

Electronic Supplementary Information

A Theoretical Study on the Mechanism of Ruthenium(II)-Catalyzed Phosphoryl-Directed *ortho*-Selective C–H Bond Activations: the Hydroxy Group of Phosphoryl Triggered Ru(II)/Ru(0) Catalytic Cycle

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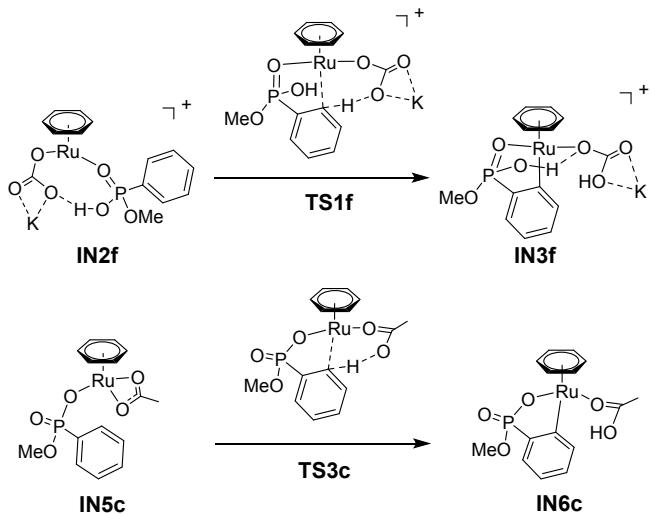
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The Effects of Different Density Functionals:

It should be noted that different density functionals may vary from each other in predicting reaction barriers. Our evaluation of three typical density functionals (B3LYP, B3PW91 and PBE1PBE) showed that they predicted similar results and led to the same discussion and conclusions for the studied catalytic systems.

Table S1. Relative free energies (kcal mol⁻¹) using different functionals



Functional	IN2f	TS1f	IN3f	IN5c	TS3c	IN6c
B3LYP	0	23.8	2.1	0	21.9	9.5
B3PW91	0	23.1	8.8	0	21.4	9.5
PBE1PBE	0	25.7	11.4	0	24.6	13.1

The Effects of real substrates and model substrates:

Comparison of some relative energy values in the C-H activation process obtained with the model substrates and the real substrates is as follows. We examined the difference between explicit-solvation and polarizable continuum model (PCM) for the K⁺-assisted transmetalation pathway. Assuming two tBuOH molecules coordinates to each potassium cation, we obtain the corresponding intermediates and transition states (**IN2f-real**→**TS1f-real**→**IN3f-real**). The activation barriers varied within 2 kcal mol⁻¹, demonstrating that the PCM approach can yield relative complexation energies comparable to the predictions based on molecular-level solvation, but at significantly lower computational cost.

Table S2. Relative free energies (kcal mol⁻¹) using model and real substrates

Substrate	IN2f	TS1f	IN3f	IN5c	TS3c	IN6c
Model	0	23.8	2.1	0	21.9	9.5
Real	0	21.8	3.2	0	19.3	9.1

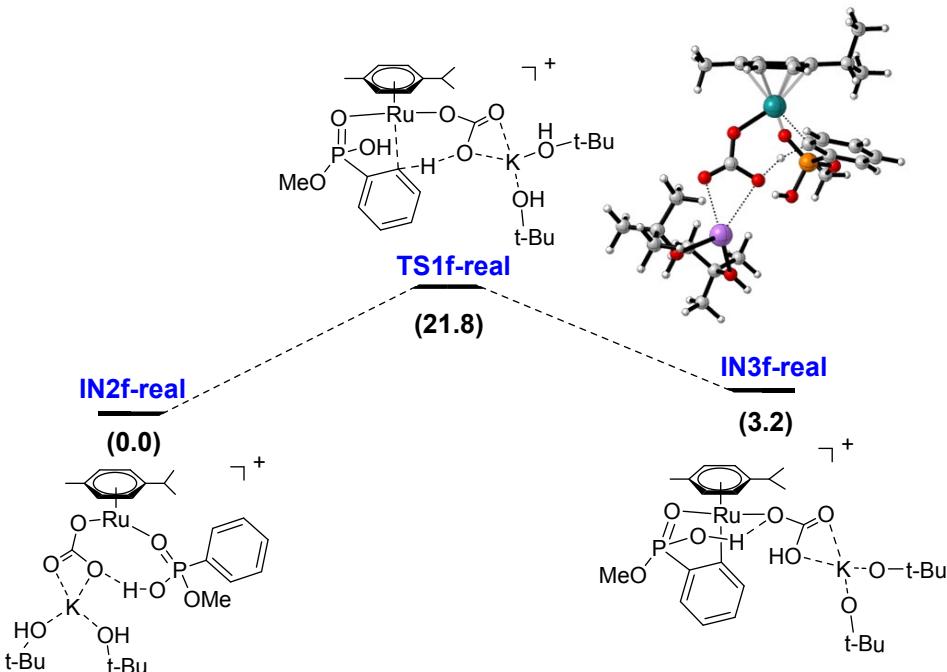


Fig. S1. Free energy profile (kcal mol⁻¹) for the C-H activation using real substrates with explicit-solvation.

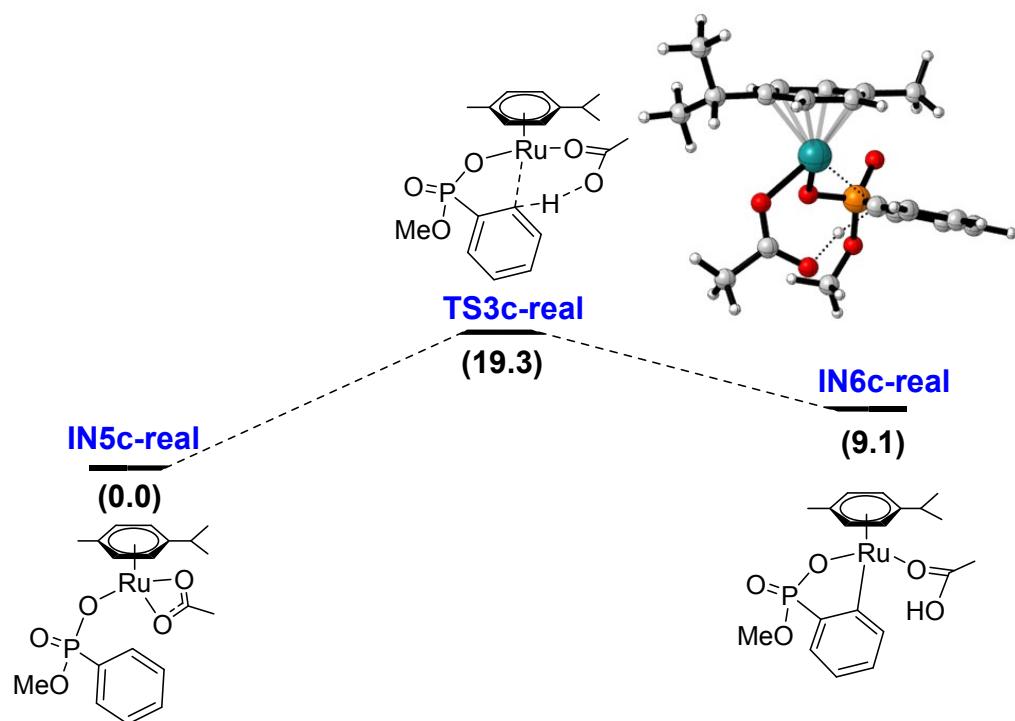
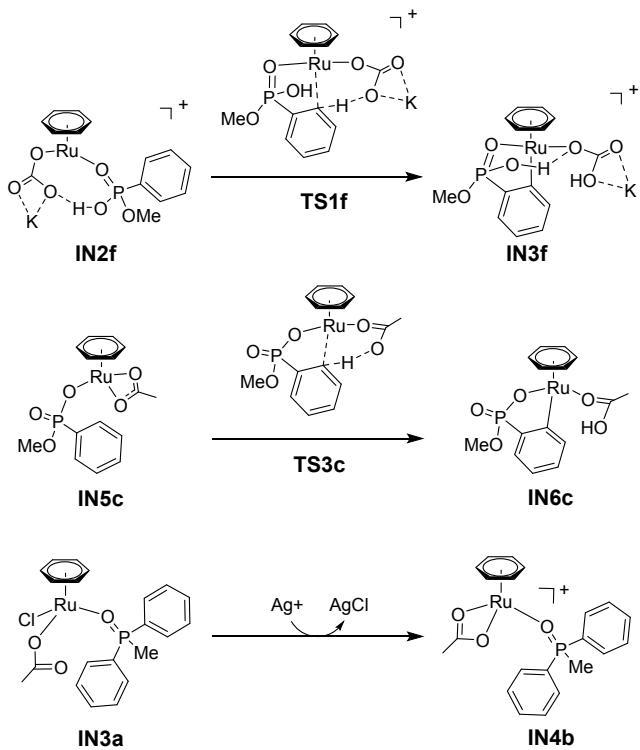


Fig S2. Free energy profile (kcal mol⁻¹) for the C-H activation using real substrates.

The Effects of different basis sets for K, Cl, P:

Table S3. Relative free energies (kcal mol⁻¹) using different basis sets for K, Cl, P



Basis set	IN2f	TS1f	IN3f	IN5c	TS3c	IN6c	IN3a	IN4b
6-31G(d)	0	23.8	2.1	0	21.9	9.5	0	-38.0
6-311G(d)	0	25.0	3.7	0	23.6	10.4	0	-42.2
TZVP	0	24.5	3.4	0	23.8	10.1	0	-42.5

The Comparison of Free Energy Profiles in Gas-phase and Solution-phase

— ESP(M06L,PCM)
— ESP(B3LYP,GAS)

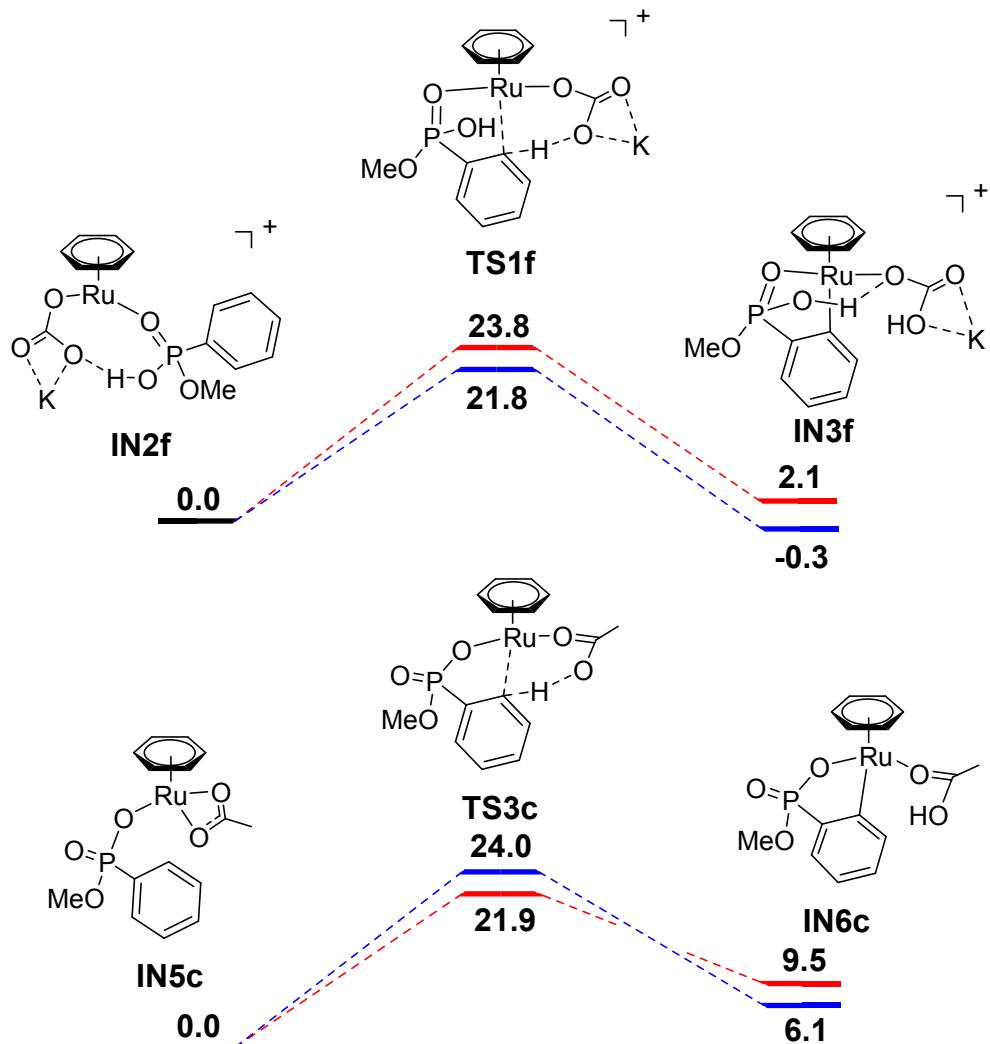
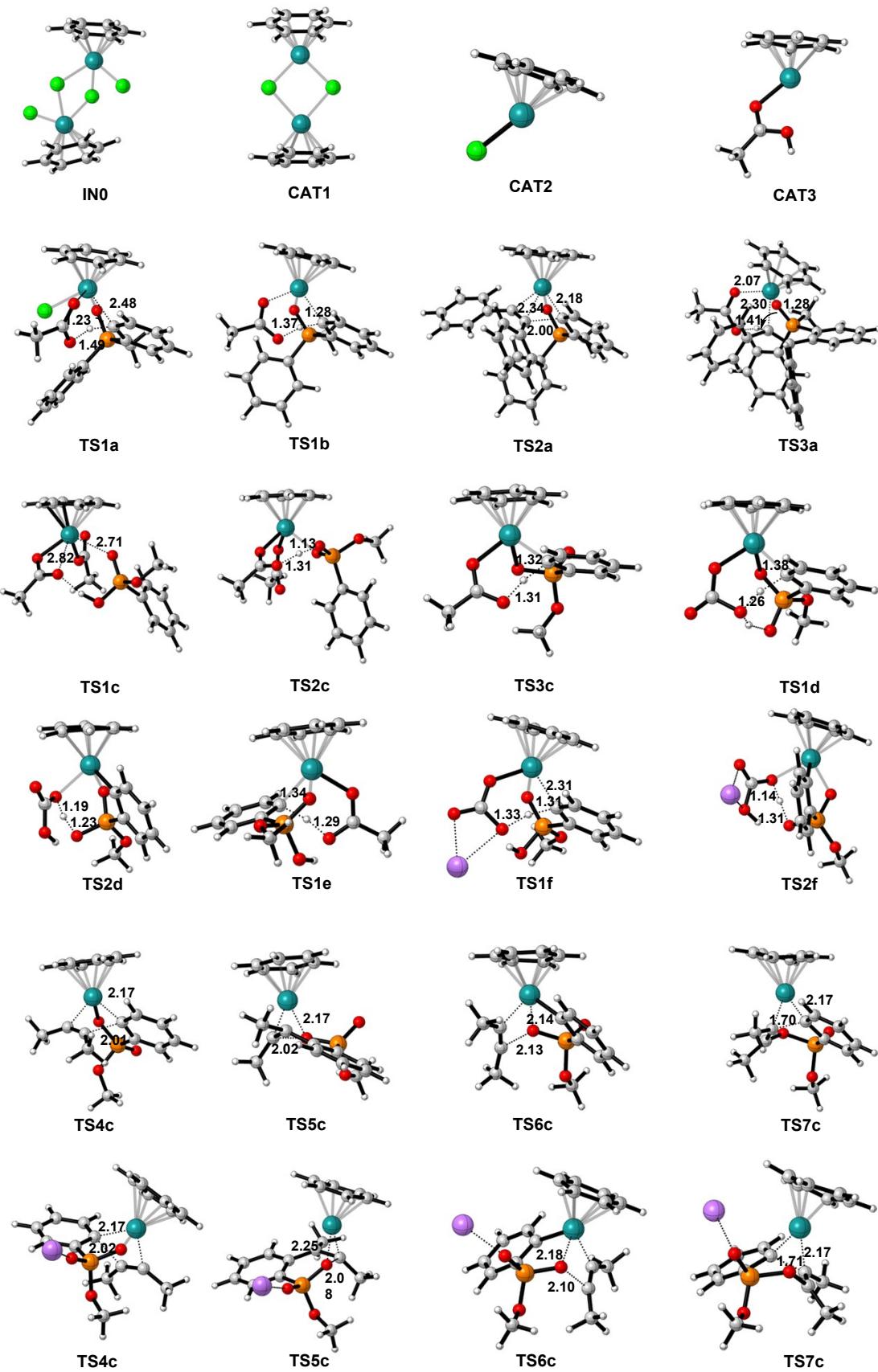
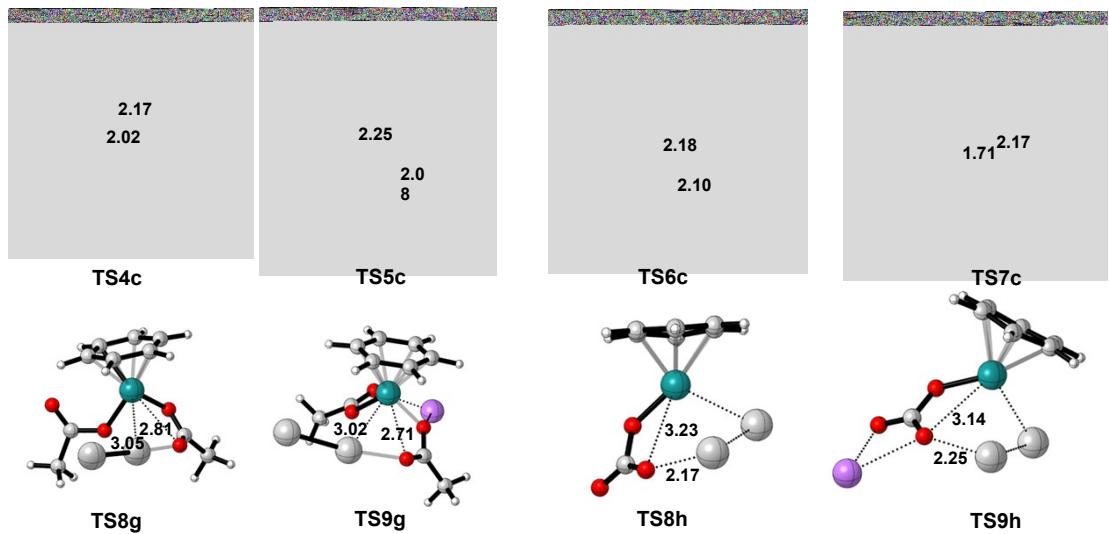


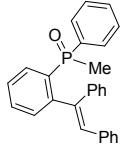
Fig. S3 Free energy profiles in gas-phase and solution-phase

3D Optimized Structures:





Energies of Intermediates and Transition States:

	Solvation Energies(Hartree)	Thermal Corrections of Gibbs Free Energies(Hartree)	Dispersion Corrections(kcal/mol)
IN0	-2495.5469513	0.160829	-61.5973
CAT1	-1574.6020208	0.160018	-47.0160
CAT2	-787.2816551	0.069590	-19.0505
CAT3	-555.9207868	0.125627	-24.2562
1,2-diphenylethyne	-539.5225444	0.154579	-29.6523
Ph ₂ P (O)Me	-919.9162392	0.183418	-40.5645
IN2a	-1707.2633696	0.275811	-70.1741
IN3a	-1935.991204	0.322841	-85.5814
TS1a	-1935.930202	0.318582	-87.2977
IN4a	-1935.983837	0.318996	-82.7257
IN4b	-1475.5880746	0.324033	-77.8730
TS1b	-1475.5409923	0.319680	-80.9897
IN5a	-1475.5634303	0.325125	-80.9265
IN6a	-1246.3973368	0.267233	-65.9178
IN7a	-1785.9520054	0.443717	-119.2570
TS2a	-1785.9348245	0.446026	-120.0636
IN8a	-1785.9690045	0.447906	-122.1540
TS3a	-2015.1002831	0.502958	-136.3040
IN9a	-2015.1625315	0.505920	-127.5954
	-1459.4887502	0.364210	-88.7592
but-2-yne	-156.0023915	0.057949	-5.7773
PhP(O)OMeOH	-839.370210105	0.115207	-24.8094
IN1c	-784.3850076	0.161617	-33.9245
IN2c	-1623.7677114	0.297911	-65.2719
TS1c	-1623.7545993	0.299727	-69.0792
IN3c	-1623.7611608	0.298546	-71.6881
TS2c	-1623.7602747	0.298655	-71.7907
IN4c	-1623.7649916	0.301431	-72.2877
IN5c	-1394.6210384	0.245662	-59.0272
TS3c	-1394.5739114	0.242468	-64.7148
IN6c	-1394.5981387	0.246736	-64.5403
IN1d	-591.1527861	0.082812	-21.7807
IN2d	-1430.5504492	0.221468	-57.9477
TS1d	-1430.4830800	0.220529	-62.4312
IN3d	-1430.5313878	0.223948	-61.1314

TS2d	-1430.5202031	0.221711	-62.0714
IN4d	-1430.5248868	0.225880	-62.5671
IN1e	-1384.2364375	0.225350	-39.5380
IN2e	-1395.0613466	0.334335	-59.9786
TS1e	-1395.0091251	0.328540	-63.9687
IN3e	-1395.0307604	0.333950	-63.2264
IN1f	-1191.0076314	0.079704	-23.9829
IN2f	-2030.3936471	0.217347	-59.9662
TS1f	-2030.348834	0.216921	-64.0230
IN3f	-2030.3850194	0.223031	-66.8834
TS2f	-2030.3739219	0.220932	-67.4418
IN4f	-2030.3778639	0.223025	-67.2914
IN7c	-1165.4278894	0.188362	-49.8973
IN8c	-1321.452021	0.268006	-69.6524
TS4c	-1321.4308835	0.269278	-69.5016
IN9c	-1321.4596653	0.270430	-68.2408
TS5c	-1321.442736	0.270187	-67.6876
TS6c	-1321.4161069	0.269191	-69.0428
IN11c	-1321.4332663	0.272618	-68.6447
TS7c	-1321.3913822	0.269305	-67.5928
IN10c	-1321.4594987	0.273055	-66.6613
IN5f	-1765.2788717	0.184363	-51.2443
IN6f	-1921.3049393	0.263197	-72.1537
TS4f	-1921.2837217	0.266039	-72.0823
IN7f	-1921.3176482	0.268783	-71.2928
TS5f	-1921.2941724	0.268245	-69.8180
IN8f	-1921.3392346	0.269630	-71.7647
TS6f	-1921.2699263	0.266171	-73.2635
IN9f	-1921.2850479	0.269506	-73.8966
TS7f	-1921.2452357	0.266995	-73.9273
IN10g	-1078.543398	0.150346	-44.0876
TS8g	-1078.534722	0.151931	-45.1980
IN11g	-1078.542005	0.150608	-46.1247
IN10h	-885.2965485	0.072450	-34.0488
TS8h	-885.2973581	0.073408	-34.0277
IN11h	-885.3314491	0.074166	-35.5428
IN9g	-2296.9870116	0.309548	-91.9935
IN12g	-1678.412137	0.148925	-54.0508
TS9g	-1678.390394	0.148097	-49.7263
IN13g	-1678.398747	0.146569	-48.184
IN9h	-2479.3964744	0.274563	-93.3682
IN12h	-1485.1637756	0.071128	-36.2218
TS9h	-1485.1641046	0.071727	-36.5532

IN13h	-1485.1896239			0.072109		-38.1584								
The Cartesian Coordinates for the Optimized Structures and the First Frequency from Calculations														
(Values in cm ⁻¹):														
IN0 (20. 21)														
6	0.631981	-0.164562	10.328812	1	2.801271	1.395707	-1.243985							
6	1.004713	-1.133083	9.336297	1	1.838453	-0.553207	-2.497283							
6	1.094661	-2.502518	9.672356	1	0.895696	-2.506253	-1.241428							
1	1.467790	-3.216823	8.948037	1	1.835863	-0.563313	2.497427							
6	0.841016	-2.922877	11.019328	8	-0.542677	1.738293	-1.089938							
6	0.502962	-1.964687	12.001154	8	-0.541054	1.740544	1.089004							
1	0.420801	-2.263676	13.040266	8	-1.539098	-0.518969	0.002769							
6	0.382922	-0.577199	11.651115	6	-0.952241	2.257688	-0.000692							
1	0.224607	0.162275	12.427601	6	-1.928128	-1.769730	-0.000115							
6	7.079441	1.143589	13.465057	8	-1.202766	-2.764157	-0.004185							
6	7.333116	1.564285	12.118790	6	-3.449512	-1.892176	0.002033							
6	7.240441	0.627010	11.063762	1	-3.865994	-1.390519	-0.878063							
1	7.314516	0.966820	10.036527	1	-3.741076	-2.944181	0.000346							
6	6.928715	-0.747505	11.334554	1	-3.863342	-1.393984	0.885333							
6	6.679843	-1.160319	12.655409	6	-1.913235	3.412192	-0.001129							
1	6.297866	-2.158217	12.834654	1	-1.777473	4.021097	0.895922							
6	6.739026	-0.204422	13.724333	1	-1.780532	4.017988	-0.900728							
1	6.431485	-0.497397	14.722208	1	-2.935908	3.017274	0.001370							
17	4.159159	-2.996091	10.858135											
17	3.386120	-0.603713	13.199510	IN2c (11. 07)										
17	3.965193	0.355357	10.129356	8	2.139431	-1.118428	1.514180							
17	4.223366	2.657997	12.637140	8	0.413714	0.179328	1.248013							
44	2.388876	-1.350165	11.038733	6	0.948035	-0.837459	1.827263							
44	5.359486	0.591207	12.205610	6	0.165003	-1.639175	2.825893							
1	1.304087	-0.799680	8.348822	1	0.729016	-2.521015	3.134599							
1	0.664940	0.892013	10.089195	1	-0.792032	-1.934115	2.382721							
1	1.024155	-3.952129	11.304270	1	-0.047463	-1.016108	3.701641							
1	7.031415	1.879833	14.258725	6	-6.474054	-0.016463	-0.411622							
1	7.475437	2.616391	11.901762	6	-5.139287	-0.227255	-0.069886							
1	6.733970	-1.434822	10.519998	6	-4.165998	-0.311899	-1.076795							
				6	-4.537360	-0.188971	-2.421534							
IN1c (25. 91)														
44	0.390898	0.137813	0.000339	6	-5.875857	0.019982	-2.758827							
6	2.476014	0.511368	0.706839	1	-6.842458	0.106198	-1.755148							
6	2.477416	0.514067	-0.701998	1	-7.227741	0.053913	0.367941							
6	1.928145	-0.601869	-1.417354	1	-4.849031	-0.318467	0.972368							
6	1.409901	-1.711378	-0.718988	1	-3.771809	-0.252780	-3.188636							
6	1.409259	-1.714206	0.713936	1	-6.162550	0.117679	-3.802355							
6	1.926594	-0.607631	1.417413	15	-7.884266	0.270498	-2.017753							
1	2.798657	1.391077	1.252700	8	-2.422994	-0.604243	-0.678380							
				8	-2.379932	-2.013945	0.183220							

8	-1.530311	-0.625731	-1.889378	1	-1.973715	1.507599	-0.904872
8	-2.136090	0.454321	0.495831	1	-3.762619	3.242207	-0.803443
1	-1.201408	0.391741	0.843362	1	-5.991495	2.663981	0.130895
8	4.106335	3.135996	1.395458	15	-1.875911	-1.267017	-0.122509
8	2.652982	1.509753	2.023731	8	-2.579431	-2.583994	-0.809708
6	3.449557	2.529588	2.240046	8	-0.657604	-0.776356	-0.873123
6	3.492239	2.915075	3.715519	8	-1.677083	-1.786870	1.375406
1	4.147812	3.776084	3.858725	1	-0.699344	-1.963788	1.551493
1	3.855118	2.070360	4.311033	8	1.401218	3.300403	-0.241733
1	2.483720	3.152500	4.070470	8	0.697579	1.395695	0.768701
44	2.285426	0.639427	0.225329	6	0.705352	2.693723	0.571152
6	2.888826	2.297542	-1.121430	6	-0.259278	3.420184	1.502314
6	3.994519	1.403707	-0.956352	1	-0.296867	4.481044	1.246833
6	3.823853	0.027795	-1.228018	1	0.077860	3.305947	2.538575
6	2.566732	-0.472148	-1.704188	1	-1.259271	2.980098	1.436770
6	1.475237	0.402649	-1.859113	44	1.833691	0.035654	-0.199595
6	1.641375	1.793976	-1.548494	6	2.217232	1.175530	-2.093411
1	2.991035	3.320957	-0.787223	6	3.311132	1.259147	-1.169888
1	4.906092	1.773660	-0.507022	6	3.930479	0.066448	-0.695755
1	4.626444	-0.667221	-1.004063	6	3.458022	-1.215972	-1.114215
1	2.426442	-1.539425	-1.835221	6	2.313640	-1.280447	-1.931882
1	0.482524	0.014143	-2.078073	6	1.711123	-0.084142	-2.448989
1	0.774776	2.446437	-1.568279	1	1.698980	2.083274	-2.371872
6	-2.439129	-3.246955	-0.547087	1	3.603575	2.226261	-0.782580
1	-1.708079	-3.253782	-1.361078	1	4.703825	0.131149	0.062072
1	-2.212003	-4.043918	0.164366	1	3.871160	-2.117784	-0.677400
1	-3.443529	-3.405550	-0.958064	1	1.832860	-2.235027	-2.113021
				1	0.778687	-0.158447	-2.993559
TS1c (89. 51i)				6	-2.872803	-2.547221	-2.209243
8	2.376822	-0.367443	1.806405	1	-1.971133	-2.336319	-2.793616
8	0.896466	-1.992022	1.525749	1	-3.258055	-3.534747	-2.472829
6	1.654537	-1.316084	2.266032	1	-3.635422	-1.791024	-2.433644
6	1.734643	-1.587940	3.754484				
1	2.641335	-1.160864	4.187769	IN3c (16. 76)			
1	1.689806	-2.663962	3.943169	8	1.263387	1.388527	1.251095
1	0.866569	-1.126450	4.240714	8	-0.351701	0.621770	2.658633
6	-5.460961	0.615533	0.547354	6	0.394025	1.512753	2.176219
6	-4.461043	-0.354466	0.487432	6	0.276247	2.924077	2.724748
6	-3.200631	-0.028377	-0.035458	1	1.267522	3.343872	2.918946
6	-2.952878	1.268455	-0.502858	1	-0.330013	2.938676	3.632242
6	-3.957695	2.236327	-0.441601	1	-0.196010	3.541128	1.952096
6	-5.209793	1.910296	0.083364	6	-5.408748	-0.292656	0.217200
1	-6.435887	0.363207	0.955651	6	-4.195112	-0.970054	0.315130
1	-4.654814	-1.361141	0.846160	6	-3.002700	-0.316666	-0.036235

6	-3.021843	1.013867	-0.480874	1	-0.301781	3.100509	3.528478
6	-4.245323	1.682127	-0.570660	1	-0.124945	3.622806	1.825863
6	-5.432666	1.033664	-0.226099	6	-5.408019	-0.346198	0.180986
1	-6.333334	-0.795022	0.488296	6	-4.183708	-0.997912	0.316584
1	-4.170133	-1.999161	0.662979	6	-2.996939	-0.332938	-0.031517
1	-2.091214	1.515778	-0.736795	6	-3.034217	0.985287	-0.510189
1	-4.266186	2.713817	-0.910665	6	-4.267523	1.628812	-0.637191
1	-6.380431	1.560976	-0.299575	6	-5.448962	0.967545	-0.296475
15	-1.419050	-1.171940	0.122278	1	-6.327676	-0.859166	0.449197
8	-1.638372	-2.688295	-0.461122	1	-4.146035	-2.017310	0.690898
8	-0.348631	-0.385749	-0.645958	1	-2.109317	1.498483	-0.763011
8	-1.067095	-1.507993	1.624161	1	-4.301210	2.651203	-1.003420
1	-0.688725	-0.618432	2.092437	1	-6.404745	1.475082	-0.399555
8	1.713113	1.350842	-1.472693	15	-1.399754	-1.155659	0.180920
8	-0.174528	2.538499	-0.965479	8	-1.598426	-2.700448	-0.341484
6	0.853725	2.336715	-1.601156	8	-0.344925	-0.393477	-0.640816
6	1.292676	3.296301	-2.712468	8	-1.038574	-1.391107	1.688549
1	1.433007	2.752332	-3.652876	1	-0.682172	-0.418489	2.133099
1	2.254578	3.753263	-2.453924	8	1.693499	1.342261	-1.478735
1	0.541734	4.077955	-2.845952	8	-0.165092	2.545146	-0.907129
44	1.715603	-0.154370	-0.080864	6	0.830154	2.326294	-1.589267
6	3.531297	-0.899613	-1.102552	6	1.209920	3.254471	-2.747644
6	3.907322	-0.323135	0.148528	1	1.226167	2.694806	-3.689545
6	3.275116	-0.784703	1.335193	1	2.215426	3.661044	-2.593293
6	2.320673	-1.841438	1.303228	1	0.489490	4.072088	-2.819375
6	2.562767	-1.926864	-1.165279	44	1.715397	-0.163952	-0.087813
6	1.933892	-2.360871	0.045342	6	3.523110	-0.901744	-1.122177
1	3.909179	-0.463876	-2.021347	6	3.912171	-0.337249	0.129705
1	4.589690	0.517772	0.181594	6	3.283898	-0.802797	1.316766
1	3.466335	-0.269040	2.270199	6	2.325830	-1.856519	1.285244
1	1.787444	-2.132767	2.199461	6	2.549688	-1.925820	-1.184730
1	2.223739	-2.302919	-2.123182	6	1.931472	-2.370152	0.027624
1	1.097942	-3.050371	-0.006326	1	3.894585	-0.460562	-2.040996
6	-1.944300	-2.842850	-1.855965	1	4.597847	0.500914	0.163953
1	-2.925069	-2.415160	-2.090454	1	3.480653	-0.291565	2.253084
1	-1.181608	-2.364833	-2.479306	1	1.793444	-2.148222	2.181922
1	-1.960892	-3.917352	-2.048908	1	2.202180	-2.293694	-2.142767
				1	1.093174	-3.056847	-0.021999
TS2c (157.75i)				6	-1.890961	-2.914250	-1.730767
8	1.289087	1.378874	1.268922	1	-2.876837	-2.512814	-1.989290
8	-0.430548	0.765182	2.627581	1	-1.132352	-2.446942	-2.367312
6	0.391095	1.594050	2.140810	1	-1.888246	-3.995584	-1.883042
6	0.316581	3.026265	2.632209				
1	1.319490	3.418701	2.822122	IN4c (28.27)			

8	1.334900	1.391464	1.319694	1	-2.777550	-2.644089	-1.777611
8	-0.582325	1.243455	2.526904	1	-1.039019	-2.518114	-2.154918
6	0.423734	1.882635	2.011440	1	-1.729501	-4.078212	-1.611260
6	0.452545	3.357346	2.309350				
1	1.481527	3.689031	2.466915				IN5c (13.81)
1	-0.173399	3.604440	3.168373	6	-4.030054	-1.242505	0.189945
1	0.067758	3.858477	1.413830	6	-5.304376	-0.859955	0.608790
6	-5.399060	-0.475467	0.129824	6	-2.987728	-0.304778	0.152606
6	-4.156108	-1.070333	0.343423	6	-3.232612	1.014765	0.557802
6	-2.980199	-0.382255	0.005496	1	-2.417851	1.731757	0.559994
6	-3.054096	0.907372	-0.541812	6	-4.508993	1.394980	0.977285
6	-4.303516	1.497322	-0.746667	8	-0.343647	0.210308	0.168099
6	-5.472661	0.809448	-0.415712	1	1.432057	4.484330	0.795204
1	-6.308117	-1.011142	0.390609	6	1.086572	3.939797	-0.086553
1	-4.095168	-2.067390	0.771318	6	1.439338	2.483910	0.025676
1	-2.141621	1.442812	-0.790268	1	-0.004051	4.035294	-0.145466
1	-4.360961	2.497992	-1.166805	1	1.517197	4.367281	-0.995359
1	-6.442061	1.273468	-0.579683	8	1.551626	1.913752	1.157376
15	-1.356504	-1.127144	0.347575	8	1.607427	1.763683	-1.015195
8	-1.499832	-2.710455	-0.121330	1	-4.692320	2.418949	1.293047
8	-0.339008	-0.397139	-0.581407	1	-3.826579	-2.269343	-0.098435
8	-1.002041	-1.174802	1.835522	1	-6.107548	-1.591849	0.636496
1	-0.662755	0.243742	2.255149	6	-5.546034	0.459843	0.999415
8	1.655400	1.272343	-1.519074	1	-6.538988	0.756693	1.327710
8	-0.098656	2.571838	-0.845521	15	-1.347601	-0.860213	-0.428149
6	0.799348	2.261138	-1.623789	8	-1.114496	-2.329834	-0.186024
6	1.030669	3.056107	-2.911508	8	-1.362131	-0.628758	-2.068409
1	0.748055	2.443528	-3.775686	44	1.707316	-0.007612	0.196998
1	2.088802	3.312693	-3.024905	6	2.963708	-1.294512	-1.078311
1	0.424164	3.964296	-2.901524	6	3.826876	-0.581680	-0.185539
44	1.705334	-0.203188	-0.092547	6	3.574949	-0.630674	1.202963
6	3.482704	-0.955664	-1.137549	6	2.497829	-1.427302	1.718763
6	3.918091	-0.410275	0.103784	6	1.902990	-2.084325	-0.578813
6	3.289087	-0.852431	1.299053	6	1.673845	-2.148809	0.832681
6	2.312156	-1.890584	1.289351	1	3.075912	-1.161151	-2.149285
6	2.476902	-1.956346	-1.180120	1	4.594056	0.075567	-0.578947
6	1.889961	-2.409224	0.044818	1	4.144773	0.000410	1.876592
1	3.838965	-0.519348	-2.064664	1	2.261457	-1.392975	2.776422
1	4.624467	0.410943	0.125221	1	1.180944	-2.543234	-1.242267
1	3.507766	-0.340438	2.230253	1	0.768401	-2.634750	1.175456
1	1.781086	-2.159079	2.194062	6	-1.451510	0.690983	-2.607774
1	2.099346	-2.311429	-2.131587	1	-1.451486	0.584618	-3.696160
1	1.036930	-3.078153	0.014493	1	-2.384762	1.182455	-2.302591
6	-1.776783	-2.992163	-1.497914	1	-0.598130	1.302419	-2.298459

				6	-2.881051	-0.376614	2.782831
TS3c (1087.76i)				6	-1.705186	-0.682743	0.694171
6	-2.915403	-1.389992	0.715093	6	-0.528091	-0.131672	1.239499
6	-2.924500	-1.920408	2.006984	1	-0.687954	1.419090	-1.443511
6	-1.848148	-0.588551	0.299729	6	-0.557325	0.305334	2.570057
6	-0.762657	-0.314126	1.168789	8	-0.440811	-0.034566	-1.498342
1	-0.422407	0.960184	1.245938	1	-0.796665	4.627216	0.267374
6	-0.794305	-0.871043	2.466805	6	0.152940	4.340042	-0.197487
8	-0.301808	0.815557	-1.324573	6	0.146256	2.856884	-0.458548
1	0.900088	4.425803	2.156363	1	0.231057	4.883638	-1.144073
6	1.226977	4.045349	1.185552	1	0.978859	4.606302	0.462636
6	0.814160	2.598935	1.025418	8	-0.732710	2.457252	-1.331621
1	0.729987	4.636519	0.407522	8	0.939703	2.105905	0.140555
1	2.306794	4.155581	1.070978	1	0.327725	0.751979	3.019032
8	-0.307790	2.242903	1.496270	1	-3.765496	-1.245018	1.012482
8	1.612099	1.822100	0.416841	1	-3.782659	-0.470651	3.382530
1	0.012553	-0.648353	3.162815	6	-1.725634	0.184735	3.333028
1	-3.723121	-1.617203	0.024265	1	-1.731761	0.531490	4.364343
1	-3.755928	-2.541115	2.331906	15	-1.510986	-1.164664	-1.048742
6	-1.863960	-1.660550	2.884737	8	-1.120233	-2.589871	-1.308658
1	-1.880916	-2.070226	3.891792	8	-2.920491	-0.818831	-1.818037
15	-1.650533	-0.015248	-1.435995	44	1.112114	-0.056660	-0.007449
8	-1.764408	-1.159807	-2.403739	6	3.454988	-0.054503	-0.490641
8	-2.835753	1.081500	-1.727626	6	3.158471	-0.119402	0.917627
44	1.087000	-0.151640	-0.111915	6	2.370685	-1.169797	1.439210
6	3.131433	-0.542090	-1.014204	6	1.739814	-2.087034	0.539181
6	3.155238	-0.898346	0.375355	6	2.860194	-0.955591	-1.369468
6	2.223141	-1.820581	0.890446	6	1.922477	-1.917859	-0.854997
6	1.223396	-2.371923	0.020858	1	4.075877	0.752265	-0.866966
6	2.140530	-1.080664	-1.855483	1	3.562482	0.634644	1.584634
6	1.175040	-2.010338	-1.340984	1	2.171435	-1.225145	2.503655
1	3.803887	0.223355	-1.385000	1	1.045085	-2.836220	0.899469
1	3.855074	-0.405684	1.041831	1	3.005711	-0.863606	-2.440079
1	2.214415	-2.057884	1.948060	1	1.316246	-2.512129	-1.530049
1	0.445643	-3.004572	0.433417	6	-3.421997	0.516358	-1.889447
1	2.042355	-0.724431	-2.874965	1	-4.459781	0.443505	-2.224965
1	0.336589	-2.313619	-1.959950	1	-3.396169	1.013636	-0.912563
6	-2.781788	2.377220	-1.122779	1	-2.852877	1.111176	-2.611681
1	-3.761839	2.834823	-1.282482				
1	-2.577890	2.321461	-0.047721				
1	-2.008932	2.990846	-1.595878	6	-2.458727	0.000167	-0.000006
				8	-1.651460	-1.094102	0.000030
IN6c (28.63)				8	-1.651368	1.094200	-0.000099
6	-2.872040	-0.811189	1.455890	8	-3.660006	0.000146	-0.000111

44	-0.014566	-0.000143	-0.000064	6	2.728441	1.932001	-1.035870
6	1.681434	-0.717879	1.216920	6	3.273153	1.779632	0.256932
6	1.753445	-1.434136	-0.000342	1	0.907391	2.298107	-2.187547
6	1.681926	-0.717191	-1.217099	1	-0.540687	2.623713	-0.181527
6	1.682045	0.718062	-1.216686	1	0.424350	2.311909	2.110196
6	1.753456	1.434228	0.000516	1	2.834673	1.754941	2.400679
6	1.681453	0.717392	1.217331	1	3.331685	1.707511	-1.908556
1	1.580486	-1.251995	2.155269	1	4.293558	1.433079	0.377128
1	1.684758	-2.515825	-0.000656				
1	1.581236	-1.250766	-2.155784	TS1d(1247.43i)			
1	1.581450	1.252144	-2.155088	6	-2.451190	2.131003	-0.218268
1	1.684948	2.515932	0.000729	6	-2.102736	3.268973	-0.953163
1	1.580529	1.251000	2.155969	6	-1.601802	1.026420	-0.233136
				6	-0.383864	1.027971	-0.963679
IN2d(17.46)				1	-0.319711	-0.167747	-1.642669
6	-3.201740	0.573375	1.106170	6	-0.082725	2.176709	-1.724712
6	-4.271977	1.465608	1.048726	8	-0.529758	-1.094422	0.961073
6	-2.735930	-0.040464	-0.066311	6	0.446755	-2.223696	-1.841984
6	-3.344409	0.251627	-1.293713	8	-0.599020	-1.262713	-2.208921
1	-2.973850	-0.228161	-2.194181	8	1.377121	-1.660668	-1.164794
6	-4.415151	1.146712	-1.347376	1	0.818491	2.196766	-2.334439
8	-0.163381	-0.559669	0.848659	1	-3.371360	2.105769	0.358784
6	2.174311	-2.010033	-0.417541	1	-2.754867	4.138685	-0.944156
8	1.537510	-1.116652	-1.353661	6	-0.931468	3.285079	-1.719781
8	2.520967	-1.283424	0.598611	1	-0.687128	4.162109	-2.314031
1	-4.887902	1.367914	-2.300585	15	-1.945414	-0.616588	0.476461
1	-2.728340	0.347525	2.057402	8	-2.911432	-0.327684	1.762992
1	-4.635566	1.935446	1.958836	8	-2.629686	-1.506016	-0.558495
6	-4.879024	1.752586	-0.178066	6	-3.922728	-1.283608	2.127057
1	-5.713730	2.447526	-0.220368	1	-4.706068	-0.727923	2.648139
15	-1.318401	-1.175745	-0.019244	1	-4.331098	-1.771171	1.238456
8	-1.933317	-2.409425	0.853416	1	-3.501426	-2.037287	2.800526
8	-0.903667	-1.586255	-1.440398	8	0.337885	-3.349743	-2.250386
6	-1.058752	-3.507648	1.180878	1	-1.480118	-1.544116	-1.775496
1	-1.700260	-4.306754	1.557721	44	1.173228	-0.093025	0.207354
1	-0.515839	-3.855274	0.296676	6	1.916667	1.869166	0.938831
1	-0.344068	-3.205275	1.951969	6	1.549203	1.098947	2.062955
8	2.299833	-3.182831	-0.649712	6	2.112044	-0.207339	2.233396
1	0.538741	-1.424030	-1.538356	6	3.046967	-0.713735	1.310056
44	1.515606	0.445358	0.075587	6	2.858655	1.363959	-0.017241
6	1.342512	2.270410	-1.194312	6	3.391932	0.069889	0.160460
6	0.524108	2.460205	-0.063548	1	1.428383	2.819795	0.756517
6	1.079269	2.286632	1.246686	1	0.783150	1.453202	2.742656
6	2.441123	1.962404	1.412018	1	1.742821	-0.845556	3.028804

1	3.400382	-1.734781	1.393016	6	2.749183	1.639190	-0.944815
1	3.095566	1.936079	-0.906441	6	2.450783	2.956216	-1.286473
1	4.007015	-0.370368	-0.616642	6	1.703870	0.759826	-0.641731
				6	0.343234	1.144539	-0.662259
IN3d(30. 16)				1	0.807318	-0.772905	1.786901
6	2.779871	1.804147	-0.710484	6	0.081960	2.486150	-0.986668
6	2.436066	3.105055	-1.063296	8	0.601335	-1.652697	-0.589670
6	1.759795	0.866833	-0.498335	6	-0.366377	0.808114	2.589153
6	0.385211	1.172201	-0.621630	8	0.815213	1.179938	3.127417
1	1.214267	-0.661990	1.973801	8	-0.295780	-0.320842	1.847107
6	0.078522	2.503662	-0.950555	1	-0.937142	2.863023	-0.994646
8	0.798968	-1.634081	-0.437267	1	3.778726	1.291963	-0.917642
6	-0.963028	0.776514	2.512284	1	3.246799	3.653001	-1.533873
8	-0.531733	0.755456	3.811741	6	1.116560	3.373769	-1.297299
8	-0.408804	-0.165145	1.774291	1	0.877198	4.404926	-1.547321
1	-0.956402	2.824556	-1.022318	15	1.883036	-0.931435	-0.082623
1	3.821553	1.513300	-0.603875	8	3.260814	-1.514567	-0.699312
1	3.208193	3.848150	-1.241665	8	1.979159	-0.998861	1.494438
6	1.083399	3.447978	-1.172661	6	3.862813	-2.703472	-0.152092
1	0.807816	4.468805	-1.428129	1	4.874113	-2.747929	-0.560243
15	2.006383	-0.809387	0.047346	1	3.898580	-2.649698	0.938933
8	3.448423	-1.307929	-0.474687	1	3.301445	-3.589624	-0.464080
8	2.139558	-0.887149	1.659015	8	-1.384015	1.426685	2.785895
6	4.011035	-2.553617	-0.015643	1	1.541072	0.638383	2.757971
1	5.000948	-2.621638	-0.469351	44	-1.066635	-0.333379	-0.232051
1	4.096155	-2.556734	1.073961	6	-2.399093	0.352175	-1.827803
1	3.394935	-3.395098	-0.346368	6	-2.216575	-1.047090	-1.960364
8	-1.788411	1.602360	2.172144	6	-2.641548	-1.941188	-0.913332
1	0.067847	-0.000126	3.919739	6	-3.105615	-1.424994	0.293222
44	-0.971222	-0.368707	-0.296744	6	-3.130948	0.001747	0.483705
6	-2.172906	0.232042	-2.040441	6	-2.878106	0.886676	-0.590865
6	-1.880218	-1.146264	-2.170974	1	-2.092813	1.015656	-2.628775
6	-2.320401	-2.076040	-1.166846	1	-1.764605	-1.449886	-2.859886
6	-2.969461	-1.621528	-0.018269	1	-2.491085	-3.008986	-1.032240
6	-3.135019	-0.207319	0.168180	1	-3.321178	-2.082284	1.128046
6	-2.821741	0.712051	-0.861055	1	-3.321236	0.411032	1.469210
1	-1.834312	0.929653	-2.798524	1	-2.945456	1.956347	-0.434063
1	-1.312400	-1.502619	-3.022902				
1	-2.060679	-3.124834	-1.268041	IN4d(41. 86)			
1	-3.228220	-2.308476	0.779301	6	2.700542	1.588971	-1.030894
1	-3.490395	0.178372	1.115494	6	2.403115	2.901913	-1.389919
1	-2.982036	1.770210	-0.698134	6	1.660796	0.720532	-0.681144
				6	0.305746	1.119905	-0.673811
TS2d(654. 97i)				1	0.537811	-0.826672	1.898011

6	0.042102	2.456623	-1.016021	1	-0.990006	-1.254351	2.247423	
8	0.521417	-1.654016	-0.464805	1	-0.989800	1.252454	2.248445	
6	-0.119372	0.910141	2.578293	1	-1.715978	2.516130	0.202040	
8	1.159178	1.151091	2.848479	1	-2.281965	1.250684	-1.872245	
8	-0.338972	-0.318482	1.959364	1	-2.281932	-1.248918	-1.873303	
1	-0.974333	2.840631	-1.001744	1	-1.716416	-2.516208	0.199922	
1	3.728381	1.235512	-1.025404	6	3.849185	0.000077	-0.029003	
1	3.197546	3.587012	-1.672844	1	4.209595	-0.010473	1.008206	
6	1.073242	3.331460	-1.370888	1	4.222344	-0.897502	-0.527331	
1	0.834476	4.360044	-1.631750	1	4.222961	0.906414	-0.510501	
15	1.866179	-0.953851	-0.062662					
8	3.137810	-1.594616	-0.848173	IN2e(22, 33)				
8	2.111210	-0.982837	1.472349	6	3.263905	0.362142	-0.986136	
6	3.866673	-2.696636	-0.281231	6	4.271480	1.309027	-0.810545	
1	4.842568	-2.706716	-0.771384	6	2.606163	-0.169121	0.137280	
1	3.988382	-2.566443	0.797235	6	2.964428	0.244806	1.429286	
1	3.346740	-3.638436	-0.485284	1	2.472515	-0.188371	2.293956	
8	-1.038447	1.637465	2.839022	6	3.974158	1.194973	1.593502	
1	1.746824	0.475466	2.410396	8	0.042918	-0.821347	-0.867411	
44	-1.112942	-0.329948	-0.186821	6	-2.482450	-1.620292	0.600911	
6	-2.449757	0.344080	-1.772537	8	-1.666678	-0.974892	1.373270	
6	-2.268156	-1.060016	-1.883560	8	-2.759188	-1.058786	-0.498680	
6	-2.702786	-1.937620	-0.825928	1	4.261302	1.508688	2.592629	
6	-3.156485	-1.399315	0.374646	1	3.004447	0.023953	-1.985257	
6	-3.168214	0.030966	0.544164	1	4.789668	1.712737	-1.675150	
6	-2.926248	0.899676	-0.546151	6	4.623908	1.726662	0.477304	
1	-2.141490	0.994032	-2.583686	1	5.413651	2.460397	0.609660	
1	-1.820996	-1.477180	-2.778909	15	1.278133	-1.354933	-0.100866	
1	-2.562155	-3.008190	-0.930221	8	1.978846	-2.531511	-0.928645	
1	-3.374873	-2.042334	1.219936	8	0.862151	-1.925933	1.347123	
1	-3.365800	0.453844	1.523191	6	1.235996	-3.683145	-1.403264	
1	-2.991076	1.971975	-0.407505	1	1.951108	-4.281577	-1.966876	
				1	0.857814	-4.258294	-0.554112	
IN1e(36, 90)				1	0.416361	-3.363035	-2.050690	
6	2.363822	0.000150	-0.008912	1	-0.075621	-1.683363	1.565411	
8	1.665782	1.082231	0.011243	44	-1.404335	0.545244	-0.138920	
8	1.665845	-1.082023	0.011281	6	-1.653471	2.306130	1.161319	
44	-0.084007	0.000004	-0.204225	6	-0.349062	2.388851	0.587643	
6	-1.362533	-0.716686	1.381634	6	-0.209609	2.319103	-0.818320	
6	-1.362359	0.715542	1.382201	6	-1.349405	2.182632	-1.658832	
6	-1.780145	1.433642	0.222877	6	-2.806678	2.211039	0.338766	
6	-2.100083	0.717546	-0.944687	6	-2.641816	2.124337	-1.071809	
6	-2.100098	-0.716551	-0.945287	1	-1.760790	2.253801	2.240006	
6	-1.780372	-1.433727	0.221686	1	0.528834	2.416372	1.222460	

1	0.783420	2.258118	-1.250474	1	-2.860198	-2.148043	-0.966141
1	-1.228787	2.046828	-2.727140	1	-4.032823	0.005944	-0.508945
1	-3.789896	2.105502	0.782589	6	-0.900076	3.566450	-2.281153
1	-3.504020	1.920880	-1.698780	1	-0.105551	4.254678	-1.971703
6	-3.050070	-2.943865	1.002030	1	-0.857982	3.489358	-3.371743
1	-2.237776	-3.659503	1.171074	1	-1.865508	3.961382	-1.964087
1	-3.592429	-2.838646	1.947650				
1	-3.720318	-3.321166	0.228465	IN3e (21.97)			
				6	-2.916763	0.933098	1.346619
TS1e (1179.39i)				6	-2.721358	1.784501	2.430708
6	2.597865	-1.950240	-0.616103	6	-1.798625	0.401546	0.686757
6	2.272719	-2.984982	-1.500144	6	-0.462664	0.684922	1.076515
6	1.677747	-0.921626	-0.425162	1	-0.450022	2.233890	-0.318170
6	0.421075	-0.880668	-1.089659	6	-0.309228	1.566999	2.163093
1	0.246799	0.362084	-1.569211	8	-0.482682	-0.653090	-1.390155
6	0.149695	-1.920426	-2.001129	6	0.932010	2.396901	-1.596613
8	0.568462	1.041280	1.042754	8	-0.223269	2.799103	-1.094026
6	-0.649679	2.213443	-1.671212	8	1.546793	1.404555	-1.187058
8	0.398385	1.565130	-2.032567	1	0.684832	1.850401	2.499712
8	-1.473676	1.754634	-0.830313	1	-3.921261	0.687842	1.012477
1	-0.774332	-1.906281	-2.573841	1	-3.573001	2.205996	2.955301
1	3.546914	-1.951398	-0.088672	6	-1.418462	2.104173	2.826751
1	2.973862	-3.799093	-1.657911	1	-1.262205	2.782459	3.661420
6	1.061209	-2.960871	-2.199228	15	-1.893620	-0.623170	-0.769785
1	0.833177	-3.753354	-2.906463	8	-2.516633	-2.029610	-0.314563
15	1.951056	0.553016	0.562760	8	-2.997991	-0.109755	-1.845606
8	3.016879	0.190697	1.693564	6	-2.929220	-3.041970	-1.272228
8	2.707096	1.683198	-0.313664	1	-3.318452	-3.866914	-0.676126
6	3.697384	1.204969	2.485988	1	-3.709440	-2.644530	-1.923685
1	4.378433	0.656516	3.135627	1	-2.072550	-3.376446	-1.863360
1	4.252898	1.877836	1.830591	1	-2.654285	0.574520	-2.445073
1	2.971490	1.760434	3.084298	44	1.070246	-0.300018	0.079068
1	2.125037	1.967378	-1.052962	6	1.332613	-1.676790	1.790607
44	-1.154881	-0.007098	0.274115	6	1.298401	-2.440044	0.601030
6	-1.699984	-2.104299	0.889220	6	2.306882	-2.273557	-0.413544
6	-1.403459	-1.370338	2.051598	6	3.238624	-1.249030	-0.291033
6	-2.097571	-0.142345	2.316228	6	2.288791	-0.621307	1.915007
6	-3.084800	0.323728	1.430679	6	3.172221	-0.365561	0.843071
6	-2.675636	-1.615726	-0.040187	1	0.593537	-1.841506	2.566393
6	-3.351119	-0.405571	0.227472	1	0.517962	-3.180786	0.465341
1	-1.132692	-2.997592	0.653739	1	2.277248	-2.888177	-1.306634
1	-0.612036	-1.697540	2.716509	1	3.945694	-1.047742	-1.088177
1	-1.808499	0.462340	3.169092	1	2.289526	0.017915	2.789955
1	-3.559480	1.283935	1.597911	1	3.835754	0.491460	0.889779

6	1.453581	3.261849	-2.704116	6	0.880804	-3.128177	1.807482
1	0.675699	3.409428	-3.459640	1	0.775269	-4.102230	2.288375
1	1.707624	4.249560	-2.303319	1	1.706728	-3.163961	1.087841
1	2.336263	2.806958	-3.152898	1	1.081442	-2.360714	2.561415
				8	3.980541	0.430709	0.446939
IN1f(27.76)				1	1.753448	-1.165120	-0.982912
6	-1.643292	-0.978422	-0.031150	44	0.079686	1.525576	0.250952
8	-0.533884	-1.698692	-0.164314	6	-1.831757	1.966979	-0.724198
8	-1.322634	0.331353	0.122376	6	-2.034014	2.165610	0.664245
8	-2.789452	-1.391231	-0.041075	6	-1.130513	2.979430	1.386535
44	0.654484	-0.117978	-0.015543	6	-0.089672	3.691671	0.701250
6	2.516368	-0.374732	1.129330	6	-0.769565	2.652954	-1.397298
6	2.757874	-0.929709	-0.150015	6	0.058380	3.573159	-0.696117
6	2.450598	-0.160480	-1.295459	1	-2.422418	1.229811	-1.256726
6	2.016241	1.199281	-1.160079	1	-2.765734	1.563262	1.189710
6	1.901740	1.792750	0.118610	1	-1.185089	3.021605	2.468995
6	2.094605	0.988764	1.263828	1	0.635073	4.259558	1.275386
1	2.605585	-0.996217	2.013933	1	-0.570169	2.433987	-2.441072
1	3.015992	-1.977974	-0.249525	1	0.900247	4.037497	-1.196453
1	2.486611	-0.615135	-2.279589	19	5.318165	-1.654338	-0.370269
1	1.735879	1.759434	-2.045603				
1	1.523308	2.803541	0.218492	TS1f(1128.80i)			
1	1.874392	1.383779	2.249633	6	-0.357875	2.952635	1.614602
19	-4.082264	0.858069	0.283572	6	-0.699976	2.764773	2.958505
				6	-0.065666	1.834274	0.836958
IN2f(15.24)				6	-0.106043	0.508490	1.349318
6	-3.216381	-1.538153	0.852985	1	0.901310	-0.198351	0.890044
6	-4.582944	-1.517693	0.574213	6	-0.418428	0.367091	2.716090
6	-2.288924	-1.614340	-0.198467	8	-0.214456	0.654547	-1.587572
6	-2.738239	-1.677390	-1.525076	6	1.848324	-1.685304	-0.327035
1	-2.012839	-1.757280	-2.328839	8	2.088295	-0.572777	0.408130
6	-4.108259	-1.653512	-1.798211	8	0.611509	-1.957120	-0.612432
8	-0.121379	-0.339818	1.023029	1	-0.417962	-0.623244	3.166103
6	2.902135	0.222161	-0.109172	1	-0.326350	3.949815	1.186060
8	2.721691	-0.972927	-0.714338	1	-0.939387	3.623500	3.579031
8	1.967241	1.124852	-0.233653	6	-0.717170	1.478287	3.508636
1	-4.455933	-1.710425	-2.825794	1	-0.960893	1.346653	4.559462
1	-2.869188	-1.512017	1.881976	15	0.459704	1.846279	-0.884768
1	-5.301009	-1.469879	1.387967	8	0.132346	3.295748	-1.479976
6	-5.028578	-1.571444	-0.750706	8	2.068172	1.733656	-0.936989
1	-6.093659	-1.558858	-0.964248	6	0.586970	3.694106	-2.799826
15	-0.509412	-1.597916	0.132814	1	0.235412	4.716523	-2.935888
8	-0.363356	-2.868422	1.143424	1	1.677520	3.658633	-2.846077
8	0.297380	-1.693221	-1.159859	1	0.149796	3.042211	-3.560119

8	2.793222	-2.409278	-0.673801	6	-3.251962	0.128866	1.203925
1	2.281940	0.835276	-0.539729	6	-3.726794	0.084577	-0.155152
44	-1.073449	-0.845610	-0.256417	6	-3.373656	-0.981603	-0.977392
6	-3.081004	-0.533264	0.729254	6	-2.526592	-2.021741	-0.456256
6	-3.214222	-0.190439	-0.626691	6	-2.190824	-2.064859	0.916262
6	-2.804326	-1.123273	-1.635579	1	-2.226569	-0.936170	2.792831
6	-2.318036	-2.398647	-1.282077	1	-3.446717	1.006569	1.810178
6	-2.542903	-1.811509	1.100145	1	-4.268704	0.933328	-0.558256
6	-2.171246	-2.736876	0.100838	1	-3.637852	-0.978722	-2.028966
1	-3.302424	0.198640	1.497645	1	-2.140237	-2.785314	-1.121389
1	-3.540416	0.803647	-0.910288	1	-1.598152	-2.886790	1.299239
1	-2.802538	-0.818039	-2.676441	19	3.167443	-2.650762	-0.496845
1	-1.940296	-3.069839	-2.044786				
1	-2.381337	-2.048631	2.145252				TS2f(570.35i)
1	-1.689655	-3.668597	0.375440	6	-2.572884	-0.818734	1.538978
19	4.733073	-1.416622	0.645812	6	-2.983286	0.278364	2.300221
				6	-1.309661	-0.801781	0.935352
IN3f(32.36)				6	-0.414900	0.290706	1.051347
6	2.560387	1.045117	1.403230	1	-0.275806	-0.842495	-1.940322
6	3.047319	0.013074	2.204783	6	-0.864949	1.385060	1.815548
6	1.278926	0.931197	0.845431	8	0.902133	-1.951928	0.030508
6	0.433846	-0.188402	1.049407	6	-0.817116	1.101397	-1.924337
1	0.433541	1.417309	-2.141257	8	-2.062237	0.579938	-2.069575
6	0.963647	-1.209758	1.863265	8	0.173583	0.209867	-1.904122
8	-1.004438	1.942521	-0.128642	1	-0.226065	2.253513	1.957516
6	0.786588	-1.226838	-1.758285	1	-3.217063	-1.687686	1.433596
8	2.037971	-0.796711	-2.183560	1	-3.942926	0.264495	2.809667
8	-0.116955	-0.308792	-1.727933	6	-2.121682	1.376249	2.438187
1	0.374736	-2.097713	2.074772	1	-2.415095	2.215713	3.066868
1	3.157131	1.936678	1.230546	15	-0.637146	-2.096856	-0.127819
1	4.023515	0.095928	2.674215	8	-1.247600	-3.492829	0.374258
6	2.237324	-1.108841	2.437141	8	-1.058716	-1.843806	-1.632672
1	2.589562	-1.897522	3.100560	6	-1.084342	-4.709229	-0.399509
15	0.511846	2.183504	-0.181453	1	-1.746551	-5.443572	0.058910
8	1.062552	3.599492	0.315598	1	-1.368684	-4.538156	-1.440259
8	1.023824	2.101827	-1.736651	1	-0.048213	-5.050914	-0.337566
6	0.720004	4.840407	-0.358236	8	-0.680632	2.302504	-1.790903
1	1.288438	5.617386	0.151994	1	-2.027028	-0.414074	-2.009550
1	1.006075	4.788578	-1.410823	44	1.413617	0.122928	0.056920
1	-0.350842	5.032639	-0.259433	6	2.556852	0.981196	1.714407
8	0.708139	-2.407910	-1.430289	6	3.177183	-0.224384	1.295876
1	2.028746	0.172984	-2.284805	6	3.715284	-0.348614	-0.034102
44	-1.391244	-0.193011	0.047738	6	3.483671	0.658694	-0.966025
6	-2.552507	-0.967559	1.759172	6	2.711584	1.811659	-0.582664

6	2. 335224	2. 023521	0. 763132	1	-3. 868066	-0. 329641	-2. 001876	
1	2. 186105	1. 073609	2. 729137	1	-2. 651991	-2. 428656	-1. 362279	
1	3. 264035	-1. 053657	1. 989021	1	-2. 037675	-2. 877390	1. 008329	
1	4. 194582	-1. 274766	-0. 331973	19	3. 087170	-2. 553976	-0. 495168	
1	3. 781221	0. 531578	-2. 000921					
1	2. 424075	2. 536810	-1. 336037	IN7c (25. 47)				
1	1. 808561	2. 928206	1. 042313	6	-3. 041632	1. 234283	0. 253945	
19	-3. 058486	2. 636358	-0. 527158	6	-3. 016106	2. 609242	0. 023854	
				6	-1. 849839	0. 500857	0. 223394	
IN4f (37. 43)				6	-0. 605644	1. 124388	-0. 022266	
6	2. 555938	0. 630389	1. 583677	6	-0. 608717	2. 515120	-0. 246109	
6	2. 891696	-0. 491398	2. 346434	8	-0. 237140	-1. 595620	0. 282272	
6	1. 308415	0. 685711	0. 948778	1	0. 322993	3. 042473	-0. 440026	
6	0. 358132	-0. 360653	1. 037853	1	-3. 981129	0. 729129	0. 464240	
1	0. 127400	0. 691932	-2. 101827	1	-3. 938328	3. 184105	0. 045180	
6	0. 734326	-1. 485207	1. 799374	6	-1. 796332	3. 247142	-0. 229474	
8	-0. 803057	1. 913737	-0. 073776	1	-1. 773549	4. 319606	-0. 409579	
6	0. 859979	-1. 102589	-1. 983900	15	-1. 800423	-1. 294021	0. 543925	
8	2. 055849	-0. 517270	-2. 049308	8	-2. 406183	-1. 746337	1. 831068	
8	-0. 208799	-0. 256861	-2. 007362	8	-2. 588492	-2. 002010	-0. 719138	
1	0. 052014	-2. 324001	1. 913639	44	1. 045262	-0. 098351	0. 004334	
1	3. 245447	1. 466898	1. 503873	6	3. 072532	-1. 147534	-0. 596783	
1	3. 835959	-0. 527562	2. 883304	6	2. 723116	0. 005685	-1. 383252	
6	1. 973792	-1. 546978	2. 451912	6	2. 603760	1. 294976	-0. 785247	
1	2. 209996	-2. 407900	3. 075250	6	2. 562238	1. 388294	0. 621211	
15	0. 755052	2. 028781	-0. 130982	6	3. 043883	-1. 053226	0. 791247	
8	1. 315709	3. 393044	0. 514136	6	2. 661082	0. 193126	1. 400136	
8	1. 290442	1. 842505	-1. 586590	1	3. 212707	-2. 107426	-1. 081568	
6	1. 343359	4. 626540	-0. 244898	1	2. 636260	-0. 090665	-2. 460588	
1	1. 996824	5. 302984	0. 306563	1	2. 412249	2. 163934	-1. 403800	
1	1. 739608	4. 448686	-1. 247329	1	2. 331977	2. 330598	1. 104942	
1	0. 336704	5. 048580	-0. 303240	1	3. 154550	-1. 939107	1. 406809	
8	0. 727118	-2. 302435	-1. 872254	1	2. 521011	0. 243122	2. 474664	
1	1. 962631	0. 503278	-1. 916173	6	-2. 095391	-1. 880952	-2. 049743	
44	-1. 451720	-0. 091071	0. 035314	1	-2. 814069	-2. 387668	-2. 699550	
6	-2. 629238	-0. 883104	1. 692879	1	-2. 018676	-0. 829455	-2. 357226	
6	-3. 163649	0. 370064	1. 286442	1	-1. 114357	-2. 357580	-2. 152162	
6	-3. 714384	0. 536814	-0. 033756					
6	-3. 565434	-0. 480640	-0. 971582	IN8c (27. 90)				
6	-2. 871227	-1. 686419	-0. 602214	6	2. 850939	1. 737204	-0. 404046	
6	-2. 499836	-1. 935435	0. 738515	6	2. 680303	3. 063734	-0. 010203	
1	-2. 252344	-1. 005788	2. 702118	6	1. 776542	0. 840476	-0. 344723	
1	-3. 181348	1. 199341	1. 984843	6	0. 499029	1. 254863	0. 071137	
1	-4. 130822	1. 495848	-0. 321927	6	0. 346775	2. 593966	0. 467821	

8	2.814698	-1.143790	-2.041720	1	-0.508980	2.802151	1.312288
1	-0.618079	2.958670	0.814738	1	3.515307	1.465705	-1.265884
1	3.812020	1.389755	-0.776074	1	3.231747	3.841783	-0.532917
1	3.511832	3.762400	-0.052692	6	1.335431	3.458493	0.429274
6	1.423899	3.486583	0.430633	1	1.185306	4.493137	0.729401
1	1.275294	4.518985	0.740838	15	1.819851	-0.905742	-0.989059
15	1.923498	-0.895207	-0.858881	8	2.450928	-1.809334	0.260625
8	2.476959	-1.700793	0.494799	8	0.308206	-1.338535	-1.005857
8	0.405715	-1.335582	-0.896786	6	3.865613	-1.990131	0.316801
6	3.883672	-1.878562	0.651909	1	4.355900	-1.116450	0.769288
1	4.346709	-0.978900	1.081016	1	4.053695	-2.864397	0.947411
1	4.029726	-2.712369	1.345549	1	4.280095	-2.155411	-0.681765
1	4.359037	-2.106181	-0.306856	6	0.116486	-0.086191	1.892719
6	-0.636966	-0.271415	2.136867	6	-0.444588	-1.190065	1.570556
6	-0.622601	-1.428382	1.681052	6	0.687045	0.629431	3.068172
6	-0.557850	0.792379	3.154311	1	1.695079	1.005843	2.867976
1	0.254040	1.490092	2.932159	1	0.067145	1.480498	3.371520
1	-1.488153	1.370557	3.209054	1	0.727722	-0.074715	3.908753
1	-0.376171	0.346351	4.139765	6	-0.596913	-2.615241	1.940265
6	-0.448044	-2.883886	1.566727	1	-0.152618	-2.823022	2.922283
1	-0.099871	-3.290228	2.524407	1	-1.648737	-2.922009	1.960882
1	-1.386840	-3.382888	1.298754	1	-0.080488	-3.226106	1.190754
1	0.296729	-3.099172	0.797185	6	-2.693965	-0.976804	-1.508694
6	-2.558382	-1.000178	-1.674144	6	-3.252282	-1.063960	-0.222417
6	-3.246382	-1.059391	-0.457667	6	-3.279047	0.103410	0.602031
6	-3.283227	0.106365	0.364431	6	-2.845065	1.348382	0.075163
6	-2.812953	1.357546	-0.118477	6	-2.413929	1.451367	-1.283543
6	-2.208449	1.420893	-1.403714	6	-2.291258	0.291146	-2.054106
6	-2.025625	0.244818	-2.151633	1	-2.536104	-1.876484	-2.092905
1	-2.391119	-1.901712	-2.253645	1	-3.564189	-2.023496	0.175393
1	-3.642776	-1.999671	-0.090731	1	-3.625339	0.039766	1.628201
1	-3.712943	0.046086	1.359135	1	-2.865690	2.232701	0.702780
1	-2.909419	2.249470	0.489650	1	-2.065461	2.403382	-1.668539
1	-1.793357	2.357442	-1.760271	1	-1.848087	0.329193	-3.042605
1	-1.469565	0.269653	-3.081747	44	-1.150714	-0.142548	-0.058964
44	-1.063469	-0.106386	-0.084979				
IN9c (28.38)							
TS4c (321.33i)				6	-3.714201	0.130777	0.162723
6	2.657013	1.764912	-0.669827	6	-4.521116	-1.001496	0.257527
6	2.484980	3.094212	-0.278861	6	-2.337915	0.016516	-0.077149
6	1.703704	0.797977	-0.337714	6	-1.753470	-1.257650	-0.224029
6	0.533562	1.155832	0.366910	6	-2.580479	-2.388314	-0.109098
6	0.373478	2.500657	0.752378	8	-0.820537	1.955542	-1.483642
8	2.675335	-1.001429	-2.220600	1	-2.142661	-3.378548	-0.215781

1	-4.142899	1.118734	0.291238	1	5.040724	1.567642	-1.545790	
1	-5.586914	-0.896243	0.442186	6	3.387793	2.715481	-0.776413	
6	-3.949147	-2.267611	0.126839	1	3.851490	3.677739	-0.961906	
1	-4.564935	-3.159915	0.207443	15	1.418980	-1.373287	-0.146028	
15	-1.256453	1.484197	-0.120180	8	2.547185	-2.149126	0.715798	
8	-2.204232	2.591364	0.657770	8	0.203691	-1.230576	0.836685	
8	-0.127424	1.120144	0.942347	6	2.562930	-3.585287	0.699259	
6	-2.107595	3.968590	0.287505	1	2.439211	-3.957192	-0.318171	
1	-1.878342	4.070798	-0.777173	1	3.530329	-3.888683	1.096437	
1	-3.074214	4.430183	0.509655	1	1.768039	-3.981485	1.335215	
1	-1.330032	4.469123	0.877422	44	-1.403128	0.026933	0.087343	
44	1.231474	-0.213212	0.233252	6	0.093653	1.491745	0.677719	
6	-0.287349	-1.499609	-0.539367	6	-0.388352	0.528772	1.623742	
6	0.567171	-1.892097	0.541409	6	-0.456999	2.890264	0.975830	
6	-0.074952	-2.063084	-1.944828	1	0.197720	3.455128	1.649447	
1	-0.719393	-2.935147	-2.125193	1	-0.569855	3.472574	0.058191	
1	-0.328743	-1.306316	-2.695504	1	-1.439351	2.826153	1.443397	
1	0.962547	-2.373637	-2.103626	6	-0.146082	0.266057	3.051846	
6	0.843003	-3.130443	1.310512	1	0.920189	0.260136	3.293990	
1	-0.058645	-3.406764	1.876407	1	-0.602867	1.100648	3.600516	
1	1.058262	-3.971167	0.633236	1	-0.613923	-0.660036	3.382598	
1	1.670136	-3.017745	2.017987	6	-3.487591	0.713150	0.001732	
6	3.389457	-0.844918	0.195358	6	-2.793169	1.208946	-1.132426	
6	2.970939	-0.535226	-1.135161	6	-2.194923	0.309175	-2.065790	
6	2.741090	0.826299	-1.515436	6	-2.229475	-1.060488	-1.792475	
6	2.766775	1.804971	-0.536383	6	-2.924312	-1.560505	-0.647795	
6	3.117557	1.477271	0.814249	6	-3.584208	-0.692093	0.230935	
6	3.520415	0.190853	1.164666	1	-3.945834	1.406942	0.693735	
1	3.672648	-1.861026	0.449780	1	-2.726114	2.275991	-1.294035	
1	2.950789	-1.312733	-1.890150	1	-1.655861	0.685233	-2.923284	
1	2.460711	1.067231	-2.534266	1	-1.653549	-1.744388	-2.400358	
1	2.457168	2.816634	-0.773032	1	-2.890477	-2.620089	-0.434067	
1	3.080747	2.255504	1.569348	1	-4.115952	-1.075222	1.090752	
1	3.852155	-0.035978	2.171821	IN10c (20.93)				
TS5c (198.25i)				6	-2.962894	-1.745264	-0.929607	
6	3.421657	0.330928	-0.858355	6	-2.922804	-3.106219	-0.641368	
6	4.052681	1.542781	-1.102806	6	-2.081921	-0.861444	-0.296217	
6	2.151144	0.270567	-0.286884	6	-1.094150	-1.308508	0.619921	
6	1.464490	1.456204	0.065277	6	-1.088507	-2.693874	0.896354	
6	2.122013	2.669207	-0.205417	8	-2.571589	1.278092	-2.091433	
8	1.129926	-2.041498	-1.437684	1	-0.364661	-3.096944	1.595834	
1	1.644063	3.607081	0.035151	1	-3.674983	-1.353637	-1.650614	
1	3.921033	-0.593739	-1.120731	1	-3.609632	-3.793845	-1.125620	

6	-1.980605	-3.568179	0.282850	1	0.629152	4.773513	0.098243
1	-1.935894	-4.627002	0.526524	15	1.844632	-0.712261	-0.637023
15	-2.158621	0.874882	-0.715857	8	1.919077	-1.231776	-2.047975
8	-3.050971	1.522691	0.498118	8	3.243570	-0.992313	0.208627
8	-0.609472	1.374843	-0.339786	6	4.133587	-2.022639	-0.238701
6	-3.608180	2.837503	0.323830	1	4.050962	-2.161703	-1.319769
1	-3.923676	2.989563	-0.711671	1	5.148321	-1.711278	0.025740
1	-4.469387	2.901355	0.992640	1	3.904630	-2.968708	0.266879
1	-2.872764	3.601087	0.600201	6	-0.780696	-0.018036	2.086596
44	1.425733	0.159821	-0.155171	6	0.221546	-0.769186	2.264961
6	-0.112089	-0.395127	1.265637	6	-1.621850	0.828280	2.995820
6	-0.019344	1.024935	0.941809	1	-1.575410	1.872316	2.667560
6	0.341203	-0.802242	2.662826	1	-2.670934	0.516695	2.949801
1	-0.507481	-0.871967	3.358931	1	-1.293823	0.778197	4.040530
1	0.842335	-1.775356	2.664099	6	1.277273	-1.584515	2.848679
1	1.056022	-0.085015	3.074162	1	1.110613	-2.651093	2.664653
6	0.000781	2.197573	1.884070	1	2.263669	-1.307903	2.465902
1	-1.006540	2.414204	2.266168	1	1.250799	-1.413948	3.935903
1	0.653933	2.007623	2.739320	44	-1.116256	-0.184497	-0.039658
1	0.371584	3.085639	1.361591	6	-1.873075	0.146351	-2.136049
6	3.386414	0.438378	0.704984	6	-1.714964	-1.240938	-1.947518
6	3.133306	-0.963605	0.530630	6	-2.466832	-1.936345	-0.939062
6	2.968721	-1.524669	-0.777312	6	-3.268479	-1.217749	-0.052912
6	2.889351	-0.648072	-1.865665	6	-3.318871	0.217610	-0.145371
6	3.099769	0.759923	-1.692440	6	-2.671792	0.888640	-1.209152
6	3.414903	1.302423	-0.432436	1	-1.309917	0.659217	-2.906985
1	3.583918	0.831280	1.697696	1	-0.993531	-1.781239	-2.550930
1	3.128055	-1.614081	1.399733	1	-2.340032	-3.007081	-0.821224
1	2.811879	-2.589658	-0.905880	1	-3.787067	-1.725204	0.754085
1	2.636051	-1.025149	-2.851104	1	-3.895777	0.785371	0.577035
1	2.992694	1.416625	-2.549580	1	-2.739006	1.967500	-1.293950
1	3.608119	2.363737	-0.319440				

IN11c (36.79)

TS6c (235.77i)							
6	2.556315	2.038011	-0.488213	6	2.497364	2.148500	-0.315820
6	2.223275	3.380573	-0.311110	6	2.162703	3.447945	0.054684
6	1.561120	1.057882	-0.397556	6	1.508265	1.154189	-0.318419
6	0.214594	1.385222	-0.130228	6	0.162003	1.409182	0.040848
6	-0.095098	2.744298	0.042663	8	0.736470	-1.390811	0.109769
8	0.663180	-1.341074	0.260034	1	-1.137272	2.986492	0.749984
1	-1.117841	3.047394	0.261284	1	3.518516	1.900992	-0.593603
1	3.585187	1.748554	-0.687589	1	2.918463	4.228494	0.062945
1	2.989609	4.148689	-0.375336	6	0.844943	3.730274	0.428840
6	0.895542	3.728175	-0.045683	1	0.576899	4.739574	0.734994

15	1. 861256	-0. 531614	-0. 821925	8	1. 839918	-1. 361490	-2. 072160
8	1. 726603	-0. 970588	-2. 245207	8	3. 388382	-0. 890319	0. 000660
8	3. 324400	-0. 845173	-0. 155404	6	4. 216583	-2. 012944	-0. 358194
6	4. 115645	-1. 926874	-0. 680997	1	3. 943132	-2. 887141	0. 242213
1	3. 918082	-2. 065595	-1. 746598	1	4. 106628	-2. 249691	-1. 418995
1	5. 162111	-1. 657840	-0. 520593	1	5. 246412	-1. 724507	-0. 136456
1	3. 888081	-2. 850751	-0. 138835	6	0. 028145	0. 322461	1. 648180
6	-0. 436873	-0. 507115	1. 846081	6	0. 657072	-0. 883760	1. 637188
6	0. 646550	-1. 229658	1. 573525	6	-0. 339626	1. 045884	2. 918281
6	-0. 948492	-0. 114064	3. 194051	1	0. 444081	1. 753807	3. 215732
1	-0. 963789	0. 980067	3. 288799	1	-1. 262403	1. 618657	2. 790556
1	-1. 980395	-0. 458342	3. 346219	1	-0. 502142	0. 345581	3. 744584
1	-0. 340013	-0. 510861	4. 018551	6	1. 204933	-1. 753849	2. 714394
6	1. 674809	-1. 969917	2. 360242	1	0. 812226	-2. 774005	2. 626008
1	1. 679355	-3. 037944	2. 102363	1	2. 299383	-1. 815105	2. 629474
1	2. 684044	-1. 579246	2. 186000	1	0. 958192	-1. 365279	3. 705175
1	1. 452984	-1. 881420	3. 428444	6	-3. 621750	-0. 840603	0. 443440
44	-1. 167517	-0. 164504	-0. 047432	6	-3. 203875	0. 527282	0. 223266
6	-2. 366063	0. 515391	-1. 947769	6	-2. 684471	0. 944534	-1. 045632
6	-2. 232025	-0. 875955	-2. 022116	6	-2. 303295	-0. 042955	-1. 994029
6	-2. 718130	-1. 719398	-0. 964404	6	-2. 399119	-1. 398076	-1. 589095
6	-3. 281024	-1. 160748	0. 186349	6	-3. 198588	-1. 799454	-0. 452549
6	-3. 283571	0. 266762	0. 341322	1	-4. 183064	-1. 105637	1. 334484
6	-2. 836505	1. 093446	-0. 724961	1	-3. 467799	1. 285604	0. 954863
1	-2. 003536	1. 149044	-2. 748866	1	-2. 537025	1. 998533	-1. 257450
1	-1. 746510	-1. 327583	-2. 880653	1	-1. 845701	0. 227695	-2. 938526
1	-2. 604881	-2. 795167	-1. 047985	1	-1. 972822	-2. 166066	-2. 226914
1	-3. 625571	-1. 796820	0. 994701	1	-3. 391684	-2. 853965	-0. 280760
1	-3. 659484	0. 716135	1. 254074	44	-1. 189241	-0. 252577	-0. 051393
1	-2. 858155	2. 171792	-0. 614055				

IN9c (20. 88)

TS7c (245. 39i)				IN9c (20. 88)			
6	2. 350802	2. 064942	-0. 879995	6	2. 962692	1. 745544	-0. 929497
6	1. 964126	3. 394399	-0. 705490	6	2. 922412	3. 106478	-0. 641187
6	1. 530670	1. 022537	-0. 450771	6	2. 081876	0. 861565	-0. 296115
6	0. 270996	1. 242383	0. 241883	6	1. 094066	1. 308449	0. 620074
6	-0. 078445	2. 629769	0. 383605	8	0. 609543	-1. 374802	-0. 340021
8	0. 824804	-1. 408436	0. 331703	1	0. 364334	3. 096723	1. 596095
1	-1. 013104	2. 883200	0. 876174	1	3. 674810	1. 354053	-1. 650549
1	3. 289272	1. 834953	-1. 379820	1	3. 609122	3. 794229	-1. 125428
1	2. 593535	4. 205732	-1. 056461	6	1. 980177	3. 568259	0. 283085
6	0. 734096	3. 653046	-0. 079475	1	1. 935323	4. 627065	0. 526804
1	0. 405400	4. 682589	0. 049322	15	2. 158704	-0. 874712	-0. 715913
15	1. 947317	-0. 679546	-0. 748237	8	2. 571807	-1. 277703	-2. 091516

8	3.050983	-1.522636	0.498042	6	2.231920	-1.437953	-2.829602
6	3.607968	-2.837531	0.323716	1	2.281019	-1.207148	-3.895202
1	2.872053	-3.601063	0.598909	1	3.232720	-1.693759	-2.465230
1	3.924537	-2.989180	-0.711519	1	1.554846	-2.284165	-2.669362
1	4.468428	-2.901939	0.993431	44	-1.390928	-0.361314	0.200307
6	0.112135	0.394884	1.265738	6	-3.380874	0.294190	-0.475964
6	0.019434	-1.025124	0.941641	6	-2.972049	-0.887793	-1.170180
6	-0.341033	0.801696	2.663057	6	-2.798554	-2.129539	-0.467538
1	0.507706	0.871156	3.359122	6	-2.794168	-2.126735	0.924039
1	-0.842052	1.774866	2.664607	6	-2.973509	-0.882213	1.620895
1	-1.055902	0.084442	3.074253	6	-3.397662	0.291665	0.934918
6	-0.000825	-2.197980	1.883635	1	-3.567875	1.207739	-1.028769
1	-0.371902	-3.085837	1.360997	1	-2.863137	-0.861547	-2.249196
1	1.006502	-2.414919	2.265541	1	-2.534477	-3.025481	-1.018520
1	-0.653805	-2.008085	2.739025	1	-2.531735	-3.021312	1.477874
6	-3.386232	-0.438062	0.705172	1	-2.862646	-0.855657	2.700052
6	-3.133064	0.963875	0.530495	1	-3.603820	1.199680	1.489102
6	-2.968652	1.524665	-0.777587	19	4.673241	-1.226239	1.724454
6	-2.889416	0.647812	-1.865743				
6	-3.099906	-0.760130	-1.692235	IN6f(11.58)			
6	-3.414880	-1.302344	-0.432072	6	-1.927000	-2.510429	0.251360
1	-3.583692	-0.830749	1.697978	6	-1.381596	-3.769960	0.020064
1	-3.127621	1.614509	1.399479	6	-1.114491	-1.369658	0.183499
1	-2.811729	2.589612	-0.906395	6	0.258906	-1.449946	-0.117288
1	-2.636149	1.024672	-2.851276	6	0.787122	-2.734203	-0.340205
1	-2.992951	-1.417007	-2.549255	8	-0.560301	1.207436	-0.045271
1	-3.608141	-2.363623	-0.318818	1	1.845098	-2.865375	-0.552316
44	-1.425635	-0.159824	-0.155202	1	-2.982112	-2.406296	0.495706
				1	-2.001935	-4.659908	0.075549
IN5f(26.22)				6	-0.019456	-3.874022	-0.278136
6	1.715856	2.590793	-0.324817	1	0.421946	-4.851334	-0.458567
6	1.119415	3.825071	-0.069619	15	-1.753976	0.295542	0.415251
6	0.947406	1.424510	-0.248819	8	-1.919483	0.396878	2.053866
6	-0.426594	1.450146	0.089170	6	-2.769330	1.386318	2.636632
6	-0.998358	2.712463	0.338648	1	-3.772376	1.351955	2.198217
8	0.436001	-1.192750	-0.126313	1	-2.829717	1.158577	3.703201
1	-2.048823	2.796262	0.604163	1	-2.356277	2.394481	2.508564
1	2.768683	2.535235	-0.590748	6	1.774381	-0.253170	1.913545
1	1.703948	4.738554	-0.131865	6	1.443974	0.944221	1.900827
6	-0.238119	3.880674	0.264134	6	2.226636	-1.545031	2.458772
1	-0.704965	4.841275	0.466147	1	1.474278	-2.324084	2.311554
15	1.621487	-0.221666	-0.547546	1	3.154362	-1.881670	1.982312
8	1.737023	-0.258783	-2.180040	1	2.414316	-1.438725	3.533657
8	2.958848	-0.533469	0.110730	6	1.087589	2.302696	2.338269

1	0.198634	2.646776	1.803561	6	-1.589093	-1.283013	2.942143
1	0.878154	2.302187	3.414646	1	-1.508977	-0.817650	3.932283
1	1.903328	3.010749	2.149710	1	-2.580034	-1.745257	2.862004
44	1.344492	0.317820	-0.264420	1	-0.847428	-2.087110	2.875875
6	1.966221	2.041099	-1.765145	6	-1.750023	-2.417428	-1.350885
6	3.032405	1.924712	-0.868980	6	-2.786247	-2.272038	-0.412710
6	3.565589	0.628281	-0.599142	6	-3.500502	-1.034892	-0.363160
6	3.161008	-0.500224	-1.358400	6	-3.235243	-0.024341	-1.323527
6	2.141079	-0.347346	-2.338571	6	-2.273852	-0.246280	-2.357495
6	1.504910	0.895577	-2.497583	6	-1.511510	-1.418148	-2.353424
1	1.463517	2.993354	-1.895986	1	-1.113666	-3.294959	-1.315437
1	3.380981	2.785198	-0.308907	1	-2.972290	-3.045797	0.323497
1	4.319433	0.509893	0.172037	1	-4.246936	-0.865783	0.405692
1	3.626943	-1.464331	-1.191707	1	-3.782681	0.910743	-1.283367
1	1.789504	-1.211166	-2.892488	1	-2.068315	0.537880	-3.078079
1	0.666914	0.994690	-3.177953	1	-0.713433	-1.559648	-3.073066
8	-3.101496	0.590523	-0.242914	44	-1.345525	-0.495228	-0.187459
19	-5.064235	0.861351	-1.675138	19	5.101759	-1.341810	-1.303660

TS4f(313.24i)

6	1.733540	2.522262	-0.644604	6	3.097830	1.672847	-0.141933
6	1.081209	3.640662	-1.164162	6	3.381455	2.928149	-0.673793
6	0.996621	1.451869	-0.129495	6	1.780766	1.244177	0.073441
6	-0.416985	1.467531	-0.138178	6	0.683128	2.100352	-0.225502
6	-1.055283	2.609547	-0.660220	6	1.004132	3.346356	-0.805398
8	3.127204	-0.373011	-0.242429	8	2.900078	-1.284826	0.347950
1	-2.140616	2.670831	-0.656476	1	0.214612	4.032065	-1.082644
1	2.819178	2.468802	-0.643911	1	3.906019	0.993811	0.110790
1	1.652463	4.477431	-1.555430	1	4.409093	3.246285	-0.822597
6	-0.317248	3.674301	-1.176393	6	2.318268	3.755273	-1.025349
1	-0.835329	4.538434	-1.584288	1	2.503113	4.731683	-1.464630
15	1.773416	-0.089959	0.407037	15	1.607775	-0.496101	0.537379
8	1.981917	0.186663	2.020381	8	1.227012	-0.395292	2.139684
8	0.664267	-1.170520	0.190583	8	0.399115	-1.087564	-0.265303
6	2.525744	-0.849088	2.839619	6	1.140489	-1.603535	2.906156
1	3.551566	-1.094527	2.537686	1	0.999356	-1.305892	3.947126
1	2.537194	-0.469704	3.863693	1	0.287996	-2.211788	2.581800
1	1.909426	-1.754818	2.795036	1	2.063364	-2.185514	2.816217
6	-1.201508	0.963300	1.657674	44	-1.499279	-0.246845	-0.143103
6	-1.372698	-0.287476	1.862908	6	-0.756497	1.805343	0.075636
6	-1.335081	2.292816	2.314798	6	-1.207951	0.999035	1.175097
1	-0.418771	2.884613	2.232015	6	-1.744632	2.924665	-0.278364
1	-2.158077	2.878914	1.892895	1	-1.478446	3.868159	0.216059
1	-1.553006	2.118890	3.375941	1	-1.781017	3.107962	-1.358034

1	-2.756610	2.667397	0.045539	1	-2.797798	2.287644	1.392067
6	-1.547569	1.283148	2.586700	6	-0.913636	0.480102	2.958808
1	-0.604924	1.404032	3.138692	1	0.050788	0.873126	3.299027
1	-2.092908	2.233411	2.675040	1	-1.698030	1.133589	3.368762
1	-2.123498	0.480582	3.056231	1	-1.071377	-0.531372	3.340701
6	-3.687770	-0.561281	0.246490	6	-3.798094	-0.788670	0.102147
6	-3.534245	0.077526	-1.019220	6	-3.521219	-0.031858	-1.076353
6	-2.976088	-0.642081	-2.127276	6	-2.735277	-0.594775	-2.133824
6	-2.424318	-1.893108	-1.897398	6	-2.131752	-1.837301	-1.927413
6	-2.479772	-2.485130	-0.591819	6	-2.363945	-2.571913	-0.717086
6	-3.190485	-1.879451	0.450137	6	-3.247997	-2.096673	0.265687
1	-4.209925	-0.049387	1.048171	1	-4.444162	-0.371433	0.867417
1	-3.953410	1.063541	-1.181211	1	-3.958352	0.953096	-1.195792
1	-2.937831	-0.183297	-3.108897	1	-2.559257	-0.033219	-3.044131
1	-1.903210	-2.415856	-2.692367	1	-1.450091	-2.239695	-2.669171
1	-1.993043	-3.440238	-0.426427	1	-1.847229	-3.513374	-0.563319
1	-3.310626	-2.375398	1.406592	1	-3.458598	-2.680906	1.154054
19	4.277025	-2.718479	-1.095468	19	4.224290	-2.575683	-1.410312

TS5f(204.58i)

6	2.630190	1.877156	-0.938043	6	0.523836	1.210265	-2.138739
6	2.526184	3.050824	-1.678374	6	-0.251278	2.117596	-2.802636
6	1.537598	1.362825	-0.227355	6	0.353153	0.972151	-0.722238
6	0.280430	2.024752	-0.240487	6	-0.717599	1.690413	-0.026443
6	0.202994	3.204151	-1.012829	6	-1.450513	2.692902	-0.759516
8	2.823849	-1.099524	-0.038740	8	2.708969	-0.560737	-0.287843
1	-0.730871	3.749454	-1.068443	1	-2.184902	3.296760	-0.236825
1	3.575929	1.344310	-0.896633	1	1.316717	0.678076	-2.658146
1	3.383492	3.445397	-2.215249	1	-0.103720	2.290599	-3.864616
6	1.295689	3.706620	-1.714638	6	-1.221054	2.893328	-2.091546
1	1.181273	4.621932	-2.288869	1	-1.779680	3.658136	-2.623904
15	1.792812	-0.198434	0.632631	15	1.813311	0.557692	0.218305
8	2.330545	0.295084	2.107471	8	2.624025	1.972769	0.317556
8	0.381092	-0.858148	0.869550	8	1.242310	0.323280	1.714330
6	2.818816	-0.679307	3.039953	6	3.750133	2.118276	1.192009
1	3.207276	-0.123346	3.895362	1	4.108247	3.141722	1.068844
1	2.013587	-1.344632	3.371108	1	3.454897	1.955097	2.233717
1	3.623396	-1.274226	2.595127	1	4.552769	1.421861	0.919942
44	-1.636259	-0.426391	-0.020943	44	-1.211273	-0.479949	0.039090
6	-0.940682	1.570834	0.492680	6	-1.050139	1.244908	1.307859
6	-1.026195	0.538255	1.486900	6	-0.217925	0.155446	1.797768
6	-2.010313	2.649842	0.724071	6	-2.150788	1.899628	2.108165
1	-1.577305	3.555142	1.168764	1	-1.785735	2.829375	2.566142
1	-2.501583	2.935731	-0.212127	1	-3.019259	2.149838	1.491598

1	-2.495437	1.254390	2.919190	1	0.934397	3.640438	-0.846691
6	-0.462637	-0.502593	3.133939	1	-0.549887	4.270897	-1.608533
1	-0.077243	0.116808	3.955320	1	-0.462459	4.134227	0.158121
1	-1.525322	-0.683105	3.308148	44	-1.341153	-0.085549	0.182666
1	0.056654	-1.465525	3.174578	6	-1.803300	-0.856132	2.305700
6	-1.488457	-2.724760	0.328727	6	-2.784439	0.164239	2.066674
6	-2.653270	-2.039088	0.782054	6	-3.583195	0.105626	0.924730
6	-3.391042	-1.210255	-0.108251	6	-3.385447	-0.952741	-0.026924
6	-2.965575	-1.061296	-1.450600	6	-2.475228	-1.999369	0.252021
6	-1.768273	-1.683961	-1.868666	6	-1.700374	-1.969170	1.453451
6	-1.043871	-2.550253	-0.998824	1	-1.142508	-0.764138	3.161087
1	-0.935545	-3.357674	1.014725	1	-2.856636	1.006655	2.745600
1	-2.981205	-2.156533	1.809005	1	-4.293074	0.897864	0.711710
1	-4.280918	-0.698496	0.242938	1	-3.965984	-0.975529	-0.942327
1	-3.505524	-0.410066	-2.128681	1	-2.360220	-2.817990	-0.449356
1	-1.391932	-1.496177	-2.868466	1	-0.992305	-2.762845	1.665003
1	-0.141648	-3.039553	-1.347172	8	2.184855	0.153755	1.795557
19	4.424313	-2.330230	-0.403283	19	3.014197	-2.215424	1.279320

TS6f(235.00i)

6	2.575220	-0.654162	-1.622532	6	2.628630	1.063366	1.477147
6	2.414304	-1.642551	-2.595081	6	2.373393	1.998664	2.478691
6	1.476646	-0.263596	-0.837431	6	1.553366	0.502807	0.765186
6	0.184229	-0.818068	-1.008101	6	0.192593	0.831230	1.019614
6	0.058342	-1.805770	-2.005653	6	-0.014377	1.770435	2.051993
8	0.128578	1.427698	0.739444	8	0.456699	-1.503238	-0.698721
1	-0.912662	-2.252785	-2.206185	1	-1.027712	2.042525	2.336190
1	3.536347	-0.156401	-1.498469	1	3.648077	0.754201	1.258293
1	3.249049	-1.937858	-3.224821	1	3.190239	2.430676	3.049108
6	1.149808	-2.217776	-2.776563	6	1.045827	2.347095	2.759104
1	1.009769	-2.977687	-3.541695	1	0.834374	3.060523	3.552047
15	1.607476	0.855140	0.571852	15	1.811357	-0.532080	-0.676692
8	2.577723	2.073690	0.066672	8	1.897113	0.232864	-1.978911
6	3.317827	2.857970	1.024650	8	3.090220	-1.464363	-0.354707
1	3.649602	2.235089	1.859040	6	3.812291	-2.129383	-1.423065
1	4.178081	3.268631	0.492709	1	3.334554	-3.086919	-1.645311
1	2.696507	3.676394	1.401808	1	3.835034	-1.502027	-2.316711
6	-1.480875	1.381848	-1.340645	1	4.822171	-2.296223	-1.047416
6	-0.744262	2.339667	-0.936634	6	-0.846121	-1.660872	1.174718
6	-2.325890	1.271935	-2.582215	6	0.138359	-2.284304	0.535168
1	-2.027133	0.383611	-3.148965	6	-1.496290	-2.073790	2.455489
1	-3.382246	1.155636	-2.317871	1	-1.378524	-1.286794	3.211631
1	-2.231332	2.147254	-3.233382	1	-2.574595	-2.232636	2.327146
6	-0.156317	3.660965	-0.780837	1	-1.071499	-2.997702	2.867531

6	0.883618	-3.566040	0.680440	6	0.679614	3.440396	-1.029203
1	0.764197	-4.195181	-0.211083	1	0.247767	4.082892	-0.252724
1	1.955463	-3.408746	0.846076	1	1.770065	3.574874	-0.997797
1	0.487352	-4.119808	1.536640	1	0.321034	3.775266	-2.004867
6	-3.503382	-0.770174	-0.371827	6	-3.603852	0.988208	0.111154
6	-3.339511	0.327550	0.534812	6	-3.263433	-0.217158	-0.600299
6	-2.749844	1.535581	0.073785	6	-2.778662	-1.371023	0.089680
6	-2.340802	1.671656	-1.289593	6	-2.437367	-1.261915	1.465044
6	-2.376763	0.540097	-2.115022	6	-2.505256	0.022479	2.061038
6	-2.985559	-0.678587	-1.667232	6	-3.203137	1.111446	1.431475
1	-3.951514	-1.695768	-0.026966	1	-4.091858	1.807367	-0.406873
1	-3.687816	0.250853	1.558401	1	-3.512441	-0.301706	-1.653396
1	-2.655270	2.375135	0.753735	1	-2.676437	-2.313666	-0.438417
1	-1.960673	2.619132	-1.658893	1	-2.125942	-2.127232	2.043430
1	-1.967886	0.583725	-3.119647	1	-2.131944	0.160678	3.071134
1	-3.014899	-1.536301	-2.330008	1	-3.342363	2.040033	1.974647
44	-1.280388	-0.109591	-0.096448	44	-1.260054	0.204240	0.145758
19	1.483200	2.756339	-1.427601	19	0.888557	-2.542861	1.699300

TS7f (261.17i)				IN10g (8.09)			
6	2.548883	-1.542833	-1.132303	8	0.572589	1.745856	0.157845
6	2.185800	-2.492244	-2.086491	6	1.051703	1.982689	1.322378
6	1.606113	-0.631504	-0.638645	8	2.114136	1.359881	1.643861
6	0.239048	-0.539903	-1.147966	6	0.365953	2.921494	2.268912
6	-0.068562	-1.547098	-2.134339	1	1.063730	3.271559	3.032526
8	0.652686	1.549865	0.524196	1	-0.062519	3.764777	1.721313
1	-1.065164	-1.566006	-2.565553	1	-0.456922	2.387796	2.759626
1	3.570469	-1.512564	-0.756518	47	-4.123225	0.046864	-0.632952
1	2.910181	-3.203701	-2.468011	6	0.737816	-2.081729	1.328452
6	0.859495	-2.479893	-2.566064	8	1.670151	-2.813099	1.018199
1	0.555666	-3.216382	-3.306430	8	0.588894	-0.827152	0.919848
15	1.948664	0.463748	0.710391	6	-0.382234	-2.544535	2.247872
8	1.886758	-0.111466	2.104103	1	-0.183220	-3.563497	2.584393
8	3.283622	1.298880	0.366838	1	-0.462196	-1.875796	3.111387
6	4.046720	1.965338	1.408183	1	-1.343633	-2.511362	1.722092
1	3.618892	2.952974	1.597541	47	-1.621244	-0.004208	0.142115
1	4.041667	1.370995	2.323920	44	2.034304	0.198897	-0.156965
1	5.060492	2.065176	1.020029	6	2.660180	0.839242	-2.173159
6	-0.228329	1.048663	-1.561282	6	3.756657	1.059774	-1.306269
6	0.331730	2.015664	-0.787909	6	4.209561	-0.015117	-0.484486
6	-0.719182	1.294622	-2.964107	6	3.629537	-1.304229	-0.582493
1	0.087226	1.149653	-3.693300	6	2.552502	-1.516551	-1.492976
1	-1.522406	0.603645	-3.231280	6	2.067007	-0.458856	-2.293158
1	-1.107328	2.311549	-3.080335	1	2.217220	1.677106	-2.701562

1	4. 165790	2. 055642	-1. 181475	1	3. 339153	3. 493359	-0. 120858
1	4. 954972	0. 177329	0. 280543	47	-3. 002062	-0. 479389	0. 088993
1	3. 902737	-2. 090372	0. 107464	6	1. 473462	-0. 284146	2. 593790
1	2. 034487	-2. 466767	-1. 471827	8	1. 881003	-1. 437642	2. 701208
1	1. 191941	-0. 599698	-2. 917138	8	1. 137230	0. 312839	1. 468118
				6	1. 301463	0. 630492	3. 798903
TS8g(82. 28i)				1	1. 665552	0. 134354	4. 700445
8	0. 631248	2. 336557	-0. 439105	1	1. 840653	1. 570196	3. 642848
6	1. 838583	2. 420689	-0. 095655	1	0. 241547	0. 881820	3. 920642
8	2. 608187	1. 402610	0. 000698	47	-1. 125578	1. 348822	-0. 099346
6	2. 436170	3. 772976	0. 226683	44	0. 992946	-0. 574060	-0. 344674
1	3. 525731	3. 748072	0. 158386	6	0. 129903	-1. 936223	-1. 915147
1	2. 027241	4. 534311	-0. 442339	6	1. 430569	-1. 575048	-2. 314195
1	2. 156972	4. 041530	1. 252442	6	2. 515878	-1. 740187	-1. 400162
47	-3. 447931	-0. 406304	-0. 209573	6	2. 300229	-2. 316744	-0. 119196
6	0. 839437	-0. 869931	2. 602148	6	0. 987514	-2. 742005	0. 255717
8	1. 108671	-2. 061874	2. 499670	6	-0. 087134	-2. 535372	-0. 629799
8	1. 006633	0. 038044	1. 654770	1	-0. 718039	-1. 706946	-2. 549775
6	0. 259725	-0. 266562	3. 871492	1	1. 588810	-1. 050943	-3. 249891
1	0. 212571	-1. 022493	4. 657294	1	3. 490800	-1. 335473	-1. 649725
1	0. 867974	0. 581693	4. 201234	1	3. 099196	-2. 359926	0. 609888
1	-0. 747363	0. 114267	3. 666008	1	0. 815502	-3. 090765	1. 264871
47	-1. 253654	1. 036206	-0. 181250	1	-1. 097582	-2. 760908	-0. 312139
44	1. 472551	-0. 339622	-0. 260057				
6	1. 106743	-1. 054076	-2. 362117	IN10h(19. 90)			
6	2. 495216	-0. 898670	-2. 192590	47	-0. 632036	-1. 884110	-0. 665571
6	3. 129999	-1. 498826	-1. 063166	6	-1. 446722	2. 243805	-0. 835777
6	2. 379765	-2. 303647	-0. 157432	8	-2. 250572	2. 016889	0. 119955
6	0. 988213	-2. 537563	-0. 390888	8	-0. 061474	1. 899698	-0. 561575
6	0. 355750	-1. 884912	-1. 463510	47	-1. 741070	-0. 011675	0. 905682
1	0. 586168	-0. 493711	-3. 130842	8	-1. 598619	2. 763858	-1. 926960
1	3. 050299	-0. 214532	-2. 824409	44	0. 952491	0. 384829	-0. 089659
1	4. 167597	-1. 268805	-0. 845099	6	3. 033005	0. 993713	-0. 646787
1	2. 833069	-2. 679352	0. 750750	6	2. 734846	1. 533245	0. 623810
1	0. 409402	-3. 073724	0. 349014	6	2. 248009	0. 665726	1. 650505
1	-0. 722900	-1. 928881	-1. 559326	6	2. 203658	-0. 744184	1. 444729
				6	2. 570908	-1. 285308	0. 190709
IN11g(17. 60)				6	2. 918339	-0. 416572	-0. 871521
8	0. 501293	2. 840532	-0. 452500	1	3. 284486	1. 653387	-1. 470838
6	1. 624605	2. 410628	-0. 799507	1	2. 744968	2. 607012	0. 776506
8	1. 955682	1. 183454	-0. 978710	1	1. 911875	1. 081013	2. 594695
6	2. 741927	3. 413993	-1. 037183	1	1. 819809	-1. 389585	2. 225456
1	3. 403105	3. 077072	-1. 839548	1	2. 482261	-2. 350036	0. 011529
1	2. 328614	4. 397618	-1. 268750	1	3. 096053	-0. 818490	-1. 862959

				6	1. 942654	-2. 333728	1. 436386
TS8h (106. 52i)				6	2. 472627	-1. 884759	2. 641894
47	-0. 957963	-1. 908222	-0. 606871	6	0. 664029	-1. 928303	1. 028295
6	-0. 878195	2. 596127	-0. 711813	6	-0. 126372	-1. 044370	1. 809561
8	-1. 496457	2. 341522	0. 388445	6	0. 441363	-0. 611413	3. 026233
8	0. 318364	1. 861962	-0. 932678	8	-1. 243069	-1. 473708	-0. 831178
47	-1. 717175	0. 218430	0. 782472	1	-0. 116144	0. 055999	3. 672495
8	-1. 132361	3. 433663	-1. 558833	1	2. 516665	-3. 011184	0. 809550
44	0. 962513	0. 288772	-0. 072726	1	3. 458367	-2. 204589	2. 963710
6	3. 102295	0. 722363	-0. 532394	6	1. 711216	-1. 018385	3. 430206
6	2. 820803	1. 098175	0. 800861	1	2. 107244	-0. 656363	4. 374517
6	2. 252368	0. 142281	1. 703875	15	0. 063432	-2. 477745	-0. 559173
6	2. 090673	-1. 217219	1. 312652	8	1. 006346	-2. 425542	-1. 730770
6	2. 339515	-1. 588928	-0. 017255	8	-0. 603907	-3. 923240	-0. 282030
6	2. 758651	-0. 595125	-0. 960268	6	-0. 972183	-4. 795702	-1. 378645
1	3. 426825	1. 465170	-1. 252711	1	-1. 921462	-4. 469036	-1. 812355
1	2. 938856	2. 130735	1. 112208	1	-0. 191078	-4. 799980	-2. 142066
1	1. 951578	0. 456402	2. 697273	1	-1. 083552	-5. 789943	-0. 945618
1	1. 651569	-1. 925800	2. 004718	6	-1. 516265	-0. 633863	1. 424523
1	2. 123628	-2. 595140	-0. 356117	6	-2. 170204	-1. 157636	0. 241664
1	2. 855456	-0. 860319	-2. 008083	6	-2. 428833	-0. 315646	2. 605364
				1	-2. 453075	-1. 145288	3. 324612
IN11h (13. 10)				1	-2. 096842	0. 576342	3. 144791
47	-1. 457249	-0. 730432	-1. 244888	1	-3. 453126	-0. 122475	2. 280690
6	-0. 248154	2. 362306	-0. 393414	6	-3. 467285	-1. 904124	0. 112918
8	0. 125949	1. 859860	0. 798162	1	-3. 844043	-1. 840564	-0. 912891
8	0. 147823	1. 507262	-1. 352527	1	-3. 325545	-2. 963371	0. 366206
47	-1. 477978	-0. 236992	1. 395684	1	-4. 225469	-1. 498930	0. 786106
8	-0. 852524	3. 397824	-0. 568521	6	-2. 216751	2. 705998	0. 578168
44	0. 940244	0. 151534	-0. 022305	6	-1. 238010	3. 091702	-0. 384875
6	2. 732108	-0. 400736	-1. 232100	6	-1. 408443	2. 633354	-1. 714763
6	3. 117646	0. 510999	-0. 203309	6	-2. 605233	1. 987278	-2. 132627
6	2. 827061	0. 194339	1. 154403	6	-3. 621209	1. 706256	-1. 202061
6	2. 185130	-1. 026909	1. 493362	6	-3. 409151	2. 030890	0. 170314
6	1. 770772	-1. 895870	0. 451021	1	-2. 088742	2. 979789	1. 619645
6	2. 088862	-1. 620466	-0. 910618	1	-0. 404780	3. 732181	-0. 116560
1	2. 880389	-0. 127099	-2. 271672	1	-0. 627790	2. 821390	-2. 444394
1	3. 566046	1. 464651	-0. 458746	1	-2. 713772	1. 681549	-3. 167729
1	3. 044481	0. 921836	1. 929700	1	-4. 539061	1. 220939	-1. 516721
1	1. 929884	-1. 245989	2. 523412	1	-4. 166308	1. 796213	0. 910526
1	1. 190701	-2. 779390	0. 692526	44	-1. 712995	0. 732532	-0. 291774
1	1. 762898	-2. 294071	-1. 694164	8	2. 945777	2. 150087	0. 811583
				8	3. 256940	0. 937625	-1. 043687
IN9g (21. 21)				6	3. 679857	1. 690277	-0. 115955

6	5. 155716	2. 064612	-0. 095699	1	3. 312617	-2. 696833	2. 285822
1	5. 369091	2. 798116	0. 682813	1	1. 776728	-3. 147614	3. 076264
1	5. 757632	1. 166274	0. 085368	1	2. 101512	-3. 682066	1. 426054
1	5. 450864	2. 464813	-1. 071263	47	-3. 806425	-0. 043983	-0. 557935
47	0. 909649	1. 417548	0. 345772	6	1. 620732	-0. 491425	-2. 341655
19	2. 949257	-0. 963066	-2. 641780	8	0. 694540	-0. 357796	-1. 445564
				8	2. 787541	-0. 071392	-2. 223020
IN12g(23. 28)				6	1. 161309	-1. 195851	-3. 606220
8	0. 702114	-2. 918814	0. 312769	1	2. 010371	-1. 653852	-4. 118431
6	-0. 487033	-2. 636837	0. 547515	1	0. 393628	-1. 941487	-3. 388055
8	-1. 047627	-1. 477033	0. 403239	1	0. 719830	-0. 452652	-4. 281136
6	-1. 404750	-3. 741891	1. 068780	47	-1. 615642	-0. 947080	0. 576644
1	-2. 284817	-3. 857630	0. 423044	44	0. 860473	0. 752282	0. 275117
1	-0. 872270	-4. 692866	1. 099914	6	0. 262800	2. 247121	1. 879773
1	-1. 742433	-3. 506254	2. 086509	6	1. 656602	2. 305575	1. 709965
47	1. 638290	1. 522634	0. 969874	6	2. 208334	2. 484000	0. 401718
6	-2. 212507	1. 862997	0. 875175	6	1. 350818	2. 631229	-0. 722637
8	-0. 972020	1. 526220	0. 719346	6	-0. 065307	2. 611912	-0. 544958
8	-3. 179967	1. 255633	0. 379560	6	-0. 598029	2. 392506	0. 743684
6	-2. 421830	3. 099088	1. 737581	1	-0. 160406	2. 009273	2. 849066
1	-3. 479509	3. 229890	1. 972625	1	2. 313561	2. 119739	2. 552910
1	-1. 836330	3. 030682	2. 659592	1	3. 283548	2. 465752	0. 259199
1	-2. 068880	3. 984158	1. 195682	1	1. 775899	2. 688703	-1. 718278
47	2. 067563	-1. 063672	0. 513584	1	-0. 725080	2. 643576	-1. 404187
44	-0. 222388	0. 181260	-0. 766765	1	-1. 666337	2. 262946	0. 864460
6	1. 073709	-0. 273388	-2. 552976	19	4. 458507	-0. 899276	-0. 576859
6	-0. 097728	-1. 054664	-2. 641841	IN13g(9. 96)			
6	-1. 386074	-0. 432137	-2. 630505	8	-0. 853994	0. 185304	-1. 992771
6	-1. 493149	0. 963907	-2. 479568	6	-1. 933902	-0. 460216	-2. 140558
6	-0. 307037	1. 753148	-2. 345128	8	-2. 811315	-0. 341506	-1. 204642
6	0. 968317	1. 147118	-2. 399236	6	-2. 157768	-1. 342428	-3. 332223
1	2. 046395	-0. 750668	-2. 562105	1	-3. 215336	-1. 363812	-3. 608588
1	-0. 016474	-2. 135454	-2. 678339	1	-1. 557261	-0. 993127	-4. 174703
1	-2. 280768	-1. 044033	-2. 679182	1	-1. 837270	-2. 363801	-3. 091470
1	-2. 466864	1. 430080	-2. 382839	47	4. 357015	0. 087936	-0. 078875
1	-0. 388912	2. 817791	-2. 155695	6	-1. 176278	-1. 793386	1. 292290
1	1. 862499	1. 748674	-2. 291558	8	-0. 544067	-0. 961315	0. 510932
19	-3. 593325	-1. 105955	1. 038390	8	-2. 358620	-1. 644685	1. 641847
TS9g(79. 04i)				6	-0. 350355	-2. 976813	1. 759606
8	0. 340548	-1. 432705	1. 783155	1	-0. 971502	-3. 674873	2. 323339
6	1. 561177	-1. 618419	1. 584677	1	0. 110210	-3. 486810	0. 907494
8	2. 268891	-0. 778716	0. 904404	1	0. 466390	-2. 623625	2. 399290
6	2. 241000	-2. 854110	2. 132380	47	1. 894771	-0. 769029	-0. 045606

44	-1.375145	0.882236	-0.057692	6	-2.292453	3.598659	-0.212550
6	-1.238181	3.072180	-0.536869	6	-1.294067	3.388000	0.789467
6	-2.489252	2.832297	0.060954	6	0.063535	3.133066	0.422625
6	-2.560362	2.173693	1.334737	6	0.338073	2.923458	-0.955760
6	-1.382897	1.782369	2.001058	6	-0.646480	3.135168	-1.956632
6	-0.112811	2.011552	1.384602	6	-1.961554	3.489793	-1.595485
6	-0.041223	2.638598	0.121822	1	-3.301777	3.855878	0.089758
1	-1.182641	3.493354	-1.534747	1	-1.560197	3.498752	1.835317
1	-3.400813	3.082991	-0.470912	1	0.866098	3.166599	1.153139
1	-3.527151	1.937712	1.766579	1	1.337489	2.618553	-1.249503
1	-1.444515	1.224157	2.928113	1	-0.389948	2.980158	-2.998986
1	0.791469	1.610994	1.830307	1	-2.714385	3.666440	-2.356506
1	0.916813	2.712125	-0.382458	44	-1.572687	1.553467	-0.403296
19	-4.488095	-1.678514	0.325336	6	2.951620	-0.737387	0.199947
				8	1.818094	-1.285486	0.492706
IN9h(8. 15)				8	3.165416	0.507138	0.530191
6	-1.293202	-3.046445	1.631837	8	3.852256	-1.405740	-0.448822
6	-1.193471	-2.969233	3.017212	47	5.309585	0.404176	-0.236321
6	-1.848367	-1.989161	0.899602	47	0.609438	0.538840	0.995045
6	-2.309807	-0.804623	1.529741	19	1.894896	-3.122280	-1.340099
6	-2.196764	-0.760017	2.934874	IN12h(19. 32)			
8	-2.126300	-0.517940	-1.343045	47	0.886961	-1.949842	-0.822171
1	-2.545610	0.113241	3.473853	6	-2.073405	1.094373	-0.384283
1	-0.945801	-3.934638	1.111212	8	-2.524198	0.295076	0.525047
1	-0.771433	-3.791356	3.586110	8	-0.762598	1.477724	-0.327121
6	-1.649158	-1.815585	3.660744	47	-0.810759	-1.089238	1.084202
1	-1.585291	-1.738033	4.742534	8	-2.761813	1.606638	-1.281757
15	-1.895077	-2.109058	-0.881049	44	1.018786	0.767174	-0.098924
8	-0.718824	-2.716114	-1.593811	6	2.298689	2.569963	-0.608711
8	-3.321319	-2.805942	-1.209159	6	1.940569	2.656462	0.750019
6	-3.611485	-3.301894	-2.537065	6	2.160045	1.529530	1.602037
1	-3.874034	-2.471871	-3.199428	6	2.870099	0.386840	1.128317
1	-2.752946	-3.844432	-2.939457	6	3.277345	0.325236	-0.223773
1	-4.464160	-3.972636	-2.427441	6	2.919294	1.378148	-1.103938
6	-2.943931	0.324960	0.778840	1	2.029241	3.364774	-1.296176
6	-3.122608	0.290736	-0.660388	1	1.389701	3.515805	1.116864
6	-4.000120	1.094356	1.566737	1	1.793193	1.544840	2.622870
1	-4.766732	0.419034	1.969930	1	3.032789	-0.457009	1.787766
1	-3.564442	1.635597	2.412365	1	3.769370	-0.559879	-0.608614
1	-4.501768	1.837096	0.943284	1	3.124370	1.283826	-2.165150
6	-4.374093	0.465725	-1.473148	19	-5.027037	0.721573	-0.405670
1	-4.119047	0.696198	-2.512436	TS9h(87. 31i)			
1	-4.976762	-0.452218	-1.457616				
1	-4.990597	1.277777	-1.081617				

47	1. 119768	-1. 958470	-0. 748381	6	-3. 431297	-0. 684564	-1. 356027
6	-1. 981101	0. 920453	-0. 770931	6	-3. 527186	-1. 430448	-0. 156578
8	-2. 207169	0. 421049	0. 420404	6	-3. 549383	-0. 746440	1. 087927
8	-0. 719955	1. 257625	-1. 091434	1	-3. 491701	-1. 306361	2. 016504
47	-0. 771456	-1. 216101	0. 986752	6	-3. 549436	0. 683818	1. 123528
8	-2. 885386	1. 159354	-1. 586529	6	-3. 531860	1. 430317	-0. 085760
44	0. 876229	0. 820818	-0. 044819	1	-3. 461850	2. 512873	-0. 054669
6	2. 016353	2. 641855	-0. 705176	6	-3. 436321	0. 746933	-1. 320947
6	1. 502954	2. 884731	0. 585293	1	-3. 293359	1. 307169	-2. 240000
6	1. 754178	1. 938874	1. 628643	6	3. 431666	0. 657547	-1. 369140
6	2. 646696	0. 844829	1. 429696	6	3. 441724	-0. 772782	-1. 303007
6	3. 150955	0. 595654	0. 144444	6	3. 534550	-1. 428029	-0. 052810
6	2. 762022	1. 447362	-0. 941424	1	3. 466093	-2. 509736	0. 002357
1	1. 734005	3. 278657	-1. 536554	6	3. 547493	-0. 654515	1. 140078
1	0. 830761	3. 718118	0. 759012	6	3. 546422	0. 774578	1. 072972
1	1. 272566	2. 066459	2. 592482	1	3. 486023	1. 354759	1. 988843
1	2. 832749	0. 146621	2. 237326	6	3. 523551	1. 430559	-0. 186230
1	3. 757009	-0. 281845	-0. 047042	1	3. 447065	2. 512011	-0. 234634
1	3. 067594	1. 198800	-1. 952373	17	-0. 000004	1. 609477	0. 324943
19	-4. 896404	0. 663962	-0. 076158	17	-0. 000400	-1. 609801	0. 324865
				44	-1. 798464	-0. 000062	-0. 013541
IN13h(21. 64)				44	1. 798658	-0. 000908	-0. 015011
47	0. 778228	-1. 712499	-1. 151645	1	-3. 453123	-2. 512898	-0. 180548
6	-1. 860840	0. 276147	-1. 076671	1	-3. 283728	-1. 197666	-2. 301553
8	-1. 677253	0. 684260	0. 181975	1	-3. 492006	1. 196841	2. 078855
8	-0. 717159	0. 275990	-1. 739398	1	3. 284389	1. 149265	-2. 326049
47	0. 392876	-1. 445353	1. 491874	1	3. 302785	-1. 353483	-2. 209891
8	-2. 956098	-0. 059909	-1. 528535	1	3. 488196	-1. 146442	2. 106328
44	0. 391200	0. 920452	-0. 081347	CAT2(16. 34)			
6	1. 452943	2. 556372	-1. 173711	6	0. 739277	-0. 864439	1. 365819
6	0. 583987	3. 146044	-0. 218439	6	0. 656884	0. 550857	1. 529549
6	0. 697413	2. 773169	1. 154731	6	1. 185380	1. 406084	0. 515211
6	1. 679209	1. 844883	1. 571036	1	1. 028373	2. 478130	0. 581792
6	2. 527562	1. 244903	0. 593309	6	1. 836943	0. 854766	-0. 624709
6	2. 443649	1. 618303	-0. 769453	6	1. 927802	-0. 544593	-0. 779803
1	1. 318731	2. 775484	-2. 228030	1	2. 327072	-0. 963657	-1. 697677
1	-0. 192351	3. 832428	-0. 537847	6	1. 358374	-1. 404464	0. 197385
1	-0. 005534	3. 171928	1. 878950	1	1. 328626	-2. 475518	0. 022987
1	1. 750660	1. 550351	2. 611232	17	-2. 459184	0. 000516	-0. 004173
1	3. 232236	0. 478471	0. 894687	44	-0. 264465	0. 000076	-0. 342696
1	3. 081597	1. 144335	-1. 506232	1	0. 254465	-1. 523726	2. 078509
19	-4. 409448	0. 368660	0. 562030	1	0. 109745	0. 971893	2. 366698
CAT1(7. 43)				1	2. 166352	1. 511488	-1. 423458

CAT3 (27. 38)				IN3a (24. 99)			
6	2.625886	-0.005778	-0.000544	1	4.110816	-0.141420	-0.232767
8	2.369131	1.294472	-0.001938	6	2.424563	-3.598022	0.313774
8	1.605374	-0.738130	0.004043	1	0.604432	-2.658171	-0.352937
44	-0.240677	0.164243	-0.209840	6	3.784999	-3.426867	0.578736
6	-1.335307	-0.860613	1.382297	1	5.446647	-2.049529	0.585000
6	-1.669793	0.527228	1.420133	1	1.955842	-4.564617	0.472003
6	-2.231342	1.172260	0.275197	1	4.375454	-4.262606	0.942507
6	-2.393321	0.454865	-0.924311	6	1.720116	1.651997	-0.251659
6	-1.991375	-0.914948	-0.991571	6	1.627562	2.855615	-0.973767
6	-1.496574	-1.587011	0.165920	6	2.092807	1.681662	1.103275
1	-0.864010	-1.331029	2.240910	6	2.374835	2.900035	1.720062
1	-1.444311	1.109929	2.309847	1	2.156569	0.761748	1.672987
1	-2.423136	2.241660	0.300929	6	2.282800	4.091738	0.997536
1	-2.710980	0.967536	-1.828406	1	1.841222	4.994778	-0.912582
1	-2.005277	-1.433804	-1.947183	1	2.665974	2.916744	2.765933
1	-1.142704	-2.611667	0.090238	1	2.505949	5.038067	1.481610
6	4.012264	-0.537630	0.010031	6	1.812142	0.202593	-2.821032
1	4.514699	-0.235387	0.939804	1	1.606692	-0.759991	-3.297670
1	3.999438	-1.626026	-0.057015	1	1.244814	0.980321	-3.338945
1	4.586405	-0.120494	-0.827878	1	2.882085	0.417375	-2.893621
1	3.160997	1.871616	-0.028032	8	-0.248479	-0.225202	-1.123488
IN2a (19. 11)				IN3a (24. 99)			
6	-3.552398	-1.485140	-0.554935	6	-2.293590	-2.932008	-0.810956
6	-3.789026	-1.115054	0.808058	6	-2.692185	-4.029619	-0.047254
6	-3.785520	0.247119	1.172450	6	-1.910727	-1.729741	-0.191001
1	-3.837869	0.530177	2.217413	6	-1.930572	-1.641482	1.213338
6	-3.506274	1.232824	0.181182	1	-1.598990	-0.738582	1.720104
6	-3.373569	0.867290	-1.195894	6	-2.337238	-2.744292	1.967643
1	-3.131018	1.625486	-1.932280	8	0.141582	-0.189187	-1.509783
6	-3.416985	-0.491291	-1.566387	1	1.732356	2.638488	1.781344
1	-3.200411	-0.785143	-2.587257	6	1.326125	2.072221	2.623985
17	-0.544747	-0.464953	1.955179	6	0.163546	1.200159	2.172930
44	-1.897065	-0.223593	0.095796	1	2.132768	1.445520	3.026195
1	-3.855663	-1.881766	1.571831	1	0.986769	2.745219	3.413999
1	-3.454666	-2.534107	-0.814772	8	-0.896784	1.174515	2.794925
1	-3.368929	2.267518	0.477446	8	0.320321	0.451815	1.102858
15	1.300437	0.083213	-1.067123	1	-2.353802	-2.666028	3.051368
6	2.264221	-1.276397	-0.347441	1	-2.287994	-3.022316	-1.892725
6	3.634218	-1.106709	-0.086123	1	-2.986920	-4.951838	-0.540746
6	1.661965	-2.526802	-0.150823	6	-2.718643	-3.934905	1.345262
6	4.389199	-2.183088	0.377872	1	-3.035353	-4.786352	1.942220

15	-1.382585	-0.306952	-1.226860	8	-0.169407	-2.369655	1.178323
44	1.840071	-0.019874	-0.194055	8	-2.427724	-2.421305	1.237847
6	4.025671	-0.123611	-0.490312	1	-1.932829	-0.596351	2.602985
6	3.747454	-0.244029	0.902804	1	1.882116	2.568660	2.707635
6	2.837725	-1.247574	1.340676	1	0.376753	2.410937	4.655807
6	2.239615	-2.147496	0.418353	6	-0.916277	0.942290	3.733670
6	3.444240	-1.008389	-1.432191	1	-1.574749	0.863485	4.595329
6	2.511658	-1.978259	-0.967688	15	1.677159	1.398832	-0.023266
1	4.614050	0.716591	-0.840856	44	-1.244116	0.417027	-0.821696
1	4.151905	0.476166	1.603686	6	-2.756638	0.143735	-2.390898
1	2.535812	-1.276113	2.382624	6	-3.190932	-0.538420	-1.212187
1	1.492019	-2.858060	0.750142	6	-3.274283	0.170553	0.006754
1	3.599437	-0.858577	-2.493651	6	-2.986957	1.573721	0.060008
1	1.946544	-2.556588	-1.691194	6	-2.400080	1.513317	-2.330127
6	-2.223714	1.192259	-0.621176	6	-2.534065	2.234980	-1.096344
6	-3.546402	1.120471	-0.159761	1	-2.559674	-0.420924	-3.294577
6	-1.582916	2.432784	-0.733366	1	-3.312003	-1.614225	-1.199563
6	-4.223699	2.287270	0.192196	1	-3.448923	-0.404577	0.907017
1	-4.044005	0.159859	-0.059061	1	-2.994301	2.089444	1.013386
6	-2.269086	3.594520	-0.376676	1	-1.962238	1.997824	-3.195869
1	-0.550176	2.483637	-1.065501	1	-2.193982	3.263488	-1.038329
6	-3.585170	3.524677	0.083690	6	2.965868	0.132784	-0.283548
1	-5.244573	2.228591	0.559604	6	2.778797	-1.187525	0.160894
1	-1.766322	4.554820	-0.450868	6	4.154637	0.479855	-0.948132
1	-4.112230	4.432734	0.364712	6	3.780938	-2.134161	-0.053582
6	-2.131200	-0.576089	-2.886976	1	1.862211	-1.502501	0.648212
1	-1.918778	0.318524	-3.478983	6	5.148201	-0.474638	-1.159211
1	-1.673497	-1.435855	-3.383823	1	4.313125	1.491110	-1.310632
1	-3.214190	-0.713195	-2.821376	6	4.962605	-1.783003	-0.707925
17	1.984974	2.301398	-0.900060	1	3.626042	-3.152937	0.289065
				1	6.062952	-0.196166	-1.675127
TS1a(590.42i)				1	5.737360	-2.527737	-0.870267
6	1.033442	1.890873	2.672220	6	2.547350	3.011066	0.078957
6	0.181553	1.808105	3.772906	1	2.911930	3.278369	-0.916731
6	0.782924	1.116619	1.530435	1	1.829739	3.771619	0.397110
6	-0.317227	0.225842	1.467529	1	3.390103	2.979988	0.774756
1	-0.311625	-0.901674	0.969800	17	-0.007539	-1.351683	-1.869404
6	-1.145824	0.154347	2.608700				
8	0.576506	1.532396	-1.122639	IN4a(17.21)			
1	-0.957162	-4.752222	0.023175	6	-1.576147	1.303914	2.458510
6	-1.219509	-4.492594	1.056061	6	-0.673721	2.114521	3.138012
6	-1.304909	-2.969254	1.174176	6	-1.103895	0.375176	1.518209
1	-2.177361	-4.954793	1.307855	6	0.270248	0.224561	1.210046
1	-0.428271	-4.886311	1.702061	1	2.122327	2.103764	-1.285087

6	1. 150051	1. 080267	1. 901909				
8	-1. 274536	-1. 505899	-0. 407334	IN4b (16. 52)			
1	4. 999355	4. 191556	-1. 301372	6	1. 180913	3. 281347	-0. 571315
6	4. 750427	3. 744159	-0. 333324	6	1. 056252	4. 393370	0. 263380
6	3. 841135	2. 550738	-0. 534262	6	1. 177642	1. 986217	-0. 026201
1	5. 661998	3. 432810	0. 178183	6	1. 049549	1. 818344	1. 365119
1	4. 234991	4. 511324	0. 254259	1	1. 036586	0. 822440	1. 796406
8	2. 716093	2. 893074	-1. 161292	6	0. 923909	2. 934691	2. 191509
8	4. 113963	1. 419758	-0. 163029	8	-0. 035130	-0. 301930	-1. 222114
1	2. 211744	1. 054990	1. 677183	1	1. 403234	-3. 084239	1. 690279
1	-2. 643706	1. 402696	2. 648550	6	0. 344194	-3. 245041	1. 920425
1	-1. 024569	2. 836429	3. 870286	6	-0. 481102	-2. 241404	1. 177444
6	0. 690278	1. 998042	2. 847838	1	0. 064223	-4. 258026	1. 625216
1	1. 404620	2. 641195	3. 357686	1	0. 210609	-3. 112331	2. 997718
15	-2. 184641	-0. 699559	0. 560079	8	-0. 550301	-1. 016954	1. 552944
44	0. 853566	-1. 165332	-0. 202251	8	-1. 150485	-2. 546030	0. 137291
6	2. 248232	-2. 478758	-1. 604721	1	0. 832157	2. 800529	3. 265424
6	2. 945224	-1. 464418	-0. 858689	1	1. 288935	3. 434485	-1. 640493
6	2. 917027	-1. 449475	0. 554492	1	1. 066830	5. 391586	-0. 163992
6	2. 044248	-2. 348811	1. 242465	6	0. 927813	4. 220715	1. 643076
6	1. 392637	-3. 346282	-0. 933137	1	0. 837107	5. 087497	2. 291345
6	1. 238279	-3. 240327	0. 494739	15	1. 290052	0. 511418	-1. 091772
1	2. 290599	-2. 475540	-2. 687880	44	-1. 811744	-0. 534064	-0. 091934
1	3. 510914	-0. 695103	-1. 368864	6	-3. 073437	0. 492577	-1. 644264
1	3. 489300	-0. 698671	1. 083340	6	-3. 692232	-0. 720445	-1. 289181
1	1. 941382	-2. 294150	2. 320896	6	-3. 964277	-1. 003590	0. 090481
1	0. 762177	-4. 033907	-1. 487097	6	-3. 621820	-0. 065496	1. 088615
1	0. 510263	-3. 865733	1. 000223	6	-2. 716838	1. 443889	-0. 634618
6	-3. 452722	0. 250304	-0. 347092	6	-2. 988223	1. 166451	0. 720392
6	-3. 095163	0. 789163	-1. 593700	1	-2. 777246	0. 663294	-2. 673076
6	-4. 741487	0. 468621	0. 163483	1	-3. 882003	-1. 476206	-2. 043301
6	-4. 023506	1. 540818	-2. 313823	1	-4. 356790	-1. 974418	0. 372673
1	-2. 095201	0. 623524	-1. 984857	1	-3. 758491	-0. 311794	2. 135656
6	-5. 663704	1. 222688	-0. 563336	1	-2. 162067	2. 336005	-0. 901249
1	-5. 037824	0. 051755	1. 121855	1	-2. 638944	1. 844738	1. 491115
6	-5. 304872	1. 758640	-1. 801803	6	2. 647413	-0. 544354	-0. 496767
1	-3. 742766	1. 956841	-3. 277342	6	2. 570714	-1. 925229	-0. 740783
1	-6. 660707	1. 387683	-0. 163995	6	3. 795813	0. 001195	0. 097428
1	-6. 024430	2. 344559	-2. 367613	6	3. 638615	-2. 751523	-0. 387525
6	-3. 083700	-1. 821862	1. 705127	1	1. 678246	-2. 345672	-1. 195379
1	-3. 768563	-2. 464858	1. 144308	6	4. 857386	-0. 832531	0. 449959
1	-2. 335819	-2. 442004	2. 207954	1	3. 862185	1. 067749	0. 291675
1	-3. 641823	-1. 267311	2. 465526	6	4. 779891	-2. 206123	0. 206917
17	0. 587711	0. 669449	-1. 832981	1	3. 580894	-3. 819046	-0. 579418

1	5.743339	-0.409881	0.914253	6	-4.231872	1.893200	-0.511513
1	5.609634	-2.851671	0.479700	1	-2.232580	1.907911	-1.331505
6	1.762249	1.050548	-2.776000	6	-5.001253	-0.233568	0.359181
1	1.861016	0.152065	-3.391874	1	-3.618869	-1.873319	0.225376
1	0.987667	1.688903	-3.210066	6	-5.223537	1.121609	0.098582
1	2.719594	1.579203	-2.764442	1	-4.407390	2.945661	-0.714437
				1	-5.770376	-0.829691	0.840843
TS1b (879.74i)				1	-6.170723	1.576103	0.373874
6	-0.738494	-3.193430	0.297830	6	-1.568830	-1.797327	-2.623627
6	-0.086814	-3.910671	1.307400	1	-1.898292	-1.128526	-3.424647
6	-0.492429	-1.826961	0.154403	1	-0.666324	-2.327177	-2.941086
6	0.422816	-1.140004	0.999639	1	-2.368670	-2.516879	-2.423162
1	0.030626	-0.007426	1.450982				
6	1.042514	-1.892245	2.017813	IN5a (14.77)			
8	-0.162004	0.324112	-1.459946	6	1.151256	3.007333	0.376651
1	-1.945427	3.382983	1.740195	6	0.561516	3.790798	1.367249
6	-0.885745	3.372851	2.017692	6	0.539815	1.813288	-0.029441
6	-0.279336	2.071318	1.548441	6	-0.694385	1.367037	0.516670
1	-0.381883	4.228473	1.566747	1	-0.185541	0.300623	2.325901
1	-0.832862	3.429018	3.108556	6	-1.254062	2.184483	1.520684
8	-0.639141	0.997024	2.100607	8	0.081773	-0.335352	-1.578516
8	0.569327	2.130636	0.591489	1	2.153238	-2.507535	2.385982
1	1.699124	-1.388364	2.722668	6	1.103155	-2.635503	2.676041
1	-1.422713	-3.713106	-0.367782	6	0.309978	-1.512194	2.077380
1	-0.277936	-4.973437	1.423110	1	0.750785	-3.591258	2.285690
6	0.797146	-3.258336	2.170020	1	1.045198	-2.612905	3.766231
1	1.284827	-3.813674	2.966115	8	0.267254	-0.423141	2.820498
15	-1.219807	-0.782385	-1.143418	8	-0.229465	-1.613206	0.966785
44	1.557822	0.471496	-0.194729	1	-2.192393	1.900578	1.989853
6	2.873922	0.840570	-1.966411	1	2.082726	3.336875	-0.077709
6	3.170966	1.823645	-1.003421	1	1.031285	4.716098	1.685784
6	3.508363	1.424044	0.329297	6	-0.638659	3.369963	1.941498
6	3.587829	0.056226	0.663115	1	-1.106600	3.968699	2.718396
6	2.970564	-0.553595	-1.640334	15	1.208208	0.710478	-1.296873
6	3.323879	-0.937879	-0.336013	44	-1.566981	-0.368219	-0.234366
1	2.506843	1.137973	-2.942799	6	-2.940878	-1.442795	-1.830191
1	3.034101	2.873588	-1.235449	6	-3.119197	-2.140696	-0.640088
1	3.635462	2.176847	1.099458	6	-3.386514	-1.408831	0.568708
1	3.803713	-0.241611	1.682643	6	-3.640860	-0.019398	0.542216
1	2.704326	-1.301832	-2.377975	6	-3.039485	-0.006604	-1.838851
1	3.322795	-1.986539	-0.061202	6	-3.450889	0.693953	-0.680643
6	-2.792497	-0.047894	-0.608943	1	-2.632674	-1.962095	-2.731182
6	-3.012549	1.313650	-0.865549	1	-2.957808	-3.211980	-0.598087
6	-3.788023	-0.822071	0.006003	1	-3.435484	-1.941511	1.512880

1	-3.914218	0.502940	1.451427	1	4.074253	1.290920	0.115156
1	-2.820090	0.539302	-2.749517	6	-2.835434	-0.587107	0.141001
1	-3.552692	1.773069	-0.705149	6	-2.725332	-1.665418	-0.749727
6	2.731571	-0.130376	-0.750157	6	-4.084741	0.013952	0.368320
6	2.762526	-1.532316	-0.785224	6	-3.860223	-2.135141	-1.410531
6	3.865020	0.585407	-0.332930	1	-1.761901	-2.138408	-0.909005
6	3.923171	-2.210243	-0.405436	6	-5.212445	-0.459365	-0.300342
1	1.883824	-2.078953	-1.110991	1	-4.190647	0.840931	1.065398
6	5.018219	-0.098413	0.048965	6	-5.100097	-1.531825	-1.189379
1	3.857730	1.671560	-0.297592	1	-3.776558	-2.974330	-2.094486
6	5.048219	-1.495601	0.011636	1	-6.178106	0.004274	-0.123342
1	3.950087	-3.295513	-0.444289	1	-5.981718	-1.900190	-1.705474
1	5.892912	0.457512	0.372932	6	-1.717801	0.324323	2.718269
1	5.950393	-2.025078	0.303878	1	-2.050650	-0.609718	3.180122
6	1.634524	1.660338	-2.799566	1	-0.812230	0.680255	3.217922
1	1.953532	0.962915	-3.580064	1	-2.501497	1.079850	2.827702
1	0.757121	2.216671	-3.141275				
1	2.451976	2.360244	-2.599057	IN7a(9.84)			
				6	1.709783	-2.649803	-2.055629
IN6a(17.78)				6	3.005325	-2.932279	-1.636042
6	-1.427289	2.705825	0.044359	6	1.089419	-1.455280	-1.650436
6	-0.828575	3.823188	-0.533043	6	1.745444	-0.502199	-0.836077
6	-0.683301	1.529624	0.203292	6	3.042944	-0.833156	-0.411569
6	0.672739	1.425415	-0.214338	8	-0.685782	0.549943	-1.725532
6	1.238715	2.580645	-0.790794	1	3.584020	-0.165445	0.251540
8	-0.172901	-1.036512	0.827649	1	1.187592	-3.352281	-2.701438
1	2.270742	2.569456	-1.129544	1	3.495466	-3.849668	-1.946978
1	-2.467764	2.755539	0.355851	6	3.663333	-2.020531	-0.805274
1	-1.396876	4.739224	-0.662591	1	4.671039	-2.235613	-0.459348
6	0.506432	3.756550	-0.947616	15	-0.574969	-0.966992	-2.108785
1	0.974442	4.627405	-1.398294	44	0.836027	1.336245	-0.458608
15	-1.337163	0.022930	0.958037	6	0.581675	3.477871	-1.477603
44	1.618933	-0.379139	0.048510	6	0.542338	3.705593	-0.099118
6	3.159134	-1.973935	0.848147	6	1.566271	3.145251	0.721017
6	2.763416	-2.388459	-0.421429	6	2.700351	2.520362	0.142753
6	2.738898	-1.433414	-1.492342	6	1.695542	2.797832	-2.071755
6	3.326848	-0.141322	-1.340030	6	2.772374	2.382477	-1.270089
6	3.535773	-0.603420	1.052068	1	-0.242664	3.796452	-2.106844
6	3.729812	0.277383	-0.055022	1	-0.307052	4.203060	0.354769
1	3.057460	-2.635648	1.701308	1	1.490899	3.226508	1.800074
1	2.349172	-3.378884	-0.574223	1	3.502063	2.155289	0.773747
1	2.325380	-1.719062	-2.454033	1	1.713105	2.624188	-3.141779
1	3.355714	0.542098	-2.180812	1	3.614790	1.868359	-1.720221
1	3.739211	-0.248459	2.056960	6	-1.843438	-1.979153	-1.276386

6	-1.567028	-3.271282	-0.804584	6	2.044076	-2.141260	0.727158
6	-3.137662	-1.450003	-1.146892	8	0.167154	0.499701	-2.025665
6	-2.582258	-4.029595	-0.218825	1	2.543821	-1.693735	1.580525
1	-0.565437	-3.683243	-0.882007	1	0.175847	-3.852540	-2.204756
6	-4.145727	-2.212620	-0.558254	1	1.714288	-5.175847	-0.790182
1	-3.352820	-0.441328	-1.486325	6	2.246046	-3.492464	0.459643
6	-3.869918	-3.502523	-0.097769	1	2.930732	-4.064309	1.079949
1	-2.366244	-5.030450	0.143431	15	-0.467161	-0.917062	-2.187850
1	-5.144180	-1.798243	-0.455343	44	1.592396	0.761256	-0.402695
1	-4.657366	-4.095092	0.358794	6	2.603504	2.497299	-1.515458
6	-0.856701	-1.168347	-3.904921	6	2.459592	2.898359	-0.176582
1	-1.854445	-0.794533	-4.154890	6	2.938146	2.040643	0.856350
1	-0.104769	-0.600898	-4.460438	6	3.647537	0.857357	0.517658
1	-0.800577	-2.224901	-4.185267	6	3.359881	1.323063	-1.853099
6	-0.673117	0.884464	1.072111	6	3.930040	0.541097	-0.845475
6	0.307781	0.208317	1.470037	1	2.143539	3.076352	-2.308792
6	1.056891	-0.720137	2.281081	1	1.901106	3.793308	0.073019
6	2.188792	-0.305245	3.007060	1	2.761549	2.288569	1.897181
6	0.621609	-2.054426	2.394308	1	4.012232	0.210464	1.307494
6	2.864907	-1.201618	3.830907	1	3.464184	1.039886	-2.894694
1	2.523441	0.725482	2.934282	1	4.480482	-0.360212	-1.090937
6	1.304452	-2.945747	3.219315	6	-2.238820	-0.946964	-1.771308
1	-0.252030	-2.377634	1.837162	6	-2.901060	-2.161698	-1.532526
6	2.426180	-2.524252	3.937324	6	-2.954044	0.258271	-1.752671
1	3.731350	-0.868060	4.394627	6	-4.271899	-2.166723	-1.279125
1	0.958360	-3.971828	3.304405	1	-2.353583	-3.101075	-1.533367
1	2.954675	-3.221989	4.580248	6	-4.326444	0.244708	-1.498829
6	-1.991310	1.455450	1.261694	1	-2.437995	1.197288	-1.922441
6	-2.559914	1.391908	2.550493	6	-4.984375	-0.964096	-1.264245
6	-2.715172	2.069745	0.224754	1	-4.783145	-3.106374	-1.091816
6	-3.819530	1.934940	2.790092	1	-4.878720	1.179495	-1.480636
1	-2.005245	0.918531	3.355148	1	-6.052432	-0.971005	-1.066961
6	-3.975319	2.611889	0.474564	6	-0.340675	-1.494897	-3.920004
1	-2.291749	2.091331	-0.772789	1	-0.838337	-0.760919	-4.561446
6	-4.530189	2.549164	1.755074	1	0.710612	-1.577262	-4.209444
1	-4.245171	1.882220	3.788016	1	-0.837961	-2.460877	-4.050536
1	-4.527493	3.083052	-0.333952	6	-0.148711	1.020223	0.653408
1	-5.510792	2.975191	1.946168	6	0.079024	-0.168284	1.121887
				6	-0.122742	-0.919848	2.363866
TS2a(294, 23i)				6	0.198099	-0.314593	3.593654
6	0.690000	-3.372373	-1.375855	6	-0.704336	-2.200182	2.364914
6	1.564139	-4.119848	-0.588453	6	-0.058082	-0.975457	4.794714
6	0.497048	-2.007452	-1.119080	1	0.643797	0.675923	3.599097
6	1.183457	-1.349565	-0.061425	6	-0.969220	-2.850791	3.567084

1	-0.959271	-2.671370	1.421317	6	-2.325566	-2.952246	-0.990304
6	-0.642670	-2.243673	4.783630	6	-1.999077	-1.088503	-2.521700
1	0.196874	-0.499424	5.737104	6	-3.665336	-3.024022	-1.367320
1	-1.431637	-3.833529	3.557198	1	-1.940937	-3.642820	-0.243752
1	-0.844756	-2.757405	5.718976	6	-3.341548	-1.170329	-2.895842
6	-1.076726	2.130666	0.794138	1	-1.351885	-0.335786	-2.959098
6	-2.004758	2.148339	1.856282	6	-4.171832	-2.135173	-2.321141
6	-1.088417	3.191948	-0.129995	1	-4.313255	-3.770646	-0.918163
6	-2.899673	3.206003	1.993306	1	-3.737504	-0.478586	-3.633179
1	-2.013322	1.333504	2.573000	1	-5.215596	-2.196035	-2.615229
6	-1.989373	4.246354	0.009559	6	0.962421	-3.500754	-1.851934
1	-0.404077	3.163455	-0.971410	1	0.785946	-3.470265	-2.931712
6	-2.894110	4.259488	1.074033	1	2.039818	-3.564787	-1.678759
1	-3.603561	3.209376	2.820676	1	0.460150	-4.380809	-1.440872
1	-1.989179	5.056081	-0.714761	6	0.069353	1.003044	0.128368
1	-3.593063	5.083363	1.185316	6	-0.695116	0.294371	0.991646
				6	-2.041550	0.680729	1.534198
IN8a(17.02)				6	-2.143002	1.436008	2.715693
6	1.284582	-3.000723	1.212765	6	-3.223368	0.276879	0.896159
6	1.349862	-3.182496	2.583231	6	-3.388800	1.774527	3.246059
6	0.579099	-1.905095	0.642472	1	-1.238159	1.772393	3.217082
6	-0.046265	-0.948900	1.513432	6	-4.469546	0.622010	1.422613
6	0.002030	-1.195468	2.902931	1	-3.167943	-0.299782	-0.020198
8	1.031034	-0.732222	-1.829559	6	-4.557146	1.367114	2.599490
1	-0.509203	-0.506150	3.565969	1	-3.445482	2.361216	4.158725
1	1.763151	-3.729882	0.568473	1	-5.374221	0.306915	0.909956
1	1.887292	-4.030887	2.995428	1	-5.527947	1.632570	3.007963
6	0.680077	-2.284338	3.429479	6	-0.275986	2.267630	-0.552160
1	0.695040	-2.439916	4.504629	6	-0.761756	3.387447	0.148958
15	0.280393	-1.939099	-1.179385	6	-0.081850	2.386816	-1.944261
44	1.947065	0.160692	-0.085530	6	-1.055317	4.576590	-0.520160
6	3.482724	1.327465	-1.137461	1	-0.912111	3.326124	1.220839
6	2.959165	2.111198	-0.075734	6	-0.390093	3.571413	-2.610562
6	2.990784	1.597067	1.253623	1	0.305802	1.534927	-2.494501
6	3.538052	0.307845	1.465918	6	-0.876276	4.673138	-1.901041
6	4.221993	0.120529	-0.867795	1	-1.428220	5.428552	0.041589
6	4.255975	-0.381973	0.426214	1	-0.247848	3.636800	-3.686029
1	3.370435	1.671616	-2.159772	1	-1.110376	5.598330	-2.419668
1	2.446226	3.041186	-0.291552				
1	2.523474	2.139104	2.067340	TS3a(1008.26i)			
1	3.468551	-0.143715	2.450273	6	-0.257218	3.142627	-2.396130
1	4.664338	-0.431775	-1.690015	6	-0.763554	2.954624	-3.679901
1	4.731072	-1.333147	0.640673	6	-0.309041	2.134449	-1.416213
6	-1.490956	-1.981958	-1.568479	6	-0.914297	0.879278	-1.719821

6	-1.426381	0.731825	-3.029676	1	-3.535056	0.652799	-0.359634	
8	1.652878	1.554814	0.501160	6	-4.905199	-2.220347	-1.557371	
1	-1.901471	-0.204099	-3.296600	1	-3.781782	-3.893950	-2.325426	
1	0.181612	4.104470	-2.158476	1	-5.735702	-0.405753	-0.738220	
1	-0.708380	3.755390	-4.410761	1	-5.872259	-2.682281	-1.733148	
6	-1.343978	1.730411	-3.996702	6	-0.520192	-2.217441	0.687071	
1	-1.747266	1.549100	-4.988636	6	0.090273	-3.431347	0.345434	
15	0.480849	2.530848	0.180059	6	-1.480087	-2.231656	1.714611	
44	2.061500	-0.395484	-0.286470	6	-0.256920	-4.623005	0.987368	
6	4.109406	0.076693	-1.170210	1	0.835917	-3.459078	-0.440122	
6	4.104553	-1.257268	-0.721341	6	-1.826457	-3.417580	2.359510	
6	3.106705	-2.173080	-1.170996	1	-1.956671	-1.302520	2.009702	
6	2.117884	-1.729809	-2.082897	6	-1.216829	-4.621367	1.998483	
6	3.087262	0.509434	-2.072168	1	0.225375	-5.551403	0.693374	
6	2.122909	-0.390606	-2.570981	1	-2.574812	-3.400033	3.147027	
1	4.819151	0.789171	-0.766257	1	-1.485986	-5.545921	2.500926	
1	4.802683	-1.568397	0.048490	8	2.423043	-0.886780	1.696306	
1	3.081660	-3.180876	-0.774703	8	0.461684	-0.088651	2.420542	
1	1.329766	-2.406311	-2.393102	1	0.254520	-0.244797	1.034751	
1	3.032553	1.556621	-2.349423	6	1.594872	-0.598557	2.628508	
1	1.345269	-0.047323	-3.241227	6	2.004065	-0.941642	4.041277	
6	-0.810243	2.699990	1.455150	1	3.090996	-0.964011	4.138220	
6	-0.443056	2.701634	2.809716	1	1.568724	-0.228309	4.744558	
6	-2.137327	2.977996	1.091143	1	1.610366	-1.936039	4.282602	
6	-1.399233	2.967892	3.788087					
1	0.578213	2.477138	3.096233	IN9a(13.08)				
6	-3.089647	3.241309	2.076858	6	1.098667	-2.995814	-2.468174	
1	-2.428940	2.998722	0.045318	6	2.089354	-3.247238	-3.413378	
6	-2.721344	3.235368	3.423622	6	1.158286	-1.867897	-1.626579	
1	-1.113446	2.962655	4.835686	6	2.238779	-0.952333	-1.761848	
1	-4.115554	3.455326	1.791959	6	3.246905	-1.256697	-2.693086	
1	-3.463414	3.441865	4.189375	8	-1.031461	-0.522493	-0.399531	
6	1.232815	4.201457	0.093050	1	4.087265	-0.575769	-2.784037	
1	1.717448	4.363732	1.060919	1	0.280273	-3.701302	-2.382507	
1	1.995042	4.249444	-0.689062	1	2.019179	-4.123003	-4.051276	
1	0.483317	4.983463	-0.053098	6	3.176495	-2.378530	-3.513797	
6	-0.163930	-0.899770	0.021385	1	3.965266	-2.569174	-4.235750	
6	-1.080305	-0.343950	-0.851611	15	-0.082500	-1.753791	-0.278782	
6	-2.398393	-1.028120	-1.096955	44	-3.046580	0.071485	-0.148980	
6	-2.488535	-2.314934	-1.651070	6	-4.745773	-0.357200	-1.504766	
6	-3.586457	-0.344078	-0.788623	6	-5.191364	0.528684	-0.472964	
6	-3.731749	-2.901116	-1.887677	6	-4.489888	1.733975	-0.240815	
1	-1.584366	-2.860246	-1.899937	6	-3.364554	2.090218	-1.054222	
6	-4.828216	-0.941822	-1.001196	6	-3.637287	-0.015179	-2.311579	

6	-2.948972	1.215279	-2.076798	1	1.700600	4.331951	2.362887
1	-5.216327	-1.328519	-1.615847	1	0.363147	6.018606	1.117942
1	-6.000743	0.232878	0.184856	8	-3.275535	-1.526791	1.254611
1	-4.752820	2.353980	0.609537	8	-2.557856	0.415654	1.900863
1	-2.776806	2.971234	-0.820957	1	0.490858	0.916829	-1.757026
1	-3.261911	-0.715220	-3.048753	6	-2.854897	-0.785093	2.210574
1	-2.034405	1.425475	-2.619299	6	-2.703767	-1.303767	3.607084
6	0.819739	-1.736399	1.307770	1	-1.642226	-1.484942	3.810634
6	0.694654	-0.640968	2.172780	1	-3.056113	-0.554144	4.321044
6	1.627481	-2.827303	1.669032	1	-3.258351	-2.235805	3.731059
6	1.370287	-0.644205	3.396068				
1	0.072223	0.201292	1.890736				
6	2.294588	-2.825107	2.893439				
1	1.747213	-3.674586	0.998609				
6	2.165882	-1.733386	3.757457				
1	1.276026	0.207383	4.063825				
1	2.914395	-3.672219	3.172231				
1	2.688364	-1.732149	4.709706				
6	-1.051619	-3.311525	-0.283339				
1	-1.772990	-3.237233	0.534029				
1	-1.606551	-3.410673	-1.220666				
1	-0.420323	-4.191476	-0.138123				
6	1.310907	1.215379	-1.110060				
6	2.346874	0.342691	-1.021784				
6	3.667456	0.645133	-0.396413				
6	4.342855	1.842430	-0.693502				
6	4.294793	-0.285568	0.449231				
6	5.596793	2.107793	-0.145268				
1	3.882515	2.561447	-1.364062				
6	5.545234	-0.014743	1.004746				
1	3.795954	-1.221980	0.679918				
6	6.200555	1.182483	0.709784				
1	6.106192	3.034956	-0.392567				
1	6.010549	-0.742497	1.663890				
1	7.178300	1.389619	1.135402				
6	1.109038	2.527810	-0.475237				
6	0.335694	3.488098	-1.156866				
6	1.593291	2.856192	0.805096				
6	0.074879	4.737962	-0.595768				
1	-0.034743	3.257517	-2.154307				
6	1.320535	4.099887	1.371824				
1	2.178334	2.129123	1.357666				
6	0.565544	5.047644	0.675158				
1	-0.501161	5.472717	-1.152285				