Electronic Supplementary Information

Mechanism, Catalysis and Predictions of 1,3,2-Diazaphospholenes: Theoretical Insight into the Highly Polarized P-X bonds

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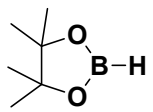
Energies of Intermediates and Transition States:

Table 1.

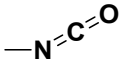
	Sum of electronic and thermal Enthalpies (Hartree)
1a	-584.498127
1b	-627.466320
1c	-2461.416116
1d	-609.665553
1e	-608.474300
1f	-876.214083
1g	-757.793769
1h	-569.713243
BEt_3	-262.268031
$HBEt_3$	-262.884167
E_a^+	583.682307
E_b^+	-626.669474
E_c^+	-2460.640499
E_d^+	-608.861673
E_e^+	-607.694899
E_f^+	-875.449302
E_g^+	-756.922129
E_h^+	-568.847066

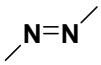
Figure 5.

	Solvation Energies (Hartree)	Thermal Corrections of Gibbs Free Energies (Hartree)	Dispersion Corrections (kcal/mol)
	-411.8269975	0.15836	-22.803

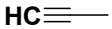
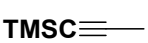
	-193.1346234	0.055448	-6.1954
TS1A	-604.9237015	0.235134	-34.3292
IN1A	-605.0262718	0.242055	-33.8982
1e	-608.6224255	0.098674	-17.0995
TS1B	-801.73121	0.175796	-29.4364
IN1B	-801.8032438	0.180145	-28.4155
TS2B	-1213.614711	0.362989	-62.9436
IN2B	-1213.620572	0.363794	-63.1285
TS3B	-1213.614711	0.360904	-60.8129
1f	-876.5081841	0.234249	-39.3022
TS1C	-1069.616207	0.310952	-51.921
IN1C	-1069.687657	0.315762	-50.5449
TS2C	-1481.498663	0.498354	-87.248
IN2C	-1481.508099	0.500097	-87.6611
TS3C	-1481.503902	0.499413	-86.0988
1g	-757.94234	0.082513	-18.5353
TS1D	-951.0203287	0.160637	-31.7026
IN1D	-951.1183204	0.163619	-30.0788
TS2D	-1362.899803	0.34477	-63.8849

Table 2.

	Solvation Energies (Hartree)	Thermal Corrections of Gibbs Free Energies (Hartree)	Dispersion Corrections (kcal/mol)
	-212.54378	0.094473	-10.4375
TS-2	-1089.008056	0.349302	-58.1328
Pro-2	-1089.093326	0.357148	-60.9599
	-207.9733977	0.023536	-3.8384

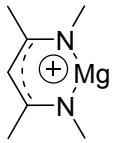
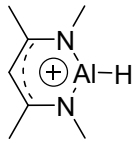
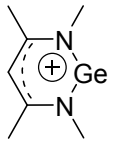
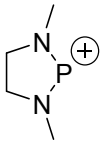
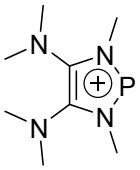
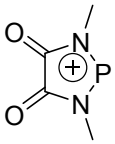
TS-3	-1084.479028	0.277961	-48.893
Pro-3	-1084.51853	0.281673	-47.2492
CO_2	-188.5822007	-0.009781	-1.0302
TS-4	-1065.081411	0.240716	-46.7699
Pro-4	-1065.114054	0.244939	-45.9705
	-189.2480911	0.05794	-5.6841
TS-5	-1065.714429	0.309026	-52.0953
Pro-5	-1065.79771	0.316652	-54.3528
	-117.8778972	0.055079	-5.0396
TS-6	-994.3324936	0.306286	-50.2793
Pro-6	-994.4389678	0.314655	-50.6708
	-116.6387985	0.031494	-3.5695
TS-7	-993.0953286	0.281714	-48.7933
Pro-7	-993.2084148	0.290531	-48.9456
	-232.4007028	0.085543	-9.1746
TS-8	-1108.833036	0.337459	-57.673
Pro-8	-1108.993525	0.343723	-55.5545

Figures 7 and 8.

	Solvation Energies (Hartree)	Thermal Corrections of Gibbs Free Energies (Hartree)	Dispersion Corrections (kcal/mol)
2a	-991.976459	0.266507	-46.3918
	-116.6387985	0.031494	-3.5695
TS4a	-1185.072914	0.347915	-62.393
IN3a	-1185.139969	0.346208	-58.7854
TS5aH	-1301.733038	0.39242	-69.4883
IN4aH	-309.7877232	0.111306	-13.7902
	-525.2953266	0.121772	-17.1493

TS5aTMS	-1710.371365	0.4955	-93.6848
IN4aTMS	-718.4609268	0.203494	-30.6997
2b	-1010.485935	0.302984	-50.881
$HNMe_2$	-135.1385095	0.067575	-5.3633
TS4b	-1203.599299	0.387089	-69.2133
IN3b	-1203.637126	0.386786	-64.5302
TS5bH	-1338.726966	0.474051	-77.2394
IN4bH	-328.2844163	0.150448	-18.2244
$TMSNMe_2$	-543.7939583	0.1574	-21.5546
TS5bTMS	-1747.377565	0.575141	-107.7116
IN4bTMS	-736.9556733	0.241725	-35.5369
2c	-1297.085607	0.296516	-54.5922
$HPMe_2$	-421.7424083	0.057263	-7.3304
TS4c	-1490.191464	0.374767	-69.3983
IN3c	-1490.245552	0.376275	-67.4734
TS5cH	-1911.93223	0.448901	-82.4244
IN4cH	-614.8921755	0.139899	-21.0393
$TMSPMe_2$	-830.3889252	0.150681	-24.5112
TS5cTMS	-2320.588232	0.552526	-110.5132
IN4cTMS	-1023.56387	0.231408	-38.1215
2d	-1314.038573	0.259099	-48.8693
HSMe	-438.6842477	0.022197	-3.2934
TS4d	-1507.148627	0.34254	-62.8476
IN3d	-1507.185542	0.342029	-61.8385
TS5dH	-1945.851141	0.37986	-72.1541
IN4dH	-631.8328405	0.105693	-15.3506
TMSSMe	-847.3498021	0.115586	-18.8793
TS5dTMS	-2354.484623	0.480362	-95.1839
IN4dTMS	-1040.502444	0.19686	-32.2159

Table S1. The NICS values of the E^+ derivatives

E^+	NICS(0)zz	NICS(1)zz
	**1.3**	**0.7**
	**-0.2**	**-4.5**
	**-1.5**	**-9.7**
	**-2.9**	**0.8**
	**-11.3**	**-27.1**
	**-2.9**	**-21.8**
	**5.6**	**3.2**
	**-10.7**	**-25.8**

The Cartesian Coordinates for the Optimized Structures and the First Frequency from Calculations

1a (61.5)

7	1.488615	0.523995	0.000125
6	2.455325	-1.719736	-0.000091
1	2.133305	-2.757308	-0.000211
1	3.080842	-1.548915	-0.878525
7	-1.488633	0.523794	0.000505
6	1.271352	-0.780081	-0.000231
6	0.000035	-1.381237	-0.000730
1	0.000141	-2.460489	-0.001187
6	-1.271402	-0.780251	-0.000204
6	-2.455250	-1.719851	-0.000191
1	-2.133314	-2.757455	-0.002416
1	-3.082132	-1.547574	-0.877342
1	-3.079475	-1.550630	0.879477
6	2.864427	1.008748	0.001274
1	3.420435	0.684340	0.886240
1	3.421970	0.684361	-0.882742
1	2.856577	2.099275	0.001223
6	-2.864352	1.008749	0.001198
1	-3.420995	0.686026	-0.884009
1	-3.421377	0.682764	0.884947
1	-2.856319	2.099265	0.003174
1	3.080850	-1.549056	0.878329
12	0.000060	1.875152	-0.001014
1	-0.001905	3.581001	-0.005355

1b (35.6)

7	1.417143	-0.466997	-0.000402
6	2.471974	1.730632	0.000263
1	2.189409	2.779621	0.000024
1	3.087978	1.533649	0.879794
7	-1.417131	-0.467004	0.000038
6	1.253447	0.844125	-0.000097
6	0.000006	1.472175	-0.000076
1	0.000016	2.550829	-0.000056
6	-1.253411	0.844141	-0.000063
6	-2.471943	1.730639	-0.000093
1	-2.189370	2.779626	-0.000279
1	-3.088305	1.533699	0.879188
1	-3.088447	1.533429	-0.879212
6	2.762822	-1.029649	-0.000102
1	3.329697	-0.736553	-0.887279
1	3.329091	-0.737031	0.887624
1	2.690703	-2.117739	-0.000450
6	-2.762843	-1.029602	0.000118
1	-3.329424	-0.736542	0.887495
1	-3.329376	-0.736890	-0.887404
1	-2.690773	-2.117695	0.000325
1	3.088833	1.533442	-0.878604
13	-0.000043	-1.745806	0.000084
1	0.000447	-2.601240	1.349368
1	-0.000310	-2.601890	-1.348782

1c (55.9)

32	0.000013	-1.513997	-0.280719
7	1.402793	-0.159452	0.183533
6	2.439047	2.040059	-0.012557
1	2.190108	3.022242	-0.405908
1	2.764271	2.159877	1.023416
7	-1.402792	-0.159497	0.183489
6	1.244752	1.122184	-0.081613
6	-0.000021	1.701772	-0.368193
1	-0.000030	2.752238	-0.616175
6	-1.244781	1.122151	-0.081661
6	-2.439106	2.039986	-0.012652
1	-2.190195	3.022153	-0.406060
1	-2.764343	2.159857	1.023311
1	-3.280341	1.633066	-0.575486
6	2.692781	-0.662665	0.632395
1	3.425640	-0.678154	-0.180688
1	3.102813	-0.070328	1.453129
1	2.559526	-1.684566	0.984787
6	-2.692746	-0.662679	0.632507
1	-3.102562	-0.070418	1.453405
1	-3.425758	-0.677999	-0.180435
1	-2.559502	-1.684636	0.984741
1	0.000091	-1.040808	-1.818137
1	3.280297	1.633190	-0.575405

1d (54.8)

6	-0.765640	1.323060	0.163105
6	0.768923	1.366207	0.027797
1	-1.250195	2.130115	-0.391414
1	1.092096	2.056009	-0.756714

15	-0.007754	-1.144268	0.055437
7	1.208126	0.013649	-0.307164
7	-1.208388	0.030286	-0.350825
1	-0.072225	-0.993806	1.507548
6	-2.582965	-0.285992	-0.020147
1	-3.246683	0.457316	-0.466703
1	-2.847645	-1.262538	-0.426637
1	-2.765239	-0.294955	1.066221
6	2.593798	-0.277357	-0.019993
1	3.236327	0.412403	-0.572748
1	2.835897	-0.183427	1.049679
1	2.834656	-1.290900	-0.342854
1	-1.046609	1.423397	1.223433
1	1.215984	1.698863	0.974959

1e (97.3)

6	-0.667745	1.350152	0.034660
6	0.667751	1.350167	0.034598
1	-1.316007	2.205074	0.154165
1	1.316003	2.205108	0.154014
15	0.000016	-1.114190	-0.081743
7	1.223129	0.100622	-0.307928
7	-1.223118	0.100600	-0.307800
1	0.000138	-1.100426	1.388361
6	-2.562706	-0.207079	0.153482
1	-3.245711	0.585798	-0.153720
1	-2.902320	-1.137728	-0.302084
1	-2.612029	-0.309274	1.246678
6	2.562660	-0.207079	0.153534
1	3.245725	0.585773	-0.153601
1	2.611824	-0.309246	1.246741
1	2.902311	-1.137749	-0.301964

1f (41.2)

6	-0.707327	0.358755	-0.035164
6	0.544609	-0.132070	-0.042803
15	-0.997088	-2.184609	-0.092966
7	0.593416	-1.525232	-0.349184
7	-1.693821	-0.612282	-0.329011
1	-0.963047	-2.134956	1.375810
6	-3.033996	-0.420983	0.197739
1	-3.378327	0.579063	-0.055249
1	-3.704060	-1.155105	-0.250775
1	-3.064102	-0.533657	1.291521
6	1.676147	-2.319941	0.202741
1	2.637659	-1.944009	-0.144002
1	1.672346	-2.319959	1.302792
1	1.577472	-3.348955	-0.146788
6	2.468503	0.706613	-1.238969
1	3.121801	1.582362	-1.227650
1	3.095973	-0.183906	-1.387109
1	1.788087	0.789425	-2.085839
6	-0.838286	2.468361	-1.157935
1	0.234074	2.677869	-1.274771
1	-1.188194	1.905702	-2.023427
1	-1.380057	3.415786	-1.119381
7	1.697734	0.673220	-0.006292
7	-1.113858	1.706072	0.054240
6	-0.679073	2.399014	1.258259
1	-1.223316	3.342750	1.337845
1	-0.915253	1.789691	2.130525
1	0.397826	2.611250	1.252725
6	2.515916	0.625443	1.195717
1	1.866205	0.575067	2.069013
1	3.210322	-0.225358	1.225012
1	3.107667	1.542479	1.258454

1g (83.3)

6	-0.771186	0.946039	0.022414
6	0.771216	0.945992	0.022435
15	-0.000038	-1.583103	0.010479
7	1.222260	-0.345456	-0.041293
7	-1.222295	-0.345401	-0.041086
1	0.000045	-1.805267	1.426060
6	-2.643069	-0.643268	-0.097203
1	-3.163485	0.271852	-0.374294
1	-2.833404	-1.412229	-0.846429
1	-3.017120	-0.980351	0.871710
6	2.643044	-0.643305	-0.097228
1	3.163396	0.271419	-0.375751
1	3.017311	-0.978970	0.872097
1	2.833229	-1.413340	-0.845382
8	1.449854	1.937243	0.036899
8	-1.449753	1.937342	0.036720

1h (297.8)

6	-1.218187	-0.663586	0.077722
6	-1.218187	0.663586	0.077722

1	-2.039581	-1.348068	0.201119
1	-2.039581	1.348068	0.201119
15	1.155554	0.000000	0.026373
1	1.065914	0.000000	1.462527
8	0.018636	1.215860	-0.199564
8	0.018636	-1.215860	-0.199564

E_a^+ (59.5)

7	-1.579653	-0.627757	-0.009560
6	-2.439017	1.656378	0.014258
1	-2.082391	2.678847	-0.057085
1	-3.122562	1.466437	-0.814304
7	1.578900	-0.628063	-0.016745
6	-1.292785	0.679719	-0.001264
6	-0.000143	1.238140	0.004694
1	0.000013	2.315899	0.014868
6	1.292398	0.679330	0.000042
6	2.438916	1.655743	0.004513
1	2.082276	2.676902	0.092447
1	3.013728	1.569778	-0.920105
1	3.119540	1.451105	0.832004
6	-2.982438	-1.049775	-0.016719
1	-3.534558	-0.633884	0.827381
1	-3.487491	-0.755110	-0.938802
1	-3.038564	-2.134939	0.057467
6	2.981653	-1.050399	-0.017783
1	3.532933	-0.620485	-0.855393
1	3.487553	-0.770992	0.908556
1	3.037537	-2.134197	-0.109852
1	-3.010712	1.554417	0.939201
12	-0.000530	-1.729421	-0.024169

E_b^+ (74.9)

7	-1.429553	-0.524954	-0.000035
6	-2.471403	1.687510	0.000149
1	-2.191458	2.736284	-0.000632
1	-3.087338	1.488681	-0.879112
7	1.429566	-0.524947	-0.000145
6	-1.257737	0.808719	-0.000006
6	-0.000001	1.416872	-0.000028
1	-0.000004	2.495444	0.000025
6	1.257744	0.808728	-0.000052
6	2.471374	1.687570	-0.000034
1	2.191383	2.736331	0.000579
1	3.086378	1.489738	-0.880185
1	3.087078	1.488801	0.879402
6	-2.792614	-1.081734	-0.000208
1	-3.344053	-0.773152	0.887694
1	-3.343412	-0.774039	-0.888821
1	-2.733005	-2.169455	0.000320
6	2.792624	-1.081757	0.000031
1	3.344124	-0.772940	-0.887748
1	3.343358	-0.774327	0.888772
1	2.732988	-2.169477	-0.000950
1	0.000098	-3.196370	0.000298
1	-3.086159	1.489682	0.880474
13	0.000001	-1.647796	0.000156

E_c^+ (77.3)

32	0.000013	-1.486480	-0.000048
7	1.387083	-0.185011	0.000104
6	2.473454	2.008813	-0.000193
1	2.206557	3.061281	0.000353
1	3.086113	1.803424	0.879624
7	-1.387118	-0.185026	-0.000106
6	1.245102	1.149509	0.000004
6	-0.000017	1.770568	-0.000085
1	-0.000016	2.849401	-0.000117
6	-1.245145	1.149482	-0.000097
6	-2.473420	2.008831	0.000224
1	-2.206407	3.061265	-0.000549
1	-3.084971	1.804403	0.881049
1	-3.086426	1.803394	-0.879313
6	2.746099	-0.755338	0.000261
1	3.297361	-0.450593	-0.888558
1	3.296991	-0.450966	0.889441
1	2.676091	-1.842688	0.000058
6	-2.746117	-0.755370	-0.000049
1	-3.297315	-0.450445	0.888754
1	-3.297091	-0.451194	-0.889244
1	-2.676100	-1.842720	0.000399
1	3.085299	1.804071	-0.880732

E_d^+ (103.9)

6	0.758873	1.367994	-0.112749
6	-0.758900	1.367990	0.112752
1	1.278840	1.989889	0.615415
1	-1.026673	1.704770	1.116877

15	0.000006	-1.139131	-0.000033
7	-1.197270	-0.033217	-0.038340
7	1.197280	-0.033214	0.038244
6	2.630328	-0.323362	0.022888
1	3.107588	0.159822	0.875148
1	2.793027	-1.397765	0.086852
1	3.070509	0.051548	-0.902051
6	-2.630320	-0.323380	-0.022772
1	-3.070315	0.051352	0.902330
1	-3.107747	0.159968	-0.874844
1	-2.793031	-1.397767	-0.086887
1	1.026508	1.704794	-1.116907
1	-1.278761	1.989909	-0.615472

E_e^+ (70.9)

6	0.681503	1.329796	-0.000024
6	-0.681503	1.329796	-0.000016
1	1.341196	2.183809	-0.000019
1	-1.341196	2.183809	-0.000005
15	0.000000	-1.133685	-0.000030
7	-1.177696	0.063604	0.000013
7	1.177696	0.063604	0.000016
6	2.624643	-0.210131	0.000024
1	3.070753	0.219497	0.894530
1	2.785586	-1.285841	-0.001410
1	3.071382	0.221950	-0.893003
6	-2.624643	-0.210131	0.000023
1	-3.070743	0.219453	0.894555
1	-3.071392	0.221994	-0.892978
1	-2.785586	-1.285841	-0.001463

E_f^+ (65.1)

6	-0.721730	-0.110466	-0.070961
6	0.663524	0.037007	0.017571
15	-0.298069	2.438293	0.013687
7	1.000635	1.366526	0.054441
7	-1.336917	1.112832	-0.057857
6	-2.788044	1.256776	-0.217736
1	-3.291524	1.130246	0.738956
1	-3.003971	2.248243	-0.609825
1	-3.131918	0.496755	-0.916710
6	2.387603	1.804643	0.239286
1	2.841789	1.203322	1.025080
1	2.950767	1.687267	-0.684390
1	2.391752	2.852174	0.532747
6	1.532667	-1.950996	1.163247
1	1.617632	-2.956134	0.743352
1	2.340032	-1.812312	1.888380
1	0.581554	-1.870656	1.687730
6	-2.281993	-1.743765	0.858847
1	-1.730936	-2.448394	1.491966
1	-2.613331	-0.912961	1.478693
1	-3.160196	-2.250519	0.458273
7	1.597010	-0.956015	0.103965
7	-1.454280	-1.260008	-0.245909
6	-0.888205	-2.316333	-1.077819
1	-1.710781	-2.887921	-1.508852
1	-0.312082	-1.877260	-1.890507
1	-0.250874	-3.002474	-0.511302
6	2.673358	-1.083418	-0.866108
1	2.496609	-0.413845	-1.707177
1	3.651359	-0.857674	-0.430716
1	2.696942	-2.106280	-1.251431

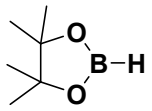
E_g^+ (89.5)

6	-0.770392	0.945572	-0.000210
6	0.770400	0.945567	0.000006
15	-0.000007	-1.528155	-0.000120
7	1.212821	-0.410813	-0.000330
7	-1.212826	-0.410805	-0.000562
6	-2.659212	-0.692834	0.000517
1	-3.104020	-0.250897	-0.888853
1	-2.813559	-1.769906	-0.000839
1	-3.102530	-0.252939	0.891628
6	2.659208	-0.692844	0.000370
1	3.103481	-0.252817	-0.890214
1	3.103063	-0.251042	0.890270
1	2.813551	-1.769917	0.001294
8	1.481754	1.886769	0.000078
8	-1.481737	1.886781	0.000006

E_h^+ (451.7)

6	0.000348	1.215795	0.670991
6	0.000348	1.215795	-0.670991
1	0.000585	2.016223	1.392899
1	0.000585	2.016223	-1.392899
15	-0.000728	-1.178649	0.000000
8	0.000348	-0.058891	-1.152633

8	0.000348	-0.058891	1.152633



(86.3)

5	-0.000028	1.944917	-0.000194
1	0.000030	3.134847	-0.000636
8	1.086066	1.201028	0.366997
8	-1.086022	1.200890	-0.367447
6	0.789150	-0.191458	0.045020
6	-0.789181	-0.191460	-0.044974
6	1.379736	-1.073498	1.143494
1	1.140751	-2.128748	0.968330
1	2.469412	-0.969753	1.148709
1	1.010564	-0.791701	2.132154
6	1.479974	-0.483875	-1.293368
1	2.549238	-0.273349	-1.193953
1	1.360476	-1.531428	-1.589079
1	1.085170	0.150259	-2.093256
6	-1.379716	-1.073966	-1.143131
1	-1.140742	-2.129145	-0.967498
1	-2.469394	-0.970242	-1.148470
1	-1.010495	-0.792604	-2.131891
6	-1.480013	-0.483334	1.293512
1	-2.549186	-0.272235	1.194279
1	-1.361034	-1.530925	1.589279
1	-1.084713	0.150635	2.093287

(36.4)

6	0.000015	0.185296	-0.000016
6	1.293123	-0.614750	-0.000010
1	1.341191	-1.267830	-0.880592
1	2.148540	0.063616	-0.000644
1	1.341744	-1.266761	0.881334
6	-1.293078	-0.614824	0.000005
1	-1.341512	-1.267229	-0.881055
1	-1.341359	-1.267474	0.880890
1	-2.148495	0.063547	0.000159
8	-0.000058	1.400975	0.000003

TS1A (602.8i)

1	-1.499233	0.320107	-1.181887
6	-2.645167	-0.000896	0.087849
8	-1.743933	-0.201868	0.980115
5	-0.643408	0.092445	-0.265560
8	0.150647	1.194971	0.103700
8	0.125047	-1.049317	-0.553068
6	1.526682	0.779282	-0.065263
6	1.425948	-0.794261	0.030881
6	-3.324178	-1.190252	-0.549041
1	-2.612296	-2.009522	-0.662527
1	-4.113090	-1.510804	0.146414
1	-3.788507	-0.942663	-1.506991
6	-3.352601	1.332894	0.047908
1	-2.660171	2.132675	0.316047
1	-3.817667	1.529845	-0.921325
1	-4.143731	1.291237	0.810144
6	1.991519	1.263872	-1.447397
1	1.827159	2.344133	-1.515602
1	3.056255	1.067036	-1.615678
1	1.418425	0.782243	-2.245841
6	2.467587	-1.561241	-0.782828
1	3.482533	-1.340345	-0.431559
1	2.299637	-2.637945	-0.672903
1	2.404273	-1.318271	-1.846167
6	1.410432	-1.307458	1.480030
1	1.118128	-2.362528	1.474981
1	2.396403	-1.226464	1.951630
1	0.685071	-0.760265	2.088329
6	2.363741	1.440614	1.029668
1	3.406433	1.103652	0.986443
1	2.354182	2.527448	0.894343
1	1.965366	1.222594	2.023125

IN1A (36.4)

1	-3.766729	-1.094417	-0.531458
6	-2.992804	-0.404338	-0.174952
8	-1.761583	-1.054905	-0.539448
5	-0.522507	-0.565680	-0.298012
8	-0.220493	0.596168	0.392772
8	0.597269	-1.233101	-0.746155
6	1.201888	0.840208	0.212373
6	1.746768	-0.604507	-0.125838
6	-3.122210	-0.272699	1.342632
1	-2.993225	-1.248974	1.822086
1	-2.370005	0.415160	1.740233

1	-4.115979	0.108227	1.605400
6	-3.154344	0.925992	-0.910620
1	-3.037660	0.780580	-1.989900
1	-4.152010	1.341440	-0.727416
1	-2.409105	1.651853	-0.571595
6	1.340668	1.827098	-0.954569
1	0.761214	2.728069	-0.729549
1	2.383417	2.120543	-1.115151
1	0.954471	1.398959	-1.885084
6	2.911190	-0.643411	-1.114339
1	3.787508	-0.123844	-0.709744
1	3.192921	-1.683778	-1.305893
1	2.643976	-0.187090	-2.070208
6	2.088577	-1.428055	1.124042
1	2.255985	-2.467949	0.827210
1	2.993322	-1.059704	1.619085
1	1.266284	-1.412348	1.846690
6	1.752100	1.461257	1.494498
1	2.836199	1.606626	1.424423
1	1.290179	2.440678	1.657015
1	1.539229	0.839813	2.367190

1e (86.5)

6	-0.671523	1.360447	0.040013
6	0.671523	1.360448	0.040007
1	-1.321690	2.221945	0.131526
1	1.321689	2.221947	0.131514
15	0.000001	-1.117769	-0.084762
7	1.231667	0.101911	-0.286234
7	-1.231666	0.101909	-0.286222
1	0.000014	-1.179292	1.395828
6	-2.585783	-0.209029	0.140944
1	-3.261387	0.597020	-0.165524
1	-2.922797	-1.130745	-0.344517
1	-2.672523	-0.337186	1.234169
6	2.585779	-0.209029	0.140948
1	3.261384	0.597029	-0.165495
1	2.672501	-0.337205	1.234173
1	2.922805	-1.130735	-0.344523

TS1B (713.2i)

6	1.907716	1.292411	0.638284
6	2.527966	0.094693	0.724383
1	2.202751	2.225348	1.099296
1	3.418398	-0.149195	1.289255
15	0.362758	-0.327986	-0.719403
7	0.774033	1.248177	-0.170091
7	1.872115	-0.864019	-0.032568
1	-0.847726	-0.874487	0.374228
6	-2.128108	-0.297719	0.129792
8	-1.920482	0.426348	-0.919283
6	2.267193	-2.263832	-0.013585
1	3.334964	-2.364242	-0.238708
1	2.066189	-2.729137	0.960558
1	1.705841	-2.808476	-0.778007
6	0.112797	2.491893	-0.576412
1	0.682483	2.987073	-1.372130
1	-0.893960	2.246758	-0.913343
1	0.051877	3.165920	0.285246
6	-2.948160	-1.576290	-0.062717
1	-3.995627	-1.299786	-0.249112
1	-2.589774	-2.116051	-0.944826
1	-2.915768	-2.237042	0.811162
6	-2.340129	0.416294	1.469084
1	-3.311611	0.929824	1.445567
1	-2.337045	-0.276713	2.317757
1	-1.567189	1.175401	1.624015

IN1B (28.4)

6	-2.322047	-0.671184	0.764465
6	-2.321405	0.672710	0.764417
1	-2.946915	-1.335887	1.345805
1	-2.945845	1.338019	1.345531
15	-0.342231	-0.000309	-0.806275
7	-1.412985	-1.195977	-0.173721
7	-1.411970	1.196526	-0.173960
1	2.277203	-0.000229	-1.265663
6	2.288531	-0.000369	-0.163744
8	0.934246	-0.001853	0.319980
6	-1.108235	2.614983	-0.227456
1	-2.037593	3.196420	-0.221879
1	-0.482618	2.947607	0.613640
1	-0.579354	2.839397	-1.159461
6	-1.110486	-2.614708	-0.226997
1	-0.582129	-2.839816	-1.159130
1	-0.484817	-2.947595	0.613950
1	-2.040339	-3.195337	-0.220939
6	2.982480	-1.270312	0.325095

1	2.974994	-1.308786	1.420292
1	2.466639	-2.160613	-0.050282
1	4.023980	-1.305323	-0.016296
6	2.980168	1.270708	0.325455
1	2.972535	1.308885	1.420662
1	4.021627	1.307695	-0.015860
1	2.462785	2.160203	-0.049723

TS2B (153.6i)

6	-3.952524	0.302338	0.736489
6	-3.271983	1.440778	0.968771
15	-2.089896	0.378030	-1.094602
7	-3.493258	-0.340248	-0.429273
7	-2.316945	1.698680	-0.022952
1	-2.022859	-1.668775	0.825660
6	-0.937211	-1.542619	0.762273
8	-0.710874	-0.565522	-0.295306
5	0.876070	0.165189	-0.848021
1	0.348051	0.712764	-1.787827
8	1.344565	0.965616	0.234550
8	1.842837	-0.819721	-1.145994
6	2.777751	0.865065	0.243644
6	3.040599	-0.570520	-0.385399
6	-1.396107	2.831337	0.058308
1	-1.079901	3.114462	-0.949254
1	-1.917673	3.683877	0.504961
1	-0.501124	2.587547	0.640046
6	-4.194382	-1.471917	-1.018059
1	-4.128517	-2.366691	-0.385009
1	-5.252365	-1.230374	-1.175038
1	-3.750295	-1.707472	-1.988964
6	-0.332005	-2.880578	0.339291
1	-0.800931	-3.230284	-0.586700
1	0.738834	-2.793087	0.154624
1	-0.502346	-3.634404	1.117848
6	-0.452479	-1.019747	2.112396
1	-0.970900	-0.090619	2.367354
1	-0.669163	-1.758489	2.893824
1	0.618698	-0.815806	2.105963
6	4.227151	-0.633099	-1.356622
1	5.171018	-0.392451	-0.852573
1	4.309543	-1.646719	-1.763273
1	4.093976	0.051836	-2.196706
6	3.325094	2.014803	-0.623148
1	2.965343	2.964169	-0.212629
1	4.420363	2.039357	-0.637378
1	2.966141	1.940118	-1.654136
6	3.217830	-1.681983	0.661193
1	3.220462	-2.651416	0.151470
1	4.167508	-1.580386	1.198785
1	2.410267	-1.690366	1.396113
6	3.275198	1.044655	1.680385
1	4.366514	0.954524	1.736413
1	3.001024	2.042977	2.038310
1	2.832977	0.312867	2.360664
1	-3.407201	2.137147	1.785615
1	-4.761746	-0.123782	1.313413

IN2B (33.2)

6	3.851082	-0.380570	0.809769
6	3.129861	-1.503086	1.003225
15	2.094211	-0.422993	-1.115136
7	3.468783	0.267083	-0.373972
7	2.218406	-1.732629	-0.030805
1	1.942430	1.860725	0.669411
6	0.854515	1.725389	0.659484
8	0.636012	0.621513	-0.259534
5	-0.713728	-0.106341	-0.628842
1	-0.260175	-0.870737	-1.494223
8	-1.259585	-0.789140	0.532161
8	-1.740223	0.776828	-1.114758
6	-2.672582	-0.862334	0.327006
6	-2.981668	0.479755	-0.464910
6	1.269394	-2.850094	0.019520
1	0.993759	-3.139504	-0.996524
1	1.758633	-3.701873	0.501623
1	0.361691	-2.567441	0.561173
6	4.219910	1.389618	-0.923474
1	4.186149	2.260088	-0.257264
1	5.266779	1.108321	-1.085432
1	3.787901	1.676629	-1.885632
6	0.223182	3.002476	0.107212
1	0.614049	3.216908	-0.893018
1	-0.859442	2.905438	0.025835
1	0.462798	3.849436	0.762046
6	0.417355	1.366623	2.078103
1	0.929860	0.460952	2.416214
1	0.674854	2.186499	2.760026

1	-0.656098	1.181384	2.130328
6	-4.069118	0.350676	-1.540694
1	-5.036639	0.070011	-1.106089
1	-4.193746	1.313628	-2.048184
1	-3.796636	-0.389038	-2.297016
6	-2.981943	-2.127930	-0.498238
1	-2.600011	-3.001541	0.041741
1	-4.057494	-2.267916	-0.654328
1	-2.491116	-2.095880	-1.475246
6	-3.351823	1.655701	0.457152
1	-3.365765	2.577264	-0.135222
1	-4.343542	1.527657	0.906929
1	-2.626083	1.785870	1.264808
6	-3.357706	-0.983572	1.691817
1	-4.449751	-0.999051	1.591702
1	-3.050432	-1.919265	2.172133
1	-3.082054	-0.161838	2.357459
1	3.203125	-2.204344	1.823269
1	4.639711	0.023507	1.429387

TS3B (91.8i)

6	3.963178	-0.240232	0.650036
6	3.307496	-1.341479	1.096419
1	4.742659	0.315115	1.154224
1	3.474603	-1.881842	2.018050
15	2.102017	-0.732462	-1.129656
7	3.493951	0.138482	-0.591802
7	2.316146	-1.749478	0.227608
1	1.553594	2.491759	0.960042
6	0.500032	2.219823	0.788327
8	0.561648	0.949103	0.146616
5	-0.549156	0.083858	-0.207249
1	0.204236	-0.850912	-0.834844
8	-1.258599	-0.563629	0.876111
8	-1.531083	0.569047	-1.136437
6	-2.543159	-0.950361	0.376885
6	-2.836973	0.146203	-0.731716
6	1.352430	-2.790153	0.602034
1	1.130321	-3.427487	-0.256410
1	1.792425	-3.409331	1.388033
1	0.427840	-2.322807	0.955739
6	3.976973	1.332913	-1.276109
1	3.670162	2.243286	-0.750068
1	5.068989	1.305237	-1.347188
1	3.560383	1.358436	-2.286429
6	-0.110544	3.293694	-0.118259
1	0.418373	3.324073	-1.077170
1	-1.161302	3.081485	-0.327170
1	-0.033678	4.282643	0.351533
6	-0.175716	2.144269	2.161144
1	0.286260	1.358440	2.766923
1	-0.073559	3.101072	2.688749
1	-1.239008	1.908313	2.069372
6	-3.583397	1.375275	-0.182041
1	-3.580347	2.158488	-0.947629
1	-4.626193	1.148354	0.069279
1	-3.093140	1.775529	0.709901
6	-3.588163	-0.369738	-1.965894
1	-4.584857	-0.747026	-1.705079
1	-3.715248	0.450213	-2.681265
1	-3.033939	-1.165139	-2.470051
6	-2.441700	-2.374143	-0.205949
1	-2.088712	-3.053724	0.578178
1	-3.410810	-2.743051	-0.559895
1	-1.732098	-2.416144	-1.037434
6	-3.530774	-0.967704	1.548191
1	-4.547259	-1.205190	1.211638
1	-3.226878	-1.733480	2.270602
1	-3.551789	-0.008071	2.070090

1f (38.2)

6	0.737609	-0.231352	0.026748
6	-0.596575	0.015080	-0.019181
15	0.543454	2.344613	-0.090501
7	-0.891932	1.389762	-0.322230
7	1.533672	0.918698	-0.245218
1	0.522874	2.412540	1.390044
6	2.876062	1.017372	0.316549
1	3.406546	0.076989	0.160348
1	3.419953	1.822613	-0.188453
1	2.864025	1.227242	1.400880
6	-2.138988	1.997960	0.116773
1	-2.993201	1.427989	-0.257393
1	-2.221344	2.072155	1.215578
1	-2.208436	3.008849	-0.300339
6	-2.251433	-1.237236	-1.303230
1	-2.719007	-2.230236	-1.279325
1	-3.039350	-0.503495	-1.550336

1	-1.509739	-1.222898	-2.105861
6	1.754529	-2.094861	-1.126223
1	0.884440	-2.578984	-1.603700
1	2.151497	-1.342588	-1.813379
1	2.525672	-2.858125	-0.964467
7	-1.589485	-0.987102	-0.027067
7	1.418717	-1.460966	0.147554
6	0.942372	-2.399236	1.154727
1	1.733871	-3.133068	1.356120
1	0.732033	-1.858056	2.081228
1	0.033133	-2.941312	0.854288
6	-2.475869	-1.093575	1.127678
1	-1.907372	-0.890346	2.038764
1	-3.341563	-0.409062	1.100635
1	-2.868893	-2.117052	1.188553

1	3.404545	-2.403507	-1.045243
1	3.477432	-0.683482	-1.501109
1	4.544373	-1.314449	-0.229143
6	2.607618	-1.809871	1.565378
1	3.601116	-1.716279	2.022150
1	1.867484	-1.443187	2.281503
1	2.423170	-2.884066	1.392831
6	2.529428	2.470145	-0.716765
1	3.458899	1.882560	-0.811951
1	2.047789	2.516207	-1.697599
1	2.799013	3.491460	-0.422224
6	2.140201	1.900934	1.623660
1	2.377853	2.930913	1.917667
1	1.380896	1.517487	2.310634
1	3.049540	1.289511	1.726467

TS1C (698.6i)

6	0.908051	0.758102	-0.145660
6	1.300226	-0.550554	-0.096478
15	-1.195404	-0.577636	-0.990434
7	-0.380187	0.899251	-0.697599
7	0.289134	-1.384999	-0.602307
1	-2.204612	-0.839344	0.394706
6	-3.375676	-0.045905	0.426166
8	-3.336025	0.581985	-0.700486
6	0.344816	-2.838617	-0.561410
1	1.288350	-3.207595	-0.973815
1	0.229849	-3.227466	0.458564
1	-0.469982	-3.238886	-1.172405
6	-0.919834	2.221693	-1.036095
1	-0.549683	2.547376	-2.016725
1	-2.007038	2.146654	-1.045434
1	-0.586915	2.938190	-0.282642
6	-4.432178	-1.146459	0.571100
1	-5.424042	-0.678211	0.645259
1	-4.433060	-1.778003	-0.322815
1	-4.277108	-1.768361	1.460398
6	-3.097643	0.752868	1.706421
1	-3.935385	1.442108	1.882971
1	-2.989747	0.108830	2.586760
1	-2.191619	1.355798	1.590253
7	1.603166	1.911825	0.265690
7	2.557887	-0.995775	0.355019
6	3.536346	-1.376955	-0.658696

IN1C (22.4)

6	1.143347	0.799150	-0.243800
6	1.191843	-0.559617	-0.196485
15	-1.189001	0.030615	-1.155266
7	-0.033886	1.267966	-0.868691
7	0.029094	-1.126699	-0.808433
1	-3.781776	-0.434269	-0.774484
6	-3.481483	-0.191835	0.257999
8	-2.108237	0.232258	0.260836
6	-0.015949	-2.478855	-1.338914
1	0.792629	-2.665556	-2.058575
1	0.048274	-3.235813	-0.546584
1	-0.968618	-2.621054	-1.859699
6	-0.293186	2.670992	-1.141631
1	-0.954262	2.753416	-2.010790
1	-0.776076	3.182112	-0.296664
1	0.647931	3.180842	-1.361514
6	-4.336535	0.968266	0.762817
1	-4.030978	1.251033	1.776706
1	-4.219015	1.843152	0.114970
1	-5.397764	0.693033	0.785266
6	-3.623865	-1.444394	1.122645
1	-3.297616	-1.235045	2.147698
1	-4.665775	-1.785860	1.152448
1	-3.004786	-2.258163	0.730138
7	2.053067	1.757343	0.238121
7	2.162615	-1.315483	0.494901
6	3.085865	-2.132240	-0.286795

1	2.669801	-3.104547	-0.604576
1	3.390739	-1.581025	-1.180271
1	3.982645	-2.339864	0.311787
6	1.709120	-1.968309	1.719306
1	2.579837	-2.240162	2.330455
1	1.086429	-1.274593	2.289789
1	1.125249	-2.889786	1.542930
6	3.474682	1.489019	0.061097
1	3.873023	0.754709	0.776683
1	3.648424	1.114955	-0.951251
1	4.028012	2.429641	0.181673
6	1.731758	2.299683	1.557888
1	2.284888	3.233429	1.717353
1	0.662227	2.517348	1.618862
1	1.987649	1.601718	2.373910

TS2C (170.8i)

6	-2.877190	-0.234263	-0.171801
6	-2.250973	0.958268	-0.407211
15	-0.836441	-0.799969	-1.730346
7	-2.275837	-1.268817	-0.961047
7	-1.203685	0.821237	-1.344827
1	-0.827212	-2.318369	0.619359
6	0.213713	-1.981283	0.698488
8	0.475722	-1.176082	-0.473822
5	2.034133	-0.200243	-0.957502
1	1.602287	-0.067185	-2.074731
8	2.065789	0.911964	-0.077406
8	3.206175	-0.958537	-0.807895
6	3.437637	1.137401	0.293849
6	4.114842	-0.288091	0.087086
6	-0.514990	1.963571	-1.943989
1	-0.208477	1.701805	-2.960321
1	-1.205499	2.808544	-1.985823
1	0.377119	2.242104	-1.374494
6	-2.930138	-2.551550	-1.174122
1	-3.111981	-3.068750	-0.226184
1	-3.892232	-2.430946	-1.688480
1	-2.286095	-3.177742	-1.798272
6	1.119048	-3.212923	0.679558
1	0.923721	-3.811291	-0.216678
1	2.171881	-2.925983	0.663563
1	0.931366	-3.839095	1.560621
6	0.327687	-1.141500	1.970348
1	-0.356504	-0.289153	1.924916
1	0.071847	-1.748493	2.847943
1	1.336417	-0.747367	2.102394
7	-3.914581	-0.589907	0.704339
7	-2.469817	2.238135	0.117480
6	-3.832082	2.680850	0.353401
1	-4.267684	2.304118	1.294629
1	-3.844935	3.777129	0.401704
1	-4.469005	2.365663	-0.476385
6	-5.300163	-0.428850	0.284048
1	-5.923136	-1.204186	0.750649
1	-5.730796	0.550170	0.554288
1	-5.370982	-0.542273	-0.800679
6	-3.699116	-0.505494	2.140052
1	-3.909218	0.494684	2.559738
1	-4.355207	-1.221373	2.654522
1	-2.663475	-0.762991	2.372888
6	-1.511629	2.687032	1.128906
1	-1.767175	2.320935	2.138676
1	-0.509985	2.328778	0.878708
1	-1.494458	3.783278	1.158163
6	5.487374	-0.248055	-0.598855
1	6.223959	0.291444	0.008546
1	5.849774	-1.271893	-0.739075
1	5.433233	0.221427	-1.583346
6	3.991480	2.217945	-0.653301
1	3.381059	3.121301	-0.550085
1	5.030421	2.478715	-0.423429
1	3.936744	1.896875	-1.697921
6	4.253856	-1.112278	1.376332
1	4.582870	-2.123351	1.114190
1	4.999516	-0.678250	2.052236
1	3.311376	-1.199368	1.920033
6	3.475499	1.670002	1.729256
1	4.505447	1.848979	2.059703
1	2.936455	2.622396	1.776654
1	3.001318	0.982486	2.433595

IN2C (22.9)

6	-2.833755	-0.234440	-0.192074
6	-2.197974	0.962441	-0.399297
15	-0.871060	-0.748386	-1.847252
7	-2.277287	-1.231975	-1.038730
7	-1.190565	0.841955	-1.379244

1	-0.699389	-2.415093	0.587867
6	0.340488	-2.081955	0.705808
8	0.569612	-1.215859	-0.422965
5	1.802525	-0.338172	-0.745078
1	1.510663	-0.019240	-1.910124
8	1.879948	0.800757	0.172144
8	3.067518	-1.026575	-0.641942
6	3.257584	1.166314	0.263403
6	4.015907	-0.219702	0.057531
6	-0.434615	1.996097	-1.876965
1	-0.094756	1.784029	-2.892472
1	-1.098017	2.862872	-1.887680
1	0.436980	2.188988	-1.247303
6	-2.854492	-2.567581	-1.145862
1	-2.970523	-3.024215	-0.159442
1	-3.837663	-2.532956	-1.629318
1	-2.192843	-3.190507	-1.753736
6	1.247695	-3.311016	0.632291
1	1.092670	-3.840683	-0.313798
1	2.297499	-3.018065	0.681780
1	1.020502	-3.999627	1.455815
6	0.432465	-1.330769	2.034205
1	-0.212120	-0.447060	2.020131
1	0.113701	-1.987781	2.853465
1	1.449813	-0.992290	2.234337
7	-3.845884	-0.612366	0.703238
7	-2.378475	2.218667	0.182906
6	-3.724035	2.724593	0.390799
1	-4.202258	2.355529	1.313830
1	-3.684982	3.819180	0.457284
1	-4.354097	2.455654	-0.460662
6	-5.236645	-0.450546	0.291491
1	-5.864448	-1.168728	0.834020
1	-5.636677	0.558770	0.483085
1	-5.331465	-0.656471	-0.778161
6	-3.610763	-0.450867	2.132144
1	-3.820733	0.566678	2.503433
1	-4.256752	-1.144641	2.686030
1	-2.570739	-0.692799	2.362006
6	-1.413442	2.599519	1.218071
1	-1.713577	2.239981	2.217015
1	-0.429461	2.183564	0.985583
1	-1.332643	3.692454	1.259300
6	5.291172	-0.125001	-0.795454
1	6.047940	0.516232	-0.326175
1	5.721444	-1.125805	-0.911195
1	5.076979	0.259885	-1.795307
6	3.567961	2.189107	-0.849076
1	2.919794	3.062817	-0.715117
1	4.607910	2.533207	-0.820311
1	3.368568	1.770956	-1.839922
6	4.379174	-0.924924	1.377412
1	4.737445	-1.934603	1.148100
1	5.173053	-0.399371	1.921293
1	3.516106	-1.020786	2.041200
6	3.494964	1.834090	1.622451
1	4.549469	2.102168	1.760230
1	2.903897	2.755034	1.684172
1	3.190686	1.186667	2.448565

TS3C (51.0i)

6	2.825522	0.212859	-0.392474
6	2.247061	-1.035440	-0.260841
15	0.897214	0.129746	-2.161386
7	2.261929	0.887335	-1.478148
7	1.245326	-1.223679	-1.211658
1	0.599654	2.492812	1.029038
6	-0.445548	2.141305	0.994882
8	-0.467796	1.183216	-0.053336
5	-1.596746	0.351388	-0.458233
1	-1.094095	-0.119162	-1.581529
8	-1.897243	-0.768505	0.440693
8	-2.859512	0.999030	-0.731544
6	-3.266235	-1.128562	0.251336
6	-3.943592	0.239110	-0.201971
6	0.423627	-2.435659	-1.266600
1	0.116666	-2.616417	-2.298736
1	1.025734	-3.274960	-0.914308
1	-0.463094	-2.301826	-0.641113
6	2.602441	2.273934	-1.785911
1	2.413781	2.919262	-0.924517
1	3.655261	2.358051	-2.069688
1	1.984025	2.604454	-2.624427
6	-1.319071	3.363340	0.685775
1	-1.038515	3.786961	-0.284834
1	-2.373536	3.086085	0.632528
1	-1.186768	4.137081	1.453331
6	-0.753973	1.529822	2.367277

1	-0.097456	0.674732	2.561799
1	-0.604506	2.273223	3.161021
1	-1.783202	1.167734	2.418226
7	3.769982	0.873510	0.401920
7	2.500397	-2.065288	0.642487
6	3.873882	-2.464429	0.903680
1	4.372819	-1.858892	1.678012
1	3.882709	-3.507098	1.245295
1	4.456850	-2.402522	-0.018715
6	5.176650	0.782154	0.023300
1	5.716841	1.654550	0.410926
1	5.673850	-0.123290	0.409778
1	5.268467	0.780450	-1.066331
6	3.525869	0.980353	1.835205
1	3.869910	0.104018	2.409179
1	4.056366	1.858864	2.224233
1	2.457316	1.117636	2.013700
6	1.585666	-2.196252	1.781118
1	1.919988	-1.604761	2.648763
1	0.585595	-1.855782	1.501255
1	1.528052	-3.247961	2.086602
6	-3.353339	-2.223131	-0.832557
1	-2.774542	-3.095424	-0.506607
1	-4.384235	-2.552595	-1.004520
1	-2.938657	-1.875938	-1.783321
6	-3.800310	-1.704534	1.568044
1	-4.864330	-1.960145	1.493739
1	-3.250908	-2.620355	1.815070
1	-3.667855	-1.004188	2.396124
6	-5.014599	0.090905	-1.293342
1	-5.861669	-0.517727	-0.952549
1	-5.397179	1.082506	-1.558902
1	-4.602984	-0.357895	-2.200541
6	-4.559508	1.031473	0.967390
1	-4.851351	2.022350	0.602767
1	-5.452727	0.542162	1.373947
1	-3.845066	1.174305	1.782688

1g (94.7)

6	-0.769384	0.950844	0.023593
6	0.769384	0.950843	0.023564
15	-0.000001	-1.589539	-0.020482
7	1.229152	-0.350483	-0.019543
7	-1.229153	-0.350481	-0.019539
1	-0.000010	-1.901569	1.387414
6	-2.655834	-0.645297	-0.077843
1	-3.176982	0.301000	-0.235882
1	-2.874964	-1.328336	-0.905371
1	-3.008618	-1.092409	0.859427
6	2.655834	-0.645298	-0.077843
1	3.176978	0.300981	-0.236006
1	3.008643	-1.092298	0.859471
1	2.874944	-1.328435	-0.905295
8	1.457645	1.951521	0.025521
8	-1.457643	1.951523	0.025505

TS1D (721.7i)

6	-1.768434	-0.941001	0.188442
6	-2.102845	0.550390	0.306411
15	0.330132	0.323655	-0.913719
7	-0.508061	-1.102139	-0.400108
7	-1.088665	1.246791	-0.296023
1	1.330083	0.963603	0.301100
6	2.363211	0.105704	0.330014
8	2.093457	-0.668500	-0.721508
6	-1.129784	2.702675	-0.326927
1	-2.041744	3.045351	-0.824828
1	-1.116601	3.116811	0.687057
1	-0.260543	3.073220	-0.878808
6	-0.082423	-2.477770	-0.701326
1	-0.549005	-2.822566	-1.630155
1	1.000768	-2.493021	-0.790441
1	-0.416571	-3.123686	0.112810
6	3.547841	1.045969	0.163703
1	4.456131	0.430233	0.113171
1	3.468544	1.592653	-0.780071
1	3.648654	1.750290	0.995740
6	2.202582	-0.518922	1.711544
1	3.009367	-1.251935	1.844302
1	2.275234	0.223913	2.512497
1	1.252623	-1.053924	1.796425
8	-3.104658	1.003504	0.825237
8	-2.490389	-1.850080	0.532363

IN1D (18.6)

6	-2.042173	0.769854	-0.291200
6	-2.042156	-0.769914	-0.291089
15	0.211806	0.000109	0.901828

7	-0.900947	1.217567	0.345224
7	-0.900892	-1.217499	0.345386
1	2.856480	-0.000656	1.123258
6	2.756642	-0.000193	0.028239
8	1.342620	0.000247	-0.309630
6	-0.636488	-2.644963	0.487288
1	-1.566198	-3.177824	0.278439
1	0.130193	-2.976434	-0.222454
1	-0.305790	-2.871152	1.506154
6	-0.636562	2.645065	0.486846
1	-0.305578	2.871388	1.505589
1	0.129909	2.976461	-0.223156
1	-1.566347	3.177867	0.278189
6	3.377016	1.272315	-0.537874
1	3.241488	1.310878	-1.624086
1	2.909398	2.161148	-0.101403
1	4.450436	1.306613	-0.320281
6	3.376471	-1.272508	-0.538909
1	3.240822	-1.310172	-1.625136
1	4.449899	-1.307389	-0.321446
1	2.908556	-2.161503	-0.103087
8	-2.924669	-1.461097	-0.755823
8	-2.924700	1.460942	-0.756058

TS2D (290.0i)

6	3.688999	-0.063481	0.275128
6	3.140826	-1.488195	0.400513
15	1.440267	-0.190378	-1.226472
7	2.824669	0.677183	-0.493654
7	2.013369	-1.611458	-0.402307
1	1.330942	2.470135	0.709908
6	0.256754	2.286705	0.625943
8	0.182875	0.991141	-0.034831
5	-0.990442	0.133822	-0.195697
1	-0.077946	-0.779862	-0.943820
8	-1.489099	-0.561874	0.907454
8	-2.007927	0.517615	-1.070862
6	-2.820773	-1.013128	0.558972
6	-3.269306	0.036590	-0.545280
6	1.282799	-2.877966	-0.421787
1	1.075846	-3.188556	-1.449961
1	1.914936	-3.623752	0.063151
1	0.340317	-2.783075	0.125526
6	3.270296	1.978988	-0.984687
1	3.440018	2.668083	-0.152032
1	4.211610	1.878749	-1.535841
1	2.509532	2.394271	-1.650752
6	-0.382897	3.362121	-0.247279
1	0.075092	3.379069	-1.241638
1	-1.453569	3.179122	-0.372341
1	-0.245333	4.348085	0.211353
6	-0.324842	2.203516	2.034589
1	0.135873	1.386056	2.595611
1	-0.129534	3.143798	2.562727
1	-1.405501	2.038231	2.015632
8	3.636795	-2.371820	1.068127
8	4.753939	0.315156	0.725586
6	-2.705245	-2.447747	0.020742
1	-2.231824	-3.074242	0.783706
1	-3.687517	-2.873963	-0.208149
1	-2.091805	-2.492148	-0.884052
6	-4.083699	-0.551187	-1.699450
1	-5.028313	-0.975125	-1.339637
1	-4.320314	0.239259	-2.419117
1	-3.530944	-1.330157	-2.229248
6	-4.009230	1.252989	0.030001
1	-4.116613	2.005991	-0.757345
1	-5.009861	0.987422	0.387490
1	-3.457999	1.707506	0.858683
6	-3.667956	-1.015699	1.832252
1	-4.703537	-1.301841	1.615380
1	-3.257888	-1.741674	2.541724
1	-3.670753	-0.037695	2.318605

(71.3)

6	0.412682	-0.057757	0.000001
6	0.360646	1.461302	-0.000002
1	-0.178551	1.834448	-0.880361
1	-0.178434	1.834447	0.880432
1	1.360454	1.903914	-0.000061
6	1.784373	-0.687619	-0.000001
1	2.358822	-0.370329	-0.881062
1	2.358826	-0.370325	0.881056
1	1.697122	-1.776008	0.000002
7	-0.606848	-0.826562	0.000001
6	-1.935275	-0.225773	0.000000

1	-2.687866	-1.019502	0.000013
1	-2.108495	0.404200	0.885732
1	-2.108503	0.404175	-0.885750

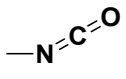
TS-2 (825.0i)

6	1.163876	0.741030	-0.270294
6	1.587329	-0.549371	-0.108893
15	-1.008612	-0.699908	-0.687409
7	-0.185124	0.809490	-0.656575
7	0.548054	-1.443036	-0.407608
1	-2.009448	-0.764400	0.784272
6	-3.144699	0.018139	0.755077
6	0.659439	-2.887058	-0.284538
1	1.366695	-3.303629	-1.010510
1	0.970580	-3.190802	0.721741
1	-0.323409	-3.327437	-0.481739
6	-0.741316	2.053371	-1.204462
1	-0.288853	2.268827	-2.179356
1	-1.820791	1.914848	-1.287963
1	-0.529737	2.892577	-0.537980
6	-4.170008	-0.946832	1.357571
1	-5.152136	-0.457156	1.422477
1	-4.289278	-1.852010	0.754962
1	-3.876536	-1.245600	2.369604
6	-2.722144	1.117664	1.730462
1	-3.568286	1.794151	1.911703
1	-2.400236	0.701891	2.692833
1	-1.906792	1.715168	1.314195
7	1.877749	1.944358	-0.124630
7	2.873174	-0.923002	0.333596
6	3.734691	-1.639654	-0.599882
1	3.544199	-2.726253	-0.644230
1	3.607357	-1.226720	-1.604116
1	4.782439	-1.502560	-0.303116
6	3.005761	-1.360002	1.719940
1	4.045738	-1.223276	2.043556
1	2.364159	-0.745981	2.356996
1	2.744590	-2.420741	1.883434
6	3.215658	2.009233	-0.699734
1	3.978954	1.497187	-0.094433
1	3.204689	1.559233	-1.696132
1	3.502676	3.063436	-0.803125
6	1.783725	2.565417	1.194660
1	2.096487	3.614493	1.128385
1	0.747734	2.539005	1.544439
1	2.415682	2.064022	1.948939
7	-3.218040	0.424978	-0.545459
6	-4.092388	-0.329708	-1.429655
1	-3.970282	0.046898	-2.452423
1	-3.900589	-1.418674	-1.463752
1	-5.156662	-0.210771	-1.164303

Pro-2 (41.9)

6	0.937475	0.764918	-0.434770
6	1.228289	-0.528338	-0.136727
15	-1.217882	-0.586850	-1.181158
7	-0.355368	0.928306	-0.988307
7	0.156978	-1.411470	-0.486464
1	-3.476498	-0.539888	1.770312
6	-2.643089	0.006538	1.303775
6	0.430213	-2.774667	-0.927904
1	1.108654	-2.819495	-1.794202
1	0.867613	-3.370156	-0.118578
1	-0.513176	-3.250822	-1.212524
6	-0.603203	2.004716	-1.946406
1	0.068881	1.958640	-2.815602
1	-1.634957	1.924447	-2.301406
1	-0.481004	2.984928	-1.476840
6	-3.022799	1.497724	1.280998
1	-2.205506	2.091403	0.860076
1	-3.916940	1.670591	0.671659
1	-3.232137	1.861747	2.294716
6	-1.410638	-0.248492	2.172999
1	-0.533940	0.284293	1.796357
1	-1.606287	0.100377	3.194099
1	-1.171357	-1.314924	2.208579
7	1.691828	1.938577	-0.234034
7	2.381064	-0.960297	0.561962
6	3.401137	-1.685629	-0.191552
1	3.197603	-2.765020	-0.303106
1	3.492408	-1.251623	-1.190358
1	4.368915	-1.584368	0.317510
6	2.170448	-1.503235	1.899077
1	3.132856	-1.543982	2.425379
1	1.499696	-0.848944	2.460167
1	1.743094	-2.522295	1.905827
6	3.136526	1.864371	-0.391157
1	3.651763	1.413915	0.470173

1	3.374246	1.274659	-1.280178
1	3.525497	2.880904	-0.537513
6	1.277526	2.764295	0.896220
1	1.694479	3.773077	0.787618
1	0.187212	2.843428	0.916092
1	1.611403	2.356545	1.867238
7	-2.528380	-0.548975	-0.062609
6	-3.810259	-1.003040	-0.603656
1	-3.680037	-1.333368	-1.638066
1	-4.211210	-1.846112	-0.021572
1	-4.565651	-0.203149	-0.597709



(46.4)

6	0.734134	-0.058647	-0.005934
8	1.898039	0.079017	0.144299
7	-0.418786	-0.318839	-0.241423
6	-1.739455	0.177465	0.047179
1	-1.873685	1.193061	-0.342376
1	-2.475124	-0.474084	-0.430089
1	-1.932486	0.184452	1.126008

TS-3 (70.1i)

6	0.840563	0.756699	-0.249483
6	1.127190	-0.588057	-0.287093
15	-1.108853	-0.312226	-1.604465
7	-0.308458	1.053373	-1.006755
7	0.219416	-1.266581	-1.124265
1	-2.301814	-0.616916	-0.204408
6	-3.165695	0.155892	0.337658
8	-3.309115	1.159819	-0.368360
6	0.148732	-2.723198	-1.157065
1	1.122400	-3.153305	-1.399803
1	-0.183960	-3.124635	-0.191842
1	-0.566455	-3.021053	-1.929021
6	-0.792397	2.422322	-1.207420
1	0.070186	3.090691	-1.236372
1	-1.334023	2.468847	-2.153608
1	-1.487166	2.710109	-0.414958
7	-3.610553	-0.311984	1.439592
6	-3.182950	-1.584576	1.954127
1	-2.413683	-2.076336	1.325509
1	-2.761504	-1.474336	2.964133
1	-4.030551	-2.280234	2.038551
7	1.523718	1.814947	0.352213
7	2.110794	-1.337198	0.370566
6	3.372176	-1.592926	-0.317258
1	4.114759	-0.789399	-0.182202
1	3.812252	-2.524521	0.059740
1	3.190482	-1.710384	-1.389166
6	2.200134	-1.253323	1.821743
1	2.644148	-2.179193	2.209809
1	2.817971	-0.413247	2.181439
1	1.197138	-1.150889	2.242954
6	2.971538	1.884854	0.231968
1	3.288237	2.926968	0.364115
1	3.510207	1.278361	0.978463
1	3.273726	1.559714	-0.766529
6	0.990308	2.324545	1.616231
1	1.340326	1.744854	2.486194
1	1.302285	3.366752	1.750392
1	-0.101275	2.291703	1.600557

Pro-3 (27.4)

6	1.177505	0.683984	-0.239243
6	1.166632	-0.675851	-0.157706
15	-1.122686	-0.040465	-1.258012
7	0.035975	1.163245	-0.942018
7	0.044913	-1.215549	-0.861109
1	-3.806612	-0.170419	-0.874725
6	-3.416759	-0.024798	0.148023
8	-2.074633	0.088102	0.230103
6	-0.298407	-2.628047	-0.777411
1	0.550534	-3.251369	-1.070652
1	-0.610821	-2.921755	0.232492
1	-1.123460	-2.825822	-1.469604
6	-0.221583	2.576647	-1.167710
1	0.717773	3.087603	-1.391279
1	-0.896201	2.683797	-2.022950
1	-0.687156	3.063094	-0.299648
7	-4.148490	0.039249	1.178334
6	-5.578635	-0.086405	0.972218
1	-5.875798	-0.229059	-0.082266
1	-5.961768	-0.935935	1.551823
1	-6.085940	0.810507	1.349913
7	2.117742	1.631157	0.192612
7	2.038673	-1.575129	0.475357
6	3.145967	-2.123544	-0.298544

1	4.039306	-1.475842	-0.308462
1	3.441309	-3.095365	0.118109
1	2.828937	-2.277898	-1.333568
6	2.306980	-1.406985	1.894694
1	2.613864	-2.370488	2.323764
1	3.107826	-0.678684	2.113987
1	1.395396	-1.079976	2.400819
6	3.523478	1.402444	-0.100308
1	4.059167	2.359789	-0.056146
1	4.019371	0.713870	0.604680
1	3.625225	0.997086	-1.110021
6	1.871045	2.262514	1.487626
1	2.209851	1.646097	2.337381
1	2.396422	3.224498	1.533514
1	0.801105	2.447878	1.610134

CO_2 (640.1)

8	0.000000	0.000000	1.169167
6	0.000000	0.000000	0.000000
8	0.000000	0.000000	-1.169167

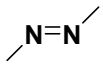
TS-4 (308.1i)

6	-0.260053	0.765715	-0.485661
6	-0.730324	-0.518079	-0.346618
15	1.627050	-0.761417	-1.383930
7	0.132465	-1.448273	-0.977050
7	0.972340	0.786880	-1.175833
8	2.495700	0.628897	1.684751
6	2.117202	-0.518081	1.532721
8	1.619707	-1.473455	2.095521
1	2.280455	-0.836505	0.214042
6	1.740213	2.009132	-1.398960
1	1.049497	2.821809	-1.632773
1	2.328584	2.271879	-0.513686
1	2.414703	1.854622	-2.245974
6	-0.013170	-2.887943	-0.763228
1	0.185447	-3.147627	0.281232
1	-1.021215	-3.210768	-1.031535
1	0.702521	-3.408382	-1.406724
7	-1.869478	-1.008132	0.297420
7	-0.823306	1.988010	-0.116960
6	-0.360682	2.579308	1.144610
1	-0.410411	3.673117	1.079354
1	-0.979608	2.256410	1.997452
1	0.668037	2.275382	1.345799
6	-2.230418	2.225575	-0.400570
1	-2.908538	1.798860	0.356715
1	-2.408076	3.307918	-0.430494
1	-2.487190	1.808744	-1.377444
6	-3.107094	-1.157127	-0.456183
1	-3.699258	-1.977277	-0.030308
1	-3.737723	-0.252280	-0.453384
1	-2.877520	-1.407452	-1.495934
6	-2.014442	-0.777911	1.729520
1	-1.031202	-0.825005	2.202911
1	-2.485352	0.190261	1.972722
1	-2.643705	-1.568923	2.157956

Pro-4 (44.8)

6	-0.470714	0.676601	-0.439454
6	-0.600595	-0.670963	-0.294372
15	1.875397	-0.303086	-1.066021
7	0.569029	-1.339829	-0.762786
7	0.807930	1.010781	-0.961512
8	1.309381	0.190507	2.119495
6	2.453553	0.020300	1.744271
8	2.887131	-0.207041	0.512375
1	3.305612	0.041360	2.450952
6	1.218834	2.382671	-1.222211
1	0.390410	2.934472	-1.672023
1	1.527176	2.904513	-0.306836
1	2.064168	2.374995	-1.916906
6	0.735649	-2.779233	-0.616703
1	0.761882	-3.081278	0.436573
1	-0.079649	-3.316696	-1.109516
1	1.677673	-3.071139	-1.091150
7	-1.619191	-1.446407	0.274727
7	-1.358165	1.728661	-0.178912
6	-1.247865	2.383925	1.125684
1	-1.572715	3.429121	1.043506
1	-1.863697	1.892040	1.896439
1	-0.211403	2.355307	1.465315
6	-2.719569	1.631720	-0.679602
1	-3.389099	1.042334	-0.029855
1	-3.145746	2.640467	-0.760585
1	-2.713741	1.179029	-1.674275
6	-2.679095	-1.948176	-0.589531
1	-3.114677	-2.854690	-0.149381

1	-3.498027	-1.225132	-0.747028
1	-2.265926	-2.209092	-1.568069
6	-2.022675	-1.156063	1.644374
1	-1.149971	-0.824780	2.210355
1	-2.805746	-0.380732	1.714568
1	-2.421929	-2.068667	2.107930



(165.9)

7	-0.426593	-0.452430	-0.000120
7	0.426733	0.452787	-0.000107
6	1.797958	-0.069344	0.000047
1	2.310589	0.329547	0.883041
1	1.828042	-1.164814	-0.000001
1	2.311098	0.329711	-0.882530
6	-1.798031	0.069104	0.000065
1	-2.310836	-0.330523	0.882651
1	-1.828519	1.164550	0.000627
1	-2.310911	-0.329531	-0.882867

TS-5 (425.7i)

6	0.864032	0.613481	-0.338692
6	1.316839	-0.652541	-0.086337
15	-1.171827	-0.959466	-0.868283
7	-0.485201	0.630009	-0.764215
7	0.371598	-1.635470	-0.463221
7	-3.146784	-0.178229	1.120445
1	-2.381148	-0.914647	0.597116
7	-3.912817	0.472527	0.267394
6	-0.994839	1.731019	-1.585765
1	-0.927920	2.678877	-1.047370
1	-0.436451	1.824713	-2.528602
1	-2.047678	1.538930	-1.795768
6	0.467530	-3.008887	0.004817
1	1.461609	-3.417078	-0.189776
1	0.263126	-3.096926	1.082157
1	-0.265559	-3.615080	-0.536950
6	-4.823651	-0.469295	-0.372593
1	-5.322036	0.032458	-1.207512
1	-4.304624	-1.366080	-0.755125
1	-5.593818	-0.827212	0.330745
6	-2.343627	0.733076	1.933922
1	-1.615730	0.147338	2.504838
1	-1.813496	1.472152	1.314428
1	-3.011740	1.261151	2.619667
7	2.523418	-1.090256	0.483009
7	1.536862	1.841369	-0.279599
6	3.592673	-1.512336	-0.414872
1	4.222875	-0.678045	-0.766698
1	4.242763	-2.232204	0.098708
1	3.161641	-2.004710	-1.290753
6	2.865841	1.954751	-0.852841
1	3.677278	1.656686	-0.167342
1	2.928717	1.336656	-1.751852
1	3.046261	2.999535	-1.139006
6	1.286594	2.701045	0.871423
1	1.914773	2.449042	1.743119
1	1.484541	3.745834	0.601555
1	0.238746	2.617593	1.171606
6	2.967192	-0.496693	1.733479
1	3.620205	-1.206475	2.258897
1	3.533598	0.442131	1.608612
1	2.100427	-0.294025	2.367601

Pro-5 (18.2)

6	0.861803	0.655352	-0.406956
6	0.877624	-0.692086	-0.208678
15	-1.566449	-0.142119	-1.117142
7	-0.377210	1.123374	-0.898238
7	-0.375220	-1.295873	-0.577695
7	-2.273931	-0.371123	1.565636
1	-1.472470	-1.001341	1.507511
7	-2.649091	-0.079476	0.221056
6	-0.438707	2.325252	-1.724377
1	-0.328189	3.238171	-1.127788
1	0.337450	2.331175	-2.500765
1	-1.418291	2.359963	-2.211154
6	-0.389578	-2.652538	-1.110331
1	0.059546	-2.730581	-2.114153
1	0.161792	-3.311684	-0.432949
1	-1.422388	-3.009321	-1.168782
6	-4.084106	-0.209752	0.000938
1	-4.296467	-0.064258	-1.063296
1	-4.451838	-1.196921	0.311489
1	-4.637710	0.552344	0.565470
6	-1.925054	0.829124	2.330173
1	-1.630258	0.514117	3.338637
1	-1.115835	1.427958	1.890352

1	-2.812252	1.464339	2.422922
7	1.825893	-1.504893	0.440051
7	1.852417	1.627638	-0.175883
6	2.911594	-2.112912	-0.312070
1	3.834915	-1.507834	-0.324987
1	3.166372	-3.090994	0.120154
1	2.597253	-2.270578	-1.346765
6	3.240593	1.280840	-0.415866
1	3.715475	0.726213	0.411123
1	3.313146	0.677611	-1.323908
1	3.816552	2.203542	-0.565408
6	1.651747	2.512154	0.966898
1	1.943117	2.048665	1.926193
1	2.246966	3.424103	0.835287
1	0.598447	2.795995	1.032012
6	2.093211	-1.299171	1.852234
1	2.410339	-2.244641	2.315475
1	2.885524	-0.554342	2.050876
1	1.180757	-0.965029	2.353303

(210.5)

6	1.235025	0.162881	-0.000014
1	1.812483	-0.150672	-0.880264
1	1.181497	1.256777	-0.000294
1	1.812201	-0.150196	0.880596
6	-0.133792	-0.455539	-0.000002
6	-1.283080	0.220404	0.000006
1	-1.305651	1.308653	0.000057
1	-2.245300	-0.284744	-0.000099
1	-0.164150	-1.546292	0.000065

TS-6 (648.5i)

6	0.681772	0.633651	-0.239116
6	1.216165	-0.606352	-0.019157
15	-1.355326	-1.034918	-0.540640
7	-0.684242	0.559349	-0.601982
7	0.260668	-1.609670	-0.260778
1	-2.635712	-0.887603	0.739235
6	-1.368165	1.710293	-1.176685
1	-1.889012	2.308903	-0.418312
1	-0.635892	2.351525	-1.674070
1	-2.113040	1.351314	-1.889836
6	0.523961	-3.007326	0.037343
1	-0.399309	-3.575065	-0.115313
1	1.293020	-3.425667	-0.622133
1	0.853160	-3.142582	1.074014
6	-4.037415	0.608930	1.611090
1	-3.578274	0.341360	2.570642
1	-3.565021	1.534961	1.262138
1	-5.097068	0.829691	1.790851
6	-3.881852	-0.504837	0.577461
6	-4.097400	-0.211379	-0.794149
1	-4.138149	0.816847	-1.139453
1	-4.453168	-0.969888	-1.482464
1	-4.320267	-1.454308	0.911993
7	1.282285	1.900384	-0.208152
7	2.491101	-0.992935	0.433411
6	3.504016	-1.320648	-0.562746
1	4.044508	-0.439501	-0.948651
1	4.243931	-2.002177	-0.123669
1	3.034847	-1.828090	-1.410072
6	2.562509	2.098298	-0.864766
1	3.432704	1.820818	-0.246103
1	2.593460	1.512580	-1.786808
1	2.672132	3.159316	-1.126155
6	1.072747	2.710780	0.987027
1	1.767806	2.459898	1.806666
1	1.205795	3.771715	0.741572
1	0.051802	2.569551	1.351187
6	3.004533	-0.408213	1.661378
1	3.740703	-1.090307	2.107981
1	3.502603	0.566914	1.521084
1	2.184418	-0.275514	2.371712

Pro-6 (34.9)

6	0.672289	0.655678	0.201170
6	1.026466	-0.650315	0.034701
15	-1.299602	-0.712460	1.150061
7	-0.520577	0.841945	1.000736
7	0.128715	-1.592288	0.614260
1	-3.164250	1.193876	-0.224068
6	-0.409000	1.668845	2.210951
1	0.445291	1.389353	2.848366
1	-0.304744	2.724522	1.940576
1	-1.325889	1.565328	2.798864
6	0.700221	-2.630056	1.484547
1	-0.105700	-3.282273	1.832026

1	1.415961	-3.233123	0.920654
1	1.219301	-2.217484	2.363817
6	-4.300426	0.122354	-1.721776
1	-5.171313	0.786733	-1.672245
1	-3.689509	0.435862	-2.577221
1	-4.664884	-0.891165	-1.930165
6	-3.491666	0.164838	-0.419943
6	-2.259872	-0.749463	-0.451551
1	-1.593987	-0.478063	-1.280668
1	-2.560353	-1.795725	-0.606064
1	-4.140337	-0.118687	0.421102
7	1.291257	1.742983	-0.467216
7	2.129321	-1.203173	-0.625002
6	1.838259	-2.067496	-1.765112
1	1.691734	-1.494419	-2.697611
1	2.669020	-2.766142	-1.922496
1	0.929387	-2.638496	-1.565500
6	0.430864	2.440190	-1.418288
1	1.044798	3.101732	-2.042753
1	-0.061001	1.711586	-2.068829
1	-0.350373	3.053220	-0.935622
6	2.098795	2.666120	0.327380
1	2.820869	3.173845	-0.325854
1	1.511521	3.448616	0.839491
1	2.655083	2.108878	1.085446
6	3.353946	-0.434552	-0.769435
1	4.180222	-1.132325	-0.960112
1	3.320627	0.298990	-1.587750
1	3.562293	0.099137	0.160400

—≡ (347.0)

6	-1.241289	-0.000007	0.000012
1	-1.638392	1.002695	-0.198693
1	-1.638395	-0.673490	-0.768963
1	-1.638260	-0.329269	0.967779
6	0.218892	0.000024	-0.000049
6	1.426163	0.000007	0.000002
1	2.492449	-0.000083	0.000084

TS-7 (1014.1i)

6	0.650112	0.656809	-0.229773
6	1.083578	-0.630509	-0.065646
15	-1.481521	-0.830936	-0.775619
7	-0.682297	0.693773	-0.714535
7	0.086987	-1.538229	-0.450958
1	-2.426805	-0.900536	0.572039
6	-1.283367	1.946531	-1.153505
1	-0.488765	2.616149	-1.489745
1	-1.975056	1.742520	-1.972163
1	-1.848825	2.440310	-0.353372
6	0.228466	-2.968013	-0.239393
1	1.000667	-3.404031	-0.884215
1	0.484937	-3.198769	0.801211
1	-0.724922	-3.448992	-0.482104
6	-4.255809	-0.171319	1.841466
1	-4.379731	-1.204918	2.188142
1	-3.579723	0.326947	2.547759
1	-5.232067	0.328543	1.895902
6	-3.720216	-0.121161	0.455583
6	-3.773740	0.231228	-0.753364
7	1.324767	1.875596	-0.055168
7	2.299068	-1.136490	0.437473
6	3.349888	-1.455070	-0.521721
1	3.955933	-0.582036	-0.819608
1	4.027561	-2.202439	-0.089336
1	2.904354	-1.881338	-1.424655
6	2.641927	2.047546	-0.643112
1	2.829734	3.117894	-0.803588
1	3.465909	1.659580	-0.020090
1	2.676208	1.543435	-1.612083
6	1.117717	2.585580	1.202047
1	1.755063	2.212759	2.022474
1	1.334549	3.652284	1.063209
1	0.073505	2.488003	1.510778
6	2.772630	-0.656445	1.724782
1	3.445822	-1.404683	2.164806
1	3.327968	0.296339	1.674912
1	1.921840	-0.522539	2.398022
1	-4.392134	0.735941	-1.475857

Pro-7 (37.2)

6	-0.855558	-0.686814	-0.150142
6	-0.762613	0.667142	-0.234808
15	1.499659	-0.207648	-1.166536
7	0.265697	-1.371846	-0.729782
7	0.334642	1.087006	-1.065216
1	4.267795	-0.096197	-0.473221
6	-0.037172	-2.444577	-1.685843

1	-0.598112	-2.095327	-2.567286
1	0.900408	-2.892966	-2.025729
1	-0.631665	-3.216565	-1.190665
6	0.787282	2.466365	-1.054578
1	-0.037775	3.147622	-1.282031
1	1.227467	2.779272	-0.094453
1	1.549230	2.583472	-1.833381
6	4.579877	0.026375	1.707043
1	5.255985	-0.836825	1.775407
1	5.218089	0.920338	1.683204
1	3.974747	0.060896	2.618754
6	3.725206	-0.057786	0.474963
6	2.386201	-0.095823	0.445469
7	-1.866058	-1.503610	0.371071
7	-1.546808	1.668315	0.369299
6	-2.625541	2.268653	-0.402637
1	-3.579262	1.717222	-0.332106
1	-2.806538	3.294012	-0.052993
1	-2.338324	2.313361	-1.456591
6	-3.259924	-1.148628	0.201128
1	-3.871089	-2.061152	0.232776
1	-3.651442	-0.467203	0.975985
1	-3.397304	-0.675574	-0.774368
6	-1.556711	-2.268106	1.571606
1	-1.724357	-1.695138	2.501267
1	-2.182119	-3.169014	1.612682
1	-0.507966	-2.573786	1.538911
6	-1.759710	1.623868	1.804421
1	-1.966518	2.638100	2.173882
1	-2.601714	0.982074	2.117285
1	-0.853468	1.258967	2.295107
1	1.818717	-0.063929	1.378266

(183.0)

8	-1.005210	-0.000412	0.832661
6	-1.243902	-0.000143	-0.581909
1	-1.672132	0.919555	-0.983236
6	0.131717	-0.000055	-0.055884
6	0.933437	1.285364	-0.049914
1	1.567331	1.356158	-0.942126
1	0.271528	2.155864	-0.021619
1	1.586522	1.324700	0.830175
6	0.934104	-1.284888	-0.050072
1	1.586660	-1.324230	0.830424
1	0.272876	-2.155941	-0.022578
1	1.568630	-1.354747	-0.941913
1	-1.671873	-0.919733	-0.983743

TS-8 (416.6i)

6	-1.532547	-0.700729	-0.204791
6	-1.139159	0.608882	-0.193317
15	0.954369	-0.717420	-1.132138
7	-0.560573	-1.531972	-0.765985
7	0.167184	0.784074	-0.726884
6	0.572507	2.036879	-1.365231
1	0.396677	2.878437	-0.688214
1	1.642518	1.959847	-1.577164
1	0.021170	2.221230	-2.298664
6	-0.794781	-2.925170	-1.094438
1	-0.115937	-3.217263	-1.902885
1	-0.616262	-3.599061	-0.242620
1	-1.827963	-3.067591	-1.424236
7	-2.724649	-1.292294	0.257768
7	-1.888534	1.669132	0.358716
6	-2.539508	2.610186	-0.549348
1	-1.882787	3.424073	-0.900331
1	-2.909937	2.071299	-1.424795
1	-3.396439	3.071733	-0.040887
6	-1.350461	2.294362	1.560815
1	-2.153383	2.837965	2.075689
1	-0.974206	1.520075	2.235126
1	-0.533910	3.012892	1.367590
6	-3.978362	-0.584132	0.032735
1	-4.142580	0.251389	0.728764
1	-3.996720	-0.193551	-0.987878
1	-4.806217	-1.296823	0.142075
6	-2.635668	-1.889322	1.588838
1	-3.478926	-2.573565	1.741895
1	-1.709257	-2.463445	1.677694
1	-2.652558	-1.134212	2.394625
8	3.093458	0.538575	-1.127033
6	3.786851	0.924988	0.005575
1	3.527583	1.933331	0.391674
6	3.269090	-0.157259	0.887692
1	1.713426	-0.982232	0.117507
6	2.351840	0.217508	2.003387

1	2.926547	0.777800	2.763120
1	1.569770	0.896982	1.641917
1	1.882663	-0.646755	2.484259
6	3.990795	-1.463293	0.881255
1	3.385365	-2.290292	1.266630
1	4.329780	-1.700152	-0.131242
1	4.890169	-1.377387	1.517192
1	4.890628	0.898004	-0.112834

Pro-8 (21.9)

6	-1.351079	-0.724494	-0.179991
6	-1.273821	0.631179	-0.095529
15	0.545058	-0.061035	-1.885531
7	-0.473527	-1.258033	-1.150065
7	-0.330875	1.162793	-1.036616
6	-0.483911	2.493927	-1.611534
1	-0.331882	3.275149	-0.857440
1	0.274330	2.632558	-2.388385
1	-1.472389	2.643649	-2.069270
6	-0.731174	-2.545067	-1.787680
1	-0.104957	-2.620423	-2.681917
1	-0.483766	-3.386878	-1.130155
1	-1.781936	-2.643548	-2.084606
7	-2.127142	-1.642898	0.549424
7	-1.905198	1.421459	0.890317
6	-2.992507	2.303863	0.475968
1	-2.655640	3.272879	0.068234
1	-3.595987	1.804120	-0.285940
1	-3.636119	2.517362	1.339657
6	-1.029647	2.023695	1.889992
1	-1.630516	2.347662	2.749766
1	-0.307040	1.279825	2.235920
1	-0.471868	2.904242	1.522893
6	-3.460776	-1.237177	0.970626
1	-3.462012	-0.568332	1.843670
1	-3.961364	-0.725409	0.144781
1	-4.037041	-2.137865	1.219488
6	-1.405636	-2.395598	1.572980
1	-1.984851	-3.283562	1.853482
1	-0.440467	-2.725225	1.179395
1	-1.221592	-1.801226	2.485580
8	2.013561	-0.204709	-1.097503
6	2.164038	-0.250312	0.327591
1	1.623869	-1.120784	0.723620
6	3.650692	-0.343676	0.678543
1	4.042244	-1.238449	0.173855
6	3.821706	-0.526420	2.193512
1	3.426794	0.338449	2.742821
1	3.298961	-1.420146	2.555750
1	4.880403	-0.628361	2.457809
6	4.427311	0.875787	0.166290
1	5.499670	0.773102	0.370488
1	4.291060	0.998593	-0.911827
1	4.080377	1.794165	0.659201
1	1.723379	0.654173	0.770101

2a (25.3)

6	-0.845213	-0.732947	-0.089942
6	-0.713712	0.609780	-0.245595
15	1.359668	-0.411714	-1.409912
7	0.136269	-1.489425	-0.805683
7	0.292351	0.945395	-1.233607
6	0.841007	2.286296	-1.337094
1	0.041111	3.023403	-1.449432
1	1.461439	2.573552	-0.472755
1	1.468058	2.338430	-2.234255
6	-0.341036	-2.571724	-1.676156
1	-1.045326	-2.224885	-2.447655
1	0.518600	-3.033597	-2.169087
1	-0.845719	-3.331277	-1.073909
7	-1.797131	-1.486051	0.605976
7	-1.477634	1.582133	0.428280
6	-2.436516	2.363393	-0.341400
1	-2.003494	3.254255	-0.830867
1	-2.880439	1.733937	-1.116760
1	-3.238952	2.714672	0.321654
6	-0.836591	2.322993	1.509067
1	-1.603155	2.675699	2.212868
1	-0.154682	1.657881	2.044263
1	-0.265484	3.204869	1.169180
6	-3.117424	-0.930518	0.847204
1	-3.148063	-0.205115	1.674596
1	-3.476244	-0.433243	-0.056880
1	-3.802739	-1.754723	1.084718
6	-1.281564	-2.283614	1.716049
1	-1.972300	-3.108161	1.929956
1	-0.308974	-2.698824	1.443054
1	-1.157802	-1.688603	2.638262

6	2.413035	-0.257221	0.051737
6	3.308120	-0.114938	0.866145
6	4.350323	0.038372	1.876227
1	5.332187	0.211223	1.418237
1	4.139170	0.884070	2.542318
1	4.428230	-0.861446	2.498965

TS4a (334.3i)

6	-1.303941	-0.928654	-0.080668
6	-1.599498	0.375532	-0.370975
15	0.858335	-0.030280	-1.292403
7	-0.055059	-1.312486	-0.595181
7	-0.589172	0.943742	-1.160894
6	3.223890	-0.526491	-0.084302
8	2.766689	-1.218350	-1.082420
6	-0.479680	2.369896	-1.389128
1	-1.440750	2.802173	-1.676611
1	-0.102476	2.886840	-0.491499
1	0.231227	2.547868	-2.201907
6	0.325979	-2.727386	-0.639731
1	-0.361018	-3.280648	-1.288881
1	1.347016	-2.783709	-1.010695
1	0.284577	-3.172931	0.358248
6	4.488194	0.289523	-0.377057
1	5.314359	-0.412983	-0.552069
1	4.349929	0.876755	-1.289088
1	4.758801	0.956729	0.447469
6	3.240406	-1.229483	1.281263
1	3.976403	-2.043612	1.234181
1	3.515461	-0.549481	2.093695
1	2.263732	-1.669201	1.501879
7	-2.064432	-1.893369	0.604080
7	-2.780005	1.038627	0.024226
6	-3.758285	1.353915	-1.011419
1	-3.537299	2.276637	-1.576526
1	-3.816541	0.525623	-1.721964
1	-4.745499	1.481587	-0.549062
6	-2.670251	2.050677	1.069413
1	-3.648601	2.179650	1.550502
1	-1.957749	1.711175	1.825802
1	-2.345276	3.041096	0.705403
6	-3.483575	-1.992686	0.287417
1	-4.093547	-1.204764	0.754399
1	-3.618775	-1.940593	-0.796222
1	-3.852874	-2.967589	0.630626
6	-1.781813	-2.000582	2.033803
1	-2.163054	-2.956817	2.412305
1	-0.701604	-1.971546	2.201708
1	-2.243225	-1.187459	2.621492
6	1.952094	0.794717	0.230284
6	1.832481	1.735383	1.027198
6	1.790378	2.816186	2.008360
1	1.915435	3.799766	1.537755
1	0.837837	2.829279	2.554038
1	2.587373	2.708273	2.758066

IN3a (9.9)

6	-1.883925	-0.527277	-0.350016
6	-1.523649	0.768941	-0.149339
15	0.640656	-0.430753	-1.040598
7	-0.854004	-1.273282	-0.967070
7	-0.200202	1.006123	-0.637306
6	2.717787	-1.080743	0.640390
8	1.289276	-1.013816	0.438428
6	0.321487	2.327431	-0.939043
1	-0.300801	2.856107	-1.673855
1	0.401536	2.953041	-0.040698
1	1.326088	2.219907	-1.357604
6	-1.001411	-2.658788	-1.375287
1	-2.034188	-2.840065	-1.682548
1	-0.337546	-2.859354	-2.222947
1	-0.749688	-3.364752	-0.570745
6	3.290974	-2.289523	-0.124025
1	2.764744	-3.197179	0.190355
1	3.158446	-2.160483	-1.202165
1	4.360352	-2.409789	0.080497
6	2.896449	-1.263110	2.157320
1	2.379873	-2.174280	2.476241
1	3.957265	-1.342524	2.417037
1	2.464118	-0.411396	2.689157
7	-3.079634	-1.196773	-0.032738
7	-2.279707	1.720493	0.567131
6	-2.834941	2.854325	-0.165337
1	-2.118916	3.678860	-0.329486
1	-3.195981	2.515294	-1.139846
1	-3.686214	3.266032	0.392989
6	-1.774595	2.078543	1.889208
1	-2.585081	2.526790	2.479343

1	-1.429479	1.176488	2.400327
1	-0.940189	2.802559	1.866019
6	-4.331742	-0.489759	-0.270754
1	-4.553066	0.274535	0.488860
1	-4.291331	-0.003312	-1.248920
1	-5.152012	-1.219571	-0.281042
6	-3.061962	-1.922960	1.236374
1	-3.879561	-2.654180	1.253884
1	-2.115784	-2.460233	1.342093
1	-3.176610	-1.255014	2.107863
6	3.400316	0.159697	0.210950
6	4.013857	1.155269	-0.103128
6	4.747260	2.356233	-0.496291
1	4.636144	2.560467	-1.568399
1	4.393702	3.239296	0.049937
1	5.819527	2.248965	-0.291055

TS5aH (554.5i)

6	-1.052487	-1.720863	0.175170
6	-1.664342	-0.753709	-0.587335
15	0.817188	-0.832095	-1.389922
7	0.270061	-1.923453	-0.221253
7	-0.783675	-0.278585	-1.564569
6	1.547431	2.219739	0.549581
8	1.198947	0.844750	0.523145
6	-1.079211	0.888892	-2.393301
1	-2.055226	0.778688	-2.870661
1	-1.058833	1.803205	-1.790638
1	-0.318708	0.965897	-3.175295
6	1.122775	-2.941368	0.405169
1	0.470772	-3.722075	0.799606
1	1.804358	-3.350975	-0.339767
1	1.725494	-2.494675	1.198901
6	2.403454	2.604425	-0.681560
1	3.301015	1.979556	-0.709607
1	1.836693	2.436812	-1.604099
1	2.696378	3.659801	-0.647469
6	2.338094	2.502432	1.849516
1	3.256434	1.906022	1.845632
1	2.600273	3.562783	1.939701
1	1.736878	2.212226	2.716233
7	-1.553576	-2.469816	1.244370
7	-2.977133	-0.296063	-0.405393
6	-3.990239	-0.680504	-1.380381
1	-4.035135	-0.017453	-2.262618
1	-3.802548	-1.700284	-1.726428
1	-4.978610	-0.656471	-0.904038
6	-3.167650	1.030002	0.178397
1	-4.087177	1.035291	0.778904
1	-2.319390	1.273161	0.821576
1	-3.259179	1.825175	-0.580914
6	-2.901043	-3.015933	1.131790
1	-3.689265	-2.270969	1.313391
1	-3.042014	-3.438737	0.133524
1	-3.011231	-3.825319	1.863837
6	-1.250652	-1.918433	2.569670
1	-1.296887	-2.717498	3.318641
1	-0.246052	-1.489152	2.571557
1	-1.960273	-1.125769	2.858386
6	0.312752	3.041281	0.551611
6	-0.651647	3.775465	0.556981
6	-1.799075	4.681499	0.589376
1	-1.721572	5.455371	-0.184751
1	-2.743524	4.147241	0.425180
1	-1.876580	5.191967	1.557569
6	3.233923	-0.685952	0.048891
1	2.143904	0.209934	0.434243
6	4.296742	-1.252865	-0.199583
6	5.569537	-1.914524	-0.492640
1	6.393801	-1.478341	0.088706
1	5.542840	-2.986936	-0.252707
1	5.844054	-1.827141	-1.553141

IN4aH (19.3)

6	-0.896560	0.000004	0.032441
8	-1.309114	-0.000040	1.412346
6	-1.421980	1.270946	-0.663499
1	-2.520031	1.274159	-0.660386
1	-1.067756	2.158976	-0.133093
1	-1.084489	1.323234	-1.703736
6	-1.422299	-1.270680	-0.663726
1	-2.520347	-1.273478	-0.660860
1	-1.084605	-1.322978	-1.703909
1	-1.068559	-2.158936	-0.133377
6	0.575419	-0.000189	0.037897
6	1.783674	-0.000088	0.003161
6	3.244072	-0.000020	-0.019735
1	3.636608	0.884064	-0.536856

1	3.652134	0.003083	0.998244
1	3.636761	-0.887125	-0.531530
1	-2.280752	-0.000519	1.407501

TMSC≡—— (20.1)

6	-0.976554	-0.000450	0.000327
6	-2.194599	-0.000326	0.000222
6	-3.654080	-0.000132	0.000007
1	-4.051258	-0.048425	1.021342
1	-4.050946	0.908646	-0.468855
1	-4.051079	-0.860469	-0.552622
14	0.860860	-0.000129	-0.000087
6	1.477315	-1.505904	-0.963917
1	1.125866	-2.439840	-0.510683
1	1.125286	-1.486130	-2.001647
1	2.573900	-1.534986	-0.982958
6	1.477217	-0.081432	1.786117
1	2.573849	-0.080523	1.821349
1	1.123207	0.776553	2.368935
1	1.127250	-0.991445	2.286721
6	1.475994	1.588149	-0.822447
1	1.123767	2.476531	-0.285872
1	2.572659	1.619889	-0.838787
1	1.123698	1.662571	-1.857560

TS5aTMS (96.8i)

6	3.044991	0.120100	-0.412933
6	2.414976	-1.091198	-0.280642
15	0.612149	0.510766	-1.332156
7	2.213259	1.048318	-1.041509
7	1.116098	-1.035302	-0.824436
6	-3.110334	-0.067598	-1.245691
8	-1.947041	-0.047374	-0.441870
6	0.255739	-2.216594	-0.942313
1	0.449179	-2.899621	-0.115727
1	-0.781228	-1.883388	-0.885787
1	0.444257	-2.733950	-1.889874
6	2.602325	2.436196	-1.242541
1	3.688020	2.483221	-1.343604
1	2.131089	2.823058	-2.150011
1	2.286100	3.052480	-0.391893
6	-2.761194	-0.780563	-2.575215
1	-1.927556	-0.262171	-3.062495
1	-2.474571	-1.820425	-2.392263
1	-3.619932	-0.781008	-3.255338
6	-3.590859	1.365533	-1.581818
1	-2.772640	1.909188	-2.066237
1	-4.452381	1.341319	-2.259460
1	-3.878843	1.908843	-0.680448
7	4.335260	0.515082	-0.027674
7	2.966843	-2.221841	0.337134
6	3.292884	-3.381634	-0.486376
1	2.444936	-4.066672	-0.651289
1	3.659280	-3.046918	-1.460792
1	4.091985	-3.954722	0.000618
6	2.548501	-2.538111	1.701504
1	3.351367	-3.092428	2.204589
1	2.368078	-1.612154	2.252429
1	1.633530	-3.151215	1.755768
6	4.428330	1.109484	1.308702
1	5.373055	1.658312	1.396533
1	3.605427	1.812033	1.464100
1	4.390143	0.352413	2.109409
6	5.432225	-0.401787	-0.327206
1	5.489335	-1.253377	0.365818
1	5.317527	-0.786486	-1.343881
1	6.375596	0.155148	-0.275264
6	-4.218073	-0.835737	-0.615078
6	-5.121317	-1.488641	-0.140824
6	-6.208608	-2.261617	0.456012
1	-6.256559	-3.277312	0.043175
1	-6.081105	-2.352574	1.541915
1	-7.182038	-1.787401	0.277757
6	-0.466200	1.802365	0.372181
6	-0.345384	3.016775	0.173746
6	-0.251620	4.451434	-0.081397
1	-1.219509	4.933057	0.111029
1	0.493762	4.944772	0.555741
1	0.004738	4.666336	-1.128380
14	-1.640119	0.498062	1.382801
6	-3.308872	1.300274	1.836531
1	-3.293768	2.378570	1.635084
1	-4.170482	0.864861	1.325055
1	-3.460660	1.179794	2.916726
6	-0.610727	1.078818	2.969972
1	-1.025133	0.635792	3.887684
1	0.442650	0.765805	2.905891

1	-0.612741	2.169782	3.089574
6	-1.570106	-1.360977	1.876009
1	-0.561109	-1.775595	1.750702
1	-1.809286	-1.458883	2.942792
1	-2.265058	-1.976797	1.298102

IN4aTMS (28.6)

6	-0.790966	1.277840	-0.046213
8	0.596033	0.987079	-0.262260
6	-1.229359	2.179773	-1.214366
1	-0.588316	3.066827	-1.243389
1	-1.128010	1.643514	-2.161982
1	-2.271530	2.493657	-1.096269
6	-0.920367	2.027630	1.293782
1	-0.287299	2.920571	1.268681
1	-1.957370	2.329946	1.473977
1	-0.596159	1.390972	2.121967
6	-1.632308	0.061666	-0.020107
6	-2.359467	-0.906028	0.004845
6	-3.229471	-2.079850	0.029293
1	-3.988130	-2.029796	-0.761139
1	-2.654410	-3.001452	-0.122367
1	-3.752844	-2.170150	0.988845
14	1.517872	-0.397025	-0.019273
6	1.246218	-1.137797	1.697639
1	1.491820	-0.416769	2.486543
1	0.207849	-1.454778	1.841321
1	1.887593	-2.016654	1.843082
6	3.289450	0.222631	-0.181376
1	4.008646	-0.598596	-0.070998
1	3.457608	0.684069	-1.161261
1	3.518892	0.973868	0.583015
6	1.176487	-1.691114	-1.351156
1	1.350085	-1.276023	-2.351157
1	1.839494	-2.557773	-1.231903
1	0.142308	-2.048215	-1.313103

2b (43.6)

6	0.743839	0.759622	-0.277271
6	0.808992	-0.595203	-0.177577
15	-1.688706	-0.062221	-0.872382
7	-0.528130	1.229063	-0.676056
7	-0.422114	-1.221932	-0.559564
6	-0.416457	-2.476542	-1.305777
1	0.241430	-2.444477	-2.187929
1	-0.100376	-3.314520	-0.672959
1	-1.434053	-2.688854	-1.649926
6	-0.657375	2.459829	-1.453614
1	-1.709164	2.590137	-1.723610
1	-0.347505	3.331644	-0.869409
1	-0.058991	2.438795	-2.375519
7	1.713720	1.738789	0.003070
7	1.876278	-1.309809	0.420750
6	2.718234	-2.130860	-0.446593
1	2.287834	-3.117733	-0.691417
1	2.903992	-1.598399	-1.382859
1	3.683465	-2.306308	0.046496
6	1.549220	-1.972660	1.679470
1	2.477502	-2.278353	2.179015
1	1.019287	-1.273760	2.332470
1	0.920452	-2.872816	1.556959
6	3.112070	1.420599	-0.242760
1	3.563578	0.787992	0.535401
1	3.201168	0.902381	-1.200946
1	3.678881	2.359167	-0.303270
6	1.500681	2.504116	1.228226
1	2.084555	3.431866	1.190204
1	0.443314	2.765874	1.320376
1	1.799573	1.946987	2.134227
6	-4.002302	-0.393781	0.517342
1	-4.681369	0.291622	1.044358
1	-4.340638	-0.481347	-0.519967
1	-4.092945	-1.384399	0.993433
6	-2.086615	0.261711	1.886217
1	-1.961393	-0.710504	2.390001
1	-1.114069	0.754929	1.833366
1	-2.751531	0.879032	2.506678
7	-2.640346	0.121514	0.548168

TS4b (227.9i)

6	1.425909	0.828391	-0.295482
6	1.676857	-0.504979	-0.193708
15	-0.828740	-0.300077	-1.058381
7	0.132254	1.099224	-0.799252
7	0.564722	-1.265100	-0.659174
6	-3.323659	0.272269	-0.044002
8	-2.765643	1.188843	-0.765398
6	0.720853	-2.597651	-1.227341

1	1.473153	-2.618957	-2.027823
1	1.005268	-3.336752	-0.468079
1	-0.235563	-2.911285	-1.657870
6	-0.210790	2.416840	-1.342485
1	0.512209	2.711446	-2.110701
1	-1.214780	2.362228	-1.756591
1	-0.210568	3.180779	-0.558372
6	-4.041574	-0.858499	-0.810344
1	-4.868033	-0.386415	-1.353274
1	-3.385761	-1.315951	-1.555532
1	-4.462084	-1.636528	-0.162288
6	-4.190971	0.761632	1.129297
1	-5.140164	1.119072	0.713076
1	-4.422114	-0.027479	1.856721
1	-3.720460	1.605276	1.639342
7	2.234812	1.929560	0.030373
7	2.822825	-1.073498	0.408426
6	3.780879	-1.761809	-0.453740
1	3.502292	-2.801775	-0.697459
1	3.889649	-1.207942	-1.389655
1	4.759001	-1.791272	0.043798
6	2.607215	-1.752483	1.680893
1	3.573721	-1.904547	2.178009
1	1.985086	-1.128035	2.328335
1	2.123622	-2.742072	1.585213
6	3.660647	1.839291	-0.252739
1	4.218831	1.245639	0.486393
1	3.806438	1.389591	-1.238227
1	4.078867	2.854145	-0.272264
6	1.940905	2.576053	1.306573
1	2.382653	3.579610	1.320220
1	0.860122	2.676993	1.433548
1	2.339091	2.012543	2.169158
6	-1.962941	-1.906681	1.115090
1	-2.681546	-2.015869	1.937706
1	-2.280731	-2.547444	0.289469
1	-0.979509	-2.248368	1.462440
6	-1.361953	0.341945	1.747013
1	-0.331120	0.054824	1.983241
1	-1.379496	1.377092	1.404175
1	-1.967776	0.247310	2.656751
7	-1.897804	-0.508952	0.677527

IN3b (30.2)

6	-1.867059	-0.702131	-0.218552
6	-1.624815	0.635707	-0.248645
15	0.577292	-0.499564	-1.139651
7	-0.817453	-1.447315	-0.799466
7	-0.358157	0.915115	-0.856066
6	2.822885	-0.623129	0.401816
8	1.398269	-0.786949	0.337882
6	-0.079642	2.156704	-1.563260
1	-0.788277	2.340309	-2.383888
1	-0.110283	3.017739	-0.884781
1	0.928801	2.101598	-1.983346
6	-0.891042	-2.874853	-1.052908
1	-1.918067	-3.154547	-1.301496
1	-0.240344	-3.123588	-1.898190
1	-0.570428	-3.475397	-0.189265
6	3.513615	-1.602022	-0.564308
1	3.070761	-2.591931	-0.421400
1	3.367172	-1.303792	-1.605955
1	4.587092	-1.682900	-0.365908
6	3.189668	-0.989554	1.851775
1	2.986069	-2.049645	2.031262
1	4.253045	-0.806351	2.045765
1	2.595833	-0.409062	2.562169
7	-2.957272	-1.417337	0.309801
7	-2.419175	1.621664	0.377895
6	-3.155259	2.551024	-0.474978
1	-2.546512	3.386962	-0.861989
1	-3.571344	2.008020	-1.327445
1	-3.986528	2.986268	0.095284
6	-1.827006	2.262296	1.547777
1	-2.613726	2.767586	2.123269
1	-1.367644	1.500402	2.183019
1	-1.057596	3.016466	1.300877
6	-4.289989	-0.858079	0.124258
1	-4.512230	-0.021041	0.802395
1	-4.392960	-0.504695	-0.905099
1	-5.030487	-1.650955	0.293486
6	-2.742820	-1.960164	1.650626
1	-3.477500	-2.749772	1.850835
1	-1.741583	-2.393718	1.717941
1	-2.837312	-1.191472	2.437554
6	4.535136	1.071335	-0.249310
1	5.208047	0.940035	0.619791
1	4.907004	0.453525	-1.069298

1	4.612011	2.117714	-0.564868
6	2.585417	1.765463	0.965661
1	2.613586	2.752317	0.489225
1	1.545690	1.518895	1.185456
1	3.144941	1.838252	1.915741
7	3.135301	0.778765	0.036529

TS5bH (62.5i)

6	-2.087350	0.885740	-0.232463
6	-2.470146	-0.415868	-0.410277
15	0.178132	-0.388564	-0.663649
7	-0.700525	1.054495	-0.378887
7	-1.358844	-1.195561	-0.755317
6	3.509854	0.794611	-0.129230
8	2.151728	0.754248	0.106659
6	-1.421279	-2.624406	-1.025175
1	-1.762405	-3.195763	-0.153873
1	-2.084895	-2.840939	-1.868606
1	-0.416202	-2.969644	-1.286936
6	-0.117821	2.405156	-0.375146
1	-0.423507	2.946388	0.523641
1	0.965307	2.278137	-0.371700
1	-0.468305	2.963006	-1.249322
6	4.187674	1.413094	1.118353
1	3.642816	2.328525	1.366332
1	4.105596	0.726361	1.968950
1	5.243525	1.673186	0.974839
6	3.812578	1.692605	-1.358026
1	3.531965	2.727851	-1.132880
1	4.874209	1.686850	-1.639808
1	3.223726	1.369911	-2.222561
7	-2.876953	2.016820	0.040424
7	-3.784876	-0.895380	-0.240897
6	-4.077639	-1.628222	0.986467
1	-3.777621	-2.690824	0.955424
1	-3.567800	-1.150210	1.826987
1	-5.158111	-1.597131	1.176800
6	-4.492103	-1.398046	-1.413912
1	-5.573688	-1.318160	-1.245355
1	-4.236548	-0.787523	-2.283919
1	-4.273366	-2.453396	-1.652213
6	-3.081325	2.318609	1.454733
1	-3.814690	1.646597	1.933743
1	-2.134135	2.235077	1.995256
1	-3.441577	3.348996	1.559501
6	-4.078160	2.202067	-0.766605
1	-4.396278	3.249431	-0.689312
1	-3.847166	1.992969	-1.814516
1	-4.916157	1.559355	-0.457158
6	5.499620	-0.765069	-0.176792
1	6.099218	-0.197145	-0.917018
1	5.828941	-0.471621	0.822495
1	5.753206	-1.825112	-0.306522
6	3.635943	-1.222072	-1.579518
1	3.829732	-2.302760	-1.537339
1	2.565186	-1.072828	-1.723800
1	4.162334	-0.832054	-2.472409
7	4.058372	-0.606245	-0.326833
7	0.826609	-0.886185	1.630784
1	1.501600	-0.118037	1.405881
6	1.546669	-2.150040	1.751791
1	0.876415	-3.001741	1.573283
1	2.359743	-2.149584	1.019895
1	1.988799	-2.275740	2.753921
6	-0.082663	-0.598551	2.727607
1	-0.534988	0.386631	2.578802
1	-0.885031	-1.346994	2.767669
1	0.424760	-0.600849	3.707533

IN4bH (104.3)

6	0.615194	-0.046405	-0.023314
8	1.140389	-1.110604	-0.819704
6	1.379835	1.244629	-0.358960
1	2.450400	1.025330	-0.323389
1	1.127320	1.587146	-1.369339
1	1.175705	2.057735	0.344866
6	0.878922	-0.464278	1.431141
1	1.955884	-0.532395	1.613319
1	0.457680	0.267353	2.129108
1	0.440575	-1.443613	1.639704
6	-1.486529	1.292295	0.106169
1	-1.570149	1.342904	1.208784
1	-0.981921	2.196040	-0.242358
1	-2.504582	1.307249	-0.298596
6	-1.612598	-1.097792	-0.096558
1	-2.548449	-1.041561	-0.664754
1	-1.064814	-1.986037	-0.416054
1	-1.875858	-1.212051	0.970830

7	-0.813072	0.094055	-0.379414
1	0.857669	-0.912338	-1.729457

$TMSNMe_2$ (23.6)

7	-1.133999	0.000074	-0.209070
6	-1.921870	-1.205730	-0.001682
1	-2.797098	-1.211352	-0.669458
1	-1.332691	-2.099461	-0.227158
1	-2.301425	-1.301087	1.031992
6	-1.922215	1.205597	-0.001569
1	-1.333292	2.099517	-0.227008
1	-2.797472	1.210999	-0.669310
1	-2.301754	1.300778	1.032127
14	0.609115	0.000055	-0.004731
6	1.151637	-0.000316	1.815649
1	2.245374	-0.001367	1.909115
1	0.777517	0.884290	2.345933
1	0.775777	-0.884000	2.346236
6	1.314534	1.543307	-0.841479
1	2.410829	1.498958	-0.840202
1	0.985931	1.617416	-1.884501
1	1.031390	2.472027	-0.332782
6	1.314481	-1.542982	-0.841970
1	2.410748	-1.498072	-0.841794
1	1.032303	-2.471594	-0.332546
1	0.984850	-1.617603	-1.884617

TS5bTMS (101.2i)

6	2.436583	-0.283569	0.918889
6	2.880787	-0.581929	-0.334467
15	0.214329	-0.855761	-0.411057
7	1.038090	-0.423009	1.039945
7	1.797731	-0.988130	-1.140855
6	-2.948319	-1.119486	0.808980
8	-1.918458	-0.244618	0.433680
6	1.964446	-1.604348	-2.449121
1	2.417515	-0.922435	-3.179127
1	2.582629	-2.507687	-2.389312
1	0.978315	-1.896815	-2.823435
6	0.424601	-0.408639	2.370465
1	0.721531	0.483750	2.924158
1	-0.651238	-0.400636	2.226862
1	0.734189	-1.288947	2.945083
6	-3.845138	-0.459179	1.881978
1	-3.205554	-0.108214	2.696105
1	-4.385713	0.401291	1.478226
1	-4.570502	-1.155862	2.316455
6	-2.352927	-2.412678	1.429184
1	-1.887028	-2.203359	2.397230
1	-3.133132	-3.165434	1.599077
1	-1.592931	-2.852411	0.777412
7	3.162434	0.121534	2.053098
7	4.213247	-0.433506	-0.774313
6	4.502541	0.695758	-1.651252
1	4.204574	0.534204	-2.703287
1	3.990103	1.587591	-1.281453
1	5.582218	0.891822	-1.641959
6	4.968967	-1.638262	-1.103669
1	6.041639	-1.435957	-0.987630
1	4.696265	-2.439853	-0.412372
1	4.811899	-2.000047	-2.134578
6	3.274205	1.565257	2.246117
1	4.003469	2.033093	1.561719
1	2.301377	2.039834	2.087336
1	3.589231	1.772839	3.275730
6	4.395620	-0.596879	2.353030
1	4.663455	-0.413603	3.401377
1	4.229806	-1.669884	2.225369
1	5.242775	-0.296475	1.718473
6	-5.121561	-2.007157	-0.134246
1	-5.121446	-2.981073	0.396664
1	-5.733458	-1.306697	0.438046
1	-5.624467	-2.167764	-1.095753
6	-3.113347	-2.283636	-1.384157
1	-3.644045	-2.210831	-2.342881
1	-2.093725	-1.922884	-1.525374
1	-3.060602	-3.357925	-1.120477
7	-3.794832	-1.464752	-0.391533
7	-0.474275	1.158530	-1.158773
6	-0.991812	0.833777	-2.505370
1	-0.208987	0.355834	-3.108653
1	-1.840076	0.153756	-2.416533
1	-1.314584	1.739597	-3.035707
6	0.715699	2.017104	-1.296082
1	1.080470	2.311203	-0.309123
1	1.507182	1.459223	-1.808665
1	0.504385	2.922468	-1.874619

14	-1.886259	1.917903	-0.124408
6	-3.646783	1.751896	-0.815059
1	-4.326433	2.281742	-0.132255
1	-3.717428	2.270731	-1.779298
1	-3.987931	0.721035	-0.921387
6	-1.623566	3.765625	-0.727350
1	-2.478799	4.347819	-0.354751
1	-0.722226	4.258357	-0.339430
1	-1.622800	3.896158	-1.818855
6	-1.533290	2.293124	1.707145
1	-2.023163	3.241913	1.960429
1	-1.856168	1.529634	2.412471
1	-0.457238	2.458260	1.853762

IN4bTMS (22.4)

6	-1.064764	0.612260	0.305051
8	0.245108	0.283922	0.761262
6	-0.999086	1.772659	-0.701332
1	-0.372316	2.563511	-0.280925
1	-0.563776	1.446596	-1.651731
1	-1.986457	2.199889	-0.900988
6	-1.828715	1.065885	1.564263
1	-1.390080	1.987929	1.958301
1	-2.884057	1.256129	1.337573
1	-1.768518	0.305396	2.347008
6	-2.856561	-0.396930	-1.107144
1	-3.724992	-0.069405	-0.503072
1	-2.705513	0.326208	-1.911735
1	-3.127239	-1.351109	-1.572764
6	-1.781902	-1.732422	0.567669
1	-1.894543	-2.646038	-0.027811
1	-0.887285	-1.831819	1.184567
1	-2.659436	-1.659934	1.236134
7	-1.635796	-0.592932	-0.335530
14	1.668686	-0.106291	-0.043527
6	1.425533	-1.309612	-1.477657
1	2.393902	-1.556088	-1.933023
1	0.964107	-2.243780	-1.139784
1	0.779938	-0.893282	-2.257591
6	2.727353	-0.899816	1.298999
1	3.721441	-1.165204	0.918377
1	2.864523	-0.218208	2.146396
1	2.261511	-1.815101	1.682442
6	2.533700	1.453855	-0.674537
1	3.541572	1.211879	-1.035698
1	1.992799	1.925391	-1.502522
1	2.639165	2.198983	0.122973

2c (42.3)

6	-1.001372	-0.723956	-0.202306
6	-0.850454	0.628781	-0.195753
15	1.400892	-0.318567	-1.117907
7	0.100781	-1.442635	-0.745013
7	0.399500	1.071063	-0.768556
6	0.370649	2.150589	-1.763540
1	-0.336294	1.959171	-2.586336
1	0.098871	3.097923	-1.286568
1	1.370258	2.268824	-2.191506
6	-0.180034	-2.512571	-1.713257
1	-0.877894	-3.228577	-1.274620
1	-0.616126	-2.136185	-2.652006
1	0.752766	-3.033268	-1.945847
7	-2.057551	-1.518960	0.264999
7	-1.755062	1.539409	0.400585
6	-2.617513	2.325732	-0.479449
1	-2.149734	3.253219	-0.853189
1	-2.908493	1.722028	-1.342464
1	-3.527930	2.613196	0.063343
6	-1.245273	2.316154	1.524284
1	-2.087909	2.792629	2.041246
1	-0.739642	1.653636	2.230601
1	-0.538313	3.112387	1.229460
6	-3.409759	-0.986929	0.294029
1	-3.603353	-0.317852	1.145170
1	-3.607800	-0.435815	-0.627858
1	-4.111365	-1.829777	0.348068
6	-1.744832	-2.382992	1.400958
1	-2.453001	-3.219694	1.435264
1	-0.734745	-2.782553	1.287843
1	-1.802509	-1.845846	2.364480
15	2.741097	-0.666902	0.667296
6	3.989032	0.678832	0.281296
1	4.727962	0.720885	1.088772
1	4.519740	0.438916	-0.645774
1	3.529911	1.669335	0.179938
6	1.866907	0.149153	2.101741
1	1.502502	1.145944	1.835521
1	1.022323	-0.469014	2.419255

1	2.563165	0.233625	2.944253

TS4c (158.4i)

6	1.609357	0.887189	-0.243826
6	1.891518	-0.446731	-0.327620
15	-0.535065	-0.167520	-1.326086
7	0.374221	1.199874	-0.845579
7	0.896207	-1.117827	-1.086512
6	-3.471276	0.409958	-0.324606
8	-2.604917	1.283454	-0.730858
6	0.785609	-2.563828	-1.130169
1	1.746149	-3.023774	-1.374352
1	0.426031	-2.986005	-0.178818
1	0.072735	-2.840041	-1.914343
6	-0.073416	2.577772	-1.037847
1	0.781797	3.185898	-1.342343
1	-0.848066	2.593832	-1.802464
1	-0.508085	2.997565	-0.124975
6	-4.088358	-0.515727	-1.384304
1	-4.751768	0.092430	-2.016125
1	-3.317372	-0.939929	-2.032451
1	-4.679718	-1.326527	-0.943051
6	-4.515345	0.905521	0.686246
1	-5.217396	1.560877	0.151064
1	-5.087994	0.087353	1.137550
1	-4.049402	1.501926	1.475022
7	2.376824	1.941956	0.275903
7	3.046651	-1.066168	0.187133
6	4.039427	-1.561311	-0.760550
1	3.830752	-2.576536	-1.142094
1	4.098614	-0.882522	-1.614823
1	5.023611	-1.592071	-0.274778
6	2.905488	-1.891737	1.381187
1	3.878653	-1.971352	1.883549
1	2.202644	-1.415393	2.069667
1	2.552623	-2.918623	1.178473
6	3.814963	1.924270	0.040070
1	4.359669	1.232396	0.699601
1	4.009980	1.639881	-0.997006
1	4.207005	2.937039	0.198428
6	2.019570	2.377462	1.624099
1	2.436734	3.374513	1.809038
1	0.933111	2.437636	1.722002
1	2.399591	1.693882	2.404105
15	-2.002686	-0.772466	0.722375
6	-2.025570	-2.408549	1.656930
1	-2.785765	-2.387448	2.448139
1	-2.270852	-3.223568	0.968762
1	-1.054089	-2.623058	2.118718
6	-1.550864	0.399289	2.088827
1	-0.542054	0.201326	2.464476
1	-1.588486	1.411414	1.679359
1	-2.256978	0.324726	2.924953

IN3c (21.1)

6	-2.105371	-0.675401	-0.154221
6	-1.816296	0.646421	-0.291017
15	0.279338	-0.634438	-1.237733
7	-1.123226	-1.498867	-0.748818
7	-0.584838	0.830161	-0.996896
6	2.626255	-0.878802	0.237994
8	1.182737	-0.866307	0.201813
6	-0.293937	2.024731	-1.777633
1	-1.049402	2.205644	-2.555303
1	-0.235581	2.914959	-1.140191
1	0.679742	1.902386	-2.259934
6	-1.234424	-2.943687	-0.839676
1	-2.285276	-3.223711	-0.945804
1	-0.682046	-3.293885	-1.718231
1	-0.827370	-3.454636	0.044784
6	3.214951	-1.826123	-0.819270
1	2.763211	-2.820117	-0.712073
1	3.027212	-1.473382	-1.837487
1	4.297451	-1.931927	-0.685019
6	2.968835	-1.386235	1.641445
1	2.599969	-2.413013	1.755355
1	4.049861	-1.392866	1.818537
1	2.488152	-0.775519	2.410114
7	-3.185309	-1.307724	0.488795
7	-2.537593	1.701820	0.308001
6	-3.281825	2.607815	-0.562185
1	-2.665433	3.402472	-1.017444
1	-3.749984	2.034411	-1.366411
1	-4.074861	3.098607	0.017520
6	-1.873601	2.381837	1.415071
1	-2.618147	2.937863	2.000096
1	-1.405561	1.639338	2.066764
1	-1.097094	3.101107	1.096394

6	-4.509049	-0.720075	0.325389
1	-4.669309	0.175241	0.943999
1	-4.656501	-0.446925	-0.722771
1	-5.263049	-1.470887	0.596343
6	-2.914656	-1.739773	1.859365
1	-3.661675	-2.482115	2.166355
1	-1.925340	-2.201818	1.913522
1	-2.942283	-0.902942	2.578938
15	3.196536	0.909428	-0.147085
6	5.033734	0.850534	0.191752
1	5.285459	0.449327	1.180053
1	5.539216	0.252921	-0.573546
1	5.429609	1.870174	0.124915
6	2.619125	1.819898	1.374206
1	2.843751	2.885539	1.256290
1	1.534050	1.706749	1.455996
1	3.085535	1.468037	2.301121

TS5cH (1059.3i)

6	-2.051454	-1.195101	0.303083
6	-2.316186	-0.223460	-0.632636
15	0.058066	-1.153037	-1.221950
7	-0.820141	-1.813828	0.066449
7	-1.277554	-0.164124	-1.575230
6	2.142019	1.517753	0.152676
8	1.529951	0.247131	0.288953
6	-1.201668	0.858152	-2.618815
1	-2.126545	0.882528	-3.199291
1	-1.005734	1.840055	-2.175951
1	-0.378192	0.607718	-3.293218
6	-0.325108	-2.903902	0.914210
1	-1.165711	-3.548536	1.177322
1	0.447844	-3.452201	0.372962
1	0.125564	-2.501263	1.826732
6	2.725337	1.720535	-1.259138
1	3.485960	0.958502	-1.462209
1	1.944241	1.630993	-2.022685
1	3.196697	2.705315	-1.368665
6	3.257781	1.650519	1.202896
1	4.025811	0.890849	1.011721
1	3.742441	2.633649	1.171978
1	2.871330	1.478999	2.211562
7	-2.829875	-1.642986	1.377701
7	-3.469802	0.573597	-0.668163
6	-4.455770	0.313690	-1.712234
1	-4.253105	0.844500	-2.658429
1	-4.499111	-0.758326	-1.921110
1	-5.445107	0.635727	-1.363292
6	-3.356479	1.980588	-0.288815
1	-4.322860	2.325176	0.101691
1	-2.601242	2.090639	0.491394
1	-3.077229	2.639585	-1.127324
6	-4.262225	-1.817670	1.157274
1	-4.825952	-0.874056	1.182595
1	-4.427498	-2.298134	0.189604
1	-4.654962	-2.479813	1.938503
6	-2.512994	-1.044145	2.675945
1	-2.919856	-1.674965	3.474398
1	-1.430017	-0.981532	2.806627
1	-2.933469	-0.030308	2.784080
15	0.693864	2.747831	0.378976
6	1.530365	4.412811	0.557387
1	2.293927	4.432564	1.343501
1	1.994071	4.704832	-0.390811
1	0.771095	5.166196	0.796717
6	0.239977	2.430814	2.161535
1	-0.672395	2.980757	2.417673
1	0.047921	1.359450	2.269883
1	1.026842	2.719476	2.867794
15	2.970933	-2.320656	-0.251610
1	2.262993	-0.673073	0.126409
6	4.096689	-1.926904	-1.706162
1	4.704507	-2.796634	-1.986222
1	3.484341	-1.663926	-2.577539
1	4.781429	-1.089501	-1.511096
6	4.264959	-2.548389	1.097188
1	3.759747	-2.719572	2.055100
1	4.900378	-3.421194	0.899364
1	4.919419	-1.673964	1.215688

IN4cH (59.0)

6	0.893230	-0.036214	0.018787
8	1.325888	-1.319673	-0.468320
6	1.736942	1.073802	-0.622568
1	2.787434	0.980219	-0.309649
1	1.695467	1.006822	-1.713739
1	1.396633	2.071128	-0.320655
6	1.014584	-0.001329	1.545831

1	2.067748	-0.128472	1.837564
1	0.676804	0.952235	1.965375
1	0.443669	-0.810955	2.009682
15	-0.878931	0.061765	-0.691555
6	-1.609462	1.468929	0.299717
1	-1.553361	1.323755	1.384471
1	-1.114951	2.411572	0.041611
1	-2.664370	1.569819	0.021319
6	-1.681330	-1.383836	0.171335
1	-2.718737	-1.466999	-0.170327
1	-1.151159	-2.295556	-0.116758
1	-1.681851	-1.302534	1.264384
1	2.269759	-1.408226	-0.252017

$TMSPMe_2$ (42.9)

15	-1.245857	0.000170	-0.737762
6	-1.970273	-1.435862	0.234130
1	-3.050869	-1.474083	0.057447
1	-1.545649	-2.377736	-0.128850
1	-1.800458	-1.367741	1.314821
6	-1.970473	1.435551	0.234936
1	-1.546248	2.377709	-0.127766
1	-3.051129	1.473483	0.058544
1	-1.800399	1.367074	1.315569
14	0.911468	0.000107	0.019533
6	1.045795	-0.002582	1.914831
1	0.575164	-0.889629	2.354501
1	2.098580	-0.001288	2.225275
1	0.571994	0.881168	2.357699
6	1.764254	-1.546624	-0.672750
1	1.699911	-1.580060	-1.766366
1	2.827197	-1.557405	-0.400367
1	1.316198	-2.468370	-0.283588
6	1.763045	1.549178	-0.668991
1	2.826122	1.559814	-0.397145
1	1.698149	1.585379	-1.762494
1	1.314662	2.469667	-0.277262

TS5cTMS (89.3i)

6	2.562658	-0.749302	0.717827
6	3.156611	-0.322926	-0.433774
15	0.573036	-0.494906	-0.971214
7	1.186118	-1.007762	0.544775
7	2.193961	-0.234944	-1.478519
6	-3.116191	-0.829780	-0.636211
8	-2.172218	0.027594	-0.062951
6	2.516989	0.170266	-2.836305
1	2.737274	1.243272	-2.917180
1	3.379360	-0.387010	-3.215528
1	1.662680	-0.052935	-3.483246
6	0.303271	-1.285964	1.676614
1	0.275181	-2.357620	1.903934
1	0.665234	-0.748756	2.558081
1	-0.701177	-0.950164	1.412035
6	-3.178868	-0.659579	-2.171615
1	-3.474240	0.370377	-2.412951
1	-2.198323	-0.847874	-2.622606
1	-3.910830	-1.326404	-2.644229
6	-4.535077	-0.630556	-0.062024
1	-4.930892	0.347752	-0.355296
1	-5.239601	-1.387501	-0.429014
1	-4.532578	-0.672369	1.030942
7	3.119810	-0.976492	1.987713
7	4.531916	-0.101538	-0.613026
6	4.984743	1.243623	-0.946993
1	4.939285	1.478414	-2.024838
1	4.377378	1.976084	-0.408587
1	6.028486	1.364780	-0.629364
6	5.321435	-1.165724	-1.225284
1	6.369739	-1.066166	-0.914396
1	4.950682	-2.135102	-0.884222
1	5.302270	-1.157209	-2.330072
6	4.125593	-0.034038	2.462488
1	5.116103	-0.179593	2.006311
1	3.795495	0.986360	2.250740
1	4.222194	-0.146941	3.549536
6	3.448330	-2.370908	2.282489
1	3.575954	-2.494210	3.364199
1	2.633287	-3.022562	1.957690
1	4.376187	-2.702625	1.784320
15	-2.471930	-2.633050	-0.314555
6	-3.704516	-3.755606	-1.176017
1	-4.750990	-3.522283	-0.942663
1	-3.568009	-3.705759	-2.260959
1	-3.509609	-4.789981	-0.868330
6	-3.035342	-2.947528	1.443621
1	-2.679572	-3.934759	1.760409

1	-2.599108	-2.201883	2.114928
1	-4.124922	-2.920766	1.559821
15	-0.307330	1.797099	-0.431744
6	-0.838897	2.334348	-2.128642
1	0.022160	2.334445	-2.806363
1	-1.589791	1.640165	-2.508082
1	-1.263506	3.343264	-2.108812
6	1.037451	3.053087	-0.095868
1	1.433804	2.907084	0.913268
1	1.857410	2.916941	-0.809712
1	0.670840	4.081846	-0.175797
14	-2.156146	2.172749	0.932656
6	-1.601432	3.869671	1.694568
1	-1.370855	4.638112	0.945197
1	-2.422036	4.264624	2.310815
1	-0.727331	3.778741	2.353181
6	-3.681018	2.723198	-0.065456
1	-3.800722	2.184341	-1.006337
1	-4.586068	2.550954	0.530498
1	-3.628675	3.797662	-0.278187
6	-2.424155	1.199173	2.538640
1	-2.821296	1.867767	3.313554
1	-3.101722	0.356693	2.398312
1	-1.474131	0.800844	2.913160

IN4cTMS (16.9)

6	-0.749601	0.616170	0.041307
8	0.389394	-0.122596	-0.415909
6	-0.751073	2.011051	-0.600425
1	0.099245	2.602628	-0.241434
1	-0.681897	1.929885	-1.689336
1	-1.666025	2.560947	-0.351157
6	-0.765483	0.725043	1.568997
1	0.102702	1.298812	1.919502
1	-1.661123	1.248637	1.918947
1	-0.732402	-0.258709	2.045950
15	-2.199554	-0.380783	-0.725737
6	-3.695960	0.368087	0.112819
1	-3.647794	0.355415	1.207785
1	-3.841946	1.399906	-0.223627
1	-4.579690	-0.201275	-0.196608
6	-2.088402	-1.981683	0.225430
1	-2.867455	-2.659402	-0.140469
1	-1.118070	-2.444068	0.023604
1	-2.212144	-1.867210	1.308556
14	2.025566	-0.153709	-0.055162
6	2.795165	-1.072316	-1.506619
1	2.633999	-0.530704	-2.445604
1	3.876545	-1.198012	-1.371193
1	2.353597	-2.068919	-1.620306
6	2.787362	1.572764	0.087314
1	2.618600	2.165961	-0.818773
1	2.393852	2.140735	0.938715
1	3.872957	1.489576	0.228475
6	2.351020	-1.104723	1.546261
1	3.429649	-1.223410	1.711155
1	1.938180	-0.594333	2.423672
1	1.911282	-2.108386	1.507245

2d (37.5)

6	0.634301	0.802540	-0.321274
6	0.782030	-0.548510	-0.248366
15	-1.649732	-0.167290	-1.196159
7	-0.594727	1.161327	-0.926789
7	-0.321749	-1.216721	-0.869103
6	-0.548687	-2.648544	-0.753804
1	0.362496	-3.202313	-0.993143
1	-0.891534	-2.944797	0.247702
1	-1.320194	-2.942590	-1.472478
6	-1.016788	2.538090	-1.126417
1	-0.133688	3.156851	-1.300249
1	-1.673840	2.593060	-1.999959
1	-1.565199	2.938550	-0.261978
7	1.519901	1.833777	0.041283
7	1.895550	-1.216489	0.291471
6	2.796766	-1.907920	-0.624402
1	2.481504	-2.935959	-0.875716
1	2.877873	-1.339064	-1.553807
1	3.794875	-1.974864	-0.171671
6	1.741482	-1.876633	1.583140
1	2.728102	-1.989254	2.051793
1	1.121520	-1.256180	2.235489
1	1.286881	-2.881214	1.523391
6	2.927302	1.667169	-0.305096
1	3.463310	0.975827	0.361912
1	3.006372	1.293235	-1.329033
1	3.418531	2.647429	-0.258075
6	1.320401	2.388577	1.378752

1	1.865420	3.335983	1.465500
1	0.258800	2.593510	1.543573
1	1.671521	1.712621	2.177894
6	-2.083722	-0.000645	2.116835
1	-1.470788	-0.878733	2.336005
1	-1.439593	0.878071	2.036993
1	-2.786929	0.153152	2.940444
16	-3.070050	-0.240123	0.580223

TS4d (179.7i)

6	1.534959	0.858146	-0.284850
6	1.757496	-0.498606	-0.299952
15	-0.696753	-0.159322	-1.243474
7	0.279134	1.175365	-0.803966
7	0.680367	-1.153623	-0.900852
6	-3.413234	0.371021	-0.133980
8	-2.449542	1.159007	-0.456328
6	0.507717	-2.601414	-0.884091
1	1.461869	-3.103705	-1.047538
1	0.062765	-2.925790	0.065164
1	-0.177523	-2.886142	-1.687111
6	-0.149108	2.568245	-0.974713
1	0.736356	3.172845	-1.178542
1	-0.854533	2.629893	-1.801854
1	-0.654904	2.930576	-0.077482
6	-4.127391	-0.389792	-1.251300
1	-4.712938	0.337539	-1.832411
1	-3.414073	-0.859072	-1.933279
1	-4.807620	-1.152298	-0.860974
6	-4.346323	0.874634	0.963369
1	-4.950596	1.692614	0.544290
1	-5.019091	0.093111	1.326347
1	-3.775071	1.283739	1.800401
7	2.366467	1.898383	0.157258
7	2.893310	-1.132361	0.236300
6	3.830580	-1.767260	-0.684287
1	3.561767	-2.801121	-0.962193
1	3.901224	-1.174468	-1.599830
1	4.824413	-1.802603	-0.220052
6	2.743129	-1.822190	1.514524
1	3.726059	-1.907402	1.995207
1	2.090871	-1.238056	2.169109
1	2.323860	-2.838961	1.426134
6	3.786928	1.815048	-0.164903
1	4.342439	1.123719	0.485237
1	3.906655	1.489873	-1.201641
1	4.226067	2.815646	-0.067246
6	2.107994	2.372478	1.517567
1	2.562880	3.360807	1.650954
1	1.031702	2.466000	1.683240
1	2.518825	1.695100	2.285624
6	-1.577429	-0.400605	2.185013
1	-0.619237	-0.845194	2.471175
1	-1.401373	0.609546	1.795852
1	-2.208218	-0.336966	3.077258
16	-2.381364	-1.406502	0.885083

IN3d (27.8)

6	-1.809296	-0.735604	-0.187045
6	-1.581283	0.602889	-0.260562
15	0.608355	-0.535239	-1.169446
7	-0.761466	-1.487114	-0.766102
7	-0.329049	0.876249	-0.902174
6	2.890796	-0.673623	0.361310
8	1.473357	-0.759051	0.309080
6	-0.074948	2.105132	-1.643389
1	-0.798911	2.258520	-2.456086
1	-0.107799	2.980307	-0.984015
1	0.927968	2.053842	-2.076220
6	-0.822315	-2.923883	-0.972250
1	-1.852377	-3.222337	-1.182334
1	-0.192676	-3.191533	-1.827388
1	-0.470164	-3.490940	-0.098719
6	3.573901	-1.650628	-0.605830
1	3.224197	-2.666532	-0.389183
1	3.336375	-1.418479	-1.647291
1	4.660986	-1.622393	-0.480566
6	3.267299	-0.987937	1.810081
1	2.937925	-2.004927	2.053240
1	4.349169	-0.918344	1.956486
1	2.768419	-0.303351	2.501074
7	-2.883948	-1.446181	0.375578
7	-2.376756	1.599437	0.344768
6	-3.135704	2.494569	-0.524811
1	-2.542530	3.326424	-0.942636
1	-3.555885	1.922143	-1.355818
1	-3.965059	2.934955	0.044015
6	-1.783067	2.277083	1.492734

1	-2.571362	2.787601	2.061184
1	-1.309693	1.537622	2.144036
1	-1.025130	3.034137	1.220561
6	-4.225082	-0.904420	0.196065
1	-4.446632	-0.055800	0.859673
1	-4.345707	-0.574139	-0.838925
1	-4.954556	-1.701094	0.392250
6	-2.645425	-1.955209	1.725782
1	-3.371985	-2.744029	1.955599
1	-1.640712	-2.381293	1.788933
1	-2.733389	-1.168158	2.494893
6	2.637999	2.090748	1.075797
1	2.728858	3.120221	0.718924
1	1.581158	1.815239	1.118070
1	3.085559	2.024141	2.070994
16	3.504565	1.033609	-0.137717

TS5dH (750.9i)

6	1.734969	1.134784	0.024961
6	2.072228	-0.085148	-0.501721
15	-0.249245	0.519416	-1.538704
7	0.526852	1.606192	-0.505514
7	1.108658	-0.486643	-1.451740
6	-2.347591	-1.503493	0.209889
8	-1.716916	-0.248784	0.114327
6	1.142925	-1.785258	-2.124193
1	2.129788	-1.962258	-2.556613
1	0.886486	-2.587251	-1.424934
1	0.410132	-1.779282	-2.935673
6	-0.008027	2.930986	-0.170556
1	0.735111	3.696285	-0.407029
1	-0.927326	3.084158	-0.740645
1	-0.251058	2.988007	0.893571
6	-2.797732	-2.039854	-1.157185
1	-3.496501	-1.324088	-1.603558
1	-1.948041	-2.162036	-1.837260
1	-3.300628	-3.007639	-1.058950
6	-3.546690	-1.383939	1.162082
1	-4.262780	-0.669667	0.738893
1	-4.041887	-2.350579	1.297290
1	-3.232542	-1.006855	2.139497
7	2.411732	1.940107	0.951250
7	3.222283	-0.820471	-0.180657
6	4.302567	-0.880156	-1.160615
1	4.191616	-1.692583	-1.899408
1	4.363747	0.068564	-1.699518
1	5.254705	-1.041175	-0.639459
6	3.070645	-2.032698	0.620243
1	4.009224	-2.228308	1.154383
1	2.276269	-1.886685	1.354643
1	2.829300	-2.928794	0.025047
6	3.851387	2.109971	0.779644
1	4.437430	1.247659	1.129635
1	4.075718	2.280999	-0.276422
1	4.166592	2.996701	1.342828
6	2.014436	1.747820	2.347319
1	2.341109	2.610275	2.939389
1	0.926278	1.674032	2.420219
1	2.452721	0.836521	2.788034
6	-0.632090	-1.956483	2.440039
1	0.306942	-2.407186	2.773010
1	-0.483907	-0.889040	2.257105
1	-1.383961	-2.099588	3.220949
16	-1.112137	-2.766339	0.873600
16	-3.395057	1.859396	-0.898053
1	-2.498064	0.592747	-0.240244
6	-3.791872	2.761493	0.657798
1	-2.905406	3.233824	1.097735
1	-4.519680	3.548756	0.439395
1	-4.229880	2.092145	1.405696

IN4dH (94.6)

6	0.676395	0.093685	0.039239
8	0.686874	0.687905	1.327328
6	1.803477	-0.935264	-0.099696
1	2.763994	-0.438297	0.074808
1	1.692059	-1.741232	0.634709
1	1.816098	-1.383807	-1.098059
6	0.833407	1.243877	-0.952413
1	1.778496	1.763659	-0.756164
1	0.837806	0.871697	-1.980077
1	0.023469	1.970071	-0.841549
6	-2.153833	0.449128	0.103668
1	-3.095519	-0.050880	0.343560
1	-1.829405	1.039491	0.964022
1	-2.307052	1.100035	-0.761194
16	-0.918709	-0.857163	-0.232343
1	0.567732	-0.027922	1.974019

TMSSMe (56.3)

16	-1.278489	0.922745	-0.000237
6	-2.444834	-0.506080	0.000413
1	-2.322097	-1.122733	0.894353
1	-3.453764	-0.087559	0.000669
1	-2.322653	-1.123064	-0.893372
14	0.662200	-0.057858	-0.000102
6	0.871618	-1.129838	1.545219
1	1.864970	-1.596757	1.557181
1	0.767933	-0.531934	2.457229
1	0.130823	-1.936774	1.586980
6	0.870919	-1.131148	-1.544586
1	0.768660	-0.533776	-2.457102
1	1.863480	-1.599761	-1.555704
1	0.128785	-1.936871	-1.586076
6	1.908769	1.360164	-0.000565
1	2.933584	0.968453	-0.000357
1	1.793319	1.993926	-0.886706
1	1.793150	1.994358	0.885248

TS5dTMS (89.0i)

6	2.408570	-0.601421	0.746177
6	2.972960	-0.234530	-0.446940
15	0.425712	-0.661462	-0.956162
7	1.052029	-0.913462	0.598264
7	2.018532	-0.312084	-1.476697
6	-3.055640	-1.122171	-0.739144
8	-2.246300	-0.203901	-0.124868
6	2.282712	0.064068	-2.862249
1	2.473541	1.138367	-2.960199
1	3.137658	-0.489226	-3.259146
1	1.404674	-0.182582	-3.465188
6	0.231879	-1.380676	1.719343
1	0.496620	-2.410540	1.976412
1	0.393997	-0.746472	2.592771
1	-0.810082	-1.322028	1.409704
6	-3.096250	-0.948566	-2.270811
1	-3.490191	0.046079	-2.508627
1	-2.089007	-1.012057	-2.693865
1	-3.727724	-1.701272	-2.754139
6	-4.482503	-1.206573	-0.167605
1	-5.033087	-0.291103	-0.400512
1	-5.032519	-2.051784	-0.594042
1	-4.464494	-1.314289	0.920475
7	2.988374	-0.704477	2.022554
7	4.312325	0.157033	-0.618436
6	4.576955	1.569247	-0.880175
1	4.466666	1.855212	-1.940503
1	3.898594	2.184572	-0.283649
1	5.606268	1.803137	-0.581068
6	5.209469	-0.759166	-1.317652
1	6.243034	-0.552033	-1.013830
1	4.970752	-1.788667	-1.039285
1	5.165821	-0.676499	-2.417410
6	3.082112	0.554969	2.761265
1	3.885444	1.211144	2.385711
1	2.133455	1.095269	2.694133
1	3.278729	0.340011	3.818014
6	4.187463	-1.531598	2.133464
1	4.351473	-1.774329	3.190261
1	4.035098	-2.468396	1.590428
1	5.091867	-1.039398	1.744734
6	-2.774268	-3.424054	1.128818
1	-2.188966	-4.314137	1.378693
1	-2.553722	-2.644538	1.864922
1	-3.836119	-3.679096	1.187842
16	-2.286784	-2.918760	-0.560095
16	-0.725105	1.826000	-0.876446
6	0.406274	3.236109	-0.526939
1	0.798852	3.199398	0.491834
1	1.238841	3.167221	-1.233689
1	-0.101337	4.190687	-0.679776
14	-2.464609	1.793257	0.613528
6	-2.124161	3.597220	1.275565
1	-2.970177	3.874350	1.921623
1	-1.219469	3.686361	1.892299
1	-2.066484	4.359274	0.488187
6	-4.109194	2.142474	-0.283205
1	-4.221822	1.602753	-1.224973
1	-4.957099	1.875689	0.360577
1	-4.184504	3.214358	-0.496848
6	-2.527953	0.965910	2.332777
1	-2.983524	1.650967	3.058973
1	-3.078107	0.022918	2.328944
1	-1.512861	0.755837	2.690922

IN4dTMS (32.3)

6	**-1.031364**	**0.683007**	**0.066880**
8	**0.056064**	**-0.075991**	**-0.423227**
6	**-1.065605**	**2.058031**	**-0.611461**
1	**-0.196382**	**2.648940**	**-0.302153**
1	**-1.040345**	**1.940420**	**-1.698082**
1	**-1.970053**	**2.610634**	**-0.336082**
6	**-0.999152**	**0.812914**	**1.594015**
1	**-0.093168**	**1.345221**	**1.911316**
1	**-1.866984**	**1.376167**	**1.947974**
1	**-1.002828**	**-0.168169**	**2.077605**
6	**-2.352166**	**-1.856296**	**0.147958**
1	**-3.153334**	**-2.468639**	**-0.274572**
1	**-1.389416**	**-2.240739**	**-0.196255**
1	**-2.410424**	**-1.908127**	**1.239077**
16	**-2.608773**	**-0.163296**	**-0.482284**
14	**1.694190**	**-0.192607**	**-0.073848**
6	**2.404635**	**-1.119618**	**-1.548589**
1	**3.480133**	**-1.297919**	**-1.426468**
1	**1.916240**	**-2.092702**	**-1.673861**
1	**2.259841**	**-0.555133**	**-2.476573**
6	**2.518392**	**1.501247**	**0.088341**
1	**2.369374**	**2.110358**	**-0.810675**
1	**2.146197**	**2.072549**	**0.946946**
1	**3.600365**	**1.378206**	**0.226565**
6	**1.985364**	**-1.185406**	**1.507663**
1	**3.058478**	**-1.360056**	**1.657976**
1	**1.607936**	**-0.671429**	**2.398653**
1	**1.496938**	**-2.165700**	**1.456008**