.6915	902.0875	986.4698
	8	-0.714332	2.561024	0.264332	1012.0422	1033.6215	1041.9939
	6	-2.692553	0.351201	-0.188125	1047.8387	1073.6072	1104.2131
	8	-3.196325	-0.946104	0.147535	1114.7294	1134.7662	1154.9634
	1	0.537348	-1.516333	1.379623	1183.7068	1218.0018	1225.7100
	1	1.597584	-0.479177	-1.323891	1228.5575	1238.5420	1253.8547
	1	1.174332	1.034911	1.307013	1261.8808	1283.8445	1319.3177
	1	-0.303884	1.318707	-1.353967	1345.6788	1348.8934	1358.2994
	1	-1.211242	0.248434	1.378668	1364.7857	1396.5642	1423.5670
	1	0.635144	-3.431859	0.298473	1440.4589	1443.3569	1469.9464
	1	3.318789	-1.316662	-0.157166	1492.2577	1513.4116	2971.6514
	1	2.873901	1.835190	-0.043101	2987.9871	3036.9954	3043.6942
	1	-0.030038	3.216312	0.074309	3074.0892	3086.6608	3111.6154
	1	-3.216538	1.151635	0.341900	3319.0690	3784.6822	3786.4785
	1	-2.741071	0.534726	-1.267838	3802.9493	3815.1721	3829.4165
	1	-4.045358	-1.101586	-0.280209			
	1	-1.550586	-1.626281	-0.109938			
$\beta - R2G_1^+$	6	1.178510	-1.046901	0.363691	64.8095	91.4192	122.6309
	6	1.564273	0.273998	-0.261561	147.0636	194.3878	214.9213
	6	0.550823	1.300504	0.217454	217.6278	256.5788	290.6226
	6	-0.852791	0.796276	-0.171892	294.1802	340.7519	369.0896
	6	-1.106604	-0.653347	0.314123	373.6049	390.2475	407.2866
	8	0.000135	-1.545691	-0.058349	425.5073	456.1257	463.4643
	8	2.296528	-1.967327	-0.172205	533.2286	536.0315	588.4546
	8	2.915628	0.454130	0.138707	590.8768	618.2056	816.0595
	8	0.879927	2.514956	-0.400935	881.2265	910.1916	965.9960
	8	-1.748246	1.695926	0.426130	996.2167	1005.5242	1027.9597
	6	-2.342370	-1.290478	-0.318769	1086.2395	1095.5425	1104.3022
	8	-3.428691	-0.429041	-0.026783	1121.6458	1130.6745	1148.2941
	1	1.321526	-1.058448	1.454126	1158.7303	1215.9348	1227.8388
	1	1.489584	0.184307	-1.354375	1238.5668	1247.3613	1257.5532
	1	0.594900	1.383362	1.315870	1276.2266	1304.0513	1332.8040
	1	-0.924447	0.815351	-1.272099	1337.9875	1355.1511	1380.3123
	1	-1.199895	-0.648138	1.407992	1391.5804	1395.3862	1422.8322
	1	2.443371	-2.770576	0.358927	1448.1355	1464.8737	1476.0744
	1	3.253691	1.288038	-0.212835	1526.0295	1593.6201	2970.9877
	1	0.202094	3.161737	-0.166390	2984.2013	3005.5641	3018.6052
	1	-2.646949	1.388138	0.235665	3032.7528	3037.5445	3057.9088
	1	-2.172698	-1.387739	-1.400439	3235.3296	3709.0400	3727.2439
	1	-2.490365	-2.294195	0.099762	3792.3948	3796.7178	3835.3141
	1	-4.231505	-0.773179	-0.430828			
	1	3.087399	-1.352600	-0.146169			
$\beta - R2G_2^+$	6	1.156462	-1.296822	0.352412	65.7389	105.1054	127.2480
	6						

	6	1.537591	0.039093	-0.257447	163.8550	183.7258	205.7185
	6	0.628794	1.150736	0.193048	234.2049	267.8861	272.0571
	6	-0.801785	0.832628	-0.237222	302.4565	335.6519	350.2601
	6	-1.138305	-0.593264	0.279155	390.9009	404.8481	424.4232
	8	-0.141511	-1.534754	-0.149594	434.3623	470.4716	475.1736
	8	2.048616	-2.228314	-0.132656	535.5028	543.8780	559.2860
	8	2.909480	0.538390	0.197115	613.6594	667.3698	811.9150
	8	1.219826	2.319000	-0.364376	888.2625	909.3158	982.1902
	8	-1.595341	1.834974	0.334241	1014.1883	1023.9130	1057.5558
	6	-2.463832	-1.112504	-0.274693	1067.0814	1087.6937	1102.0550
	8	-3.451382	-0.147366	0.059859	1108.6401	1126.8384	1149.8874
	1	1.141514	-1.249446	1.454912	1163.2971	1191.8351	1225.8079
	1	1.603260	-0.050280	-1.342904	1231.2260	1254.8094	1268.0766
	1	0.634036	1.215823	1.291389	1281.1341	1307.7069	1325.5821
	1	-0.856456	0.833223	-1.338766	1340.1783	1348.2844	1364.8685
	1	-1.186254	-0.558156	1.377971	1384.4253	1400.3065	1422.7677
	1	1.876100	-3.090975	0.264571	1450.7984	1471.6651	1478.9840
	1	2.853138	1.517113	-0.001683	1525.7003	1567.3677	2968.3356
	1	0.729007	3.098829	-0.074027	2973.3251	3002.6257	3010.2291
	1	-2.520358	1.558388	0.235632	3015.0443	3061.5076	3130.0599
	1	-2.367778	-1.240198	-1.361873	3260.4726	3696.7943	3710.0042
	1	-2.683773	-2.091294	0.168861	3795.8443	3802.9616	3837.2822
	1	-4.301654	-0.416489	-0.301256			
	1	3.648158	0.098819	-0.261066			
	6	1.278949	-1.235708	0.287299	69.6467	96.1326	124.6150
	6	1.681881	0.166704	-0.247736	139.3591	176.8392	212.5612
	6	0.595141	1.087291	0.213289	239.2067	274.2404	278.8512
	6	-0.785675	0.698736	-0.240055	308.9642	336.6911	354.0411
	6	-1.055133	-0.718979	0.317044	389.7975	404.4256	409.8385
	8	-0.028610	-1.575872	-0.156997	424.7304	446.1786	462.9213
	8	2.194757	-2.108782	-0.252786	516.7739	561.0491	588.5392
	8	2.885556	0.648206	0.290872	610.0911	660.6810	790.8256
	8	0.770171	2.500474	-0.371627	858.7630	913.1451	989.4680
	8	-1.605776	1.746219	0.236783	1008.9311	1020.9651	1054.3115
	6	-2.383221	-1.272669	-0.194474	1071.5882	1079.9575	1095.5274
	8	-3.368355	-0.283713	0.092913	1107.9431	1122.3017	1153.4523
	1	1.301571	-1.228099	1.391807	1172.7187	1187.0860	1232.5288
	1	1.705218	0.096697	-1.344003	1237.4259	1245.7066	1254.8601
	1	0.630835	1.245593	1.293910	1290.1927	1306.7263	1331.4691
	1	-0.813892	0.635854	-1.338448	1339.3919	1351.1573	1369.0320
	1	-1.070167	-0.673697	1.417321	1379.4688	1403.3547	1427.4562
	1	2.126028	-2.969217	0.177745	1453.6078	1463.9026	1472.7766
	1	3.592100	0.032093	0.059564	1525.2993	1566.7512	2951.9488
	1	-0.103125	2.936193	-0.192970	2990.9605	3006.0174	3021.1184
	1	-2.530531	1.456688	0.145186	3030.7608	3075.4084	3106.1011
	1	-2.296644	-1.460549	-1.273010	3398.6274	3653.3052	3704.2821
	1	-2.602573	-2.222034	0.306954	3797.7210	3808.2668	3837.2095
	1	-4.232332	-0.592993	-0.196691			
	1	1.519922	2.978963	0.027170			
$\beta - R2G_3^+$	6	1.359498	-1.181571	0.266078	68.9263	106.6585	118.3815

	6	1.693738	0.250441	-0.190153	198.4703	202.5771	235.7680
	6	0.567976	1.219725	0.194852	266.6805	289.2162	321.4582
	6	-0.715446	0.657017	-0.368928	356.5085	363.1840	375.3074
	6	-0.967584	-0.735575	0.232624	398.0631	403.2758	416.8157
	8	0.054900	-1.574341	-0.227294	433.4467	443.4044	458.9867
	8	2.304429	-2.008949	-0.285998	492.0781	543.9998	580.2463
	8	2.848518	0.749563	0.436137	610.5671	653.2063	878.3567
	8	0.734328	2.518241	-0.309438	904.0338	965.6893	983.9550
	8	-1.873318	1.552283	-0.062882	996.4445	1018.8228	1035.3746
	6	-2.322823	-1.306979	-0.174781	1038.0298	1102.3695	1123.8537
	8	-3.291511	-0.340254	0.334898	1137.4872	1142.5355	1156.2730
	1	1.336680	-1.231477	1.368011	1193.5067	1203.5735	1226.5209
	1	1.794374	0.231115	-1.285544	1234.5497	1249.4196	1269.7264
	1	0.504926	1.232689	1.298268	1291.5480	1316.4635	1325.3644
	1	-0.691072	0.620676	-1.459365	1346.9373	1361.6144	1373.4947
	1	-0.957368	-0.649379	1.333334	1384.0560	1414.8135	1426.0727
	1	2.279659	-2.875575	0.136036	1433.5131	1456.9856	1470.8613
	1	3.609444	0.243094	0.128079	1501.6565	1539.3017	2125.1284
	1	1.626390	2.811642	-0.080454	2944.5312	2962.1639	2970.2549
	1	-2.690422	0.900111	0.204579	3013.5817	3067.5466	3121.3384
	1	-2.407570	-1.397383	-1.261999	3137.3205	3733.8974	3781.8995
	1	-2.496805	-2.277601	0.293535	3804.4177	3808.4816	3810.3449
	1	-4.174583	-0.506586	-0.018347			
	1	-1.644590	2.307968	0.502336			
$\beta - R2G_6^+$	6	1.510976	-1.166609	0.355843	54.9825	84.0824	104.8784
	6	1.693590	0.200148	-0.275616	139.3031	176.3781	235.1109
	6	0.624742	1.185635	0.204721	243.6186	255.3620	268.2785
	6	-0.796868	0.792006	-0.211351	275.2301	314.5495	365.0068
	6	-1.169487	-0.587981	0.352364	374.0245	403.6858	407.2046
	8	-0.083384	-1.572829	0.054434	420.5114	450.0273	474.1236
	8	2.205626	-2.119960	-0.244001	505.2068	524.0266	572.1978
	8	2.973961	0.594587	0.133075	585.5468	603.9657	623.9216
	8	0.995519	2.418786	-0.355726	701.9414	913.1813	934.4517
	8	-1.628316	1.781124	0.336823	1009.9217	1023.0454	1027.9753
	6	-2.453238	-1.200000	-0.217720	1099.4929	1103.0150	1112.6251
	8	-3.460168	-0.228895	-0.044428	1127.2429	1132.4691	1151.0113
	1	1.487752	-1.178405	1.446491	1170.3285	1206.2538	1235.4588
	1	1.630641	0.089205	-1.371596	1253.1124	1259.5616	1264.6449
	1	0.652514	1.230189	1.306976	1276.8605	1287.2238	1318.6634
	1	-0.854681	0.768339	-1.312978	1331.4223	1345.8343	1369.0735
	1	-1.203021	-0.551008	1.443135	1383.5230	1396.4307	1406.0268
	1	2.368983	-2.879934	0.332656	1424.8573	1447.2438	1475.6235
	1	3.028025	1.552321	0.003617	1520.9163	1524.5917	2950.0765
	1	0.352196	3.083084	-0.077588	2962.2166	2967.2430	2983.3103
	1	-2.546155	1.573439	0.112178	3043.9233	3118.6734	3134.2428
	1	-2.296389	-1.431498	-1.286456	3677.6362	3755.5687	3760.2434
	1	-2.681714	-2.137081	0.306165	3767.3922	3795.4065	3826.9979
	1	-4.312486	-0.586318	-0.315613			
	1	-0.109861	-1.854034	-0.877855			
II	6	2.032112	-0.419678	0.333616	43.7786	79.2870	93.4185
	6	1.282262	0.706079	-0.410236	162.8570	214.5128	245.6052
	6	-1.109042	1.253730	0.343775			

	6	-0.202609	0.254382	-0.366567	275.2584	307.0592	318.6211
	6	-0.126570	-1.134486	0.331549	335.3604	356.3113	382.6329
	8	1.198487	-1.572978	0.163330	384.9423	400.7777	432.3249
	8	3.262102	-0.609880	-0.243880	443.1946	458.7202	498.3604
	8	1.420486	1.986613	0.185915	532.3677	563.2703	614.2279
	8	-1.203718	2.477929	-0.266434	647.2219	718.3962	843.2672
	8	-2.524797	0.748308	0.257636	872.6919	950.4289	970.9942
	6	-1.065514	-2.176830	-0.257215	994.2960	1019.2458	1027.6777
	8	-2.411819	-1.672289	-0.035658	1075.1367	1087.1216	1111.1446
	1	2.098187	-0.180465	1.409222	1123.4888	1144.6683	1179.1776
	1	1.645688	0.712382	-1.442978	1187.5399	1210.3533	1231.3577
	1	-0.925903	1.312661	1.422034	1242.1632	1247.3931	1266.7147
	1	-0.575439	0.150809	-1.390748	1283.2196	1309.6176	1323.4824
	1	-0.365899	-1.019986	1.404231	1336.2318	1344.9082	1373.2077
	1	3.799712	-1.193510	0.303894	1385.9996	1400.8803	1421.5619
	1	2.321757	2.302998	0.053825	1433.3194	1453.6961	1478.4129
	1	-0.307500	2.858559	-0.263768	1516.5171	1714.5158	1923.8099
	1	-2.574985	-0.317923	0.058462	2944.9904	2963.1863	3052.9898
	1	-0.880639	-2.306678	-1.327770	3064.8310	3065.8356	3075.0684
	1	-0.959065	-3.134357	0.256974	3133.0807	3664.6850	3697.4504
	1	-3.080664	-2.248579	-0.422995	3810.8640	3811.6392	3822.5761
	1	-2.985020	1.303284	-0.397186			
I2	6	-0.778992	-1.749822	0.221963	50.0973	89.6377	108.1299
	6	0.397566	-1.158435	-0.561215	130.5907	169.4820	201.9212
	6	1.500389	1.112540	-0.143968	234.1217	268.5708	279.2234
	6	0.197674	0.367074	-0.476114	305.9446	336.2807	351.8656
	6	-0.905894	0.533469	0.609680	391.7823	404.5750	429.7153
	8	-1.076575	-0.772061	1.183547	441.2512	482.4555	503.9352
	8	-1.775780	-1.951350	-0.732280	538.2479	575.3045	645.3141
	8	1.688997	-1.548880	0.128804	685.2989	778.0777	809.3957
	8	2.510205	0.496099	-0.977592	837.9468	930.2418	955.9191
	8	1.820597	0.897385	1.204513	977.4030	998.0299	1005.1647
	6	-2.192283	1.123943	0.034515	1063.0811	1073.5469	1082.5755
	8	-1.794770	2.391012	-0.464120	1101.0082	1111.6253	1125.0325
	1	-0.528236	-2.669510	0.764553	1180.2887	1194.2116	1202.5608
	1	0.517562	-1.576264	-1.556437	1224.0883	1236.3968	1248.6766
	1	1.424827	2.176030	-0.382478	1260.4617	1285.5411	1302.1854
	1	-0.153288	0.734500	-1.441323	1336.1286	1342.7063	1356.7982
	1	-0.565109	1.180893	1.418185	1376.5373	1379.2235	1404.1623
	1	-2.552744	-2.327670	-0.300875	1443.8730	1451.9511	1484.8474
	1	2.361816	-0.902433	-0.320388	1527.5193	1668.7481	2177.7894
	1	3.337847	0.994329	-0.950423	3007.1077	3040.8459	3058.4978
	1	1.650834	-1.250609	1.063440	3066.0765	3095.8914	3133.4953
	1	-2.594412	0.475111	-0.754008	3142.3298	3746.8895	3795.6918
	1	-2.938072	1.204150	0.836204	3810.9730	3820.8194	3836.7375
	1	-2.565209	2.854101	-0.807115			
	1	2.312036	1.637128	1.578527			
I3	6	-4.903399	0.321756	-0.924444	50.8222	82.7179	113.6893
	6	-5.317698	0.176933	0.539318	163.6310	199.1470	216.5658
	6	-6.846813	0.178638	0.432502	236.1783	249.6506	321.9399

	6	-7.111518	0.788611	-0.923730	334.3423	347.7232	393.5561
	8	-5.882083	1.136630	-1.504917	421.8302	433.0082	465.7756
	6	-3.541221	0.945129	-1.171196	493.0346	568.4318	598.7139
	8	-2.520244	0.101604	-0.682889	687.8792	773.9708	836.1921
	6	-4.794318	-1.055971	1.243986	868.8045	899.6315	966.3341
	8	-3.443165	-0.923101	1.634789	995.9918	1033.5987	1051.1732
	8	-5.343039	-1.179844	2.542540	1081.5613	1104.9114	1112.7491
	8	-7.608732	-0.152839	-1.856734	1135.8907	1145.1556	1215.9805
	1	-4.952271	-0.674610	-1.427721	1234.5927	1249.1478	1270.6740
	1	-5.035417	1.096823	1.105581	1281.4611	1298.6473	1303.8019
	1	-7.282235	-0.843354	0.508191	1316.1751	1332.7354	1344.7086
	1	-7.784917	1.669974	-0.896291	1392.4638	1422.5750	1432.5929
	1	-3.358377	1.075711	-2.261640	1462.0234	1475.7587	1526.4156
	1	-3.439012	1.932527	-0.669237	1640.5645	2945.2289	3011.0636
	1	-1.684482	0.326858	-1.096012	3038.5098	3063.6525	3074.6906
	1	-4.927568	-2.006375	0.688619	3103.9076	3170.9650	3671.3489
	1	-2.871474	-0.920039	0.867983	3732.5482	3792.3505	3824.2696
	1	-4.596675	-1.228131	3.145815			
	1	-7.287239	0.109290	-2.722978			
I4	6	0.297171	1.712865	0.163905	71.6341	106.1919	123.5637
	6	-0.741144	0.915881	-0.623048	182.4050	183.6215	235.6934
	6	-1.817258	-0.561317	0.357809	245.3023	302.2649	330.4032
	6	-0.427742	-0.564174	-0.297327	348.4351	378.7480	424.9250
	6	0.763554	-0.512021	0.656823	461.4145	544.6856	594.5256
	8	0.795843	0.836599	1.154362	722.3762	783.9384	853.1985
	8	1.293881	2.114905	-0.750478	874.4017	916.9645	956.2379
	8	-2.703569	-1.391984	-0.313832	976.8410	983.1575	995.4942
	8	-2.003591	0.839642	0.064390	1036.9833	1057.9662	1076.9198
	6	2.086371	-0.887965	-0.013670	1080.0411	1087.8340	1103.5513
	8	2.016927	-2.276828	-0.299521	1143.4809	1194.6675	1201.6935
	1	-0.133524	2.569863	0.695109	1215.8105	1243.3680	1246.4146
	1	-0.835082	1.251669	-1.657598	1267.1705	1293.7001	1303.1027
	1	-1.857004	-0.724222	1.444863	1333.1902	1356.8791	1380.2967
	1	-0.313233	-1.281001	-1.107001	1387.5273	1433.2004	1451.7531
	1	0.624170	-1.166632	1.524068	1462.8617	1529.7508	2987.9082
	1	2.006470	2.512319	-0.238067	2995.9153	3035.6663	3046.4468
	1	-3.572283	-1.304810	0.093955	3059.9824	3096.3262	3153.1666
	1	2.224991	-0.285258	-0.921038	3807.7746	3812.6414	3840.6479
	1	2.906876	-0.652100	0.680736			
	1	2.786982	-2.518122	-0.821350			
I5	6	1.663402	-0.048986	0.256926	60.5915	115.5304	201.2173
	6	1.151797	1.275474	-0.243570	233.3516	245.2724	311.8434
	6	-0.156196	1.352471	-0.033978	404.5779	427.3014	519.8890
	6	-0.631789	0.108488	0.663790	589.1743	743.8400	791.5080
	8	0.561200	-0.627124	0.940879	823.2828	865.6403	934.5680
	8	2.070815	-0.819358	-0.851904	964.2799	965.6566	1056.5192
	6	-1.588510	-0.739363	-0.179922	1059.7328	1076.2033	1091.7470
	8	-2.774856	0.020633	-0.351966	1104.8358	1138.4877	1222.5830
	1	2.489035	0.024193	0.980742	1226.1166	1239.8352	1306.9281
	1	1.788067	1.989699	-0.748017	1340.9560	1371.7056	1381.8579
	1	-0.828779	2.147243	-0.325544			
	1	-1.126440	0.338559	1.617653			

	1	2.449394	-1.638158	-0.513255	1446.5352	1451.6059	1523.1715
	1	-1.099557	-0.972998	-1.136511	1689.7758	2986.0461	2988.3545
	1	-1.779573	-1.685144	0.348672	3009.0014	3034.6718	3222.5730
	1	-3.381652	-0.485114	-0.899281	3246.9207	3806.0374	3839.3020
I6	6	-1.494296	-0.702527	0.448156	60.3437	88.6918	89.0499
	6	-1.042580	-1.305080	-0.755987	112.7080	146.0460	190.3812
	6	0.312143	-1.227042	-0.717856	201.2904	228.3038	316.2155
	6	0.722884	-0.556680	0.534924	324.5764	415.2699	531.1805
	8	-0.540542	-0.316304	1.219631	553.0156	772.5786	821.8089
	8	-1.898440	1.703794	-0.432596	845.3634	870.1884	969.6046
	6	1.447230	0.798928	0.315805	988.6363	989.9934	1044.0088
	8	2.549661	0.473865	-0.489843	1072.1140	1085.9498	1105.0699
	1	-2.504953	-0.569911	0.813706	1131.8097	1182.3862	1231.8167
	1	-1.678898	-1.716358	-1.524519	1283.7641	1298.6484	1327.6686
	1	1.024016	-1.555639	-1.462864	1388.4525	1436.5810	1474.7923
	1	1.324163	-1.196330	1.189710	1532.3555	1596.3501	1661.1293
	1	-2.237228	2.394579	0.149058	3025.9891	3077.1898	3091.8547
	1	0.744332	1.486270	-0.172025	3247.9493	3255.0839	3275.7447
	1	1.723785	1.203395	1.295882	3785.7126	3837.2975	3880.3040
	1	3.278123	1.076824	-0.310632			
	1	-2.231051	1.940731	-1.306098			
I7	6	1.892602	-0.448922	-0.205682	110.0474	159.2973	205.9641
	6	1.674875	0.947793	-0.207967	249.8434	397.3016	521.0874
	6	0.394575	1.117994	0.231524	544.6675	771.3091	823.2143
	6	-0.200123	-0.200802	0.506057	844.9564	871.6527	948.5797
	8	0.877587	-1.130666	0.205673	982.3178	1009.5077	1042.4919
	6	-1.456328	-0.544071	-0.379696	1052.3931	1090.9276	1104.7387
	8	-2.421894	0.428159	-0.134848	1128.6675	1153.5128	1231.9200
	1	2.771094	-1.015240	-0.500318	1273.9161	1319.3869	1362.1578
	1	2.391822	1.693999	-0.515667	1384.7179	1420.8751	1466.3851
	1	-0.154096	2.043988	0.344616	1508.7366	1580.9889	3053.8465
	1	-0.459382	-0.352147	1.560145	3076.2847	3116.1028	3218.8141
	1	-1.153361	-0.504036	-1.430593	3249.1462	3272.9424	3825.3554
	1	-1.768135	-1.564913	-0.139777			
	1	-3.107087	0.086454	0.449580			
I8	6	1.955877	-0.458468	0.070307	52.8005	98.6669	125.4446
	6	1.355866	0.914511	-0.284074	148.2861	169.4206	238.2368
	6	-1.079080	1.618139	-0.394687	241.6520	292.4551	310.4550
	6	-0.109449	0.508672	-0.475020	353.3140	357.0203	386.5063
	6	-0.305087	-0.567291	0.656186	431.3230	456.6059	515.6425
	8	0.982497	-1.076023	0.911370	542.2686	591.9257	726.7170
	8	2.112934	-1.135795	-1.135825	754.5579	817.6683	924.6068
	8	1.344484	1.821781	0.794716	938.3429	974.9217	988.0226
	8	-2.304502	1.427122	-0.239845	998.4405	1051.1662	1085.4857
	6	-1.268506	-1.680193	0.251084	1097.3359	1106.1850	1133.8924
	8	-2.508153	-1.029903	-0.125503	1141.2473	1176.6968	1204.5737
	1	2.878797	-0.404013	0.656241	1209.5299	1224.0236	1252.3947
	1	1.816957	1.324399	-1.188095	1271.6201	1277.5744	1325.0641
	1	-0.763636	2.660971	-0.465327	1348.5151	1354.8205	1376.2655
	1	-0.239131	0.025102	-1.454249	1387.2034	1405.8609	1427.5922
	1	-0.680910	-0.081752	1.566119			
	1	2.572431	-1.969585	-0.982814			
	1	2.227716	2.175442	0.948032			

	1	-2.531014	0.387210	-0.166939	1444.1817	1515.3047	1636.2063
	1	-0.875460	-2.242519	-0.600927	1670.9911	2142.4519	3022.9206
	1	-1.441449	-2.356122	1.091434	3033.1643	3067.1983	3072.5501
	1	-3.280110	-1.588807	0.014447	3078.2667	3132.8062	3155.7766
					3810.4861	3818.3333	3833.3349
I9	6	-1.863093	-0.445635	0.019892	32.1310	68.0460	98.8511
	6	-1.188011	0.923708	0.178092	110.5351	175.0686	204.1581
	6	1.255458	1.617473	-0.038891	218.1069	256.2471	266.2270
	6	0.288477	0.499617	0.305311	279.4105	302.3386	385.9304
	6	0.355900	-0.723991	-0.630519	393.4959	442.3727	486.1165
	8	-0.989529	-1.209906	-0.772693	538.3601	580.2518	720.6516
	8	-2.027706	-0.985706	1.310118	802.5508	871.5458	918.9456
	8	-1.320354	1.706244	-0.996440	965.0827	985.8903	1012.0463
	8	1.829096	2.277885	0.786837	1033.4934	1078.9367	1080.5994
	6	1.253094	-1.836682	-0.107253	1083.9927	1108.4657	1132.3401
	8	2.568122	-1.307032	-0.091251	1139.1137	1200.1467	1207.1462
	1	-2.821054	-0.396372	-0.517320	1228.8640	1245.8362	1274.9294
	1	-1.545889	1.451533	1.068509	1296.5916	1322.6434	1349.5834
	1	1.392114	1.799757	-1.125149	1374.5317	1392.7727	1401.8967
	1	0.470203	0.206591	1.341389	1428.0546	1443.4527	1453.3142
	1	0.711144	-0.428373	-1.626065	1525.7129	1831.9967	2912.8066
	1	-2.289117	-1.906877	1.203423	2982.2034	3007.5590	3013.7382
	1	-2.235959	1.991209	-1.074630	3034.6495	3056.0217	3099.2762
	1	0.909669	-2.131772	0.895688	3813.1242	3825.9441	3844.1076
	1	1.170246	-2.712967	-0.767350			
	1	3.150665	-1.931535	0.349145			
I10	6	-1.837332	-0.624537	0.068295	61.9943	79.2761	125.8300
	6	-1.375279	0.799517	0.417620	144.1627	164.1330	195.9084
	6	1.036531	1.822847	0.532374	239.7377	258.4523	347.5943
	6	0.120222	0.602760	0.547967	365.7278	377.6492	396.7662
	6	0.421286	-0.465490	-0.553294	416.3406	454.5243	502.8906
	8	-0.917160	-0.909545	-0.980808	555.7297	568.3900	672.5897
	8	-1.686231	-1.378590	1.208003	740.1667	781.7597	822.6589
	8	-1.576926	1.550725	-0.930230	882.2177	906.6396	945.7570
	8	2.203095	1.710968	0.271596	958.6957	994.7980	1005.9089
	6	1.337294	-1.622080	-0.128793	1047.0562	1078.2300	1093.1692
	8	2.683609	-1.266588	-0.286281	1100.1307	1125.8038	1165.4343
	1	-2.841786	-0.689944	-0.367686	1182.8266	1212.9492	1258.8385
	1	-1.915064	1.381094	1.160749	1269.4985	1303.5092	1328.9212
	1	0.590085	2.797401	0.813486	1334.6873	1348.9842	1371.3394
	1	0.250367	0.148963	1.541472	1396.7626	1414.4460	1428.1003
	1	0.882160	-0.005004	-1.431239	1448.6971	1512.6343	1604.9492
	1	-2.050700	-2.263730	1.079687	1826.6949	2941.3124	2990.3298
	1	-2.465900	1.936457	-1.041487	3026.1430	3052.1151	3086.9473
	1	1.089527	-1.949087	0.892849	3096.5965	3179.8177	3242.7904
	1	1.150259	-2.462116	-0.804108	3690.7869	3770.7231	3797.4656
	1	2.869829	-0.446454	0.189184			
	1	-1.426208	0.818553	-1.596165			
I11	6	0.542079	-0.658013	-0.258994	63.4292	68.7794	124.3648
	6	-0.309196	0.506989	0.258021	172.4372	210.8648	240.2446
	6	-1.741462	0.172656	-0.240884			

	6	-1.663356	-1.331202	-0.287200	252.7000	322.0433	371.2763
	8	-0.509440	-1.800373	-0.288176	386.3817	452.0810	478.6963
	6	1.776669	-1.105674	0.529292	494.9778	545.8041	625.8642
	8	2.901555	-0.454146	0.020423	711.3883	727.1349	800.4128
	6	0.232002	1.884543	-0.134172	909.2607	956.8592	1011.7284
	8	1.409002	2.078668	-0.274627	1024.1303	1076.2361	1089.3386
	8	-2.828668	0.700261	0.431858	1116.2244	1129.9166	1169.1606
	1	0.816717	-0.557314	-1.312366	1184.1071	1228.6337	1266.2868
	1	-0.321004	0.484594	1.359288	1271.6014	1289.7540	1318.0673
	1	-1.853293	0.481688	-1.297367	1353.2539	1356.1831	1391.3393
	1	-2.504295	-2.028134	-0.316152	1400.7084	1409.3498	1431.9023
	1	1.920978	-2.178986	0.368821	1499.6148	1632.5770	1821.9994
	1	1.620323	-0.941229	1.605982	2959.2947	2976.7927	2998.7019
	1	2.807451	0.501380	0.142775	3003.2972	3089.2551	3108.4757
	1	-0.520090	2.687652	-0.245744	3151.5263	3748.5684	3781.7640
	1	-2.766798	0.539277	1.382563			
I12	6	0.140325	-0.580752	-0.631172	55.8537	95.9856	153.7675
	6	0.166658	0.874127	-0.214452	207.9362	217.2785	249.4739
	6	-1.082468	1.322911	-0.057107	287.0277	297.2369	388.4812
	6	-2.052241	0.194520	-0.280953	447.4787	485.3665	535.2467
	8	-1.258227	-0.860058	-0.785456	577.5052	611.2609	719.7078
	6	0.801900	-1.563522	0.355962	803.4579	825.7115	881.1312
	8	2.197290	-1.619174	0.198645	937.0547	990.5095	1021.1711
	6	1.362522	1.672021	0.062251	1038.0230	1056.0587	1084.4814
	8	2.490003	1.226854	0.150491	1098.4327	1103.2445	1195.7240
	8	-2.647828	-0.107742	0.956722	1209.0033	1231.6674	1293.3036
	1	0.625766	-0.724998	-1.605384	1313.8406	1369.8541	1375.7489
	1	-1.386748	2.311705	0.261745	1388.5127	1421.2365	1449.0098
	1	-2.826376	0.413222	-1.031820	1463.7134	1510.5591	1684.8494
	1	0.409280	-2.559474	0.128241	1766.5370	2931.5867	2975.0195
	1	0.492767	-1.312350	1.383549	2991.5880	3027.8346	3081.1519
	1	2.540793	-0.715619	0.274263	3224.0506	3689.1396	3807.7687
	1	1.174235	2.754331	0.211579			
	1	-3.299791	-0.801697	0.807442			
I13	6	0.203321	-0.543583	-0.640735	35.6512	59.5696	140.2683
	6	0.190879	0.902766	-0.229611	176.8715	208.1832	212.9493
	6	-1.070127	1.347384	-0.117637	250.2982	297.5486	350.7772
	6	-1.974220	0.205520	-0.417834	385.9577	407.5732	477.9545
	8	-1.226431	-0.838610	-0.802010	549.5210	591.1222	658.5418
	6	0.860945	-1.552866	0.334397	715.0244	756.9406	804.6028
	8	2.231963	-1.643224	0.133998	816.1262	865.3106	931.7852
	6	1.406487	1.706349	0.073702	952.4859	1010.1632	1039.4529
	8	2.488189	1.203172	0.256808	1052.6086	1067.5459	1131.0489
	8	-2.698111	-0.143137	0.916874	1144.5211	1206.7511	1228.3010
	1	0.657787	-0.689191	-1.625613	1279.6451	1308.9483	1352.2026
	1	-1.413236	2.337924	0.149811	1380.9383	1389.2435	1394.3529
	1	-2.859531	0.361824	-1.038045	1420.0665	1443.1428	1502.3871
	1	0.431287	-2.533690	0.107843	1651.0563	1659.7601	1790.0645
	1	0.584344	-1.294047	1.372896	2934.2154	2986.9695	3083.1135
	1	2.639510	-0.787341	0.333211			
	1	1.250851	2.797614	0.146176			
	1	-2.077586	-0.289024	1.657970			

	1	-3.282010	-0.923093	0.836699	3089.8305 3605.2895	3114.4801 3699.7720	3238.2051 3725.2196
I14	6	0.223352	-0.600201	0.448625	94.2192	116.6938	172.3660
	6	0.345470	0.834381	0.115676	198.5800	246.5433	273.7050
	6	1.640457	1.096850	-0.249543	370.2462	467.8573	522.4605
	6	2.328633	-0.132069	-0.133350	525.2313	596.9920	701.0395
	8	1.578794	-1.093570	0.281642	800.9760	871.4142	877.3281
	6	-0.768811	-1.482478	-0.459074	928.5135	942.0524	992.2516
	8	-2.044408	-1.418931	0.041372	1019.4659	1035.8537	1080.3829
	6	-0.790895	1.805721	0.061586	1144.8660	1154.6018	1180.0737
	8	-1.936846	1.434696	0.019350	1234.5517	1269.5252	1330.1261
	1	-0.069170	-0.815089	1.481240	1345.7865	1385.4223	1426.5076
	1	2.071187	2.030087	-0.583123	1432.1978	1479.5745	1504.7002
	1	3.366477	-0.372900	-0.341942	1579.0483	1785.7517	3009.4515
	1	-0.403659	-2.507193	-0.356358	3035.6293	3091.5760	3124.0460
	1	-0.662404	-1.156586	-1.500789	3220.5984	3257.7780	3738.7209
	1	-2.442238	-0.560915	-0.167377			
	1	-0.509754	2.871811	0.025919			
I15	6	2.212943	-0.671349	0.393855	53.3120	91.7024	103.7407
	6	0.859900	-0.377587	-0.230888	127.1610	171.9917	202.5752
	6	0.315979	0.993147	0.176014	243.3593	263.6829	295.4545
	6	-1.161864	0.820511	-0.129311	311.2611	339.4793	378.5849
	6	-1.364861	-0.622426	0.396630	395.9957	431.6683	450.7881
	8	-0.097225	-1.306360	0.209004	475.1796	482.2417	505.1458
	8	2.845280	-1.702880	-0.173423	526.1054	565.9656	578.9582
	8	3.066656	0.658885	0.033068	600.8099	653.4858	677.8357
	8	1.058775	1.986186	-0.552187	901.8366	947.7748	966.4071
	8	-1.918153	1.793828	0.525331	1008.9907	1016.5796	1073.6257
	6	-2.487082	-1.356008	-0.321843	1077.4787	1100.4316	1116.3298
	8	-3.606915	-0.492095	-0.186276	1127.0559	1135.7943	1162.4576
	1	2.229454	-0.636298	1.484237	1192.4746	1214.2937	1228.8302
	1	0.992651	-0.411625	-1.325442	1242.6690	1243.1694	1260.2757
	1	0.429311	1.166584	1.254939	1287.7244	1304.6815	1318.4350
	1	-1.308840	0.843297	-1.221051	1338.2212	1348.0080	1354.1394
	1	-1.583855	-0.572826	1.469713	1387.5961	1403.0283	1418.1290
	1	3.472578	-2.123733	0.430403	1451.2100	1470.5902	1517.4387
	1	2.400376	1.414789	-0.262090	1525.6713	1669.0418	2368.6892
	1	0.780069	2.873913	-0.288591	2975.6237	2986.1598	2998.9198
	1	-2.848043	1.559025	0.400011	3030.3212	3044.4413	3061.2705
	1	-2.211489	-1.511146	-1.375372	3129.2381	3716.2903	3768.3000
	1	-2.661327	-2.337171	0.137167	3777.9334	3781.2045	3839.9603
	1	-4.389980	-0.913879	-0.552519			
	1	3.661669	0.430829	-0.702275			
I16	6	-1.857253	-1.472537	-0.326612	28.9894	43.3766	59.4376
	6	-0.719552	-0.846992	0.461979	85.1051	125.4490	132.0159
	6	-0.527223	0.650357	0.134207	155.5620	184.3506	214.0230
	6	0.990561	0.795421	0.234754	225.3118	243.6656	273.7003
	6	1.459578	-0.542431	-0.344390	309.9999	334.2301	369.1597
	8	0.500716	-1.500638	0.105407	374.4588	421.1509	458.3759
	8	-2.974569	-1.620192	0.095874	469.2874	485.4506	504.4905
	8	-3.581665	1.233055	-0.717598			
	8	-1.264082	1.444404	1.045956			

	8	1.433553	1.934455	-0.459093	534.0499	565.1447	619.4287
	6	2.847301	-0.951956	0.122178	677.1416	912.8524	930.3207
	8	3.713304	0.110529	-0.272603	979.2331	1014.2589	1051.0615
	1	-1.560829	-1.786711	-1.352123	1063.4205	1074.3217	1090.4241
	1	-0.922071	-0.960638	1.533686	1126.7847	1133.4607	1141.7089
	1	-0.836537	0.866929	-0.897820	1159.2164	1204.9147	1232.6378
	1	1.256883	0.842042	1.304251	1240.5350	1260.8117	1295.4977
	1	1.454275	-0.470941	-1.442803	1305.2537	1322.6669	1333.8902
	1	-3.085658	1.360240	0.102968	1355.8781	1401.4308	1409.9902
	1	-1.071889	2.366183	0.835154	1425.1805	1448.8787	1464.8711
	1	2.397140	1.872583	-0.491305	1523.9402	1694.9840	1830.4832
	1	2.834486	-1.082150	1.213860	2892.9545	2963.9386	2991.5877
	1	3.143051	-1.905850	-0.335116	2998.6320	3020.1810	3042.2567
	1	4.601214	-0.075008	0.044736	3048.1192	3749.2304	3772.8762
	1	-3.988598	0.369248	-0.591723	3797.0751	3844.8557	3862.7407
I17	6	-2.279383	-1.092008	-0.438447	46.3261	74.2509	90.4637
	6	-1.459546	-0.215415	0.549078	138.5004	192.7752	202.8668
	6	-0.925658	1.028167	-0.180553	204.7623	229.8041	234.6999
	6	0.591488	0.881801	-0.163184	293.6755	328.4281	367.4727
	6	0.727709	-0.638105	0.108053	407.9395	437.5653	506.2817
	8	-0.324065	-0.877294	1.044319	524.0921	572.3402	655.4104
	8	-1.889023	-2.152075	-0.822178	701.2610	774.7642	793.1516
	8	-1.379253	2.324642	0.585703	834.4349	886.7001	923.3592
	8	1.144323	1.380448	-1.334410	969.3318	1000.8515	1024.3729
	6	2.078863	-1.003262	0.700829	1075.4565	1089.4053	1107.3136
	8	3.022086	-0.391289	-0.170276	1120.0812	1146.2349	1170.3429
	1	-3.251583	-0.648904	-0.744978	1213.0795	1238.4536	1245.1824
	1	-2.131717	0.038212	1.379717	1262.3992	1287.1363	1294.8403
	1	-1.342797	1.236902	-1.165516	1326.7545	1346.3743	1372.0248
	1	0.976156	1.394703	0.741196	1397.8543	1402.4039	1425.7052
	1	0.559673	-1.191455	-0.823849	1471.1543	1526.0466	1651.3215
	1	-1.089198	3.131559	0.116141	1862.1909	2901.1717	2909.4764
	1	-1.089198	3.131559	0.116141	3005.2521	3036.5094	3052.7779
	1	2.059881	1.060928	-1.363650	3076.5990	3142.9225	3617.9201
	1	2.149983	-0.607679	1.724457	3704.9756	3722.6372	3842.1302
	1	2.194038	-2.092049	0.739665			
	1	3.907356	-0.715263	0.021168			
	1	-1.025185	2.350518	1.495732			
I18	6	-2.452357	-0.914797	-0.468533	39.6242	62.3889	81.5526
	6	-1.277241	-0.431115	0.364361	131.4746	185.3921	212.3185
	6	-0.773596	0.954675	-0.094121	230.4620	243.6893	300.5255
	6	0.737027	0.821329	0.115067	325.4044	335.6908	373.1230
	6	0.969748	-0.643190	-0.265790	418.8766	468.3864	487.5877
	8	-0.186936	-1.341075	0.195089	503.8584	536.6226	618.6078
	8	-3.605599	-0.809065	-0.149947	677.1529	912.8669	932.1590
	8	-1.405428	1.962966	0.653495	979.5015	1014.0704	1050.2651
	8	1.439412	1.755074	-0.668425	1062.0423	1072.4260	1093.6339
	6	2.213934	-1.245539	0.366855	1127.8991	1133.2936	1148.0761
	8	3.300458	-0.430203	-0.069898	1158.2281	1202.4480	1228.0053
	1	-2.137727	-1.380787	-1.431388	1240.4853	1252.0561	1294.1178
	1	-1.578177	-0.375924	1.416813	1305.3518	1323.2487	1332.8508

	1	-0.946292	1.090023	-1.174744	1357.5177	1401.3684	1409.5915
	1	0.940597	0.958469	1.190223	1422.9279	1453.2099	1463.9255
	1	1.055648	-0.710846	-1.361483	1523.6579	1842.4852	2866.6491
	1	-1.099463	2.810556	0.313273	2963.0825	2972.9853	2989.8253
	1	2.371196	1.506973	-0.610030	2998.0869	3041.3728	3053.5803
	1	2.105172	-1.226056	1.460711	3774.1217	3815.4748	3844.9287
	1	2.341015	-2.290203	0.051811			
	1	4.107684	-0.731952	0.355268			
I19	6	2.753924	-0.624799	0.091538	41.6863	96.9966	125.2210
	6	1.351236	-0.170382	0.026298	155.7615	182.9197	209.2505
	6	0.869162	1.027738	-0.322366	244.2487	332.2722	365.7519
	6	-0.632774	0.970343	-0.288673	382.1517	399.9143	494.9618
	6	-0.856388	-0.403443	0.404933	554.2675	598.2777	670.6671
	8	0.405056	-1.102698	0.368450	732.6480	812.5614	867.8886
	8	3.697481	0.063427	-0.217540	969.6486	994.9202	1030.4725
	8	-1.206498	2.046714	0.426072	1039.2002	1062.9188	1081.1679
	6	-1.938380	-1.250218	-0.238346	1102.7926	1127.5422	1191.8673
	8	-3.117266	-0.456355	-0.171721	1223.7728	1240.0599	1247.3284
	1	2.873977	-1.666728	0.456029	1253.9986	1316.0518	1348.9878
	1	1.460360	1.874723	-0.634041	1385.5973	1418.2387	1437.3711
	1	-1.034021	0.954488	-1.316569	1464.8835	1524.4745	1679.0109
	1	-1.110718	-0.205764	1.454287	1806.6251	2917.3083	2946.3145
	1	-2.162420	1.936661	0.358204	2989.5217	3023.3379	3041.9189
	1	-1.655641	-1.476568	-1.277360	3264.6648	3795.2242	3843.4828
	1	-2.053752	-2.201529	0.299431			
	1	-3.828654	-0.919419	-0.622382			
I20	6	2.865990	-0.541790	0.102351	54.1830	93.1524	124.1135
	6	1.415542	-0.174834	0.031186	154.0535	168.7005	215.5824
	6	0.884522	1.029851	-0.277198	253.4348	313.9960	351.8634
	6	-0.556962	0.814589	-0.397538	363.5730	402.8913	474.9163
	6	-0.756090	-0.539288	0.307571	550.3784	571.6437	647.0059
	8	0.521163	-1.171442	0.254777	730.4138	749.1452	804.8199
	8	3.717323	0.275959	-0.118046	836.0762	924.7307	967.5129
	8	-1.535054	1.749483	0.472226	1014.2539	1019.9276	1029.8735
	6	-1.935807	-1.319772	-0.245390	1065.0510	1078.8603	1125.9674
	8	-2.985354	-0.337037	-0.134288	1164.2218	1181.9193	1221.4448
	1	3.072364	-1.594192	0.369643	1243.3796	1273.5705	1317.0564
	1	1.453840	1.891099	-0.590815	1339.8761	1379.9728	1396.4159
	1	-1.001634	0.946076	-1.386429	1421.1711	1452.4852	1524.1926
	1	-0.959969	-0.320543	1.364528	1617.2166	1637.8685	1819.2401
	1	-2.397564	1.241073	0.381416	2984.3834	3027.7107	3052.2082
	1	-1.783853	-1.614130	-1.289647	3094.7494	3116.4846	3145.4049
	1	-2.148974	-2.205341	0.359139	3266.4680	3710.0548	3837.4067
	1	-3.855110	-0.737928	-0.233395			
	1	-1.626900	2.645636	0.102309			
I21	6	2.526064	-0.652785	-0.085556	64.0383	107.1809	135.5400
	6	1.141035	-0.089046	0.123657	195.6040	212.2147	260.0330
	6	0.726723	1.257537	-0.017296	278.9193	356.4326	516.3841
	6	-0.609660	1.259541	0.253951	530.0985	642.7823	722.1007
	6	-1.043394	-0.113972	0.563280	782.2315	844.1207	854.0106
	8	0.182853	-0.889647	0.470826	939.7361	951.8879	987.0771
	8	3.408171	0.097145	-0.396328			
	6	-2.115768	-0.697584	-0.437717			

	8	-3.232019	0.129883	-0.390951	1018.7294	1030.1675	1051.6389
	1	2.637079	-1.739092	0.067488	1100.8182	1119.2110	1149.2920
	1	1.372742	2.075060	-0.299355	1230.5077	1244.5554	1320.3561
	1	-1.294060	2.097624	0.225128	1359.0459	1379.0546	1389.6733
	1	-1.418177	-0.238211	1.585836	1431.0674	1472.9111	1508.4946
	1	-1.686586	-0.675623	-1.444074	1569.8185	1809.7025	3020.3308
	1	-2.307318	-1.736890	-0.154556	3053.9398	3073.4713	3116.9986
	1	-3.925719	-0.264063	0.149247	3247.4663	3275.1979	3822.3073
I22	6	-0.443361	1.205443	0.502163	37.2059	85.3922	96.8205
	6	-0.565000	-0.143421	-0.218305	107.5933	181.1882	194.3189
	6	-1.868259	-0.849254	0.025418	236.8706	247.0969	263.1407
	6	0.688958	-0.855847	0.307163	306.7690	331.4693	362.3288
	6	1.689625	0.329836	0.396260	370.0928	399.0392	437.9129
	8	0.898032	1.539963	0.420945	451.3410	483.8964	509.5930
	8	-1.266781	2.137611	-0.200204	536.6414	578.4722	591.2734
	8	-3.002109	0.316283	-0.306796	620.6145	671.5667	765.8778
	8	-2.105248	-1.848051	-0.829206	857.5385	909.7392	940.5661
	8	0.336020	-1.380319	1.575315	996.0852	1030.3936	1047.3487
	6	2.669898	0.395605	-0.769365	1068.4400	1090.7541	1095.1340
	8	3.419390	-0.799640	-0.695192	1104.2433	1130.6517	1138.4563
	1	-0.778365	1.153911	1.550245	1174.8610	1209.0782	1221.2057
	1	-0.458466	0.043400	-1.292264	1225.6219	1248.7090	1256.3294
	1	-2.114409	-1.038413	1.068330	1288.3968	1292.0182	1306.8109
	1	1.058853	-1.631513	-0.368395	1312.8082	1338.3492	1350.2309
	1	2.248866	0.250077	1.334329	1365.7698	1411.7839	1423.7266
	1	-1.282036	2.987192	0.261057	1449.1404	1458.2410	1520.5125
	1	-3.355603	0.127664	-1.193175	1523.4476	1659.6946	2656.2268
	1	-2.724907	-2.494965	-0.464101	2975.6372	2988.3945	3040.1614
	1	1.084642	-1.867208	1.937225	3065.3704	3072.1051	3088.9525
	1	2.119336	0.484276	-1.719965	3164.5494	3721.7550	3773.1366
	1	3.289801	1.295084	-0.660436	3783.4032	3817.9507	3837.8908
	1	4.157496	-0.753190	-1.310313			
	1	-2.510806	1.222746	-0.321426			
I23	6	-0.840708	1.422175	0.110655	48.0702	62.5048	92.1913
	6	-1.213987	0.043106	-0.457565	123.2165	183.4737	196.1035
	6	-2.098213	-0.725740	0.509572	226.0211	237.6777	308.0220
	6	0.185659	-0.588839	-0.581472	344.8858	364.1040	416.5308
	6	0.940774	0.014674	0.624594	427.0060	451.2014	478.8161
	8	0.235351	1.199277	1.004989	533.8505	576.5316	682.1118
	8	-0.463753	2.231317	-0.976535	791.4992	856.1952	924.5442
	8	-3.206298	-1.107926	0.240754	961.0145	982.5082	1028.8335
	8	0.122103	-1.996934	-0.557246	1040.7776	1060.8325	1066.8654
	6	2.396686	0.317318	0.304410	1107.9298	1113.2538	1124.1578
	8	2.961951	-0.934787	-0.076803	1151.4756	1211.6870	1225.0206
	1	-1.634435	1.901254	0.697771	1237.4826	1244.0618	1263.1915
	1	-1.735918	0.132316	-1.410125	1311.1638	1322.6656	1359.9534
	1	-1.659676	-0.896667	1.517023	1377.6449	1399.7262	1419.2917
	1	0.645837	-0.233281	-1.512639	1436.6512	1442.7209	1457.0796
	1	0.902486	-0.700927	1.456347			
	1	-0.183458	3.081722	-0.619863			
	1	1.035563	-2.307848	-0.572345			

	1	2.440638	1.051809	-0.512829	1524.4708	1837.5277	2891.2683
	1	2.905467	0.742463	1.180725	2993.1608	3012.9443	3020.9696
	1	3.867399	-0.794583	-0.366503	3030.3409	3042.6724	3125.9246
					3791.0552	3806.4256	3843.8847
I24	6	0.587517	-0.628363	0.688656	43.6375	78.0250	100.6192
	6	0.842774	0.302378	-0.496070	155.8473	173.2168	231.5015
	6	2.323449	0.554061	-0.625836	245.7350	282.3009	324.4737
	6	-0.212039	1.368695	-0.224088	331.0983	338.4385	360.7956
	6	-1.391004	0.473193	0.253218	408.8611	478.7620	544.7647
	8	-0.735157	-0.706459	0.886699	589.4753	608.0388	660.1649
	8	1.212723	-1.970730	0.192801	734.1826	789.8068	812.0307
	8	3.065908	-0.406158	-0.467161	863.1883	970.8341	988.6077
	8	0.325506	2.173735	0.800738	1002.8091	1007.6870	1071.7491
	6	-2.364065	-0.006485	-0.819368	1090.3010	1104.5141	1111.3890
	8	-3.395470	-0.781703	-0.271798	1142.5767	1176.5357	1202.1462
	1	1.162204	-0.425169	1.598081	1219.3479	1237.0737	1262.7359
	1	0.553874	-0.253886	-1.399118	1277.0104	1287.1705	1344.4749
	1	2.728085	1.544938	-0.869694	1352.2670	1381.3439	1395.8101
	1	-0.483308	1.943993	-1.116654	1399.0270	1417.5226	1419.7015
	1	-1.945184	0.953674	1.062492	1450.8719	1485.0832	1563.0113
	1	1.280009	-2.635765	0.901249	1736.3915	2433.4992	2975.2682
	1	-0.265631	2.909348	0.997766	3028.8752	3054.7515	3073.9759
	1	-2.836855	0.875217	-1.266949	3075.0184	3076.9501	3107.1761
	1	-1.823559	-0.532580	-1.623155	3702.3029	3813.3129	3819.3706
1	-3.034263	-1.624416	0.023386				
1	2.156758	-1.605721	-0.096701				
I25	6	-0.457683	-1.207478	-0.300357	52.1904	74.5118	92.4461
	6	-1.021605	-0.179356	0.585844	153.4534	188.2708	221.4108
	6	-2.563632	0.001943	0.371643	256.4480	270.7562	300.9731
	6	-0.117279	1.046441	0.297541	340.3882	362.0553	519.6175
	6	1.158925	0.406566	-0.291499	546.3284	614.5182	696.5900
	8	0.661510	-0.940394	-0.793094	745.3907	752.5456	861.2175
	8	-3.241211	-0.913413	0.019487	889.8066	942.2323	971.6982
	8	-0.809321	1.807930	-0.658806	998.4035	1041.7623	1066.9416
	6	2.310033	0.143182	0.662269	1099.5513	1119.2558	1137.2917
	8	3.278178	-0.562393	-0.059366	1170.6758	1200.0917	1228.7883
	1	-0.926697	-2.149767	-0.582804	1248.1681	1269.7529	1286.3900
	1	-0.931535	-0.537037	1.624369	1290.3395	1333.6897	1339.4760
	1	-2.937504	1.011748	0.603434	1395.7088	1426.1411	1465.7247
	1	0.113204	1.610798	1.206957	1506.3339	1620.8123	1848.4624
	1	1.504223	0.896014	-1.202582	2964.0202	3002.3572	3010.5987
	1	-0.465636	2.707875	-0.698468	3024.4828	3067.9097	3140.3077
	1	2.654657	1.131366	1.007673	3182.6205	3813.8095	3824.1291
	1	1.949886	-0.406100	1.548915			
	1	4.073602	-0.666524	0.474080			
	I26	6	1.155715	0.351886	-0.294148	48.0729	117.1602
6		-0.150406	1.020534	0.214088	160.9940	188.7730	234.5179
6		-1.139987	-0.108803	0.068807	262.2159	285.9280	341.1034
6		-0.533775	-1.119554	-0.582012	367.7267	410.6682	514.3551
8		0.757926	-0.930087	-0.883209	556.5879	606.5186	734.9285
6		2.174340	0.041495	0.794475			

	8	3.302397	-0.638703	0.293087	771.3612	820.7754	918.4766
	6	-2.536756	-0.083577	0.482786	965.8504	1009.5637	1018.5262
	8	-3.317750	-1.002367	0.337508	1032.9815	1055.0487	1096.7027
	8	-0.576108	2.117970	-0.585790	1109.3350	1184.8859	1209.8853
	1	1.610045	0.934903	-1.099001	1224.8978	1232.6144	1254.7300
	1	-0.032779	1.344604	1.259072	1301.2191	1339.4931	1375.2729
	1	-0.956779	-2.063709	-0.899033	1397.2982	1423.3193	1427.8946
	1	1.676194	-0.522927	1.600248	1446.3754	1494.9711	1649.5855
	1	2.534715	0.982803	1.224405	1777.7233	2892.0791	2972.2245
	1	2.978187	-1.435230	-0.142320	2985.8245	3068.6180	3095.7702
	1	-2.855971	0.867357	0.962260	3239.0923	3805.7628	3808.5444
	1	-0.100110	2.905802	-0.302381			
I27	6	2.841863	0.480344	-0.781064	37.9786	58.1534	88.1020
	6	1.327201	-0.437318	1.068743	98.9097	141.8383	170.6920
	6	1.501167	0.138091	-0.218280	197.1565	213.5972	227.1883
	6	0.237188	0.263668	-0.729166	250.2986	310.2867	332.8565
	6	-0.733058	-0.206026	0.263530	421.9967	430.1834	468.3451
	8	0.096819	-0.660162	1.368128	553.6385	560.1504	736.7028
	8	3.840487	0.255453	-0.151196	799.5635	847.0969	918.1834
	8	-2.727152	1.873118	0.436100	981.4336	998.4351	1023.5469
	6	-1.734885	-1.308958	-0.145072	1038.1542	1061.5612	1080.3843
	8	-2.583703	-0.673286	-1.072259	1104.9904	1194.5489	1214.1379
	1	2.844570	0.939216	-1.786050	1254.1763	1269.5598	1292.9803
	1	2.082087	-0.695559	1.804640	1338.4932	1384.3097	1413.9355
	1	-3.270187	2.266440	1.128312	1440.8552	1473.0860	1526.2362
	1	-0.054300	0.662031	-1.693092	1608.2902	1639.3790	1811.0835
	1	-1.355988	0.652356	0.628303	2725.5345	2985.1839	3019.9729
	1	-3.333247	1.374319	-0.126182	3070.6165	3225.4945	3241.4832
	1	-1.201733	-2.165571	-0.575796	3775.9376	3822.3482	3881.7918
	1	-2.258161	-1.635851	0.762550			
	1	-3.101510	-1.337160	-1.541020			
I28	6	1.060767	0.291924	-0.513792	64.0783	106.0941	134.8936
	6	-0.165332	1.092707	-0.370296	189.9291	231.9942	294.9196
	6	-1.221030	0.266944	-0.105806	307.5773	360.1113	510.0372
	6	-0.677199	-1.049525	-0.105123	524.9552	577.0219	733.1224
	8	0.583686	-1.082054	-0.340859	774.4671	794.9104	893.5008
	6	2.222437	0.552369	0.519236	934.3218	987.4273	998.9136
	8	3.330766	-0.209597	0.197285	1018.5942	1051.0293	1067.7637
	6	-2.670475	0.543443	0.144047	1129.3237	1158.4198	1193.2998
	8	-3.425275	-0.364579	0.365016	1233.5162	1262.0672	1289.6419
	1	1.511193	0.335268	-1.512820	1381.2138	1385.5765	1400.8315
	1	-0.185930	2.172988	-0.456567	1419.3451	1469.4147	1490.8691
	1	-1.187105	-1.992220	0.070131	1614.2380	1810.8831	2992.0961
	1	1.835822	0.384366	1.531328	3037.9283	3070.5050	3103.2700
	1	2.481055	1.610767	0.410913	3220.5677	3228.0794	3821.6701
	1	3.315574	-1.051736	0.665152			
	1	-2.979030	1.603237	0.110736			
Furfuryl alcohol	6	0.168512	0.270023	0.211527	64.0004	149.1237	274.8935
	6	-0.800711	1.179007	-0.078344	351.7762	418.3320	614.3024
	6	-2.022083	0.443348	-0.228650	641.5151	743.0901	758.0287
	6	-1.700979	-0.859554	-0.024714	814.7941	855.3777	901.6705
	8	-0.374852	-0.985896	0.248930			

	6	1.634682	0.349587	0.459836	925.9378	978.1019	1035.2116
	8	2.416216	-0.232088	-0.578456	1041.5109	1107.4850	1178.5173
	1	-0.662075	2.244442	-0.176140	1194.7714	1240.5676	1270.2539
	1	-3.000503	0.835042	-0.458075	1370.0824	1416.2789	1418.0931
	1	-2.266570	-1.776648	-0.034388	1490.0964	1538.2129	1640.5628
	1	1.873759	-0.111471	1.431186	2980.1537	3100.3626	3251.5228
	1	1.925689	1.401858	0.512811	3262.7077	3285.0554	3815.7444
	1	2.122263	-1.143815	-0.677119			
5- (hydroxymethyl)furan -2-carbaldehyde	6	2.518401	-0.633219	-0.000008	24.5427	114.8366	141.8100
	6	1.204259	-0.020277	0.000001	200.1482	241.1108	253.9646
	6	0.774115	1.280343	0.000008	271.0019	373.6502	567.8059
	6	-0.645575	1.240870	0.000016	633.5408	647.2878	685.0112
	6	-0.985269	-0.083940	0.000013	768.8692	826.7576	891.6014
	8	0.116431	-0.861769	0.000004	975.1646	999.6602	1030.6239
	8	3.559247	-0.009880	-0.000012	1036.7200	1044.7338	1106.5043
	6	-2.301493	-0.785627	0.000022	1201.2310	1225.2783	1233.9461
	8	-3.309227	0.204276	-0.000049	1235.6334	1271.4217	1388.9600
	1	2.494587	-1.744486	-0.000012	1436.3152	1464.3013	1510.1074
	1	1.416263	2.146844	0.000007	1563.0176	1627.8412	1779.2804
	1	-1.337868	2.066139	0.000022	2900.0045	2960.0959	2979.3587
	1	-2.363905	-1.441083	-0.884646	3266.9857	3284.0756	3845.5649
	1	-2.363943	-1.440992	0.884754			
	1	-4.163358	-0.236329	0.000023			
5- (hydroxymethyl)furan -3-carbaldehyde	6	1.017688	-0.217481	-0.263922	56.2146	89.7068	157.0619
	6	-0.052393	-1.037545	-0.115953	179.9775	252.7931	287.1190
	6	-1.213520	-0.192024	-0.022085	347.5274	392.0074	508.9579
	6	-0.744017	1.089839	-0.116570	625.2374	657.8332	746.8466
	8	0.593118	1.093498	-0.266372	775.5812	811.3612	842.6100
	6	2.488098	-0.420689	-0.392964	915.6327	985.4219	1014.1155
	8	3.218784	0.015614	0.745600	1040.4622	1044.6213	1147.7598
	6	-2.614562	-0.585806	0.141480	1175.5535	1190.8178	1246.3714
	8	-3.541504	0.190081	0.214066	1304.3482	1370.8871	1377.5301
	1	-0.029208	-2.115764	-0.074192	1415.4376	1451.9778	1487.7056
	1	-1.236150	2.047866	-0.094813	1567.3977	1639.6822	1792.1532
	1	2.852013	0.072415	-1.307620	2886.4826	2987.3802	3103.3619
	1	2.683707	-1.491180	-0.494471	3254.7436	3286.4948	3816.2908
	1	3.058997	0.959760	0.847898			
	1	-2.780305	-1.684416	0.196929			
5- (hydroxymethyl)furan -4-carbaldehyde	6	-0.244156	-0.608019	0.130870	87.1581	138.4023	204.6156
	6	-0.351660	0.764000	0.012737	230.1311	272.9943	308.8859
	6	-1.758190	1.043174	-0.135887	414.3618	500.1288	619.3244
	6	-2.384501	-0.153174	-0.099754	664.2137	665.8470	738.1177
	8	-1.468729	-1.161656	0.061118	758.6020	778.2424	839.4322
	6	0.927043	-1.526192	0.330989	908.3918	973.8532	1036.6255
	8	2.004434	-1.241620	-0.522748	1061.7567	1098.2067	1126.6868
	6	0.728744	1.731860	0.058977	1163.6965	1214.5502	1273.8376
	8	1.918122	1.468696	0.140166	1294.8120	1377.5671	1414.8505
	1	-2.218580	2.011214	-0.259103	1458.9159	1482.6810	1484.4935
	1	-3.411548	-0.468102	-0.172077	1543.9835	1595.7685	1751.2786
	1	0.594510	-2.548516	0.125473	2926.3764	2951.0766	3082.7225
	1	1.221904	-1.490588	1.394374			
	1	2.276774	-0.328392	-0.324870			
	1	0.402644	2.791127	0.020317			

					3256.1021	3294.0922	3621.9446
$TS_{G_5^+ \leftrightarrow G_6^+}^{R1 \leftrightarrow R1}$	6	0.585816	-1.460980	0.395278	-92.1805	79.7432	86.4397
	6	1.523400	-0.441818	-0.261325	125.2465	175.7459	226.9762
	6	1.175741	0.988132	0.167186	252.8039	273.3775	277.0265
	6	-0.279674	1.310772	-0.167570	328.5240	349.4087	380.3236
	6	-1.191737	0.297631	0.516367	383.9966	400.6879	419.3982
	8	-0.815652	-1.032482	0.135976	439.2370	456.5537	475.3946
	8	0.749585	-2.685747	-0.182331	480.7476	540.1491	601.4878
	8	2.847782	-0.676155	0.153543	652.8558	700.8403	814.1092
	8	1.951136	1.942966	-0.513309	884.2152	908.1356	977.4899
	8	-0.684488	2.573290	0.289399	1020.8192	1030.4768	1044.7158
	6	-2.675688	0.405571	0.056315	1056.8531	1074.0232	1103.3735
	8	-3.017418	-0.968475	-0.414074	1124.9239	1135.8693	1160.2029
	1	0.704832	-1.466938	1.485753	1168.6936	1197.4716	1222.8093
	1	1.409936	-0.533103	-1.351246	1237.4778	1239.5698	1250.2387
	1	1.317034	1.069256	1.258216	1271.3281	1311.0173	1348.1281
	1	-0.402226	1.218294	-1.261181	1349.0383	1356.9020	1363.1569
	1	-1.126983	0.412560	1.603715	1375.5335	1389.6120	1424.8762
	1	0.534345	-3.391967	0.438164	1441.8561	1448.9856	1453.3060
	1	3.190135	-1.455458	-0.298639	1487.2961	1508.3485	2094.9281
	1	2.881042	1.768246	-0.323694	2953.0288	2974.5236	3016.9199
	1	-0.014838	3.213017	0.013736	3050.0404	3064.6564	3122.3302
	1	-3.367219	0.634293	0.863354	3198.4157	3762.6322	3784.5538
	1	-2.802773	1.100672	-0.772485	3802.0490	3806.1961	3815.4999
	1	-3.384408	-0.981052	-1.311181			
	1	-2.013579	-1.410848	-0.335638			
$TS_{G_6^+ \leftrightarrow G_1^+}^{R1 \leftrightarrow R1}$	6	-0.610070	-1.481585	-0.371350	-1497.5902	51.0832	93.8633
	6	-1.604819	-0.501616	0.209175	102.8583	125.9750	171.5647
	6	-1.224025	0.914691	-0.240218	187.2720	233.9276	246.2177
	6	0.178452	1.285649	0.259572	266.0114	282.3911	316.4382
	6	1.234075	0.329184	-0.317990	340.2027	370.6510	388.2205
	8	0.762574	-1.078769	-0.238564	398.3269	422.3689	440.1446
	8	-0.371988	-2.635514	0.513567	452.0896	501.8222	543.6929
	8	-2.861965	-0.902254	-0.252538	605.1263	646.2376	680.2103
	8	-2.210730	1.748873	0.307626	893.9162	931.5381	971.3360
	8	0.455206	2.591266	-0.209092	1004.3799	1025.2783	1044.4721
	6	2.576977	0.364234	0.385288	1076.0651	1093.7281	1099.0858
	8	3.405199	-0.587823	-0.234071	1110.6672	1122.5068	1143.0147
	1	-0.858028	-1.808275	-1.383176	1157.7659	1161.3084	1219.1178
	1	-1.533642	-0.544381	1.308480	1225.7260	1244.4503	1250.7375
	1	-1.227885	0.964010	-1.342110	1268.1188	1274.2058	1299.3449
	1	0.180147	1.241419	1.357058	1311.1693	1348.6398	1355.9916
	1	1.365248	0.521170	-1.386017	1363.7006	1376.7302	1382.0055
	1	0.728178	-2.088857	0.509623	1428.9101	1439.8746	1459.3152
	1	-3.484365	-0.189888	-0.053089	1468.1866	1511.8453	2098.6661
	1	-2.047609	2.649853	0.002605	2969.5962	2972.0123	2986.5359
	1	0.880526	3.109341	0.480996	3026.7711	3029.7280	3103.0021
	1	2.953280	1.392407	0.285595	3125.9601	3725.5399	3780.7395
	1	2.434880	0.158701	1.459532	3801.4039	3829.6043	3840.0749
	1	4.313074	-0.463127	0.061028			
	1	-0.433701	-3.491954	0.057188			

$TS_{G_1^+ \leftrightarrow G_2^+}^{R1 \leftrightarrow R1}$	6	0.648818	-1.248765	0.316314	-940.4442	71.2459	103.1352
	6	1.516879	-0.138191	-0.261924	118.1460	159.0066	181.9738
	6	1.009756	1.187601	0.241848	216.0960	252.8302	294.8139
	6	-0.484023	1.249230	-0.184238	296.9461	307.6128	329.1366
	6	-1.287583	-0.010313	0.231536	384.3498	399.0087	407.2597
	8	-0.601476	-1.232016	-0.214632	433.7569	472.0291	542.3615
	8	1.443469	-2.419323	-0.097992	560.1328	585.6914	596.5628
	8	2.844446	-0.600771	0.155214	630.9854	665.1271	717.4661
	8	1.772383	2.204417	-0.342938	856.6938	950.6949	970.3173
	8	-0.993966	2.403788	0.448672	999.6211	1015.7212	1026.2676
	6	-2.687057	-0.071423	-0.372204	1070.8534	1083.8354	1095.5923
	8	-3.431495	-1.149997	0.128576	1100.2585	1116.5323	1129.3183
	1	0.648228	-1.234452	1.417442	1155.8978	1197.1262	1203.6992
	1	1.472941	-0.176461	-1.355099	1229.5381	1239.0190	1245.7764
	1	1.055056	1.221194	1.341988	1272.5632	1311.3053	1342.5711
	1	-0.505336	1.346548	-1.279327	1351.4579	1361.1901	1394.4208
	1	-1.369835	-0.045223	1.326225	1405.7698	1415.8222	1421.9592
	1	1.322064	-3.191164	0.477243	1427.3188	1432.8383	1444.8108
	1	3.554954	-0.219414	-0.382019	1474.3549	1489.5732	1966.3600
	1	1.393149	3.050725	-0.073308	2990.4034	2997.2347	3002.2830
	1	-1.678301	2.806796	-0.095206	3011.6223	3038.0516	3081.6484
	1	-3.217745	0.840854	-0.082002	3089.9361	3749.1101	3766.1530
	1	-2.605926	-0.085759	-1.469745	3792.2026	3826.6926	3832.3757
	1	-3.106967	-1.960944	-0.276004			
	1	2.470097	-1.810326	0.006627			
$TS_{G_2^+ \leftrightarrow G_3^+}^{R1 \leftrightarrow R1}$	6	0.473978	1.508458	-0.329462	-961.7692	68.6177	101.7167
	6	1.437194	0.487818	0.268806	136.8044	150.5098	182.6281
	6	1.052637	-0.899239	-0.220143	215.7207	258.0126	279.4477
	6	-0.311252	-1.314710	0.277082	283.3346	309.7724	351.1761
	6	-1.264012	-0.180097	-0.213423	357.6035	382.7253	414.9505
	8	-0.779813	1.108580	0.202123	432.8799	479.0127	495.5106
	8	0.822155	2.752042	0.129844	528.8963	589.6479	607.8557
	8	2.885574	0.536632	-0.010872	633.2048	663.5825	704.5278
	8	2.226815	-1.662217	0.232576	874.5283	939.1130	957.2283
	8	-0.587773	-2.558147	-0.323024	1027.6575	1032.3832	1042.7133
	6	-2.680205	-0.305757	0.347231	1058.7039	1062.0130	1096.0543
	8	-3.546173	0.641008	-0.217932	1103.7229	1121.1754	1134.7462
	1	0.446439	1.447519	-1.433963	1152.2408	1172.9343	1202.1644
	1	1.380046	0.574816	1.354725	1222.2720	1231.4897	1260.1326
	1	1.049715	-0.943941	-1.316542	1285.7566	1309.0550	1331.9280
	1	-0.319071	-1.365120	1.374763	1349.0189	1365.2633	1376.6090
	1	-1.315370	-0.225722	-1.311604	1395.3053	1406.7251	1416.3288
	1	0.240684	3.419940	-0.254436	1427.0383	1445.7968	1466.0355
	1	2.966121	-0.694043	0.039751	1478.1377	1490.9131	1943.8931
	1	2.349063	-2.485673	-0.263244	2931.9502	2990.8902	3008.9208
	1	-1.306715	-2.999273	0.141350	3024.9125	3047.0637	3083.0848
	1	-3.077333	-1.291371	0.083169	3130.4423	3746.9673	3767.5815
	1	-2.636127	-0.235722	1.445190	3801.3772	3820.4207	3831.6543
	1	-3.295576	1.510490	0.112065			
	1	3.101802	0.966079	-0.853493			
$TS_{G_3^+ \leftrightarrow G_4^+}^{R1 \leftrightarrow R1}$	6	-0.523255	-1.514943	-0.213132	-909.5269	74.0165	95.9100
	6	-1.612294	-0.502922	0.236201	137.6804	144.6267	181.9221

	6	-1.122779	0.840130	-0.242464	219.5089	260.4548	295.5602
	6	0.267798	1.143304	0.292456	314.6575	355.5363	367.8884
	6	1.258800	0.123557	-0.268019	375.5350	404.6470	412.5802
	8	0.771754	-1.111906	0.252698	427.6699	485.8902	531.4192
	8	-0.859380	-2.714199	0.367577	566.6098	585.0570	603.3662
	8	-2.849346	-0.740511	-0.375012	637.0189	678.1489	721.4799
	8	-1.849260	2.037224	0.205004	885.4183	938.6056	971.1858
	8	0.370445	2.569307	-0.113859	998.8723	1017.9861	1029.5791
	6	2.699289	0.285043	0.217139	1062.0321	1086.7041	1101.0962
	8	3.532008	-0.688955	-0.345709	1107.9567	1121.8832	1137.0762
	1	-0.506864	-1.565078	-1.315659	1145.6065	1182.9656	1215.7033
	1	-1.665058	-0.534364	1.334047	1218.5484	1234.8667	1251.0279
	1	-1.121768	0.858338	-1.338501	1288.7861	1323.3874	1330.6948
	1	0.283310	1.113463	1.385795	1340.9143	1372.2415	1384.7150
	1	1.244908	0.127582	-1.367869	1402.4765	1408.8388	1419.8644
	1	-0.373357	-3.435569	-0.049029	1428.3859	1448.4881	1460.4533
	1	-3.154556	-1.618300	-0.113787	1470.6985	1492.3289	1956.9887
	1	-2.645713	2.201137	-0.322264	2963.7662	2985.2785	3014.2677
	1	0.946577	3.087798	0.467796	3020.3358	3059.6624	3068.3224
	1	3.083315	1.257355	-0.113114	3090.8212	3762.1366	3765.8379
	1	2.708905	0.266614	1.318532	3800.0316	3808.8089	3814.0822
	1	3.284337	-1.544729	0.021987			
	1	-0.819162	2.733063	0.033397			
$TS_{G_4^+ \leftrightarrow G_4^+}^{R1 \leftrightarrow R2}$	6	0.950681	-1.404211	0.224428	-90.1157	73.5322	126.3696
	6	1.735591	-0.141284	-0.186792	140.3986	197.4969	213.3618
	6	0.902690	1.061473	0.228216	225.7123	249.7843	259.7020
	6	-0.482992	0.935628	-0.363073	280.6826	326.6752	351.1047
	6	-1.206275	-0.312002	0.131316	366.2314	398.8042	405.1750
	8	-0.375899	-1.366484	-0.335538	425.0714	448.1300	467.1833
	8	1.625530	-2.476408	-0.306480	487.4173	551.0879	568.8355
	8	2.960504	-0.018168	0.484598	601.8346	642.8618	790.5976
	8	1.351843	2.337860	-0.221660	891.6423	910.5060	975.0134
	8	-1.103042	2.264121	0.110179	1002.8546	1017.6814	1037.7976
	6	-2.633742	-0.505480	-0.432547	1056.3686	1071.2721	1101.6037
	8	-3.591563	-0.657628	0.582815	1103.6127	1122.6025	1138.9225
	1	0.867825	-1.452023	1.324101	1174.4544	1197.3500	1217.0926
	1	1.855305	-0.165230	-1.280047	1230.5906	1236.7260	1254.0919
	1	0.832332	1.061245	1.326385	1294.0286	1309.3202	1328.4186
	1	-0.471909	0.998768	-1.453421	1339.1634	1366.2423	1376.1120
	1	-1.273010	-0.293777	1.228988	1394.2183	1404.2893	1421.6048
	1	1.305858	-3.299118	0.081911	1428.9944	1451.6269	1467.2523
	1	3.528017	-0.754058	0.224766	1487.6087	1590.3197	2963.0466
	1	2.203722	2.547726	0.183068	2999.6464	3003.0707	3013.0944
	1	-1.848456	2.577295	-0.431104	3020.1048	3067.6671	3114.1475
	1	-2.934499	0.375054	-1.018485	3114.3162	3720.3967	3795.1179
	1	-2.598548	-1.349839	-1.130512	3804.7089	3810.0523	3832.4188
	1	-3.697815	-1.592075	0.786569			
	1	-0.303528	2.874936	0.037184			
$TS_{G_5^+ \leftrightarrow G_4^+}^{R1 \leftrightarrow R2}$	6	1.354661	-1.172341	0.265229	-472.0636	69.4163	90.3196
	6	1.711632	0.257037	-0.169532	107.1477	185.0076	234.1032
	6	0.602014	1.271621	0.169453	247.5733	270.6979	278.9163
	6	-0.737465	0.709077	-0.278945	288.5818	335.9311	348.5472

	6	-0.957643	-0.726698	0.237768	370.8213	399.5961	414.9319
	8	0.054374	-1.547100	-0.255288	441.7301	455.6275	479.5400
	8	2.297968	-2.005189	-0.281101	532.3101	542.1192	575.8404
	8	2.862403	0.696142	0.498026	602.9761	650.0660	739.2745
	8	0.944860	2.505046	-0.426288	873.7300	933.7808	974.9230
	8	-1.875277	1.487111	0.317129	987.5642	1010.6134	1020.1174
	6	-2.291115	-1.306631	-0.242923	1052.0693	1067.0218	1117.8973
	8	-3.361064	-0.343556	0.076096	1122.6091	1136.2817	1139.2116
	1	1.311155	-1.236510	1.365523	1157.2175	1179.3182	1200.8077
	1	1.840490	0.241793	-1.262255	1213.8060	1243.0374	1260.6019
	1	0.575502	1.390028	1.263826	1306.4556	1308.6359	1327.3623
	1	-0.849190	0.748460	-1.368224	1334.6658	1347.8862	1364.6278
	1	-0.956676	-0.689879	1.342115	1377.3117	1404.2622	1408.0657
	1	2.279458	-2.865326	0.153622	1417.6933	1441.3471	1470.5603
	1	3.611112	0.179852	0.177712	1492.5011	1506.3393	1832.6556
	1	0.202762	2.926692	-0.866654	2952.7549	2971.6369	2996.6054
	1	-2.008411	2.356925	-0.087111	3012.5027	3069.0621	3101.7311
	1	-2.299481	-1.430444	-1.327082	3169.5004	3766.0800	3792.0279
	1	-2.510902	-2.261338	0.234152	3812.1665	3813.8286	3848.0986
	1	-3.906278	-0.643734	0.815762			
	1	-2.768155	0.751464	0.243722			
$TS_{G_3^+ \leftrightarrow G_3^+}^{R1 \leftrightarrow R2}$	6	-0.829089	-1.456704	-0.271181	-92.4997	59.1073	88.3388
	6	-1.645989	-0.232708	0.189706	130.9511	146.0192	210.8249
	6	-0.868293	0.981227	-0.224935	234.6907	256.5178	275.2191
	6	0.518285	1.067852	0.338218	278.7197	294.3291	314.9556
	6	1.232562	-0.240983	-0.111958	344.1866	380.2269	401.8005
	8	0.462470	-1.364803	0.309804	409.5359	417.1629	436.8861
	8	-1.493205	-2.556668	0.221973	484.0898	538.4742	564.3956
	8	-2.914181	-0.068628	-0.411910	603.0644	647.8097	779.4969
	8	-1.707710	2.175471	0.277002	839.6422	903.7841	966.7094
	8	1.054582	2.253624	-0.206471	999.8103	1025.9990	1046.8187
	6	2.654604	-0.369536	0.486074	1062.0696	1068.5743	1089.5243
	8	3.656867	-0.423511	-0.498015	1094.3746	1104.7715	1142.7081
	1	-0.744157	-1.469357	-1.372732	1146.8070	1188.9936	1221.7079
	1	-1.717111	-0.300341	1.283727	1230.0638	1244.6780	1263.7396
	1	-0.861931	1.107794	-1.310484	1279.6847	1310.0041	1330.9523
	1	0.484456	1.092104	1.437040	1344.7991	1357.7681	1372.0762
	1	1.331835	-0.215734	-1.207697	1380.5149	1406.3947	1416.4915
	1	-1.120056	-3.364115	-0.151053	1438.5471	1450.1041	1465.7676
	1	-3.482935	-0.808655	-0.164523	1493.0835	1556.6794	2951.7052
	1	-2.634441	1.998374	-0.004652	3000.6434	3015.9223	3023.1775
	1	1.953765	2.396421	0.110954	3035.4002	3067.7608	3105.5743
	1	2.883293	0.502943	1.111070	3521.0919	3689.5340	3800.4625
	1	2.651427	-1.242592	1.149478	3809.5333	3813.6716	3829.1326
	1	3.771198	-1.334409	-0.786537			
	1	-1.358415	3.018799	-0.069203			
$TS_{G_4^+ \leftrightarrow G_3^+}^{R2 \leftrightarrow R2}$	6	1.383036	-1.141184	0.278580	-1023.5361	79.9361	102.9443
	6	1.688445	0.278199	-0.289007	152.6042	172.3603	200.5946
	6	0.563082	1.139824	0.216605	221.0406	270.0344	279.2761
	6	-0.781056	0.579011	-0.194456	293.6364	334.8245	358.4246
	6	-1.002412	-0.804635	0.404763	389.0537	403.2847	424.0568
	8	0.072061	-1.591301	-0.085825	437.5447	466.0628	525.0481
	8	2.314558	-1.975967	-0.291515			

	8	2.889851	0.794710	0.210273	581.5070	616.4104	627.1994
	8	0.416124	2.512866	-0.322361	632.3627	679.9207	693.8380
	8	-1.641762	1.668822	0.237993	919.9042	936.0284	995.6881
	6	-2.307859	-1.415353	-0.108999	1003.1913	1017.0306	1028.4276
	8	-3.284377	-0.371981	-0.062089	1060.6387	1081.2070	1088.2712
	1	1.458249	-1.110292	1.379985	1116.9697	1125.1091	1146.5045
	1	1.675402	0.208603	-1.386033	1155.4689	1183.4718	1216.2728
	1	0.630178	1.236877	1.305516	1226.7027	1240.6537	1257.4808
	1	-0.841098	0.504302	-1.286060	1268.9427	1297.6663	1316.0085
	1	-1.001504	-0.744642	1.503358	1335.8633	1348.7743	1373.0016
	1	2.323564	-2.825506	0.165129	1395.6430	1405.2144	1419.6903
	1	3.605859	0.203838	-0.054626	1428.1704	1455.0173	1465.8278
	1	0.979697	3.154505	0.135872	1469.4943	1524.1123	1969.1045
	1	-2.549725	1.507134	-0.081901	2955.5273	3005.5292	3022.7472
	1	-2.144085	-1.766505	-1.135793	3029.6524	3059.8280	3076.0484
	1	-2.601203	-2.268076	0.511748	3088.6044	3640.1428	3764.1578
	1	-4.145357	-0.727521	-0.303886	3798.9704	3807.9643	3836.6074
	1	-0.781026	2.514920	-0.090041			
$TS_{G_3^+ \leftrightarrow G_2^+}^{R2 \leftrightarrow R2}$	6	1.146549	-1.336011	0.375816	-935.7893	65.6095	108.0112
	6	1.561204	-0.014074	-0.253666	145.1986	175.4770	210.0543
	6	0.631753	1.089735	0.208189	229.8351	266.6771	272.5693
	6	-0.786992	0.857213	-0.253035	297.4791	338.1993	344.8603
	6	-1.144998	-0.569875	0.277248	390.9892	405.4435	441.5924
	8	-0.170438	-1.539363	-0.117486	465.6247	515.4600	556.4421
	8	1.987840	-2.307840	-0.108672	562.0921	584.3218	616.7935
	8	2.859590	0.579300	0.121533	660.1967	672.0204	716.4782
	8	1.350991	2.263794	-0.311720	895.9822	952.7105	970.2554
	8	-1.569202	1.867851	0.315127	1008.2468	1017.0745	1064.5633
	6	-2.477077	-1.066219	-0.282758	1067.8613	1086.1577	1093.6261
	8	-3.449076	-0.079005	0.033733	1094.8748	1121.4906	1141.2175
	1	1.137764	-1.279925	1.477971	1160.4690	1186.8373	1214.5933
	1	1.547051	-0.137951	-1.339614	1220.5679	1241.6266	1254.2998
	1	0.638768	1.169791	1.301303	1285.1962	1304.8361	1314.8025
	1	-0.831589	0.853041	-1.354159	1337.7276	1359.5556	1369.0191
	1	-1.210596	-0.507096	1.374406	1393.1701	1409.3760	1416.5955
	1	1.784840	-3.156202	0.304047	1438.9308	1450.9368	1476.6153
	1	3.593498	0.232143	-0.408183	1483.2441	1525.4239	1964.7546
	1	1.115170	3.073945	0.164474	2968.2191	2983.6352	3000.5778
	1	-2.496290	1.591889	0.228279	3014.3410	3060.4013	3064.1871
	1	-2.375442	-1.208125	-1.367476	3102.5162	3684.6519	3760.9095
	1	-2.717617	-2.035490	0.170533	3768.5345	3805.4618	3837.2449
	1	-4.300927	-0.332714	-0.334793			
	1	2.455097	1.694175	-0.107666			
$TS_{G_2^+ \leftrightarrow G_1^+}^{R2 \leftrightarrow R2}$	6	1.163964	-1.070962	0.352328	-905.3143	66.5106	100.6718
	6	1.520376	0.268338	-0.281032	132.8557	171.3009	204.9237
	6	0.562132	1.311648	0.228493	227.3367	261.8700	289.5450
	6	-0.850952	0.789265	-0.144497	302.2652	342.2922	375.3206
	6	-1.101189	-0.683498	0.286158	396.8393	401.1185	426.3862
	8	-0.009300	-1.563398	-0.126039	465.8503	531.0452	543.2835
	8	2.331241	-1.862990	-0.075423	550.3611	586.6938	607.3901
	8	2.936840	0.359469	0.084232			

	8	0.856568	2.530382	-0.393341	629.4954	664.0610	721.8774
	8	-1.736648	1.669325	0.493312	907.0190	959.8287	974.7631
	6	-2.351207	-1.278382	-0.359871	1000.1556	1005.0611	1022.6968
	8	-3.427801	-0.419576	-0.022366	1081.5504	1089.2109	1091.7940
	1	1.193980	-1.022219	1.452099	1114.3099	1130.8675	1140.1118
	1	1.454774	0.183366	-1.370446	1157.5855	1204.1318	1209.0803
	1	0.624973	1.385758	1.325699	1233.7446	1248.8435	1256.9389
	1	-0.936101	0.847149	-1.242880	1280.2829	1306.1635	1314.2094
	1	-1.191573	-0.716321	1.380683	1339.3988	1354.0163	1390.7731
	1	2.534608	-2.604346	0.516531	1392.7618	1420.6158	1422.5602
	1	3.424920	0.971494	-0.486356	1430.2754	1440.8223	1468.8763
	1	0.154856	3.154480	-0.166314	1481.3374	1525.8201	1971.9771
	1	-2.637446	1.361089	0.309850	2966.5523	2992.2884	3002.4196
	1	-2.194384	-1.333346	-1.446375	3006.8327	3027.8724	3058.6009
	1	-2.505064	-2.296741	0.018620	3081.8264	3714.2162	3749.4635
	1	-4.237039	-0.738765	-0.433881	3769.4871	3788.1152	3835.8806
	1	3.047545	-0.915758	-0.029696			
$TS_{G_1^+ \leftrightarrow G_6^+}^{R2 \leftrightarrow R2}$	6	1.330614	-1.157572	0.445111	-1513.1969	56.2537	91.6214
	6	1.678921	0.147745	-0.237051	111.4230	145.0309	202.7046
	6	0.690128	1.220154	0.231218	216.6508	236.6649	243.1409
	6	-0.737564	0.846315	-0.182428	284.9759	317.8879	331.0550
	6	-1.155503	-0.503395	0.431678	377.4834	396.4402	408.8611
	8	-0.066709	-1.505374	0.319172	418.7692	436.1978	448.4813
	8	1.703951	-2.360712	-0.301240	504.3776	508.9402	535.0927
	8	3.008330	0.427313	0.083727	592.1940	625.6184	766.2093
	8	1.123986	2.404342	-0.383199	911.9610	930.5313	973.6825
	8	-1.560196	1.869748	0.310960	1001.6492	1011.7739	1036.3834
	6	-2.373879	-1.143715	-0.234283	1072.6708	1093.6879	1108.4642
	8	-3.385729	-0.159796	-0.184217	1116.6415	1124.4520	1130.8170
	1	1.686728	-1.246661	1.471301	1156.8402	1167.3117	1215.2550
	1	1.535766	0.024427	-1.327327	1238.7087	1252.3795	1258.6887
	1	0.727138	1.304005	1.330269	1264.4543	1276.6230	1287.1273
	1	-0.778750	0.780980	-1.281915	1318.4932	1345.5857	1355.6704
	1	-1.323825	-0.373027	1.503996	1357.4953	1374.3576	1397.3253
	1	0.464389	-2.337241	-0.437802	1420.8893	1448.0325	1455.0812
	1	3.162584	1.362660	-0.110752	1473.9985	1526.1995	2106.1270
	1	0.514819	3.113193	-0.139969	2931.1829	2972.6728	2983.6206
TS1	1	-2.473085	1.672882	0.057166	2988.3660	3045.0629	3099.7016
	1	-2.116810	-1.413603	-1.270751	3152.7013	3717.1882	3753.6212
	1	-2.655543	-2.057999	0.304110	3766.2050	3794.4064	3832.1399
	1	-4.211096	-0.519674	-0.525107			
	1	2.282302	-2.171301	-1.060315			
	6	-1.550641	-1.128366	-0.303703	-245.5247	42.8165	82.4127
	6	-1.788720	0.270773	0.268428	85.9592	127.8152	157.7384
	6	-0.268709	1.477329	-0.327902	197.7677	209.0889	244.6166
	6	0.507822	0.576334	0.365912	257.1563	267.0315	286.8601
	6	0.785957	-0.792941	-0.215351	296.3274	305.2788	329.9133
	8	-0.313713	-1.614047	0.175811	356.9133	358.7017	408.7104
	8	-2.571536	-1.895453	0.209125	434.1146	448.1719	467.6646
	8	-2.792221	0.940051	-0.303797	499.5414	514.0603	553.6773
	8	-0.570594	2.672931	0.207002	607.2341	647.2845	694.1816
	8	2.620218	1.657668	0.004706			

	6	2.042757	-1.492602	0.307027	909.5838	924.0913	991.2848
	8	3.165777	-0.963252	-0.381930	1019.9406	1032.3182	1041.9574
	1	-1.546403	-1.093355	-1.406904	1071.4823	1093.5976	1106.7287
	1	-1.756059	0.297002	1.358094	1130.1546	1174.0340	1178.6060
	1	-0.388021	1.363699	-1.403561	1202.2657	1216.0869	1245.7998
	1	0.689219	0.740228	1.422601	1264.0437	1275.1463	1299.0245
	1	0.854423	-0.729846	-1.310983	1315.4061	1327.1433	1346.6489
	1	-2.560835	-2.768864	-0.201309	1374.8964	1414.6954	1424.5326
	1	-3.193947	1.566530	0.312649	1460.0288	1498.9675	1517.7412
	1	-0.955064	3.254874	-0.458625	1649.6000	1656.3472	2967.1461
	1	3.155027	0.865882	-0.186748	3010.0357	3020.7018	3077.2181
	1	2.127755	-1.364457	1.394711	3131.8281	3155.0637	3211.2565
	1	1.913754	-2.560096	0.096951	3615.9299	3786.5575	3802.2739
	1	3.934198	-1.518884	-0.214638	3819.6148	3829.7176	3845.7724
	1	3.051696	2.100952	0.743959			
TS2	6	-1.178707	-1.636844	0.193705	-61.9619	81.1243	109.3773
	6	0.178468	-1.355877	-0.449370	123.8391	175.7158	197.0466
	6	1.651810	0.795455	-0.399489	210.1016	240.4226	279.9405
	6	0.228490	0.175261	-0.527674	331.8123	337.9991	344.2370
	6	-0.764328	0.611732	0.593718	412.9557	436.9640	449.3765
	8	-1.292184	-0.608087	1.148560	467.1755	505.5052	555.7337
	8	-2.098388	-1.565381	-0.847740	592.5865	653.9631	675.5895
	8	1.254138	-1.838014	0.486324	764.7163	785.3685	810.8594
	8	2.580472	-0.263335	-0.746930	862.5173	907.6120	948.3157
	8	1.991296	1.175577	0.896565	989.8619	994.2250	1015.4208
	6	-1.833527	1.563116	0.068236	1053.0936	1073.6959	1079.9233
	8	-1.083299	2.669198	-0.415223	1090.7653	1121.5406	1124.4470
	1	-1.226071	-2.587558	0.737544	1134.6650	1204.2833	1218.7458
	1	0.372673	-1.900106	-1.369265	1227.7754	1243.2749	1252.5812
	1	1.774115	1.617322	-1.108748	1259.7812	1295.6627	1325.6674
	1	-0.168303	0.461196	-1.503295	1339.3777	1354.9637	1362.8680
	1	-0.236725	1.110083	1.406661	1387.4732	1392.6249	1433.3285
	1	-2.974879	-1.796214	-0.517116	1445.2873	1453.6889	1464.2616
	1	2.090311	-1.287596	0.100443	1532.0409	1587.9039	2179.1787
	1	3.485323	0.054427	-0.611468	3015.3497	3059.2573	3061.3203
	1	1.044684	-1.556096	1.397569	3093.2311	3109.5459	3123.5792
	1	-2.420694	1.081033	-0.724184	3181.5775	3656.0726	3763.3332
	1	-2.509158	1.843862	0.886204	3807.2329	3818.7606	3834.2359
	1	-1.685797	3.348900	-0.732821			
	1	1.944999	2.134030	0.991271			
TS3	6	0.099882	1.639562	0.244933	-1021.6563	82.0162	97.5645
	6	-0.569368	0.781446	-0.806350	105.5442	139.7004	166.8222
	6	-1.974177	-0.493698	0.300781	210.0454	218.5575	237.0651
	6	-0.167283	-0.554425	-0.589577	249.1875	295.8330	410.7591
	6	0.841425	-0.550125	0.537531	449.0558	508.9336	528.3626
	8	0.639475	0.728805	1.175301	574.7240	634.4021	671.4558
	8	1.089768	2.375842	-0.444756	769.8904	791.5004	826.1625
	8	-2.708345	-1.614646	0.234679	878.5176	940.0967	945.2534
	8	-2.428811	0.552879	-0.318410	997.8472	1039.1677	1060.8806
	6	2.299244	-0.712122	0.097932	1066.3086	1079.2360	1088.7924
	8	2.421404	-2.026466	-0.423987			
	1	-0.576905	2.304641	0.792502			

	1	-0.868966	1.236538	-1.739320	1098.3494	1118.4517	1195.6880
	1	-1.501205	-0.432576	1.287415	1207.9405	1226.4277	1242.3079
	1	-0.105930	-1.286838	-1.383365	1293.3133	1300.0805	1325.8681
	1	0.632441	-1.313604	1.299618	1331.6406	1371.1632	1386.3505
	1	1.596882	2.857251	0.218734	1428.8400	1432.9187	1453.6609
	1	-3.272835	-1.516139	-0.547427	1489.4897	1525.3855	2977.0919
	1	2.537522	0.055988	-0.650695	3006.3855	3035.4336	3042.6956
	1	2.952281	-0.557434	0.971168	3053.9660	3213.8793	3232.8488
	1	3.320466	-2.142956	-0.742754	3738.9511	3808.0766	3839.7030
TS4	6	-1.550641	-1.128366	-0.303703	-245.5247	42.8165	82.4127
	6	-1.788720	0.270773	0.268428	85.9592	127.8152	157.7384
	6	-0.268709	1.477329	-0.327902	197.7677	209.0889	244.6166
	6	0.507822	0.576334	0.365912	257.1563	267.0315	286.8601
	6	0.785957	-0.792941	-0.215351	296.3274	305.2788	329.9133
	8	-0.313713	-1.614047	0.175811	356.9133	358.7017	408.7104
	8	-2.571536	-1.895453	0.209125	434.1146	448.1719	467.6646
	8	-2.792221	0.940051	-0.303797	499.5414	514.0603	553.6773
	8	-0.570594	2.672931	0.207002	607.2341	647.2845	694.1816
	8	2.620218	1.657668	0.004706	909.5838	924.0913	991.2848
	6	2.042757	-1.492602	0.307027	1019.9406	1032.3182	1041.9574
	8	3.165777	-0.963252	-0.381930	1071.4823	1093.5976	1106.7287
	1	-1.546403	-1.093355	-1.406904	1130.1546	1174.0340	1178.6060
	1	-1.756059	0.297002	1.358094	1202.2657	1216.0869	1245.7998
	1	-0.388021	1.363699	-1.403561	1264.0437	1275.1463	1299.0245
	1	0.689219	0.740228	1.422601	1315.4061	1327.1433	1346.6489
	1	0.854423	-0.729846	-1.310983	1374.8964	1414.6954	1424.5326
	1	-2.560835	-2.768864	-0.201309	1460.0288	1498.9675	1517.7412
	1	-3.193947	1.566530	0.312649	1649.6000	1656.3472	2967.1461
	1	-0.955064	3.254874	-0.458625	3010.0357	3020.7018	3077.2181
	1	3.155027	0.865882	-0.186748	3131.8281	3155.0637	3211.2565
	1	2.127755	-1.364457	1.394711	3615.9299	3786.5575	3802.2739
	1	1.913754	-2.560096	0.096951	3819.6148	3829.7176	3845.7724
	1	3.934198	-1.518884	-0.214638			
	1	3.051696	2.100952	0.743959			
TS5	6	-1.239873	1.351368	0.438126	-295.9312	67.3426	90.1228
	6	-1.251753	0.151376	-0.374801	105.1043	130.5261	176.9727
	6	-0.589896	-1.106106	0.115296	196.8049	202.6649	234.1008
	6	0.930016	-0.899873	-0.093526	252.1340	266.0493	272.1907
	6	1.194416	0.577097	0.239659	297.6436	364.8078	381.9253
	8	0.079543	1.301207	-0.370373	383.8406	421.0816	450.4730
	8	-2.026940	2.349017	0.047756	461.9283	481.1479	485.4744
	8	-3.293956	-0.735912	0.214040	522.3912	533.4528	546.4511
	8	-1.106655	-2.194212	-0.608944	611.6762	636.7813	721.0360
	8	1.595735	-1.812524	0.720323	915.2236	953.8526	980.3941
	6	2.481224	1.112506	-0.384571	1038.4543	1048.4556	1085.1868
	8	3.480216	0.192099	0.018580	1093.4409	1110.0276	1119.7518
	1	-1.008958	1.268328	1.500656	1143.4399	1152.5524	1159.3331
	1	-1.659975	0.214603	-1.374106	1207.4179	1233.6104	1248.7406
	1	-0.765049	-1.220273	1.194477	1262.3842	1272.1781	1297.1535
	1	1.138326	-1.057404	-1.164059	1321.9195	1329.0761	1336.5063
	1	1.188876	0.729926	1.324535			
	1	-1.935144	3.122406	0.619812			
	1	-3.151062	-1.637355	-0.108884			

	1	-0.610963	-2.983365	-0.354439	1353.5669	1390.4955	1419.5100
	1	2.545221	-1.687577	0.581412	1458.0245	1466.2535	1525.4936
	1	2.361684	1.143222	-1.476911	1570.9319	1631.8878	2987.4172
	1	2.686964	2.129740	-0.029100	3007.0902	3017.9532	3052.2545
	1	4.338210	0.481160	-0.308367	3070.4912	3129.5014	3255.5985
	1	-4.096472	-0.419027	-0.217183	3743.9768	3761.7253	3789.9356
					3791.1279	3833.2858	3860.4160
TS6	6	1.095379	-1.164681	0.207144	-220.7398	59.8559	86.5945
	6	1.379114	0.232836	-0.284046	113.9002	124.0956	167.8924
	6	0.769939	1.336042	0.285861	186.6727	195.7597	210.8390
	6	-0.954817	0.726707	-0.482249	217.5325	259.5549	296.2454
	6	-1.190233	-0.630624	0.160750	315.5144	339.3971	361.1356
	8	-0.206287	-1.517751	-0.297217	380.7746	383.9063	403.8542
	8	2.027870	-2.013344	-0.342663	407.5023	443.4954	481.2775
	8	3.562261	0.148239	0.528028	498.7143	519.5652	531.4894
	8	1.016081	2.551861	-0.248414	571.2080	589.3656	672.4695
	8	-1.763073	1.741561	-0.167690	897.9681	932.9586	969.3350
	6	-2.599533	-1.148184	-0.156222	1027.9400	1033.7488	1058.9930
	8	-3.448323	-0.268294	0.573880	1063.5299	1094.6278	1127.9250
	1	1.066918	-1.208354	1.307187	1141.3081	1151.7692	1180.7316
	1	1.783130	0.314153	-1.288198	1218.5421	1227.0035	1250.3194
	1	0.472287	1.302237	1.333805	1268.8151	1284.3212	1316.1829
	1	-0.716192	0.716765	-1.544676	1329.6923	1335.6381	1349.1564
	1	-1.152924	-0.519649	1.257443	1377.7987	1409.1751	1447.9460
	1	1.867808	-2.912000	-0.028040	1467.5646	1474.1069	1523.5068
	1	4.167281	0.796214	0.146365	1623.6908	1629.2189	2972.1649
	1	0.421070	3.210517	0.131423	2991.7387	3029.7025	3081.6639
	1	-2.404621	1.442951	0.507511	3128.5885	3147.7940	3207.5630
	1	-2.798736	-1.121120	-1.234535	3588.3461	3758.6889	3799.9291
	1	-2.683199	-2.183375	0.193431	3800.5642	3830.3024	3867.5186
	1	-4.361489	-0.378800	0.288705			
	1	3.831327	-0.710288	0.174760			

Table S3. Total electronic energies (E_{298K}) at B3LYP/6-31G(2df,p) and SMD/B3LYP/6-31G(2df,p) methods, enthalpies (H_{298K}) and Gibbs free energies (G_{298K}) at G4MP2 method of all optimized geometries. All energies are in Hartree.

Species	G4MP2		B3LYP/6-31G(2df,p)	SMD/B3LYP/ 6-31G(2df,p)
	Enthalpy, H_{298K} (Hartree)	Free energy, G_{298K} (Hartree)	Total energy, E_{298K} (Hartree)	Total energy, E_{298K} (Hartree)
$\alpha - R1$	-686.369583	-686.420966	-687.2204402	-687.2513520
$\alpha - R2$	-686.370855	-686.421942	-687.2221990	-687.2506828
$\beta - R1$	-686.368040	-686.419718	-687.2185992	-687.2509532
$\beta - R2$	-686.369134	-686.420448	-687.2203019	-687.2498582
$\alpha - R1G_1^+$	-686.678497	-686.732440	-687.5596561	-687.6701322
$\alpha - R1G_2^+$	-686.671570	-686.723248	-687.5486175	-687.6702909
$\alpha - R1G_3^+$	-686.678201	-686.730451	-687.5555862	-687.6759590
$\alpha - R1G_4^+$	-686.670068	-686.722149	-687.5471095	-687.6694727
$\alpha - R1G_5^+$	-686.682371	-686.733369	-687.5595485	-687.6729008
$\alpha - R1G_6^+$	-686.685887	-686.737738	-687.5631742	-687.6722600
$\alpha - R2G_1^+$	-686.682979	-686.735736	-687.5654886	-687.6692236
$\alpha - R2G_2^+$	-686.685103	-686.736156	-687.5639260	-687.6727030
$\alpha - R2G_3^+$	-686.685146	-686.737191	-687.5618831	-687.6717621
$\alpha - R2G_4^+$	-686.691172	-686.741901	-687.5692466	-687.6802519
$\alpha - R1G_6^+$	-686.671837	-686.725173	-687.5526181	-687.6643188
$\beta - R1G_1^+$	-686.664823	-686.717635	-687.5411477	-687.6631807
$\beta - R1G_2^+$	-686.673193	-686.725662	-687.5490172	-687.6714241
$\beta - R1G_3^+$	-686.675000	-686.728344	-687.5510101	-687.6733213
$\beta - R1G_4^+$	-686.668416	-686.720577	-687.5454483	-687.6698823
$\beta - R1G_5^+$	-686.681099	-686.732561	-687.5572269	-687.6719848
$\beta - R1G_6^+$	-686.686574	-686.738403	-687.5641768	-687.6729887
$\beta - R2G_1^+$	-686.669438	-686.721366	-687.5470630	-687.6618299
$\beta - R2G_2^+$	-686.679281	-686.730886	-687.5564393	-687.6702707
$\beta - R2G_3^+$	-686.683881	-686.735702	-687.5608469	-687.6721940
$\beta - R2G_4^+$	-686.690432	-686.741225	-687.5684225	-687.6796130
$\beta - R1G_6^+$	-686.672719	-686.725488	-687.5522434	-687.6679404
$TS_{G_5^+ \leftrightarrow G_6^+}^{R1 \leftrightarrow R1}$	-686.680152	-686.730190	-687.5559199	-687.6687739
$TS_{G_6^+ \leftrightarrow G_1^+}^{R1 \leftrightarrow R1}$	-686.639957	-686.692803	-687.5140646	-687.6285533
$TS_{G_1^+ \leftrightarrow G_2^+}^{R1 \leftrightarrow R1}$	-686.661568	-686.712360	-687.5375717	-687.6577751
$TS_{G_2^+ \leftrightarrow G_3^+}^{R1 \leftrightarrow R1}$	-686.663579	-686.714472	-687.5396613	-687.6620111
$TS_{G_3^+ \leftrightarrow G_4^+}^{R1 \leftrightarrow R1}$	-686.667951	-686.718410	-687.5445589	-687.6649880
$TS_{G_4^+ \leftrightarrow G_3^+}^{R2 \leftrightarrow R2}$	-686.679276	-686.729239	-687.5556478	-687.6612932
$TS_{G_3^+ \leftrightarrow G_2^+}^{R2 \leftrightarrow R2}$	-686.675854	-686.725830	-687.5529187	-687.6635456

$TS_{G_2^+ \leftrightarrow G_1^+}^{R2 \leftrightarrow R2}$	-686.666895	-686.716926	-687.5440442	-687.6567024
$TS_{G_1^+ \leftrightarrow G_6^+}^{R2 \leftrightarrow R2}$	-686.639186	-686.690938	-687.5148854	-687.6265342
$TS_{G_4^+ \leftrightarrow G_4^+}^{R1 \leftrightarrow R2}$	-686.667951	-686.718410	-687.5445589	-687.6649880
$TS_{G_5^+ \leftrightarrow G_4^+}^{R1 \leftrightarrow R2}$	-686.671487	-686.723116	-687.5462520	-687.6668542
$TS_{G_3^+ \leftrightarrow G_3^+}^{R1 \leftrightarrow R2}$	-686.673081	-686.725917	-687.5471289	-687.6662300
I1	-686.697931	-686.749476	-687.5779091	-687.6851751
I2	-686.700344	-686.752365	-687.5786158	-687.6885843
I3	-609.993867	-610.041591	-610.7645516	-610.7896235
I4	-420.752510	-420.794986	-421.3434753	-421.4444910
I5	-420.439932	-420.481786	-421.0021884	-421.0181551
I6	-420.772428	-420.819796	-421.3596514	-421.4508899
I7	-344.403662	-344.441867	-344.9133980	-345.0103527
I8	-610.339205	-610.388228	-611.1363707	-611.2368759
I9	-610.007846	-610.059026	-610.7767521	-610.8026937
I10	-610.289475	-610.338976	-611.0853871	-611.2162694
I11	-533.934274	-533.981247	-534.6499970	-534.7673392
I12	-533.646269	-533.691906	-534.3383050	-534.3563136
I13	-533.937046	-533.982187	-534.6532455	-534.7772510
I14	-457.593189	-457.635679	-458.2314871	-458.3326978
I15	-686.680300	-686.732398	-687.5613230	-687.6720464
I16	-686.354295	-686.412413	-687.2072325	-687.2359950
I17	-610.281250	-610.332349	-611.0768274	-611.2075416
I18	-609.995907	-610.046778	-610.7670825	-610.7899044
I19	-533.634011	-533.681216	-534.3246651	-534.3409934
I20	-533.934846	-533.982222	-534.6518311	-534.7591777
I21	-457.594738	-457.638512	-458.2304116	-458.3287834
I22	-686.691309	-686.744315	-687.5713416	-687.6817864
I23	-686.363841	-686.421309	-687.2157945	-687.2485370
I24	-610.306570	-610.356418	-611.1039198	-611.2174785
I25	-533.949477	-533.997397	-534.6623291	-534.7697866
I26	-533.639547	-533.686232	-534.3326684	-534.3534643
I27	-533.961357	-534.013344	-534.6770231	-534.7739334
I28	-457.593981	-457.637576	-458.2291856	-458.3348026
TS1	-686.640664	-686.695935	-687.5218240	-687.6272575
TS2	-686.662741	-686.713320	-687.5408493	-687.6436180
TS3	-609.909915	-609.958903	-610.6833155	-610.7068634
TS4	-686.640664	-686.695935	-687.5218240	-687.6272575
TS5	-686.655033	-686.708882	-687.5303504	-687.6313957
TS6	-686.642901	-686.697708	-687.5259595	-687.6259348
FAL	-344.092030	-344.128350	-344.5739176	-344.5811077
5HMF2	-457.296424	-457.339755	-457.9099429	-457.9215319
5HMF3	-457.297463	-457.341618	-457.9074526	-457.9187467
5HMF4	-457.301344	-457.342822	-457.9154243	-457.9230521
HCOOH	-189.563644	-189.591842	-189.7752894	-189.7821222
H ₂ O	-76.352071	-76.373498	-76.42607790	-76.4368389