

Supporting Information

Mechanistic Study of Nickel-Catalyzed Intramolecular [4+2] Cycloaddition of Cyclobutanone with Allene: Origin of Selectivity and Ligand Effect

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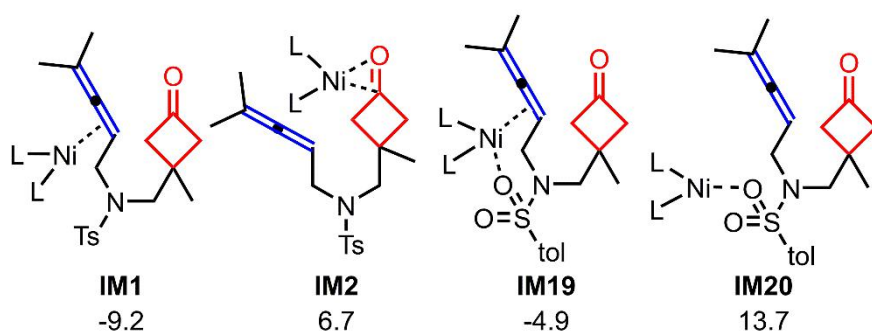


Fig. S1 Comparison of different coordination modes.

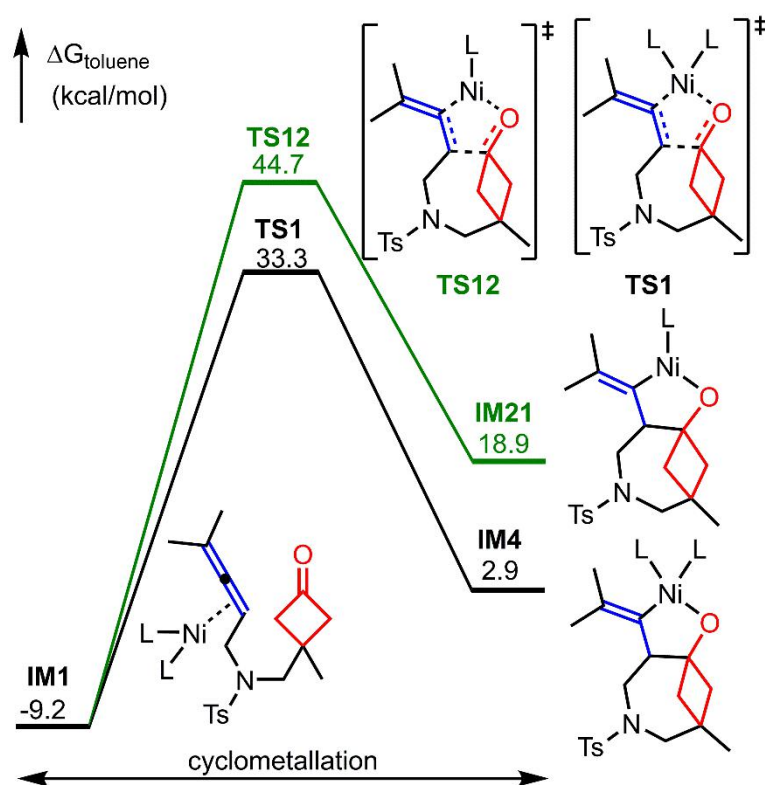


Fig. S2 Energetic comparison of cyclometallation step with one PPh_3 coordination or two PPh_3 coordination.

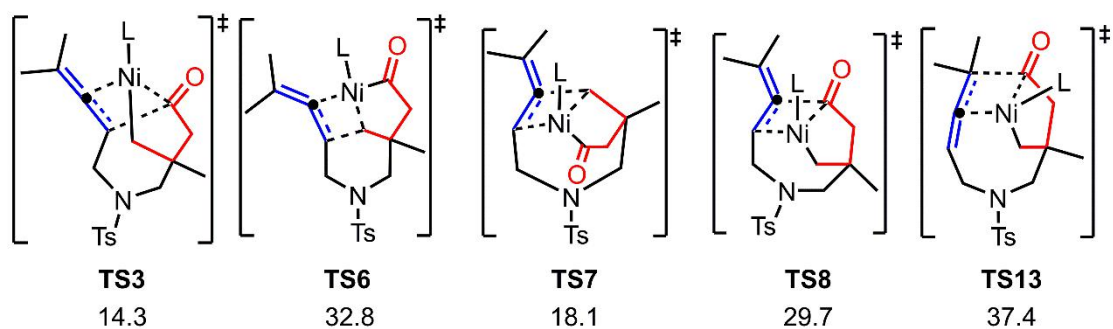


Fig. S3 All possible migratory insertion transition states that were considered.

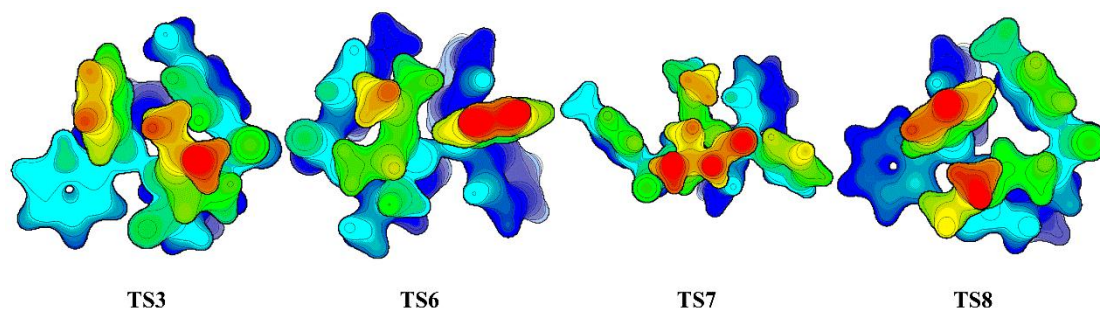


Fig. S4 Two-dimensional (2D) contour maps of transition states TS3, TS6, TS7, TS8.

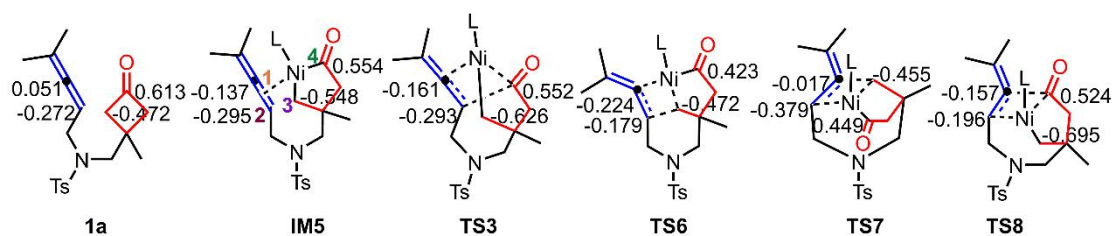
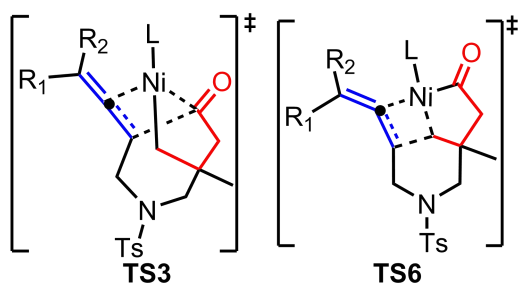
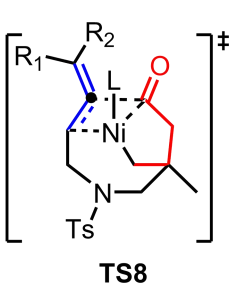
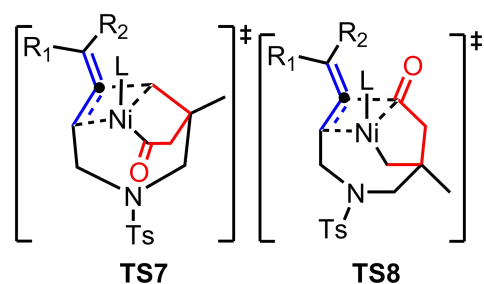
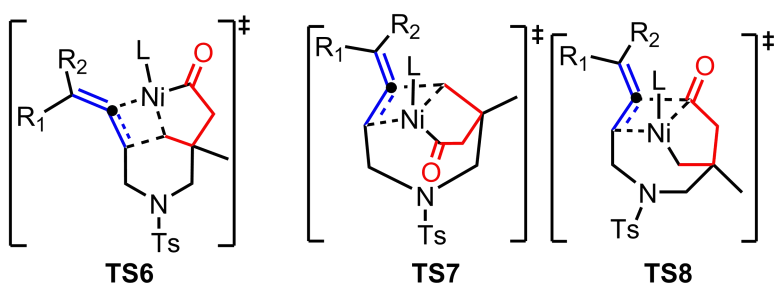


Fig. S5 Calculated natural atomic charges (in e) of the substrate **1a**, intermediate **IM5**, and migratory insertion transition states **TS3**, **TS6**, **TS7**, **TS8**.

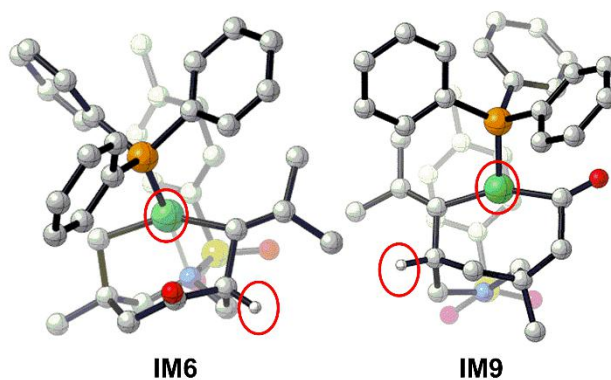
(a) 1,2-migratory insertion



(b) 2,1-migratory insertion

**Table S1.** The examination of substituent effect on regioselectivity.

	TS3	TS6	TS7	TS8
$R_1=R_2=CH_3$	0.0 ^a	18.5	3.8	15.4
$R_1=R_2=N(CH_3)_2$	0.0	13.9	3.1	3.2
$R_1=R_2=CF_3$	0.0	15.1	1.4	14.8

^a Relative Gibbs free energies are in kcal/mol.**Fig. S6** Optimized geometric structures of **IM6** and **IM9**. The circled H atoms are far away from the nickel centers, which are unlikely to undergo β -H elimination.

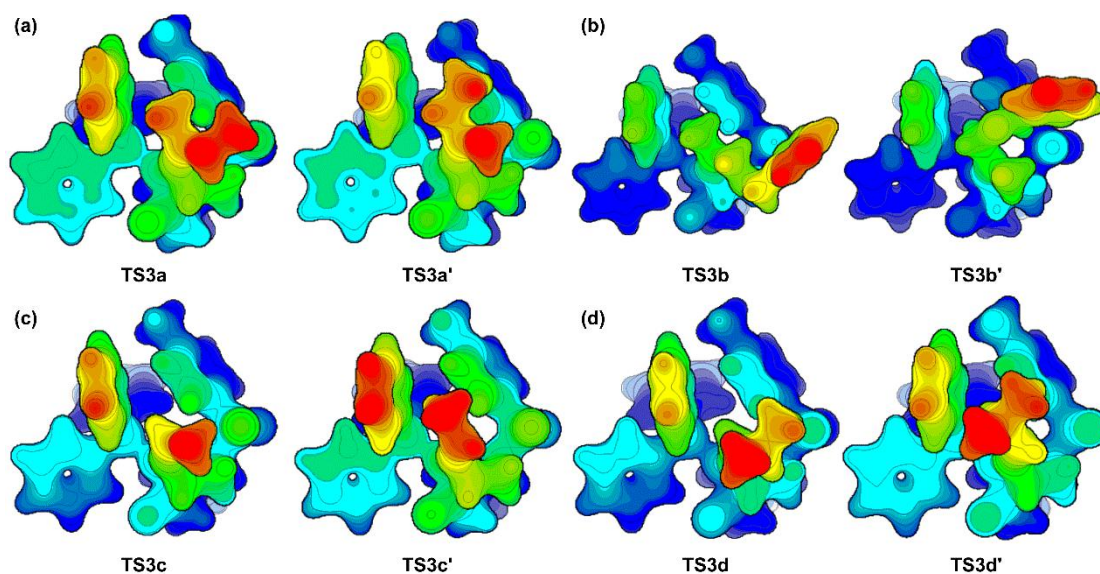


Fig. S7 Two-dimensional (2D) contour maps of *Z/E* selectivity determining transition states. The substituents at the terminal of allene are (a) $R_1=\text{Me}$, $R_2=\text{Et}$. (b) $R_1=\text{Me}$, $R_2=\text{CH}_2\text{OBn}$. (c) $R_1=\text{H}$, $R_2=\text{Me}$. (d) $R_1=\text{H}$, $R_2=i\text{Pr}$.

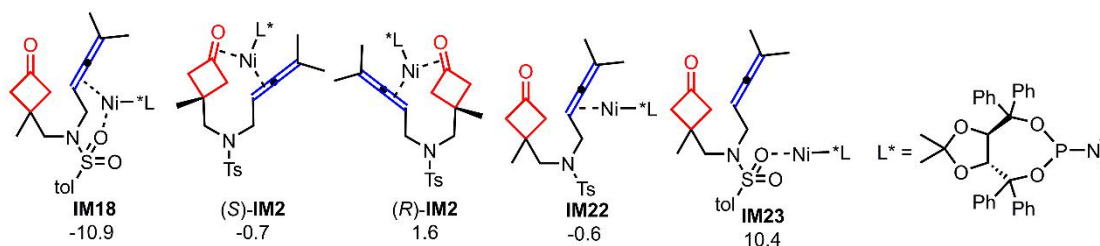


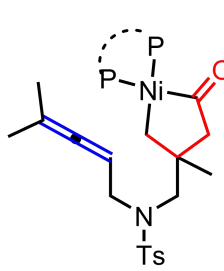
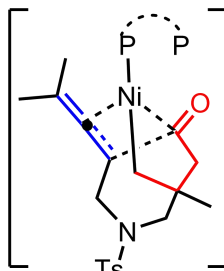
Fig. S8 Comparison of different coordination modes for the chiral TADDOL-derived phosphoramidite system

The Gibbs free energies of the C–C bond oxidative addition transition states were employed in estimating the Boltzmann distribution, which in turn, was used in the computation of the enantiomeric excess in accordance with the following equation. Using the following equation, %ee can be computed, if $\Delta G^\ddagger$, which is the difference in the Gibbs free energies between the enantiomeric transition states, is known.

$$ee = \frac{1 - e^{-\Delta G^\ddagger_{R/S}/RT}}{1 + e^{-\Delta G^\ddagger_{R/S}/RT}} \times 100$$

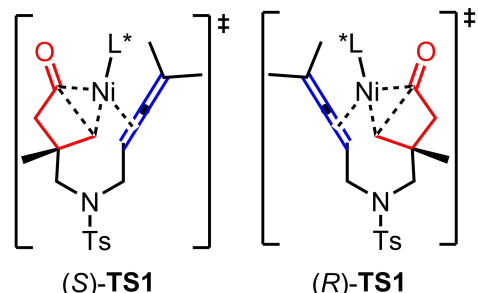
Fig. S9 The equation for the calculation of ee value.

Table S2. The examination of ligand effect and the atomic charge of Ni-center on the reactivity.

 IM3_L  TS2_{dppp}			
Entry	Ligand	$\Delta G^\ddagger(\text{TS2}_{\text{dppp}} - \text{IM3}_L)$	NPA Charge (Ni of TS2 _{dppp})
1	PPh ₃	11.1 ^a	0.055 ^b
2	P(4-MeOC ₆ H ₄) ₃	14.6	0.053
3	P(4-CF ₃ C ₆ H ₄) ₃	16.2	0.038
4	Ph ₂ P—CH ₂ CH ₂ CH ₂ —PPh ₂ (dppp)	24.9	0.075
5	Ar ₂ P—CH ₂ CH ₂ CH ₂ —PAr ₂ (Ar=4-MeOC ₆ H ₄)	24.6	0.131
6	Ar ₂ P—CH ₂ CH ₂ CH ₂ —PAr ₂ (Ar=4-CF ₃ C ₆ H ₄)	23.8	0.131

^a Activation barrier of free energies in kcal/mol; ^b NPA charges (in *e*).

Table S3. Comparison of activation barrier difference ($\Delta\Delta G^\ddagger$) of the rate- and enantioselectivity-determining step under different DFT levels.

	
DFT level ^a	$\Delta\Delta G^\ddagger [(R)\text{-TS1}] - [(S)\text{-TS1}]^b$
M06	3.7
M06L	2.2
TPSS	2.3
PBE0	1.7
ω B97X-D	1.2
M06L//B3LYP-D3(BJ)	1.6

^aThe calculations were run at DFT/BSII-SMD//DFT/BSI. ^bValues are given in kcal/mol

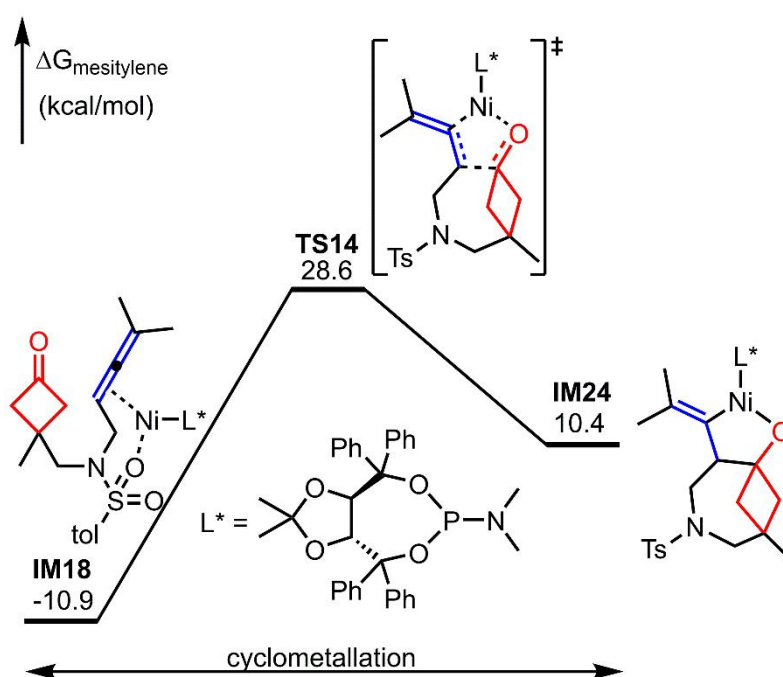


Fig. S10 The activation barrier of the cyclometallation step in the Ni/TADDOL-derived phosphoramidite ligand system.

2. Absolute Calculation Energies, Enthalpies, and Free Energies.

Table S1. Calculated absolute energies (in Hartree) of all structures under the level of M06-L/6-311++G(d,p)(SDD basis set for Ni atom)//B3LYP-D3(BJ)/6-31G(d,p)(LANL2DZ basis set for Ni atom).

Geometry	$E_{(\text{elec-B3LYP-D3(BJ)})}^1$	$H_{(\text{corr-B3LYP-D3(BJ)})}^2$	$G_{(\text{corr-B3LYP-D3(BJ)})}^3$	$E_{(\text{solv-M06-L})}^4$	$IF(i)^5$
1a	-1417.668613	0.433550	0.346682	-1417.729268	
2	-1417.749437	0.436936	0.359107	-1417.800177	
(R,R)-2a	-1417.749437	0.436937	0.359105	-1417.796905	
(S,S)-2a	-1417.749437	0.436938	0.359112	-1417.796905	
3	-1417.737583	0.436874	0.357186	-1417.784355	
4	-1417.745551	0.436482	0.359667	-1417.795538	
Cat	-2554.291422	0.780460	0.659623	-2555.928846	
Cat1	-2456.670444	0.832087	0.711781	-2458.351901	
Cat_{dppp}	-2208.880619	0.673772	0.570176	-2210.527819	
CAT-P	-2146.172835	0.639746	0.534411	-2146.229612	
cod	-312.075686	0.189149	0.149256	-312.071836	
L	-1036.390196	0.291163	0.227720	-1036.390906	
PCy₃	-1047.312557	0.505341	0.436188	-1047.272400	
P(4-Me OC₆H₄)₃	-1379.982862	0.397082	0.315927	-1380.016689	
P(4-CF₃ C₆H₄)₃	-2047.508191	0.316465	0.222306	-2047.703446	
IM1	-3659.905109	1.023982	0.860358	-3661.604304	
IM1_{dppp}	-3314.491189	0.918954	0.770703	-3316.195925	
IM2	-3659.878096	1.024247	0.856048	-3661.574662	
IM2_{dppp}	-3314.463800	0.919328	0.765522	-3316.166939	
(R)-IM2	-3562.275343	1.076764	0.917978	-3564.014805	
(S)-IM2	-3562.276121	1.076916	0.919289	-3564.019775	
IM3	-3659.897136	1.023876	0.860005	-3661.584142	
IM3_{PPh3-O} CH₃	-4347.091728	1.235893	1.038404	-4348.84385	
IM3_{PPh3-O} CF₃	-5682.144086	1.074614	0.853323	-5684.217021	
IM3_{PCy₃}	-3681.729865	1.454476	1.281219	-3683.346337	
IM3_{dppb}	-3353.808993	0.949047	0.798325	-3355.495231	
IM3_{dppe}	-3275.157180	0.888273	0.743294	-3276.853815	
IM3_{dppp}	-3314.485444	0.918678	0.770903	-3316.177645	
IM3_{dppp-O} CH₃	-3772.613526	1.059688	0.890168	-3774.348638	
IM3_{dppp-O} CF₃	-4662.6534	0.952309	0.770029	-4664.60154	
(R)-IM3	-3562.267873	1.076161	0.914669	-3564.01234	

(S)-IM3	-3562.270113	1.076016	0.915186	-3564.016925	
IM4	-3659.917853	1.026754	0.872928	-3661.597565	
IM4 _{dppp}	-3314.451060	0.918004	0.775568	-3316.155547	
IM4 _{PCy3}	-2634.364343	0.944147	0.817169	-2636.046211	
IM4 _{dppb}	-3353.770231	0.948226	0.797752	-3355.47755	
IM4 _{dppe}	-3275.127843	0.887515	0.745098	-3276.836169	
(R)-IM4	-3562.292525	1.077476	0.916279	-3564.019272	
(S)-IM4	-3562.294190	1.078617	0.917745	-3564.017506	
IM5	-2623.440444	0.729002	0.607440	-2625.164297	
IM5 _{dppp}	-3314.480952	0.920796	0.779557	-3316.168239	
(R)-IM5	-3562.338359	1.080243	0.923023	-3564.067156	
(S)-IM5	-3562.336919	1.080182	0.919158	-3564.062081	
IM6 _{dppp}	-3314.521461	0.921222	0.779625	-3316.203205	
IM6	-2623.475785	0.732079	0.616543	-2625.177685	
IM7 _{dppp}	-3314.546114	0.922356	0.778853	-3316.235199	
IM7	-3659.924399	1.026574	0.870659	-3661.598922	
IM8	-3659.957652	1.027883	0.870488	-3661.636541	
IM9	-2623.464474	0.730801	0.612535	-2625.169489	
IM10	-2623.480496	0.731610	0.607719	-2625.186192	
IM11	-2623.470110	0.730873	0.611630	-2625.167479	
IM12	-2623.487446	0.731364	0.609264	-2625.205209	
IM13	-3659.917080	1.026252	0.870575	-3661.597125	
IM14	-3659.902331	1.023309	0.868664	-3661.587736	
IM15	-3659.890534	1.023472	0.867511	-3661.579411	
IM16	-3659.928741	1.028902	0.872038	-3661.613448	
IM17	-3659.963108	1.026752	0.867465	-3661.649605	
IM18	-3562.293227	1.076641	0.915142	-3564.031913	
IM19	-3659.899640	1.023240	0.859918	-3661.596989	
IM20	-3659.874633	1.023207	0.856784	-3661.564087	
IM21	-2623.437461	0.731144	0.608021	-2625.143914	
IM22	-3562.261735	1.076390	0.906643	-3564.007086	
IM23	-3562.245366	1.076809	0.907451	-3563.97925	
IM24	-3562.273552	1.078363	0.916133	-3563.998952	
TS1	-3659.859839	1.022829	0.868055	-3661.544260	-323.58
TS1 _{dppp}	-3314.463060	0.917803	0.769762	-3316.158121	-314.16
(R)-TS1	-3562.243978	1.075141	0.917807	-3563.987727	-273.47
(S)-TS1	-3562.243504	1.074877	0.918607	-3563.991103	-307.44
TS2	-3659.875196	1.022815	0.859713	-3661.565416	-311.87
TS2 _{dppp}	-3314.441054	0.916919	0.776011	-3316.143072	-301.72
TS2 _{dppp} -O CH3	-3772.565734	1.058221	0.893685	-3774.312988	-302.23
TS2 _{dppp} -CF 3	-4662.599924	0.95076	0.769943	-4664.563489	-301.64
(R)-TS2	-3562.262722	1.075603	0.917909	-3564.004047	-252.37

(S)-TS2	-3562.260595	1.075166	0.917271	-3564.005216	-273.59
TS3	-2623.436460	0.728626	0.612433	-2625.155636	-199.73
TS3a	-2662.756709	0.758809	0.639189	-2664.470104	-206.23
TS3a'	-2662.757080	0.758917	0.639882	-2664.470071	-196.30
TS3b	-2969.041906	0.850416	0.717179	-2970.767762	-214.4
TS3b'	-2969.038860	0.850819	0.716852	-2970.766451	-154.33
TS3c	-2584.116101	0.698902	0.584794	-2585.833208	-242.44
TS3c'	-2584.109342	0.698961	0.585967	-2585.829317	-202.47
TS3d	-2662.762766	0.758546	0.639051	-2664.471386	-250.18
TS3d'	-2662.754972	0.758673	0.639973	-2664.466321	-201.05
TS3 _{dppp}	-3314.494255	0.919865	0.779232	-3316.179089	-436.20
(R)-TS3	-3562.281110	1.076456	0.918048	-3564.010478	-272.55
(S)-TS3	-3562.281129	1.077002	0.917631	-3564.010394	-353.65
TS3 _{NCH3}	-2812.766691	0.82434	0.696769	-2814.479248	-251.88
TS3 _{CF3}	-3218.870355	0.685911	0.559511	-3220.719018	-238.25
TS3 _{PPh3-O} CH3	-2967.031464	0.834512	0.700361	-2968.78171	-198.49
TS3 _{PPh3-C} F3	-3634.554402	0.753994	0.608324	-3636.465014	-193.10
TS4	-2623.459912	0.729119	0.610463	-2625.156357	-330.86
TS5	-3659.905664	1.025261	0.870443	-3661.584402	-422.10
TS6	-2623.411777	0.729041	0.611622	-2625.125345	-264.84
TS6 _{NCH3}	-2812.739957	0.824713	0.693412	-2814.453673	-264.88
TS6 _{CF3}	-3218.847134	0.686558	0.558272	-3220.69371	-224.71
TS7 _{NCH3}	-2812.753242	0.824241	0.693853	-2814.471384	-289.86
TS7 _{CF3}	-3218.86353	0.686007	0.555888	-3220.714707	-198.45
TS7	-2623.418886	0.728122	0.605233	-2625.142463	-264.80
TS8	-2623.409298	0.727091	0.608043	-2625.126676	-471.77
TS8 _{NCH3}	-2812.75391	0.824001	0.6951	-2814.472417	-382.52
TS8 _{CF3}	-3218.845603	0.685517	0.558408	-3220.694284	-247.22
TS9	-3659.893837	1.021654	0.869609	-3661.580494	-688.61
TS10	-3659.874985	1.02179	0.866879	-3661.567128	-778.50
TS11	-3659.920733	1.027235	0.873251	-3661.602576	-211.12
TS12	-2623.369150	0.727870	0.601646	-2625.096384	-537.98
TS13	-2623.392219	0.728372	0.610374	-2625.116766	-149.82
TS14	-3562.228060	1.075283	0.911549	-3563.965369	-444.56

¹The electronic energy calculated by B3LYP-GD3(BJ) in gas phase. ²The thermal correction to enthalpy calculated by B3LYP-GD3(BJ) in gas phase. ³The thermal correction to Gibbs free energy calculated by B3LYP-GD3(BJ) in gas phase. ⁴The electronic energy calculated by M06-L in toluene, mesitylene solvent. ⁵The B3LYP-GD3(BJ) calculated imaginary frequencies for the transition states.

3. Cartesian coordinates of DFT-optimized structures for all intermediates and transition states.

1a				6	-0.504235	4.091083	0.139387
				6	-1.278262	4.117345	1.439419
8	-0.099877	-2.791208	-0.483444	1	-2.316409	4.424059	1.260870
16	0.522659	-1.651548	-1.165240	1	-1.285110	3.140588	1.927736
7	-0.508756	-0.345257	-0.935732	1	-0.843570	4.847837	2.132891
8	0.846853	-1.681006	-2.593146	6	-0.431687	5.389558	-0.633007
6	2.031701	-1.267382	-0.286137	1	0.036804	6.173094	-0.024571
6	2.122968	-1.537443	1.080063	1	0.140350	5.279137	-1.556169
6	3.074789	-0.633581	-0.963358	1	-1.439342	5.740960	-0.887327
1	1.320040	-2.065812	1.580890	1	1.633205	1.624575	-0.473106
6	3.265050	-1.145662	1.773601				
6	4.209772	-0.249604	-0.253974	2			
1	2.992343	-0.458647	-2.030000				
1	3.341926	-1.354198	2.837012	8	-0.160129	-3.311399	0.300933
6	4.320944	-0.493574	1.122204	16	-0.223784	-2.229487	-0.686218
1	5.025154	0.242990	-0.776285	7	1.143051	-1.296215	-0.463174
6	5.565876	-0.099961	1.876015	8	-0.333305	-2.486135	-2.124663
1	6.305546	-0.909462	1.855206	6	-1.618216	-1.200721	-0.242912
1	6.036678	0.783463	1.435891	6	-2.086420	-1.208704	1.071277
1	5.346360	0.114757	2.925498	6	-2.222657	-0.402673	-1.213933
6	-0.151588	0.918407	-1.617832	1	-1.628161	-1.868253	1.799506
1	-1.075839	1.388456	-1.957030	6	-3.162685	-0.393510	1.413680
1	0.418785	0.646562	-2.508138	6	-3.300936	0.401877	-0.855753
6	-3.229700	-1.848116	-0.196178	1	-1.869388	-0.440398	-2.237686
6	-2.747880	-0.411820	0.200091	1	-3.536664	-0.402410	2.433662
1	-3.786028	-1.944502	-1.133440	6	-3.780672	0.427143	0.460761
6	-3.453105	-0.561418	1.593009	1	-3.783002	1.016064	-1.611241
6	-4.074712	-1.868420	1.076791	6	-4.916040	1.338462	0.849845
1	-2.763819	-0.735562	2.428164	1	-5.502293	0.919879	1.672520
1	-4.160654	0.220804	1.884177	1	-5.588774	1.522802	0.007797
8	-4.943780	-2.589281	1.496909	1	-4.533281	2.311368	1.182904
1	-2.427427	-2.593250	-0.192477	6	1.606727	-0.436640	-1.543808
6	-1.231959	-0.258669	0.341688	1	2.518738	-0.848749	-1.997085
1	-0.996486	0.704407	0.808626	1	0.841294	-0.423195	-2.318583
1	-0.864864	-1.041150	1.008298	6	0.929571	0.892371	1.322789
6	-3.380579	0.677229	-0.663626	6	2.139001	-0.042274	1.511307
1	-3.063089	0.579982	-1.705691	1	1.021129	1.705859	2.054458
1	-4.472790	0.597679	-0.645808	6	3.392370	0.680764	0.990186
1	-3.108579	1.678175	-0.309244	6	3.270090	1.091969	-0.465123
6	0.613593	1.892803	-0.745742	1	4.297706	0.074907	1.105328
6	0.075679	2.997324	-0.291508	1	3.557788	1.597567	1.572955

8	4.229553	1.425864	-1.132326	1	-0.841445	0.422984	-2.318616
1	0.014366	0.349226	1.584348	6	-0.929618	-0.892280	1.322841
6	1.919998	-1.392803	0.768006	6	-2.138936	0.042509	1.511368
1	1.391174	-2.088177	1.419391	1	-1.021216	-1.705698	2.054575
1	2.896091	-1.849922	0.548279	6	-3.392437	-0.680371	0.990346
6	2.328195	-0.366542	2.999702	6	-3.270295	-1.091721	-0.464940
1	1.413151	-0.791587	3.425857	1	-4.297661	-0.074341	1.105461
1	2.582176	0.533701	3.568464	1	-3.557994	-1.597096	1.573194
1	3.135795	-1.092552	3.144905	8	-4.229856	-1.425515	-1.132054
6	1.866794	1.020684	-1.063587	1	-0.014330	-0.349212	1.584283
6	0.806066	1.475909	-0.082155	6	-1.919765	1.392955	0.767994
6	-0.180116	2.334108	-0.401011	1	-1.390781	2.088269	1.419314
6	-1.196592	2.797985	0.615725	1	-2.895789	1.850252	0.548314
1	-0.926231	3.790137	1.002960	6	-2.328023	0.366853	2.999764
1	-1.297331	2.120923	1.464402	1	-1.412913	0.791806	3.425872
1	-2.183360	2.896145	0.152737	1	-2.582084	-0.533345	3.568560
6	-0.395027	2.936822	-1.765721	1	-3.135533	1.092962	3.144974
1	-1.353773	2.592580	-2.175541	6	-1.867034	-1.020712	-1.063450
1	0.381885	2.693413	-2.490714	6	-0.806290	-1.475969	-0.082058
1	-0.460702	4.030081	-1.698314	6	0.179782	-2.334268	-0.400948
1	1.905187	1.643875	-1.956817	6	1.196407	-2.798114	0.615636
(R,R)-2a				1	0.926818	-3.790822	1.001982
				1	1.296466	-2.121668	1.464876
				1	2.183333	-2.895094	0.152725
8	0.160303	3.311407	0.300591	6	0.394487	-2.937126	-1.765626
16	0.223942	2.229372	-0.686413	1	0.460165	-4.030381	-1.698106
7	-1.142899	1.296106	-0.463210	1	1.353183	-2.592953	-2.175612
8	0.333428	2.485816	-2.124888	1	-0.382532	-2.693818	-2.490536
6	1.618334	1.200615	-0.242985	1	-1.905529	-1.643898	-1.956676
6	2.086558	1.208711	1.071197	(S,S)-2a			
6	2.222720	0.402421	-1.213925				
1	1.628325	1.868339	1.799371				
6	3.162833	0.393549	1.413651	8	0.161051	-3.311838	0.299504
6	3.301014	-0.402087	-0.855697	16	0.224262	-2.229281	-0.686960
1	1.869439	0.440043	-2.237678	7	-1.142764	-1.296479	-0.463139
1	3.536880	0.402580	2.433606	8	0.333704	-2.484967	-2.125588
6	3.780817	-0.427179	0.460795	6	1.618500	-1.200501	-0.243130
1	3.783045	-1.016357	-1.611141	6	2.086409	-1.208656	1.071157
6	4.916257	-1.338393	0.849915	6	2.222988	-0.402151	-1.213873
1	5.502323	-0.919853	1.672743	1	1.628155	-1.868447	1.799173
1	5.589142	-1.522522	0.007940	6	3.162415	-0.393284	1.413963
1	4.533589	-2.311406	1.182773	6	3.301055	0.402508	-0.855310
6	-1.606793	0.436620	-1.543767	1	1.869885	-0.439744	-2.237688
1	-2.518807	0.848787	-1.996993	1	3.536155	-0.402283	2.434032

6	3.780466	0.427645	0.461327	6	-2.700978	-0.518332	-0.240048
1	3.783185	1.016920	-1.610574	6	-3.316417	-0.999453	0.918509
6	4.915553	1.339132	0.850844	6	-3.369729	0.343865	-1.104965
1	5.588158	1.524192	0.008853	1	-2.785197	-1.685092	1.569410
1	4.532463	2.311711	1.184483	6	-4.614391	-0.598731	1.209312
1	5.502012	0.920294	1.673243	6	-4.671800	0.738526	-0.795022
6	-1.607668	-0.437206	-1.543447	1	-2.875707	0.683652	-2.007912
1	-2.520043	-0.849609	-1.995732	1	-5.100735	-0.970845	2.106870
1	-0.843015	-0.423783	-2.318982	6	-5.311299	0.276841	0.360105
6	-0.929390	0.892369	1.322668	1	-5.199435	1.411213	-1.465086
6	-2.138303	-0.042866	1.511679	6	-6.725887	0.686240	0.683719
1	-1.021196	1.705945	2.054203	1	-7.061575	1.506106	0.043899
6	-3.392246	0.679419	0.990938	1	-6.817683	1.007340	1.726321
6	-3.270539	1.091596	-0.464175	1	-7.417797	-0.152234	0.542091
1	-4.297046	0.072700	1.105833	6	0.758585	-0.801639	1.436118
1	-3.558505	1.595759	1.574180	1	0.931387	-0.100487	2.260014
8	-4.230264	1.426396	-1.130547	1	0.226086	-1.661499	1.845698
1	-0.013858	0.349728	1.584094	6	2.208592	0.536659	-1.010951
6	-1.918833	-1.393382	0.768588	6	1.437907	1.733606	-0.408245
1	-1.389072	-2.088210	1.419796	1	2.958744	0.941329	-1.699892
1	-2.894730	-1.851288	0.549631	6	2.418110	2.216676	0.681395
6	-2.326842	-0.367023	3.000198	6	3.099756	0.960128	1.200776
1	-1.411462	-0.791590	3.426105	1	1.975029	2.798171	1.494621
1	-2.581033	0.533188	3.568913	1	3.201632	2.837289	0.223589
1	-3.134064	-1.093378	3.145780	8	3.615560	0.845234	2.293799
6	-1.867603	1.020255	-1.063335	1	1.561919	-0.125670	-1.586576
6	-0.806497	1.475724	-0.082412	6	0.067887	1.306919	0.215804
6	0.179355	2.334101	-0.401776	1	-0.735241	1.611492	-0.457828
6	1.196227	2.798374	0.614347	1	-0.091899	1.853508	1.153795
1	0.926754	3.791332	1.000137	6	1.159730	2.815018	-1.457738
1	1.296398	2.122427	1.463973	1	0.558514	2.402818	-2.274872
1	2.183072	2.895017	0.151190	1	2.092344	3.203159	-1.879431
6	0.393571	2.936779	-1.766622	1	0.611406	3.659678	-1.024579
1	0.459369	4.030032	-1.699254	6	2.086198	-1.275658	0.836859
1	1.352076	2.592470	-2.176948	6	2.942893	-0.169494	0.161169
1	-0.383739	2.693442	-2.491207	6	4.265773	-0.787470	-0.296566
1	-1.906399	1.643297	-1.956640	6	5.422300	-0.618610	0.350088
				1	5.500718	-0.034705	1.258350
3				1	6.328936	-1.092219	-0.015914
				6	4.183651	-1.644705	-1.538255
8	-0.845859	-2.412126	-0.209757	1	3.452263	-2.452551	-1.422414
16	-1.020685	-1.008363	-0.597897	1	5.152817	-2.096632	-1.762160
7	-0.127159	-0.112246	0.493553	1	1.872126	-2.064112	0.110597
8	-0.734542	-0.556333	-1.967569	1	3.869229	-1.064945	-2.413083

1	2.686643	-1.711751	1.641803	6	5.435801	-0.048844	-1.026670
4				1	5.743229	-0.601873	-0.132862
				1	5.666872	0.995663	-0.814356
				1	6.036754	-0.397081	-1.872344
				6	3.731222	-1.193687	-2.471595
8	-1.681222	-1.730569	2.399195	1	4.125470	-0.747463	-3.393904
16	-1.333890	-1.786686	0.976884	1	2.690118	-1.464648	-2.639235
7	0.169487	-1.088659	0.827061	1	4.298226	-2.119489	-2.315743
8	-1.275263	-3.043042	0.225716	1	1.425021	-0.030358	-2.056196
6	-2.493607	-0.726628	0.119640	Cat			
6	-3.234227	0.207485	0.841121				
6	-2.609685	-0.811273	-1.270644				
1	-3.154939	0.229964	1.921885				
6	-4.080066	1.080820	0.158025	28	0.008762	-1.149952	-0.083541
6	-3.453727	0.071009	-1.936946	6	-0.975303	-2.728754	1.565791
1	-2.064186	-1.575854	-1.811920	1	-1.482483	-2.005600	2.198294
1	-4.663516	1.805966	0.718082	6	-1.878247	-3.578724	0.700460
6	-4.195069	1.035037	-1.236161	1	-2.819938	-3.041104	0.580891
1	-3.549511	0.005995	-3.017433	1	-2.129171	-4.510136	1.231826
6	-5.095325	1.991782	-1.976200	6	-1.336799	-3.938477	-0.707849
1	-5.775868	1.457130	-2.647027	1	-0.785960	-4.884209	-0.660197
1	-4.510615	2.683206	-2.593950	1	-2.202376	-4.131357	-1.349775
1	-5.698010	2.588073	-1.286825	6	-0.457700	-2.895151	-1.379811
6	0.968311	-1.307294	-0.380510	1	-0.872567	-2.418306	-2.262859
1	1.809748	-1.968519	-0.142972	6	0.913160	-2.794800	-1.207273
1	0.348018	-1.828886	-1.110048	1	1.471729	-2.263573	-1.975621
6	0.561860	1.168272	-0.514293	6	1.771700	-3.649527	-0.299808
6	0.709611	1.374129	0.999576	1	2.712445	-3.121887	-0.136641
1	0.805456	2.101587	-1.034750	1	2.039225	-4.586601	-0.814888
6	2.114219	1.945885	1.229395	6	1.161395	-4.000186	1.077315
6	3.248996	1.139762	0.600436	1	0.522417	-4.883432	0.988986
1	2.348047	2.052318	2.293518	1	1.979419	-4.287282	1.747767
1	2.168345	2.955063	0.797029	6	0.364461	-2.887857	1.720026
8	4.367708	1.228575	1.096747	1	0.878447	-2.263330	2.446531
1	-0.470177	0.914813	-0.774009	15	1.782819	0.103477	0.036578
6	0.600086	-0.013887	1.717152	15	-1.773412	0.117977	-0.080524
1	-0.091831	0.023757	2.558682	6	1.884114	1.278599	1.460296
1	1.574986	-0.305079	2.129495	6	1.831252	2.673636	1.331069
6	-0.349230	2.347443	1.526930	6	1.881934	0.736759	2.757753
1	-1.356476	1.958152	1.357869	6	1.792346	3.495994	2.459040
1	-0.274014	3.316099	1.020346	1	1.813676	3.123952	0.346172
1	-0.224510	2.520323	2.601628	6	1.876009	1.556502	3.883468
6	1.493741	0.041101	-0.968835	1	1.855251	-0.340366	2.887411
6	2.954520	0.297650	-0.594817	6	1.825611	2.944029	3.738512
6	3.969137	-0.265593	-1.306904	1	1.740812	4.573633	2.332793

1	1.888515	1.110578	4.873958	1	-4.719227	-2.630948	-2.960357
1	1.801314	3.585992	4.613682	1	-6.571695	-2.800179	-1.305016
6	1.974667	1.167182	-1.458710	6	-2.163357	0.987651	1.502764
6	1.091180	0.965476	-2.524811	6	-3.166587	1.967063	1.589434
6	3.011190	2.102242	-1.602365	6	-1.400291	0.700156	2.636846
6	1.213445	1.706459	-3.700303	6	-3.406972	2.627221	2.791570
1	0.302954	0.229292	-2.409088	1	-3.750961	2.214814	0.708813
6	3.127390	2.852569	-2.770933	6	-1.634496	1.365409	3.841942
1	3.731597	2.235180	-0.801278	1	-0.601224	-0.025120	2.553975
6	2.224709	2.658658	-3.820406	6	-2.640479	2.325997	3.922147
1	0.508011	1.551058	-4.510002	1	-4.185667	3.382435	2.847580
1	3.927274	3.580998	-2.868421	1	-1.018697	1.143269	4.707434
1	2.316812	3.244436	-4.730447	1	-2.823545	2.847774	4.856993
6	3.469741	-0.673306	0.025528				
6	3.998432	-1.082113	-1.211589	Cat1			
6	4.176762	-1.007247	1.188676				
6	5.183815	-1.811240	-1.279609	28	-2.483063	-0.440467	-0.463382
1	3.479492	-0.825509	-2.128563	6	0.791931	0.968345	0.885502
6	5.365617	-1.734778	1.119997	6	2.043928	0.286402	0.310287
1	3.814360	-0.688779	2.157863	6	2.659535	1.532906	2.177762
6	5.871968	-2.146814	-0.112596	1	0.079697	0.221119	1.256765
1	5.570219	-2.116487	-2.247835	1	2.367423	0.792867	-0.603220
1	5.898314	-1.975630	2.035676	6	3.437469	2.783154	1.780587
1	6.794842	-2.716539	-0.163975	1	3.093721	3.642669	2.360840
6	-1.775348	1.597024	-1.198745	1	4.503499	2.629987	1.970958
6	-2.406921	1.641045	-2.446639	1	3.293020	3.003812	0.722189
6	-1.001766	2.699967	-0.800449	6	2.889037	1.110909	3.620608
6	-2.252955	2.750456	-3.281976	1	3.948302	0.897781	3.787501
1	-3.034538	0.819359	-2.770255	1	2.581288	1.911842	4.297769
6	-0.851506	3.805861	-1.630736	1	2.307290	0.212125	3.832864
1	-0.515561	2.689775	0.168252	8	1.254623	1.740218	1.978680
6	-1.470809	3.832936	-2.881917	8	3.017943	0.443660	1.330534
1	-2.753854	2.767264	-4.245951	6	1.872580	-1.224849	-0.026706
1	-0.242520	4.644019	-1.304611	6	0.049784	1.818933	-0.197482
1	-1.348034	4.691200	-3.535570	8	0.093069	1.041504	-1.396342
6	-3.380742	-0.705978	-0.475480	8	0.791572	-1.410052	-0.960404
6	-4.431844	-0.809998	0.446679	15	-0.559356	-0.514195	-1.348462
6	-3.503227	-1.385254	-1.700230	7	-0.491426	-0.860172	-3.014138
6	-5.570483	-1.562052	0.149796	6	-1.549065	-0.243841	-3.811498
1	-4.359369	-0.313130	1.406675	1	-1.274559	0.771606	-4.139083
6	-4.646520	-2.119923	-2.004654	1	-1.745560	-0.849662	-4.703329
1	-2.685148	-1.357839	-2.410850	1	-2.466383	-0.175244	-3.223586
6	-5.685579	-2.215928	-1.076178	6	0.787786	-0.885036	-3.722738
1	-6.368855	-1.635524	0.882741	1	1.536396	-1.405110	-3.129165

1	0.657249	-1.420420	-4.669833	1	6.335269	-1.113347	-1.595933
1	1.150915	0.129174	-3.951098	1	6.109454	-3.337547	-2.682055
6	0.800057	3.116355	-0.504254	6	-3.467539	-1.996107	-1.379411
6	0.681889	4.242630	0.318799	1	-3.020500	-2.080600	-2.366515
6	1.669266	3.175009	-1.601046	6	-3.231009	-3.216692	-0.510180
6	1.427282	5.391579	0.062651	1	-2.213156	-3.566353	-0.716869
1	0.005956	4.225818	1.163401	1	-3.899575	-4.036291	-0.817746
6	2.418422	4.325169	-1.855261	6	-3.380514	-3.006265	1.021586
1	1.745858	2.318769	-2.258778	1	-4.430210	-3.116536	1.307900
6	2.304698	5.436860	-1.021561	1	-2.845401	-3.816751	1.528435
1	1.321936	6.253666	0.714661	6	-2.867732	-1.672773	1.522037
1	3.087895	4.349719	-2.710101	1	-1.868983	-1.644860	1.942729
1	2.886906	6.332093	-1.218374	6	-3.626336	-0.546155	1.601561
6	-1.397868	2.090889	0.215813	1	-3.181753	0.325647	2.073218
6	-1.708730	2.469910	1.530922	6	-5.091583	-0.425863	1.248664
6	-2.422361	2.077526	-0.750852	1	-5.331366	0.638614	1.212059
6	-3.002947	2.868503	1.864318	1	-5.707834	-0.847996	2.057441
1	-0.933045	2.455547	2.288431	6	-5.499319	-1.076247	-0.096592
6	-3.727112	2.444194	-0.396215	1	-5.790317	-2.118787	0.069079
1	-2.178148	1.873254	-1.785461	1	-6.404554	-0.575259	-0.457875
6	-4.015831	2.862095	0.901865	6	-4.436584	-1.018912	-1.181166
1	-3.222350	3.177094	2.882161	1	-4.640285	-0.349613	-2.015204
1	-4.507468	2.421898	-1.150277	Cat_{dpp}			
1	-5.022813	3.170116	1.165333				
6	1.607101	-2.070421	1.221679	28	-0.089478	-0.900287	-0.395222
6	2.609818	-2.251107	2.185962	6	0.591396	-0.814238	-2.429714
6	0.383627	-2.719929	1.392447	1	0.921426	0.208547	-2.590326
6	2.370697	-3.029796	3.315802	6	1.678793	-1.860855	-2.557633
1	3.575287	-1.783658	2.046003	1	2.618058	-1.402649	-2.237720
6	0.147399	-3.506734	2.522700	1	1.822161	-2.140407	-3.614130
1	-0.379028	-2.608248	0.634755	6	1.451812	-3.141066	-1.715392
6	1.135392	-3.657828	3.492738	1	0.914453	-3.888382	-2.308028
1	3.156201	-3.155117	4.055358	1	2.429185	-3.581608	-1.491086
1	-0.811570	-4.002602	2.639183	6	0.711832	-2.910876	-0.407751
1	0.952474	-4.268738	4.371690	1	1.315615	-2.975646	0.492294
6	3.104572	-1.777262	-0.756262	6	-0.660838	-2.970662	-0.257107
6	2.989365	-3.037491	-1.360786	1	-1.036212	-3.112829	0.754286
6	4.319803	-1.093434	-0.845714	6	-1.675204	-3.201121	-1.357459
6	4.060125	-3.594601	-2.052365	1	-2.649856	-2.874955	-0.983157
1	2.046864	-3.569204	-1.290208	1	-1.776476	-4.277465	-1.573353
6	5.397009	-1.657196	-1.536311	6	-1.377309	-2.437774	-2.668845
1	4.443975	-0.134405	-0.358714	1	-0.714590	-3.031545	-3.306144
6	5.271807	-2.903669	-2.144145	1	-2.313357	-2.333875	-3.229510
1	3.951339	-4.569268	-2.518910				

6	-0.768431	-1.062586	-2.455707	6	2.877310	4.341243	-0.909332
1	-1.426678	-0.214018	-2.614146	1	4.535719	4.162297	0.459402
15	-1.707514	0.096023	0.683217	1	1.126100	4.230771	-2.164702
15	1.538525	0.155215	0.601750	1	3.166544	5.329773	-1.254324
6	-1.807526	1.878463	0.219916	6	1.129353	0.606704	2.380099
6	-1.401908	2.933219	1.046470	1	0.828235	1.657936	2.383279
6	-2.183182	2.182958	-1.102013	1	2.040528	0.537511	2.982018
6	-1.361479	4.245588	0.570287	6	0.016812	-0.276928	2.966927
1	-1.100350	2.744167	2.069692	1	0.062679	-0.232630	4.062471
6	-2.162377	3.492623	-1.573340	1	0.197049	-1.321120	2.685972
1	-2.493585	1.381738	-1.764623	6	-1.409899	0.098097	2.537928
6	-1.742032	4.532034	-0.738400	1	-1.712319	1.056397	2.972961
1	-1.026835	5.043044	1.227033	1	-2.103912	-0.646131	2.938585
1	-2.464763	3.701575	-2.595428				
1	-1.709485	5.552381	-1.107871				
6	-3.488587	-0.409560	0.678461				
6	-3.782698	-1.725857	1.074887	28	-1.535497	-2.222942	0.471676
6	-4.549219	0.420986	0.294429	6	-0.368678	0.670676	0.762050
6	-5.093299	-2.197333	1.085333	6	0.945134	1.022054	0.049600
1	-2.976498	-2.387351	1.376460	6	0.493793	2.642345	1.651249
6	-5.862546	-0.054304	0.295508	1	-0.226666	-0.262663	1.315696
1	-4.356124	1.446036	0.001013	1	0.761426	1.423124	-0.951507
6	-6.140512	-1.362646	0.688722	6	0.044223	3.929249	0.966054
1	-5.296123	-3.218084	1.396238	1	-0.801396	4.365515	1.502699
1	-6.670546	0.606811	-0.004836	1	0.867197	4.649402	0.951283
1	-7.162515	-1.729405	0.689163	1	-0.272288	3.727872	-0.058578
6	3.115124	-0.771982	0.796775	6	1.015238	2.856349	3.062476
6	4.126974	-0.675683	-0.171338	1	1.875015	3.531543	3.048644
6	3.268931	-1.708573	1.830819	1	0.233223	3.295610	3.686983
6	5.256953	-1.489622	-0.106698	1	1.321005	1.896987	3.483855
1	4.034021	0.050369	-0.972424	8	-0.590465	1.705582	1.699190
6	4.399955	-2.522656	1.896211	8	1.522980	2.009919	0.889130
1	2.500029	-1.810902	2.590490	6	1.917205	-0.193228	-0.084949
6	5.397605	-2.418573	0.926103	6	-1.546306	0.449515	-0.234198
1	6.030562	-1.395279	-0.863353	8	-0.957466	-0.175750	-1.401461
1	4.500473	-3.239260	2.706332	8	1.308839	-1.239537	-0.877279
1	6.276970	-3.053459	0.975383	15	-0.273406	-1.694538	-1.085530
6	2.134397	1.786940	-0.016121	7	-0.096234	-2.307030	-2.637897
6	3.277598	2.417221	0.500518	6	-1.123231	-3.228183	-3.107435
6	1.371416	2.452856	-0.981954	1	-1.933032	-2.708987	-3.641956
6	3.647673	3.684760	0.055090	1	-0.677950	-3.964135	-3.786741
1	3.883402	1.908228	1.244162	1	-1.558826	-3.758213	-2.255971
6	1.738154	3.724500	-1.424957	6	0.560595	-1.532210	-3.687071
1	0.477008	1.977078	-1.364713	1	1.364288	-0.937484	-3.252877

CAT-P

1	0.995412	-2.216807	-4.423913	1	4.964367	2.758514	-2.175057
1	-0.145228	-0.866164	-4.204245	1	6.421747	0.883835	-2.909374
6	-2.155599	1.762461	-0.680413	cod			
6	-3.033463	2.440780	0.173995				
6	-1.819914	2.336219	-1.909940				
6	-3.555593	3.678966	-0.190321				
1	-3.296543	1.998029	1.127807	6	-1.195316	1.235396	-0.507082
6	-2.344719	3.578599	-2.274608	1	-1.786648	1.832310	-1.202100
1	-1.154825	1.801552	-2.576866	6	-1.920663	0.012422	-0.006979
6	-3.209165	4.255149	-1.415074	1	-2.446785	-0.431924	-0.863361
1	-4.233339	4.196193	0.482355	1	-2.717348	0.329912	0.683260
1	-2.077099	4.014193	-3.232848	6	-1.084510	-1.091023	0.672282
1	-3.616015	5.221378	-1.698126	1	-0.647507	-0.713493	1.598060
6	-2.594901	-0.527615	0.331106	1	-1.774187	-1.887060	0.975530
6	-2.622617	-0.996346	1.690348	6	-0.032281	-1.689407	-0.232248
6	-3.722687	-0.819333	-0.495009	1	-0.338548	-2.599479	-0.747347
6	-3.708832	-1.801189	2.126909	6	1.195327	-1.235392	-0.507070
1	-1.940373	-0.595055	2.433770	1	1.786679	-1.832321	-1.202059
6	-4.768118	-1.596730	-0.035519	6	1.920661	-0.012404	-0.006985
1	-3.736675	-0.418511	-1.503123	1	2.446740	0.431963	-0.863383
6	-4.759713	-2.114947	1.278008	1	2.717381	-0.329885	0.683219
1	-3.716321	-2.148255	3.156197	6	1.084494	1.091010	0.672308
1	-5.606672	-1.809390	-0.692222	1	0.647471	0.713441	1.598058
1	-5.580789	-2.732150	1.627571	1	1.774156	1.887044	0.975598
6	2.292343	-0.747059	1.292039	6	0.032290	1.689404	-0.232244
6	3.163681	-0.025238	2.119705	1	0.338589	2.599455	-0.747360
6	1.776146	-1.961348	1.754831	L			
6	3.480707	-0.492745	3.393333				
1	3.589757	0.903312	1.762157				
6	2.096316	-2.430599	3.031009				
1	1.126148	-2.548114	1.116660	15	0.000621	0.000941	-1.279062
6	2.943291	-1.695438	3.857870	6	-1.299844	1.014687	-0.448756
1	4.155682	0.081041	4.021631	6	-2.584000	0.999374	-1.015632
1	1.684666	-3.376599	3.370695	6	-3.626986	1.720618	-0.436908
1	3.193394	-2.059650	4.849882	6	-3.396365	2.483497	0.709697
6	3.180143	0.169690	-0.872390	6	-2.120544	2.516156	1.274113
6	4.011848	-0.881976	-1.283374	6	-1.078735	1.784774	0.701536
6	3.535393	1.480931	-1.199843	6	-0.228031	-1.632261	-0.448915
6	5.168553	-0.628963	-2.013414	6	0.436059	-2.734887	-1.009119
1	3.734658	-1.899605	-1.031472	6	-1.015677	-1.827835	0.694123
6	4.700633	1.733794	-1.930098	6	1.528822	0.618953	-0.447618
1	2.925239	2.310674	-0.866534	6	2.081254	0.044232	0.705596
6	5.518093	0.684130	-2.341155	6	2.161869	1.735204	-1.016441
1	5.799574	-1.455595	-2.326455	1	-0.091392	1.810205	1.149883
				1	1.038283	-2.598289	-1.903583
				1	-1.538469	-0.987066	1.137142

1	1.606583	-0.821277	1.155163	1	-1.295725	-2.472376	-1.382623
1	1.750956	2.180478	-1.918806	1	-2.164616	-1.691819	-0.072517
6	0.331605	-3.998779	-0.430775	6	1.261838	-3.575559	0.480504
6	-0.454514	-4.182546	0.708607	1	1.296803	-2.472152	-1.381803
1	-0.544016	-5.168069	1.155889	1	2.164677	-1.691538	-0.071045
6	-1.129476	-3.095909	1.266187	6	0.000112	-4.399341	0.200855
6	3.235650	0.579402	1.279153	1	-2.159762	-4.154464	0.232554
6	3.849517	1.697317	0.712662	1	-1.318249	-3.352733	1.554542
1	4.747369	2.112259	1.161009	1	2.159937	-4.154194	0.233862
6	3.308239	2.276463	-0.436835	1	1.317521	-3.352591	1.555350
1	-4.205528	3.052876	1.157350	1	-0.000011	-5.316906	0.800777
1	-2.763985	0.417257	-1.915701	1	0.000450	-4.711443	-0.852874
1	3.653931	0.123307	2.171922	6	-1.461002	1.149762	-0.386017
1	3.783749	3.143373	-0.886211	6	-2.695860	0.957218	-1.291617
1	-1.934887	3.109929	2.164606	6	-1.845207	0.986868	1.095707
1	-4.616175	1.694668	-0.884591	1	-1.127877	2.189598	-0.525817
1	-1.744418	-3.233572	2.151012	6	-3.847274	1.889923	-0.891845
1	0.855627	-4.840947	-0.873206	1	-3.040377	-0.083080	-1.228508
PCy₃				1	-2.414482	1.122897	-2.336930
				6	-2.999427	1.922930	1.487067
				1	-2.151504	-0.048645	1.287186
				1	-0.983854	1.178507	1.741051
15	0.000020	0.148091	-1.056377	6	-4.221617	1.716861	0.584965
6	1.461110	1.149812	-0.386373	1	-4.718482	1.707886	-1.532225
6	1.844651	0.987944	1.095617	1	-3.542210	2.931638	-1.065636
6	2.696253	0.956418	-1.291397	1	-3.267959	1.765300	2.538595
1	1.128229	2.189608	-0.527087	1	-2.660824	2.965217	1.402599
6	2.998934	1.924004	1.486783	1	-5.022790	2.412004	0.861904
1	2.150547	-0.047519	1.288024	1	-4.617073	0.703014	0.740529
1	0.983004	1.180325	1.740335	P(4-MeOC₆H₄)₃			
6	3.847659	1.889218	-0.891804				
1	3.040615	-0.083869	-1.227442				
1	2.415286	1.121435	-2.336925				
6	4.221411	1.717061	0.585266	15	0.000571	-0.000561	-1.773577
1	3.267044	1.767038	2.538518	6	-1.085704	-1.238026	-0.945238
1	2.660592	2.966307	1.401473	6	-1.164393	-2.524180	-1.510552
1	4.719086	1.706612	-1.531725	6	-1.944244	-3.516978	-0.936283
1	3.542833	2.930866	-1.066398	6	-2.688383	-3.242461	0.220937
1	5.022632	2.412215	0.862036	6	-2.635060	-1.966301	0.791467
1	4.616591	0.703232	0.741652	6	-1.834792	-0.980928	0.207120
6	0.000001	-1.415650	-0.011345	6	-0.528416	1.559027	-0.945675
6	-1.257998	-2.256748	-0.305978	6	-1.604259	2.268593	-1.510577
6	1.258297	-2.256566	-0.305175	6	0.069311	2.080747	0.205653
1	-0.000337	-1.152365	1.054534	6	1.615452	-0.322606	-0.945782
6	-1.261884	-3.575716	0.479735	6	2.769858	0.243559	-1.517352

6	1.766098	-1.090867	0.212736	6	1.359662	0.932455	-1.061211
1	-1.798793	0.003837	0.660974	6	1.738896	2.168417	-1.608348
1	-2.077366	1.891995	-2.413692	6	2.025014	0.464794	0.080398
1	0.904872	1.558206	0.659312	6	0.099373	-1.626528	-1.082874
1	2.681926	0.833741	-2.425752	6	0.987841	-2.562191	-1.636263
1	0.893985	-1.544305	0.671897	6	-0.650140	-1.989604	0.044434
6	-2.074988	3.440205	-0.936755	1	-0.473031	1.792911	0.512633
6	-1.464675	3.948957	0.219543	1	1.239027	2.538076	-2.499211
6	-0.384762	3.266440	0.789513	1	1.745484	-0.486755	0.518324
6	4.019793	0.064512	-0.943525	1	1.560505	-2.301437	-2.521793
6	4.152902	-0.708197	0.219818	1	-1.347122	-1.283779	0.481848
6	3.019650	-1.291178	0.796907	6	2.745927	2.928289	-1.021170
1	-0.602989	-2.745826	-2.414413	6	3.399885	2.449851	0.116712
1	-3.204587	-1.728221	1.681690	6	3.042104	1.217081	0.664740
1	-2.005181	-4.510759	-1.367161	6	1.141995	-3.821918	-1.065780
1	0.106709	3.642036	1.678862	6	0.390707	-4.168759	0.059712
1	-2.906207	3.988586	-1.367237	6	-0.507616	-3.254459	0.611857
1	4.911885	0.501931	-1.379190	1	-2.798156	-0.152203	-2.540363
1	3.097323	-1.896604	1.691893	1	-2.550253	2.686785	1.516668
8	-1.991066	5.109739	0.704822	1	-4.874445	0.722417	-1.511688
8	-3.431301	-4.277916	0.706534	1	3.549335	0.854840	1.552101
8	5.421353	-0.834420	0.704646	1	3.025686	3.888112	-1.440907
6	-1.401127	5.672037	1.864628	1	1.828383	-4.540926	-1.498895
1	-1.960401	6.584229	2.076813	1	-1.094834	-3.533580	1.479702
1	-1.474909	4.994273	2.724889	6	0.592841	-5.509394	0.709588
1	-0.345896	5.924458	1.699400	6	-5.102152	2.235884	0.724658
6	5.610730	-1.615191	1.872541	6	4.533085	3.236947	0.714153
1	5.297633	-2.655707	1.718127	9	-0.520392	-5.933420	1.345790
1	6.680550	-1.588945	2.083972	9	1.581977	-5.465629	1.632375
1	5.062547	-1.201424	2.728743	9	0.936612	-6.456656	-0.189914
6	-4.211947	-4.047545	1.867117	9	-6.091469	2.425041	-0.175327
1	-4.957006	-3.258574	1.702855	9	-5.562281	1.345299	1.634024
1	-4.723669	-4.987292	2.079037	9	-4.913624	3.402986	1.377542
1	-3.587132	-3.774154	2.727176	9	5.716138	2.912631	0.143957
				9	4.658764	3.009048	2.039676
				9	4.364889	4.566415	0.541943
P(4-CF₃C₆H₄)₃							
15	-0.005544	0.022091	-1.907529	IM1			
6	-1.488104	0.744298	-1.077301				
6	-2.740537	0.456977	-1.642768	15	2.275647	-1.397012	-0.101302
6	-3.910187	0.946116	-1.069167	6	3.005671	-1.906169	-1.710552
6	-3.838405	1.748597	0.071947	6	2.236999	-1.726883	-2.869881
6	-2.599372	2.055181	0.636561	6	2.755312	-2.062190	-4.119933
6	-1.431308	1.553423	0.065773	6	4.049634	-2.575105	-4.226600

6	4.822114	-2.755808	-3.077787	1	-5.081305	0.062095	-0.785760
6	4.304338	-2.422272	-1.826180	6	-3.972155	3.349847	-0.561091
6	1.775347	-2.956364	0.735483	1	-4.461418	4.322043	-0.686250
6	0.773588	-2.858360	1.711200	1	-3.177598	3.278390	-1.310981
6	2.352407	-4.203657	0.469819	1	-3.505354	3.343014	0.426205
6	3.773682	-0.940773	0.874930	1	-6.570368	1.472843	0.693222
6	3.967701	-1.401026	2.184586	6	-1.295119	0.434391	-0.806192
6	4.679193	-0.008501	0.344772	6	-0.923876	-0.889043	-1.103455
1	4.917675	-2.542329	-0.939360	6	-1.347934	-1.989412	-1.731790
1	0.308684	-1.893474	1.894409	6	-2.720785	-2.065457	-2.363813
1	3.120572	-4.293092	-0.291041	1	-3.258236	-1.121191	-2.290514
1	3.286175	-2.129529	2.609514	1	-3.327120	-2.843893	-1.887068
8	-5.522981	-0.211132	1.779494	1	-2.639339	-2.333488	-3.426477
6	-7.018489	2.856144	-0.955751	6	1.926102	-5.336012	1.164661
16	-4.089151	-0.499555	1.643457	6	0.936907	-5.229045	2.144581
8	-8.072047	3.423707	-1.104415	1	0.610444	-6.111186	2.687121
7	-3.490454	0.541780	0.491905	6	0.364433	-3.985627	2.422835
8	-3.177914	-0.422006	2.791152	6	5.027863	-0.920668	2.954307
6	-3.987784	-2.172472	1.014084	6	5.908382	0.023801	2.427437
6	-2.027484	0.823392	0.464750	1	6.727030	0.404035	3.030872
6	-2.784188	-2.870735	1.120452	6	5.734115	0.471856	1.116835
6	-5.115938	-2.773224	0.457581	6	-0.549017	-3.256171	-1.888729
1	-1.608220	0.309474	1.328257	1	-0.302520	-3.441252	-2.943133
1	-1.891319	1.892842	0.640096	1	-1.137862	-4.117500	-1.549838
1	-1.921765	-2.396509	1.566678	1	0.376373	-3.239100	-1.320031
6	-2.715230	-4.181793	0.665660	1	-1.324618	1.176119	-1.607941
6	-5.028172	-4.086306	-0.005323	1	4.456281	-2.830335	-5.200720
1	-6.050474	-2.225753	0.421963	1	1.233832	-1.322365	-2.777769
1	-1.780411	-4.725318	0.761604	1	2.368910	-6.302508	0.942816
6	-3.830837	-4.805876	0.087136	1	-0.412146	-3.896300	3.176272
1	-5.905363	-4.560729	-0.436260	1	5.162815	-1.285954	3.968255
6	-3.724606	-6.213430	-0.442334	1	6.415698	1.201401	0.690242
1	-4.710126	-6.656839	-0.606795	1	5.830466	-3.151388	-3.155880
1	-3.169401	-6.857447	0.246807	1	2.149787	-1.919001	-5.010104
1	-3.189365	-6.228117	-1.399670	28	0.601374	0.030801	-0.313846
6	-5.924824	2.398801	-1.931456	15	1.421299	2.064104	0.095548
1	-6.192834	1.453996	-2.420841	6	2.094140	2.470955	1.751790
1	-5.623495	3.117220	-2.699683	6	2.508409	3.760952	2.123228
6	-4.981790	2.214087	-0.692139	6	2.200187	1.429911	2.680971
6	-6.210082	2.409707	0.259190	6	3.047714	3.990315	3.387100
1	4.563431	0.339765	-0.673523	1	2.390090	4.586608	1.428972
1	-6.108359	3.140233	1.067088	6	2.743521	1.658509	3.945158
6	-4.314522	0.835625	-0.681663	1	1.861170	0.439679	2.401722
1	-3.667151	0.758656	-1.561465	6	3.172235	2.937218	4.297715

1	3.366294	4.990675	3.664844	16	-3.914332	1.247431	-0.809896
1	2.831260	0.837237	4.648967	8	-6.979454	-3.674280	0.454026
1	3.593699	3.118310	5.281976	7	-3.181227	0.153565	0.197677
6	0.353951	3.522668	-0.264018	8	-3.394856	1.015349	-2.163582
6	0.203772	3.982820	-1.579711	6	-3.332626	2.866738	-0.317669
6	-0.393156	4.132757	0.754982	6	-1.852282	-0.382039	-0.172873
6	-0.656915	5.042633	-1.865898	6	-2.068327	3.293085	-0.730599
1	0.775288	3.525042	-2.380604	6	-4.137178	3.680719	0.475903
6	-1.247017	5.197303	0.467528	1	-1.522479	0.179377	-1.045099
1	-0.297277	3.785040	1.778263	1	-1.977960	-1.415039	-0.504350
6	-1.380075	5.657823	-0.842989	1	-1.462053	2.657424	-1.361870
1	-0.755348	5.392911	-2.889209	6	-1.609323	4.543690	-0.335753
1	-1.811599	5.663675	1.269252	6	-3.663452	4.934966	0.861850
1	-2.046306	6.485409	-1.065860	1	-5.124408	3.338228	0.763620
6	2.829608	2.313787	-1.069548	1	-0.625132	4.871903	-0.656192
6	2.767062	1.604147	-2.278974	6	-2.395436	5.380685	0.470941
6	3.974265	3.068868	-0.787012	1	-4.289644	5.576713	1.475264
6	3.830105	1.631246	-3.180417	6	-1.865142	6.717880	0.922399
1	1.895442	0.991444	-2.485460	1	-2.660194	7.349324	1.327346
6	5.037364	3.099902	-1.689978	1	-1.387006	7.256201	0.097924
1	4.057733	3.599620	0.153532	1	-1.108855	6.590609	1.706426
6	4.971895	2.377589	-2.883838	6	-5.690722	-2.144167	1.988300
1	3.774643	1.046633	-4.093337	1	-6.294817	-1.250131	2.181459
1	5.925472	3.678943	-1.453798	1	-5.653803	-2.755554	2.894498
1	5.809751	2.390276	-3.574410	6	-4.342560	-1.820134	1.250763
IM1_{dppp}				6	-5.020174	-2.192408	-0.108649
				1	-4.464123	-2.825880	-0.804750
				6	-3.879754	-0.354624	1.373884
15	2.874475	0.640914	-0.538822	1	-3.222279	-0.245095	2.244908
6	4.171754	0.839247	0.740513	1	-4.749291	0.283364	1.531819
6	3.752521	0.909751	2.078362	6	-3.265494	-2.834093	1.649435
6	4.687797	1.012678	3.106987	1	-3.660436	-3.854652	1.600822
6	6.052637	1.037578	2.812319	1	-2.929005	-2.655319	2.676965
6	6.479279	0.960330	1.485568	1	-2.394190	-2.797904	0.993989
6	5.544252	0.860570	0.454648	1	-5.389074	-1.306168	-0.636612
6	2.680504	2.295434	-1.316841	6	-0.815113	-0.296656	0.926233
6	1.433469	2.586185	-1.888586	6	-0.094295	0.887125	1.168922
6	3.699023	3.254970	-1.374127	6	-0.153276	2.051998	1.817484
6	3.747060	-0.295278	-1.899859	6	-1.359041	2.425997	2.651407
1	5.889676	0.790431	-0.571820	1	-2.134956	1.661558	2.596950
1	0.635425	1.855186	-1.798480	1	-1.790174	3.375198	2.314694
1	4.661887	3.051449	-0.916050	1	-1.076384	2.561492	3.705031
8	-5.356795	1.204238	-0.526248	6	3.471811	4.483676	-1.995089
6	-6.141498	-2.842859	0.698536	6	2.232691	4.758640	-2.577729

1	2.060541	5.714596	-3.063186	1	4.291019	-1.127942	-1.440959
6	1.213431	3.805204	-2.528782				
6	0.935190	3.092966	1.793509	IM2			
1	1.344781	3.265096	2.798656				
1	0.533465	4.056102	1.452115	15	2.621916	1.634019	0.166354
1	1.753323	2.816631	1.130469	6	2.101822	3.396361	0.312368
1	-0.881190	-1.056647	1.706551	6	1.404460	3.927921	-0.782761
1	6.781709	1.111631	3.613689	6	0.992954	5.259167	-0.786187
1	2.689378	0.870614	2.297785	6	1.262870	6.075785	0.314209
1	4.262410	5.227778	-2.023577	6	1.961286	5.557554	1.405256
1	0.245449	4.014918	-2.974146	6	2.387379	4.227853	1.402361
1	7.539991	0.973475	1.252997	6	4.177430	1.831502	-0.795811
1	4.351544	1.066709	4.138178	6	4.194038	1.351704	-2.111509
28	0.997208	-0.277825	0.081473	6	5.313866	2.473242	-0.286232
15	1.340516	-2.238341	-0.858189	6	3.176316	1.177672	1.856059
6	-0.007586	-3.473699	-1.048274	6	4.347502	0.434192	2.061243
6	-0.163240	-4.540728	-0.152179	6	2.314140	1.393727	2.943742
6	-1.000678	-3.258239	-2.017979	1	2.937554	3.839107	2.252026
6	-1.275811	-5.379642	-0.234958	1	3.309914	0.850424	-2.497352
1	0.586891	-4.717751	0.611041	1	5.304675	2.861369	0.727517
6	-2.109666	-4.098765	-2.101386	1	5.015664	0.229963	1.234298
1	-0.924670	-2.415921	-2.699961	1	1.392882	1.948116	2.801018
6	-2.251216	-5.163582	-1.208512	8	-0.493908	-0.413411	-1.062089
1	-1.380563	-6.201761	0.466785	8	-3.898447	-0.911307	2.544449
1	-2.866975	-3.915714	-2.857585	6	-0.588890	0.684404	-0.369518
1	-3.119062	-5.812850	-1.267973	16	-4.369192	-1.257798	1.199762
6	2.644203	-3.148634	0.068001	6	-1.090795	0.762228	1.085603
6	3.142684	-2.573100	1.244453	7	-3.653350	-0.189117	0.135838
6	3.189902	-4.361507	-0.379671	8	-4.188344	-2.605757	0.647214
6	4.184516	-3.179393	1.947581	6	-6.125510	-0.908654	1.148842
1	2.716620	-1.638962	1.594978	6	-2.147825	1.803320	0.605566
6	4.222390	-4.974256	0.327964	1	-0.366971	1.194692	1.780062
1	2.798570	-4.833193	-1.276556	1	-1.467264	-0.173834	1.497638
6	4.726473	-4.379694	1.488684	6	-3.675588	-0.524237	-1.303561
1	4.571778	-2.707673	2.845537	6	-6.918056	-1.531918	0.182189
1	4.636871	-5.913732	-0.025627	6	-6.669856	0.035189	2.018907
1	5.537739	-4.854638	2.032335	1	-3.858848	-1.597746	-1.371732
6	2.068567	-2.158577	-2.585080	1	-2.676805	-0.352100	-1.704795
1	2.792734	-2.972670	-2.690891	1	-6.481243	-2.283579	-0.465589
1	1.260224	-2.359384	-3.293780	6	-8.262998	-1.189047	0.081977
6	2.728132	-0.813082	-2.935599	6	-8.018956	0.366340	1.905082
1	3.229813	-0.928705	-3.903185	1	-6.045369	0.483415	2.783072
1	1.950054	-0.055852	-3.089600	1	-8.883856	-1.673076	-0.667071
1	4.480521	0.357586	-2.382328	6	-8.833119	-0.234103	0.936876

1	-8.447822	1.100056	2.582006	6	1.107520	-2.369324	0.915324
6	-10.298404	0.107938	0.836416	6	-0.124005	-2.993258	0.674071
1	-10.510307	1.089536	1.268697	6	1.385349	-1.884216	2.203596
1	-10.909400	-0.627418	1.373889	6	-1.061268	-3.125720	1.697650
1	-10.636468	0.111841	-0.204101	1	-0.368008	-3.342162	-0.322136
6	-3.570864	1.219320	0.552946	6	0.449801	-2.027676	3.226794
1	-4.199706	1.826257	-0.109933	1	2.321613	-1.379428	2.405174
1	-3.988617	1.285655	1.558750	6	-0.779997	-2.638315	2.975006
6	-1.424057	1.906272	-0.782299	1	-2.027859	-3.568315	1.484964
1	-2.032719	1.774383	-1.680551	1	0.679723	-1.638189	4.214218
1	-0.861893	2.837945	-0.869197	1	-1.528216	-2.712018	3.757537
6	-4.718257	0.255202	-2.075793	6	1.843623	-3.106583	-1.802482
6	-4.408229	1.177043	-2.952336	6	2.550099	-4.311227	-1.915612
6	-4.042834	2.094766	-3.814464	6	0.822411	-2.813880	-2.720419
6	-3.811946	1.773290	-5.274077	6	2.238850	-5.213798	-2.932162
1	-4.470269	2.376097	-5.912457	1	3.343671	-4.540045	-1.211737
1	-3.992529	0.718009	-5.487480	6	0.507704	-3.726414	-3.727587
1	-2.780054	2.013345	-5.559551	1	0.271862	-1.883787	-2.619051
6	-2.177898	3.118343	1.382239	6	1.216417	-4.924205	-3.837897
1	-2.867469	3.838666	0.923939	1	2.792788	-6.144472	-3.015618
1	-1.183561	3.576140	1.397602	1	-0.289628	-3.498871	-4.429265
1	-2.496827	2.959053	2.419080	1	0.974424	-5.629636	-4.627589
6	2.622895	0.892284	4.206235	6	3.895908	-2.276357	0.037575
6	3.790098	0.149507	4.399874	6	4.202001	-3.085345	1.139510
1	4.023716	-0.253386	5.380677	6	4.946567	-1.696285	-0.689760
6	4.648552	-0.078025	3.323930	6	5.529753	-3.282663	1.522946
6	6.459102	2.602201	-1.070161	1	3.401251	-3.543412	1.708952
6	6.472396	2.110589	-2.378337	6	6.272012	-1.897579	-0.311135
1	7.365178	2.214026	-2.987965	1	4.723772	-1.061997	-1.539396
6	5.335529	1.493654	-2.902227	6	6.566787	-2.684432	0.805395
6	-3.818397	3.530060	-3.391122	1	5.752712	-3.904052	2.385535
1	-4.003228	3.669444	-2.324191	1	7.069825	-1.427060	-0.878082
1	-4.475320	4.207313	-3.951326	1	7.598211	-2.833115	1.111327
1	-2.785410	3.833164	-3.603512	15	2.184444	-1.872690	-0.488220
1	-5.763819	0.046071	-1.848104				
1	0.931513	7.109814	0.320323	IM2_{dppp}			
1	1.182433	3.283232	-1.628354				
1	5.339334	1.114954	-3.920053	15	2.879527	1.608357	-0.295356
1	7.340448	3.089471	-0.663581	6	2.180122	3.090850	-1.116693
1	0.452175	5.655214	-1.640642	6	1.737333	2.997498	-2.445904
1	2.180559	6.189850	2.260774	6	1.101254	4.075639	-3.059805
1	1.944374	1.070204	5.035090	6	0.888365	5.260016	-2.352214
1	5.550241	-0.667609	3.455098	6	1.314146	5.357880	-1.026599
28	1.273270	0.172097	-0.629019	6	1.952683	4.280937	-0.410930

6	3.934957	2.308075	1.029214	1	-2.598343	-3.347680	-3.658794
6	4.965818	3.223087	0.769872	1	-1.303093	-2.389859	-4.410713
6	3.720312	1.870498	2.342868	6	-1.913010	3.307645	-0.309259
1	2.281122	4.367240	0.619485	1	-2.500817	3.471124	-1.221542
1	5.128868	3.579550	-0.243231	1	-0.909642	3.702536	-0.486448
1	2.920447	1.159515	2.533536	1	-2.372594	3.891877	0.496875
8	-0.048561	-0.841501	0.567423	6	4.526525	2.336570	3.382858
8	-4.303083	1.148192	2.953065	6	5.553801	3.242160	3.115009
6	-0.223736	0.432199	0.305772	1	6.183158	3.604267	3.922483
16	-4.457008	-0.096869	2.194862	6	5.772316	3.686512	1.807869
6	-0.898624	1.457854	1.236003	6	-2.590904	0.118542	-4.215343
7	-3.411608	-0.004064	0.889754	1	-2.969488	0.962230	-3.635350
8	-4.253312	-1.408031	2.817578	1	-3.055219	0.140113	-5.209390
6	-6.108704	-0.099018	1.501014	1	-1.511801	0.257566	-4.358695
6	-1.851213	1.824567	0.049631	1	-5.098945	-1.349773	-1.074083
1	-0.253865	2.292605	1.528010	1	0.389282	6.098150	-2.828640
1	-1.379866	1.033645	2.120249	1	1.884764	2.077033	-3.003363
6	-3.203735	-1.240316	0.104803	1	0.767772	3.988655	-4.089675
6	-6.718318	-1.315846	1.190265	1	1.147600	6.274012	-0.467750
6	-6.735124	1.110954	1.200986	1	4.352111	1.993061	4.397960
1	-3.465553	-2.072712	0.760488	1	6.569771	4.393914	1.600260
1	-2.138029	-1.334031	-0.103479	28	1.638324	-0.041860	0.258991
1	-6.223727	-2.243549	1.454694	6	3.248115	-2.869629	1.453452
6	-7.959005	-1.313218	0.558235	6	4.285741	-3.801345	1.595497
6	-7.976224	1.095507	0.568697	6	2.151623	-2.914744	2.327296
1	-6.260662	2.045337	1.477736	6	4.236158	-4.756837	2.608471
1	-8.437588	-2.258148	0.315628	1	5.128638	-3.789715	0.910450
6	-8.604356	-0.111427	0.234475	6	2.103223	-3.877387	3.337351
1	-8.468128	2.035490	0.333876	1	1.339057	-2.205124	2.192585
6	-9.961182	-0.119504	-0.423761	6	3.145307	-4.793699	3.481653
1	-10.125287	0.787573	-1.012107	1	5.043778	-5.475184	2.716033
1	-10.759520	-0.172296	0.326576	1	1.250586	-3.909603	4.008973
1	-10.078813	-0.982721	-1.085148	1	3.108225	-5.540019	4.269867
6	-3.289240	1.305049	0.230741	6	3.034686	-2.526352	-1.416302
1	-3.788538	1.271612	-0.746728	6	4.112213	-3.035056	-2.152587
1	-3.819026	2.024763	0.855589	6	1.724247	-2.724169	-1.884362
6	-0.972954	0.970662	-0.923252	6	3.886862	-3.731044	-3.341193
1	-1.479610	0.220708	-1.533639	1	5.129795	-2.893218	-1.801141
1	-0.360918	1.599576	-1.576194	6	1.503084	-3.434295	-3.063811
6	-4.015066	-1.291854	-1.173956	1	0.892806	-2.313411	-1.315299
6	-3.466894	-1.252833	-2.362340	6	2.582779	-3.933673	-3.796261
6	-2.863843	-1.200390	-3.525671	1	4.727929	-4.118223	-3.909175
6	-2.385387	-2.446185	-4.236956	1	0.487167	-3.595104	-3.412056
1	-2.862148	-2.542156	-5.220796	1	2.409021	-4.478437	-4.719623

15	3.208616	-1.585837	0.147464	1	-5.698668	1.432059	-1.117405
6	4.933614	-0.910638	0.134752	1	-4.502033	2.581273	-0.548223
1	5.687199	-1.704438	0.124165	6	-4.818636	1.198544	-3.422761
1	5.015384	-0.420900	1.110373	1	-5.392780	0.280959	-3.265862
6	5.256662	0.108112	-0.986620	1	-4.280978	1.116133	-4.373360
1	5.682859	-0.431052	-1.839013	1	-5.522655	2.035002	-3.508372
1	6.047292	0.763215	-0.606937	6	-2.629479	2.060444	1.544478
6	4.119032	0.991110	-1.548045	6	-2.217193	3.055853	0.662728
1	3.525181	0.411227	-2.262110	6	-2.068342	4.354006	0.410081
1	4.558445	1.829321	-2.098267	6	-2.814623	5.396902	1.212957
(R)-IM2				1	-2.113499	6.088825	1.698581
				1	-3.438705	4.939598	1.984180
				1	-3.457939	6.007291	0.564450
8	-5.229182	-1.225152	-1.118108	6	-1.138181	4.885720	-0.652879
16	-5.118032	-0.744615	0.265228	1	-0.348054	5.491732	-0.190106
7	-4.197842	0.672647	0.176548	1	-1.665388	5.543574	-1.357467
8	-6.336480	-0.551732	1.067564	1	-0.664726	4.077460	-1.211112
6	-4.044318	-1.840625	1.189358	1	-2.195830	2.072096	2.546241
6	-2.822061	-2.246765	0.655012	28	-1.349380	1.459850	0.137159
6	-4.489483	-2.334200	2.416722	6	2.359974	-0.321932	-1.292761
1	-2.484936	-1.878214	-0.303700	6	3.224797	-0.164846	-0.034792
6	-2.031470	-3.142157	1.369731	6	4.575059	-0.015263	-1.940417
6	-3.692574	-3.239804	3.112464	1	1.742114	0.562275	-1.471561
1	-5.449802	-2.010543	2.801289	1	3.214177	-1.094923	0.539969
1	-1.064008	-3.429638	0.971655	6	5.621179	-1.038063	-2.355575
6	-2.453906	-3.654730	2.602356	1	5.628448	-1.148392	-3.443234
1	-4.036999	-3.630807	4.066022	1	6.612075	-0.711596	-2.029368
6	-1.591550	-4.621415	3.374727	1	5.388775	-2.003030	-1.902055
1	-0.718183	-4.926830	2.793078	6	4.821676	1.372520	-2.521220
1	-2.151254	-5.522514	3.646499	1	5.758056	1.781985	-2.135342
1	-1.232529	-4.171871	4.307822	1	4.883029	1.309829	-3.611351
6	-3.960087	1.323062	1.479908	1	4.011964	2.050469	-2.249088
1	-4.800589	1.989202	1.728320	8	3.290788	-0.493171	-2.346902
1	-3.952670	0.538591	2.240112	8	4.541890	0.045815	-0.506652
6	-2.674675	0.392353	-2.186706	6	2.730097	0.982975	0.895227
6	-3.849386	1.408272	-2.265932	6	1.419461	-1.553573	-1.168207
1	-2.462473	-0.061884	-3.158775	8	0.774444	-1.474891	0.124577
6	-2.792133	2.550821	-2.455429	8	1.290350	0.979557	0.863524
6	-1.743829	1.564222	-1.940917	15	0.090662	-0.155520	0.876946
1	-2.945259	3.495523	-1.937567	7	0.022712	-0.857853	2.396418
1	-2.604965	2.745754	-3.520116	6	-1.062108	-0.511448	3.300333
8	-0.505745	1.624246	-1.725776	1	-1.436687	-1.414453	3.793219
1	-2.719353	-0.392024	-1.440044	1	-0.734052	0.199410	4.072515
6	-4.628502	1.565633	-0.926154	1	-1.881486	-0.071388	2.737533

6	1.076761	-1.656030	3.006301	6	3.973853	0.500051	5.012059
1	1.928467	-1.746837	2.337590	1	2.262509	1.730051	5.476256
1	1.428372	-1.185909	3.931632	1	5.602344	-0.676313	4.233616
1	0.705285	-2.663102	3.239025	1	4.272478	0.378706	6.048960
6	2.220199	-2.861446	-1.152962				
6	2.810239	-3.325669	-2.337304				
6	2.372100	-3.615795	0.013715				
6	3.558773	-4.499618	-2.342424				
1	2.681752	-2.763012	-3.252737	8	5.513979	1.542192	1.023553
6	3.118341	-4.797000	0.006304	16	5.111145	1.079672	-0.310658
1	1.893528	-3.285328	0.924371	7	4.162929	-0.302294	-0.055753
6	3.720377	-5.240089	-1.168720	8	6.122386	0.831631	-1.348901
1	4.012359	-4.840598	-3.268317	6	3.957184	2.270716	-0.969828
1	3.223897	-5.368873	0.923711	6	3.143784	2.986269	-0.088024
1	4.301585	-6.157289	-1.175804	6	3.958947	2.550254	-2.333412
6	0.380710	-1.643209	-2.283406	1	3.186896	2.779499	0.974701
6	0.482274	-0.905486	-3.464951	6	2.319991	3.984802	-0.590307
6	-0.637819	-2.597673	-2.163972	6	3.118348	3.551357	-2.820684
6	-0.413594	-1.131867	-4.513734	1	4.632101	2.010090	-2.989355
1	1.275725	-0.179141	-3.586863	1	1.697121	4.555164	0.089758
6	-1.543904	-2.809030	-3.198767	6	2.293289	4.284193	-1.960924
1	-0.696765	-3.194612	-1.261061	1	3.119010	3.779436	-3.882964
6	-1.427065	-2.080890	-4.386090	6	1.413296	5.392733	-2.479671
1	-0.315604	-0.559829	-5.431611	1	1.769321	6.369199	-2.130859
1	-2.333584	-3.544876	-3.083803	1	1.400974	5.415452	-3.572517
1	-2.123420	-2.251774	-5.201339	1	0.384723	5.278886	-2.124642
6	3.144812	2.350763	0.354794	6	3.937901	-1.085970	-1.285977
6	4.432715	2.842220	0.597087	1	4.849262	-1.646490	-1.546227
6	2.259674	3.105888	-0.422349	1	3.778386	-0.364542	-2.090423
6	4.835019	4.062849	0.059868	6	2.293861	-0.015847	2.057124
1	5.122133	2.266302	1.202944	6	3.619813	-0.758373	2.410135
6	2.666758	4.329259	-0.959509	1	1.917552	0.581347	2.897664
1	1.259016	2.740214	-0.607240	6	2.776054	-2.022914	2.772979
6	3.954080	4.810534	-0.724388	6	1.610866	-1.388634	2.021167
1	5.838067	4.430772	0.254959	1	3.150925	-2.999207	2.475159
1	1.968194	4.903150	-1.561021	1	2.522558	-2.047426	3.841529
1	4.268253	5.762390	-1.142424	8	0.411788	-1.744502	1.849583
6	3.193374	0.800084	2.335237	1	2.272030	0.588005	1.150329
6	2.459870	1.410121	3.360152	6	4.517431	-1.051786	1.167969
6	4.331901	0.056680	2.659163	1	5.559962	-0.864856	1.437538
6	2.843971	1.257859	4.689754	1	4.437747	-2.105414	0.901889
1	1.578164	1.986387	3.102456	6	4.429123	-0.154008	3.551632
6	4.718295	-0.093001	3.993822	1	4.881464	0.790647	3.241000
1	4.925204	-0.397580	1.872404	1	3.794776	0.025202	4.426697
				1	5.236560	-0.829601	3.858010

(S)-IM2

6	2.741207	-2.032651	-1.256104	6	-3.794740	-0.498152	-2.814277
6	2.503260	-3.012714	-0.293272	6	-5.599179	-2.586592	-2.448157
6	2.729654	-4.252524	0.131925	1	-4.237123	-3.294768	-0.945355
6	3.773278	-5.119602	-0.538080	6	-4.958694	-0.559729	-3.583673
1	3.314550	-6.029826	-0.947805	1	-3.083536	0.303679	-2.967236
1	4.275643	-4.591251	-1.351509	6	-5.867216	-1.600463	-3.400422
1	4.534502	-5.449995	0.181834	1	-6.296377	-3.406106	-2.301547
6	1.987230	-4.896577	1.275157	1	-5.149940	0.207273	-4.328485
1	1.529105	-5.836807	0.947148	1	-6.772602	-1.648962	-3.997979
1	2.671384	-5.157692	2.094899	6	-1.572192	-2.730593	-0.919522
1	1.199697	-4.247980	1.659822	6	-1.774985	-3.645589	0.117740
1	2.363153	-2.239133	-2.261023	6	-0.769873	-3.095620	-2.009798
28	1.247941	-1.619218	-0.017732	6	-1.205742	-4.917826	0.048048
6	-2.654258	-0.823893	0.445408	1	-2.389749	-3.371270	0.967504
6	-3.003179	0.666472	0.320166	6	-0.191280	-4.360533	-2.068504
6	-4.689913	-0.430724	1.519429	1	-0.616062	-2.383936	-2.813196
1	-1.800843	-0.993967	1.109745	6	-0.419217	-5.280022	-1.044260
1	-3.199556	0.908152	-0.724915	1	-1.371208	-5.622714	0.856945
6	-6.080946	-0.654327	0.944542	1	0.435794	-4.628843	-2.913200
1	-6.451394	-1.642700	1.229113	1	0.025093	-6.269337	-1.092574
1	-6.769672	0.103513	1.327328	6	-1.858281	1.627572	2.361930
1	-6.041873	-0.592557	-0.144362	6	-2.695538	2.485505	3.086857
6	-4.643960	-0.470275	3.041739	6	-1.047751	0.727917	3.053941
1	-5.241775	0.344347	3.457769	6	-2.714401	2.443538	4.479122
1	-5.043415	-1.422992	3.400368	1	-3.338646	3.181058	2.561380
1	-3.616108	-0.360662	3.390073	6	-1.067011	0.685712	4.449648
8	-3.812310	-1.427414	0.984741	1	-0.420561	0.047210	2.500601
8	-4.198931	0.835105	1.056812	6	-1.898318	1.543755	5.168185
6	-1.895565	1.630735	0.834021	1	-3.369352	3.114833	5.026619
6	-2.290583	-1.388176	-0.959266	1	-0.431203	-0.025158	4.969748
8	-1.433191	-0.390548	-1.545935	1	-1.913152	1.513062	6.253631
8	-0.582683	1.179859	0.367584	6	-2.098042	3.057544	0.333822
15	-0.043335	0.143845	-0.794624	6	-1.083943	3.989031	0.596897
7	0.480184	1.178915	-2.028989	6	-3.248676	3.479926	-0.335962
6	1.136524	0.485913	-3.139001	6	-1.201299	5.306923	0.168502
1	0.406897	0.085751	-3.859996	1	-0.201196	3.657805	1.131634
1	1.798006	1.184358	-3.658226	6	-3.365887	4.804462	-0.769339
1	1.730190	-0.341658	-2.758291	1	-4.070240	2.793124	-0.501553
6	-0.400468	2.244102	-2.505841	6	-2.343287	5.718468	-0.526990
1	-0.763576	2.836844	-1.671440	1	-0.408404	6.018301	0.380151
1	0.176376	2.897261	-3.164835	1	-4.264352	5.118207	-1.292063
1	-1.258633	1.852594	-3.071276	1	-2.436973	6.746569	-0.863215
6	-3.527590	-1.475874	-1.850759				
6	-4.438188	-2.526623	-1.681604				

IM3

				6	-0.090279	1.453392	-2.169895
15	1.145992	1.705746	0.666402	1	-2.203508	1.560361	-2.522715
6	0.136721	3.241147	0.805210	1	-1.236904	1.334754	-3.969434
6	-0.982553	3.269490	1.650892	8	0.481981	2.493040	-2.470495
6	-1.794061	4.401353	1.716457	1	-0.122992	-2.074489	-2.037457
6	-1.499851	5.520351	0.936750	6	-2.607125	-0.978297	-1.844291
6	-0.396061	5.494414	0.082714	1	-2.754428	-2.043510	-2.019476
6	0.416375	4.364065	0.013660	1	-3.536379	-0.454889	-2.110293
6	2.864778	2.334075	0.491419	6	-1.871453	-1.107979	-4.173752
6	3.255529	2.677464	-0.815401	1	-1.869481	-2.202921	-4.143804
6	3.791666	2.447508	1.532443	1	-1.155339	-0.791144	-4.937840
6	0.944302	0.982708	2.335843	1	-2.869633	-0.778030	-4.491012
6	0.336120	-0.277423	2.409972	6	-3.818617	1.197767	0.016220
6	1.287087	1.643300	3.526410	6	-4.050563	2.129406	-0.874207
1	1.266217	4.356363	-0.656269	6	-4.263371	3.047463	-1.785364
1	2.537602	2.582420	-1.625726	6	-4.724895	2.678777	-3.178386
1	3.534270	2.131563	2.534034	1	-5.666218	3.187742	-3.420039
1	0.017920	-0.776066	1.502939	1	-4.875143	1.602297	-3.283753
8	-2.347486	-1.890583	1.907424	1	-3.983342	2.998014	-3.921079
16	-2.933066	-2.087139	0.574923	6	4.541886	3.155411	-1.061083
7	-2.365418	-0.837214	-0.395297	6	5.456318	3.282367	-0.014422
8	-2.708161	-3.336417	-0.162904	1	6.460571	3.648387	-0.207051
6	-4.700489	-1.880200	0.750485	6	5.078545	2.921221	1.278188
6	-5.214552	-1.373028	1.943080	6	0.120748	-0.896396	3.641770
6	-5.535297	-2.156922	-0.333731	6	0.520278	-0.257380	4.815022
1	-4.542149	-1.174213	2.769643	1	0.366133	-0.737505	5.776982
6	-6.582535	-1.128703	2.041429	6	1.093955	1.017163	4.756191
6	-6.898149	-1.900945	-0.219693	6	-4.026897	4.514755	-1.513365
1	-5.123344	-2.572198	-1.246063	1	-4.938603	5.094853	-1.704433
1	-6.990015	-0.733314	2.967695	1	-3.247783	4.901421	-2.181688
6	-7.442035	-1.381531	0.964027	1	-3.703167	4.684992	-0.486745
1	-7.553048	-2.108636	-1.061287	1	-4.627160	0.874866	0.669061
6	-8.924409	-1.133607	1.083467	1	-2.126768	6.405444	0.992296
1	-9.351769	-0.805516	0.131570	1	-1.213100	2.412428	2.273265
1	-9.142647	-0.372715	1.837604	28	0.697028	0.192023	-0.970103
1	-9.450516	-2.049603	1.378636	1	-0.162208	6.358828	-0.531603
1	1.686966	2.650949	3.492714	1	-2.652896	4.407503	2.381159
6	-2.473095	0.521029	0.191214	1	5.791644	2.989673	2.093797
1	-2.226309	0.425990	1.249287	1	4.829075	3.424634	-2.073512
1	-1.681906	1.110944	-0.268091	1	-0.368560	-1.863553	3.664653
6	-0.087340	-1.030749	-2.368873	1	1.377343	1.528617	5.671476
6	-1.474767	-0.519340	-2.801058	15	2.348410	-1.375838	-0.376868
1	0.593176	-0.988571	-3.228280	6	3.150746	-1.779001	-1.979128
6	-1.345437	1.014057	-2.925678	6	3.532311	-3.072251	-2.350660

6	3.365606	-0.716623	-2.872101	1	-2.780521	0.738738	-2.331628
6	4.129300	-3.298600	-3.592296	1	-0.281172	1.158669	-0.402328
1	3.355185	-3.903515	-1.677413	8	-0.911566	2.401340	1.471865
6	3.975343	-0.942977	-4.104241	16	-0.676040	1.504319	2.611961
1	3.038252	0.282751	-2.601357	7	-1.027487	-0.054141	2.086208
6	4.356922	-2.236704	-4.467823	8	0.643708	1.446793	3.254391
1	4.414658	-4.307720	-3.874925	6	-1.868297	1.939050	3.869290
1	4.139063	-0.112877	-4.785082	6	-3.003885	2.665823	3.507781
1	4.821498	-2.416400	-5.432833	6	-1.690217	1.484749	5.176987
6	3.795548	-0.938722	0.682997	1	-3.109467	3.022074	2.489660
6	5.015094	-0.520241	0.136692	6	-3.975810	2.925238	4.470051
6	3.666066	-1.003812	2.080271	6	-2.674538	1.751560	6.124767
6	6.084587	-0.186749	0.967580	1	-0.788729	0.947782	5.447538
1	5.135106	-0.458481	-0.938338	1	-4.861102	3.491831	4.195628
6	4.736044	-0.668677	2.906829	6	-3.830157	2.469805	5.788083
1	2.734210	-1.331273	2.524564	1	-2.542635	1.400471	7.144245
6	5.951747	-0.262927	2.353390	6	-4.876078	2.778484	6.828889
1	7.022463	0.136575	0.526395	1	-4.902891	2.011714	7.607903
1	4.616644	-0.729105	3.984628	1	-5.872344	2.851456	6.384092
1	6.787174	-0.005024	2.997694	1	-4.665547	3.736717	7.319102
6	1.861218	-2.987521	0.346096	1	-0.194000	0.668665	-4.681443
6	2.798835	-3.887886	0.878738	6	-2.238736	-0.202514	1.244506
6	0.501483	-3.314783	0.384787	1	-2.338958	0.721294	0.670994
6	2.374775	-5.094620	1.431139	1	-2.029881	-0.998463	0.529174
1	3.854106	-3.635938	0.873394	6	1.143521	-2.090713	1.629758
6	0.076351	-4.521870	0.940626	6	-0.071554	-2.410948	2.521022
1	-0.224926	-2.623519	-0.019262	1	1.801579	-2.966841	1.582042
6	1.013526	-5.412105	1.463499	6	-1.021083	-3.284795	1.674664
1	3.105785	-5.785499	1.841296	6	-0.658331	-3.096556	0.198599
1	-0.984299	-4.744242	0.957127	1	-2.079178	-3.039317	1.813423
1	0.687120	-6.351427	1.900579	1	-0.918129	-4.351739	1.909729

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				8	-0.961496	-3.939267	-0.634500
				1	1.736305	-1.260143	2.032962
				6	-0.738705	-1.124035	3.064025
15	-0.441458	-1.068898	-2.190229	1	-0.045761	-0.697632	3.788623
6	-2.225817	-1.341443	-2.520927	1	-1.664693	-1.388921	3.591474
6	-2.711755	-2.646123	-2.700902	6	0.360628	-3.192390	3.781056
6	-4.075541	-2.873014	-2.859045	1	1.106406	-2.629840	4.353142
6	-4.971125	-1.802681	-2.823663	1	0.808961	-4.148400	3.494291
6	-4.500766	-0.502839	-2.630225	1	-0.487187	-3.405007	4.444897
6	-3.135937	-0.274232	-2.481042	6	-3.514571	-0.497993	2.003353
6	-0.247440	0.729527	-2.516174	6	-4.247407	-1.561529	1.785426
6	-0.219911	1.573931	-1.398937	6	-4.973389	-2.626972	1.549498
6	-0.149133	1.293746	-3.796098	6	-4.765604	-3.916084	2.313566

1	-5.699758	-4.228902	2.795934	6	0.415967	-1.914659	-3.607474
1	-3.995432	-3.816208	3.080738	1	0.265746	-1.346630	-4.530640
1	-4.469183	-4.720168	1.629047	1	-0.089882	-2.874662	-3.739790
6	-0.097948	2.953580	-1.544678	6	-6.438771	-2.036922	-3.036319
6	0.026375	3.498081	-2.822805	6	0.241995	4.977664	-2.989049
6	0.000545	2.669762	-3.948890	6	2.795814	5.229964	0.158533
6	-6.059681	-2.632689	0.499157	6	7.396635	-3.861577	1.012996
1	-7.028353	-2.875757	0.953582	9	8.570172	-3.273356	0.692373
1	-5.860566	-3.398939	-0.257491	9	7.362454	-3.963819	2.361359
1	-6.146779	-1.670205	-0.004974	9	7.424877	-5.121166	0.524116
1	-3.830447	0.233355	2.746347	9	3.522800	5.965186	-0.707027
1	-2.031617	-3.487455	-2.665245	9	3.195161	5.554833	1.407920
28	0.535786	-1.670351	-0.240543	9	1.506462	5.636679	0.045583
1	-5.199811	0.325271	-2.590395	9	1.556845	5.301402	-2.895937
1	-4.446463	-3.883169	-2.990473	9	-0.408279	5.691324	-2.051956
1	-0.080821	3.583777	-0.664770	9	-0.176201	5.412411	-4.199959
1	0.081383	3.104918	-4.938603	9	-7.193488	-1.173570	-2.315512
15	2.509632	-0.745402	-0.984904	9	-6.809434	-3.288964	-2.682584
6	3.995682	-1.630269	-0.375058	9	-6.791926	-1.873963	-4.331609
6	5.200205	-0.975791	-0.089097				
6	3.914391	-3.021770	-0.215144				
6	6.307807	-1.700033	0.346065				
1	5.271404	0.100762	-0.202336	15	-0.135140	-2.118188	1.308514
6	5.023683	-3.748905	0.205861	6	1.534031	-2.721422	1.759099
1	2.972731	-3.527978	-0.401562	6	2.022412	-3.924189	1.233006
6	6.220345	-3.086080	0.488679	6	3.323801	-4.352194	1.496509
1	7.240732	-1.193561	0.567087	6	4.169681	-3.560041	2.280350
1	4.962056	-4.825303	0.321288	6	3.700326	-2.345300	2.796590
6	2.842403	1.018974	-0.650929	6	2.398815	-1.935964	2.541051
6	3.323526	1.919682	-1.609314	6	-0.470675	-0.845886	2.583327
6	2.442650	1.501147	0.605291	6	-0.303545	0.499108	2.212261
6	3.351786	3.286187	-1.337786	6	-0.871516	-1.123125	3.894050
1	3.650466	1.569880	-2.581953	1	2.049099	-0.996550	2.954948
6	2.482205	2.861084	0.884372	1	-0.010949	0.748588	1.201429
1	2.047230	0.824592	1.353054	8	1.041311	2.815879	0.641151
6	2.914903	3.754969	-0.098869	16	1.084043	2.783114	-0.826543
1	3.682100	3.988467	-2.092577	7	1.339631	1.185598	-1.276167
1	2.132966	3.217648	1.846019	8	-0.046186	3.277073	-1.623108
6	2.696914	-0.934884	-2.838101	6	2.527324	3.720879	-1.317962
1	2.325260	-0.024357	-3.315364	6	3.531151	3.966569	-0.379927
1	3.760301	-1.024734	-3.076454	6	2.668201	4.132528	-2.643926
6	1.916192	-2.161639	-3.353716	1	3.389531	3.650658	0.647218
1	2.365890	-2.500086	-4.293677	6	4.692500	4.619491	-0.784182
1	2.022178	-2.990962	-2.646118	6	3.837947	4.781282	-3.031171

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1	1.867108	3.960409	-3.352994	28	-0.639628	-1.347992	-0.761750
1	5.476796	4.813956	-0.057863	1	4.372069	-1.743108	3.399171
6	4.866517	5.031449	-2.112847	1	3.667346	-5.287857	1.072701
1	3.953888	5.102213	-4.062622	1	-0.396705	2.560403	2.802670
6	6.117079	5.760055	-2.535643	1	-1.470003	-0.345281	5.801947
1	6.342287	5.587078	-3.591651	15	-2.766402	-0.829145	-0.013656
1	6.981577	5.444942	-1.944580	6	-4.046667	-1.051639	-1.300876
1	6.003599	6.842297	-2.397922	6	-5.206081	-0.274147	-1.356320
1	-0.986836	-2.148847	4.229520	6	-3.871062	-2.065737	-2.259435
6	2.305940	0.417406	-0.457733	6	-6.178363	-0.494441	-2.334163
1	2.222286	0.790524	0.564595	1	-5.352383	0.522519	-0.633548
1	1.955688	-0.614813	-0.446735	6	-4.835507	-2.304950	-3.227123
6	-0.805509	-0.491642	-2.571012	1	-2.958268	-2.653461	-2.251811
6	0.585966	-0.344943	-3.216642	6	-5.995757	-1.517510	-3.271816
1	-1.428728	-1.142338	-3.196808	1	-7.061112	0.132841	-2.356292
6	1.355452	-1.646039	-2.908831	1	-4.708610	-3.083332	-3.971999
6	0.686281	-2.337386	-1.713724	6	-3.083166	0.813680	0.705222
1	2.412894	-1.482716	-2.677252	6	-3.779210	1.024969	1.898672
1	1.328902	-2.345970	-3.754008	6	-2.452717	1.913961	0.093888
8	0.859012	-3.533815	-1.517629	6	-3.814996	2.284564	2.499103
1	-1.321156	0.474003	-2.495954	1	-4.280965	0.202169	2.396115
6	1.315456	0.932099	-2.731231	6	-2.494229	3.172185	0.669783
1	0.790716	1.776393	-3.177310	1	-1.878561	1.778453	-0.815069
1	2.345882	0.929796	-3.112749	6	-3.153372	3.358937	1.893814
6	0.469226	-0.167940	-4.746777	1	-4.333432	2.409337	3.441651
1	-0.151455	0.700636	-4.993362	1	-1.967512	4.002673	0.215158
1	0.000708	-1.051577	-5.190589	6	-3.338161	-2.042493	1.294182
1	1.448894	-0.031986	-5.223865	1	-3.094551	-1.633844	2.277912
6	3.744601	0.482434	-0.925616	1	-4.426071	-2.133684	1.227827
6	4.426387	-0.577505	-1.280720	6	-2.663625	-3.416951	1.108968
6	5.081911	-1.658967	-1.624625	1	-3.300169	-4.191747	1.551861
6	5.121783	-2.144596	-3.056800	1	-2.594032	-3.650826	0.040840
1	6.159432	-2.248734	-3.397873	6	-1.260998	-3.536248	1.736519
1	4.601400	-1.462701	-3.731930	1	-1.329167	-3.643786	2.823818
1	4.651811	-3.132567	-3.136684	1	-0.770781	-4.437714	1.359012
6	-0.529786	1.530919	3.109871	8	5.463839	-3.872389	2.582290
6	-0.975877	1.237585	4.403369	8	-1.234543	2.313782	5.205600
6	-1.140257	-0.095681	4.800878	8	-3.080168	4.610927	2.424817
6	5.815992	-2.501253	-0.606842	8	-6.878230	-1.821056	-4.265626
1	6.874940	-2.599637	-0.877859	6	-3.487937	4.777645	3.774632
1	5.388185	-3.510606	-0.585890	1	-2.941921	4.091855	4.433264
1	5.745507	-2.084319	0.397967	1	-3.247279	5.809254	4.036154
1	4.223176	1.460854	-0.933069	1	-4.568270	4.622903	3.895740
1	1.401480	-4.515264	0.571267	6	-8.055962	-1.038942	-4.370183

1	-7.823833	0.018132	-4.552087	1	8.006841	-2.857242	2.168315
1	-8.609163	-1.437768	-5.221547	6	9.638115	-2.006532	0.156841
1	-8.675365	-1.117998	-3.467438	1	10.017030	-1.732174	1.145413
6	-1.668265	2.064786	6.532249	1	9.991921	-1.265393	-0.564625
1	-1.807587	3.043334	6.993867	1	10.091074	-2.968765	-0.110811
1	-2.619285	1.516882	6.550663	1	-0.271319	2.584837	-3.333133
1	-0.920056	1.499785	7.102152	6	3.392595	0.305262	0.487013
6	5.971535	-5.114910	2.125084	1	3.313234	0.197988	-0.596669
1	5.983902	-5.169251	1.029574	1	2.605990	0.991213	0.797445
1	6.994640	-5.178699	2.498150	6	0.581722	-1.003556	2.803879
1	5.388296	-5.957280	2.518099	6	1.953260	-0.574600	3.359144
IM3_{PPh3}-OCF₃				1	-0.176527	-0.880562	3.586539
				6	1.929622	0.968568	3.411089
				6	0.787857	1.454671	2.521452
15	-0.120054	1.688478	-0.430205	1	2.859599	1.433292	3.069223
6	1.000201	3.146312	-0.499300	1	1.750481	1.347319	4.424931
6	2.195610	3.076462	-1.228943	8	0.252277	2.536761	2.718678
6	3.092570	4.141225	-1.224979	1	0.572847	-2.059326	2.509814
6	2.805013	5.286261	-0.482854	6	3.133074	-1.154126	2.537849
6	1.621902	5.363248	0.255850	1	3.163789	-2.224028	2.740735
6	0.725758	4.299874	0.249654	1	4.072002	-0.709375	2.894183
6	-1.800179	2.437429	-0.457205	6	2.160649	-1.130184	4.785631
6	-2.321653	2.812189	0.794755	1	2.081293	-2.222406	4.794361
6	-2.590526	2.591999	-1.599595	1	1.395864	-0.732044	5.459074
6	0.189772	0.900447	-2.054375	1	3.142482	-0.857729	5.193572
6	0.680080	-0.410862	-2.027800	6	4.753801	0.841364	0.880922
6	0.031966	1.544634	-3.292452	6	4.931900	1.875927	1.664756
1	-0.181103	4.366180	0.835636	6	5.115399	2.898397	2.464461
1	-1.704901	2.700860	1.682458	6	5.201595	2.716316	3.964439
1	-2.230704	2.273006	-2.567613	1	6.155476	3.104112	4.341973
1	0.867504	-0.898767	-1.080163	1	5.114172	1.667078	4.253593
8	3.105246	-2.126142	-1.205351	1	4.403149	3.279832	4.462483
16	3.566351	-2.347417	0.172174	6	-3.608620	3.332088	0.891748
7	3.053680	-1.017084	1.069943	6	-4.391020	3.472532	-0.256802
8	3.144037	-3.542991	0.913076	6	-3.879826	3.109537	-1.501399
6	5.350056	-2.329188	0.136419	6	0.955826	-1.096138	-3.209637
6	6.006308	-1.866580	-1.003737	6	0.733572	-0.465954	-4.433042
6	6.060525	-2.696030	1.281270	6	0.284007	0.858943	-4.476190
1	5.428726	-1.597874	-1.880537	6	5.238428	4.312160	1.947095
6	7.395022	-1.759285	-0.986681	1	6.146062	4.783298	2.343448
6	7.446500	-2.577348	1.280818	1	4.389813	4.922457	2.275510
1	5.535600	-3.074964	2.150496	1	5.281853	4.345141	0.859465
1	7.913951	-1.400228	-1.870803	1	5.623397	0.313283	0.494294
6	8.134017	-2.105273	0.152693	1	2.427646	2.192800	-1.811678

28	0.038012	0.205733	1.283967	9	-1.023506	-7.608214	-1.688745
1	1.406464	6.250816	0.840754	9	0.316346	-6.525962	-3.013356
1	4.014668	4.079885	-1.791095	9	1.035043	-7.222046	-1.084083
1	-4.499364	3.198823	-2.383961	9	-5.621490	-3.158884	5.773729
1	-4.007962	3.621965	1.857858	9	-3.904693	-2.328902	6.816880
1	1.348016	-2.104548	-3.163303	9	-5.497731	-1.013884	6.145664
1	0.138211	1.346978	-5.433529	9	-6.322222	1.860879	-3.168580
15	-1.669049	-1.254171	0.589766	9	-5.601463	0.459763	-4.674064
6	-2.631111	-1.576850	2.120985	9	-7.134961	-0.148166	-3.252130
6	-3.134480	-2.834547	2.466669	9	0.243888	-0.791953	-6.722396
6	-2.842313	-0.489897	2.984965	9	2.326767	-0.914927	-6.115644
6	-3.844493	-3.004996	3.654565	9	0.952743	-2.516023	-5.591784
1	-2.968712	-3.685632	1.816321	9	-6.308638	4.407505	-1.285154
6	-3.564022	-0.654040	4.162040	9	-6.623632	2.877919	0.229198
1	-2.423229	0.480548	2.737868	9	-5.971843	4.862423	0.820373
6	-4.063283	-1.915685	4.497752	9	4.983189	6.117472	-0.902891
1	-4.233819	-3.980550	3.922968	9	3.306494	7.427610	-1.350341
1	-3.734908	0.188963	4.822383	9	3.846819	7.036953	0.715576
6	-2.989950	-0.732835	-0.589860				
6	-4.204624	-0.191950	-0.146328				
6	-2.760886	-0.841819	-1.970557				
6	-5.171031	0.220226	-1.057821	15	-0.679275	1.639806	-0.494088
1	-4.402071	-0.090105	0.913659	6	0.341411	3.165010	-0.592526
6	-3.728281	-0.433653	-2.885183	6	1.477208	3.220424	-1.418220
1	-1.830972	-1.258582	-2.337620	6	2.310826	4.329866	-1.416520
6	-4.934709	0.096612	-2.428445	6	2.028678	5.417450	-0.580988
1	-6.094301	0.663165	-0.703402	6	0.904053	5.379400	0.249619
1	-3.543970	-0.524846	-3.949218	6	0.073992	4.258183	0.238630
6	-1.242825	-2.910013	-0.071417	6	-2.397340	2.272932	-0.399590
6	-2.182290	-3.742429	-0.702364	6	-2.892923	2.568453	0.885956
6	0.083549	-3.337980	0.041767	6	-3.251415	2.427280	-1.492146
6	-1.792448	-4.976591	-1.211931	6	-0.424874	0.903808	-2.146419
1	-3.212645	-3.420679	-0.806715	6	0.125776	-0.387458	-2.204129
6	0.479505	-4.572526	-0.468702	6	-0.675577	1.567501	-3.354483
1	0.812010	-2.706671	0.529799	1	-0.784422	4.238200	0.897965
6	-0.460387	-5.387993	-1.097383	1	-2.236790	2.456911	1.745137
1	-2.516845	-5.622731	-1.695228	1	-2.919546	2.165607	-2.487600
1	1.512397	-4.880831	-0.366667	1	0.389815	-0.899328	-1.287973
6	-0.030798	-6.690268	-1.716095	8	2.857445	-1.938504	-1.642720
6	-5.993504	0.560013	-3.387327	16	3.424688	-2.102671	-0.298547
6	-4.777024	-2.105712	5.807586	7	2.836567	-0.839647	0.639823
6	-5.820252	3.915778	-0.130556	8	3.200371	-3.340615	0.459875
6	1.061311	-1.178522	-5.717471	6	5.194055	-1.890564	-0.454687
6	3.736469	6.463857	-0.505706	6	5.720878	-1.405112	-1.650750

IM3_{PPh3}-OCH₃

6	6.016571	-2.140476	0.645376	6	-0.462512	0.940379	-4.581891
1	5.057697	-1.226323	-2.489297	6	4.541638	4.545278	1.690064
6	7.088788	-1.155317	-1.736744	1	5.437114	5.101271	1.994881
6	7.379402	-1.879301	0.543533	1	3.698068	4.946922	2.265962
1	5.595007	-2.538608	1.560948	1	4.352773	4.736634	0.634879
1	7.505923	-0.776115	-2.665499	1	5.097041	0.842593	-0.408395
6	7.935695	-1.381067	-0.643562	1	1.709476	2.389891	-2.074914
1	8.024484	-2.065584	1.397680	28	-0.266163	0.144135	1.173032
6	9.418077	-1.126384	-0.748614	1	0.665353	6.205806	0.907613
1	9.829348	-0.769146	0.199924	1	3.188730	4.375103	-2.052123
1	9.642195	-0.384858	-1.520113	1	-5.211254	2.930928	-2.193831
1	9.954732	-2.046354	-1.010670	1	-4.594102	3.217046	2.047373
1	-1.021416	2.595736	-3.346697	1	0.800441	-2.010851	-3.442399
6	2.932517	0.508580	0.026995	1	-0.675089	1.479102	-5.497198
1	2.698029	0.389811	-1.031500	15	-1.887828	-1.453853	0.582275
1	2.130297	1.097970	0.466848	6	-2.688585	-1.915478	2.164638
6	0.545877	-1.040960	2.593053	6	-3.185731	-3.197973	2.439946
6	1.916754	-0.484899	3.027084	6	-2.826768	-0.921406	3.140743
1	-0.135829	-1.019882	3.451748	6	-3.806996	-3.473689	3.650469
6	1.752229	1.050690	3.111532	1	-3.075537	-3.989320	1.706445
6	0.462147	1.423965	2.380202	6	-3.461852	-1.180267	4.355657
1	2.580715	1.603778	2.658391	1	-2.417930	0.067849	2.955699
1	1.674416	1.403999	4.147565	6	-3.953864	-2.465408	4.614137
8	-0.180194	2.412753	2.713474	1	-4.186683	-4.464336	3.877260
1	0.615411	-2.084665	2.266693	1	-3.551438	-0.386689	5.087140
6	3.066333	-0.946631	2.093740	6	-3.341106	-0.993421	-0.451675
1	3.227127	-2.005562	2.293860	6	-4.535266	-0.540232	0.131856
1	3.985225	-0.403903	2.356550	6	-3.259792	-1.025695	-1.848971
6	2.311876	-1.027908	4.418802	6	-5.603865	-0.131210	-0.651358
1	2.330461	-2.123182	4.419079	1	-4.629763	-0.502712	1.210464
1	1.582410	-0.703977	5.167184	6	-4.328079	-0.614847	-2.648416
1	3.300513	-0.670264	4.736451	1	-2.355318	-1.375852	-2.332417
6	4.273282	1.193162	0.210355	6	-5.501629	-0.153139	-2.046045
6	4.495182	2.145893	1.080841	1	-6.519261	0.235101	-0.199436
6	4.713564	3.072864	1.981875	1	-4.221215	-0.645959	-3.725813
6	5.118257	2.706308	3.393592	6	-1.360860	-3.022632	-0.188472
1	6.071600	3.180729	3.657612	6	-2.251400	-3.918743	-0.809383
1	5.220655	1.626398	3.518486	6	0.001422	-3.334024	-0.188887
1	4.367597	3.065160	4.108727	6	-1.785628	-5.081283	-1.405569
6	-4.200260	3.001114	1.059611	1	-3.311810	-3.691619	-0.841786
6	-5.052549	3.130086	-0.045873	6	0.485892	-4.497226	-0.784205
6	-4.566105	2.860762	-1.327647	1	0.702890	-2.655989	0.277656
6	0.358828	-1.021938	-3.415570	6	-0.411935	-5.375183	-1.398926
6	0.044506	-0.367633	-4.613988	1	-2.461876	-5.776645	-1.891720

1	1.550742	-4.681988	-0.756411	6	-6.928374	-2.675515	-0.492717
8	-6.589070	0.326008	-2.727679	1	-4.959208	-3.169851	-1.233109
8	-0.050345	-6.531139	-2.021043	1	-7.559063	-0.900044	2.331946
8	-4.580866	-2.834420	5.766837	6	-7.677010	-2.039404	0.506750
8	-6.339664	3.489438	0.224420	1	-7.443523	-3.192141	-1.297663
8	2.915710	6.455420	-0.639240	6	-9.183965	-2.084956	0.488897
8	0.286580	-1.067961	-5.756464	1	-9.568597	-2.184571	-0.529760
6	-7.253389	3.530404	-0.862833	1	-9.615808	-1.183178	0.932091
1	-8.225398	3.770275	-0.429318	1	-9.554800	-2.941622	1.064699
1	-6.981184	4.310076	-1.586471	6	-3.024585	0.807898	0.239266
1	-7.308184	2.564918	-1.380308	1	-3.036332	0.650420	1.318675
6	-6.515433	0.360180	-4.142582	1	-2.179538	1.461202	0.027948
1	-6.389293	-0.644598	-4.565061	6	-0.409737	-1.020495	-2.174002
1	-7.462401	0.778493	-4.486774	6	-1.668139	-0.278026	-2.694882
1	-5.690004	0.996506	-4.487938	1	0.196740	-1.328775	-3.034273
6	-4.738707	-1.854067	6.779093	6	-1.330160	1.241014	-2.703534
1	-5.344938	-1.007923	6.431103	6	0.149594	1.281927	-2.340248
1	-5.253222	-2.350471	7.602992	1	-1.891684	1.799823	-1.949684
1	-3.769802	-1.477727	7.131042	1	-1.513226	1.724915	-3.671449
6	1.332951	-6.851146	-2.058358	8	0.973616	1.848800	-3.046984
1	1.744104	-6.977837	-1.049424	1	-0.701085	-1.926131	-1.635933
1	1.409306	-7.793600	-2.602393	6	-2.908848	-0.628039	-1.849357
1	1.909587	-6.078576	-2.581647	1	-3.154359	-1.670274	-2.055914
6	0.000563	-0.443691	-6.996514	1	-3.762531	-0.014972	-2.162090
1	0.603385	0.461784	-7.142530	6	-2.002964	-0.721952	-4.133169
1	0.254352	-1.172575	-7.767233	1	-2.122625	-1.810051	-4.184426
1	-1.062099	-0.182213	-7.081955	1	-1.189548	-0.440519	-4.808985
6	2.704754	7.554508	0.231297	1	-2.925260	-0.257699	-4.506296
1	2.728326	7.244251	1.283469	6	-4.312028	1.449340	-0.227884
1	3.522470	8.251391	0.042297	6	-4.362700	2.621407	-0.808781
1	1.749148	8.053941	0.027373	6	-4.402489	3.792173	-1.397835
IM3_{PCy3}				6	-4.257350	3.925243	-2.897905
				1	-5.141359	4.410196	-3.330145
				1	-4.119249	2.954852	-3.377889
15	1.272957	1.815809	0.528796	1	-3.391790	4.554303	-3.138887
8	-2.671159	-1.542523	1.908540	6	-4.610378	5.072515	-0.620072
16	-3.099232	-1.846323	0.536639	1	-5.550367	5.551654	-0.921465
7	-2.746310	-0.499508	-0.387673	1	-3.804909	5.784744	-0.829765
8	-2.574117	-3.014025	-0.180459	1	-4.643241	4.892432	0.456261
6	-4.881252	-1.995642	0.567761	1	-5.227444	0.877586	-0.073831
6	-5.601854	-1.363556	1.583032	28	0.721451	0.139032	-0.964506
6	-5.536026	-2.660568	-0.469931	15	1.976070	-1.780997	-0.310950
1	-5.071329	-0.872942	2.390907	6	0.887280	-3.155328	0.358665
6	-6.993220	-1.389073	1.543847	6	1.298871	-4.615068	0.095271

6	0.574741	-2.885745	1.844175	1	4.598809	-2.109671	3.354388
1	-0.053673	-2.999286	-0.177939	1	6.341586	0.268507	0.919528
6	0.272818	-5.592578	0.687325	1	5.063203	0.215326	2.128721
1	2.281965	-4.830744	0.527115	1	6.884886	-1.341745	2.785407
1	1.382156	-4.784976	-0.982766	1	6.795066	-2.142441	1.220380
6	-0.394698	-3.917452	2.436535	6	3.021029	2.481094	0.428391
1	1.496362	-2.885562	2.438457	6	3.492548	2.518149	-1.040252
1	0.137652	-1.889375	1.931841	6	3.362535	3.809895	1.128126
6	0.081890	-5.351385	2.188598	1	3.595099	1.697870	0.940856
1	0.593377	-6.623875	0.496197	6	4.993586	2.815999	-1.135961
1	-0.690272	-5.454316	0.178875	1	2.930318	3.283992	-1.584352
1	-0.517862	-3.725626	3.509122	1	3.247687	1.578668	-1.540697
1	-1.376962	-3.782754	1.978168	6	4.872715	4.083882	1.049393
1	-0.637986	-6.067516	2.602058	1	2.831376	4.632022	0.637302
1	1.035089	-5.526184	2.709644	1	3.038959	3.804167	2.170609
6	2.632528	-2.399273	-1.958137	6	5.361053	4.112556	-0.403932
6	3.064975	-1.225051	-2.864076	1	5.293831	2.872505	-2.188634
6	3.726617	-3.483435	-1.973733	1	5.557284	1.982919	-0.693269
1	1.727978	-2.831969	-2.408208	1	5.106361	5.030539	1.551008
6	3.313401	-1.704976	-4.299226	1	5.408922	3.296474	1.598152
1	3.988451	-0.783059	-2.470168	1	6.443824	4.280618	-0.439542
1	2.312008	-0.434251	-2.856395	1	4.893198	4.962121	-0.920829
6	3.972178	-3.980511	-3.407312	6	1.127179	1.091323	2.255506
1	4.661292	-3.063040	-1.584823	6	1.828215	1.798517	3.428826
1	3.469605	-4.324640	-1.328775	6	-0.345186	0.750816	2.556235
6	4.355513	-2.829302	-4.345371	1	1.636934	0.129236	2.128822
1	3.630172	-0.861794	-4.923746	6	1.640253	1.016905	4.737748
1	2.365600	-2.068637	-4.720615	1	1.437828	2.811929	3.562946
1	4.753854	-4.749737	-3.406489	1	2.897512	1.898464	3.215994
1	3.057114	-4.463264	-3.778448	6	-0.512853	0.021399	3.895216
1	4.480711	-3.197886	-5.370355	1	-0.947674	1.666302	2.580234
1	5.330362	-2.426499	-4.035237	1	-0.744490	0.134276	1.746865
6	3.445078	-1.669747	0.860631	6	0.155871	0.785064	5.042216
6	4.088860	-2.947557	1.431500	1	2.127763	1.552092	5.561155
6	4.544120	-0.765496	0.274652	1	2.144695	0.043658	4.652174
1	3.018896	-1.131430	1.718441	1	-1.577888	-0.140822	4.088801
6	5.121837	-2.583283	2.511154	1	-0.060856	-0.974782	3.824696
1	4.579777	-3.508491	0.629708	1	0.040719	0.237013	5.984540
1	3.336424	-3.609099	1.863441	1	-0.340515	1.756643	5.180369
6	5.565682	-0.376020	1.349394	6	0.102349	3.291022	0.474153
1	5.064890	-1.301204	-0.526634	6	-0.051183	4.177418	1.725629
1	4.105198	0.118549	-0.186564	6	0.334557	4.185996	-0.762095
6	6.195306	-1.624013	1.981475	1	-0.865476	2.797306	0.320752
1	5.587537	-3.494294	2.905051	6	-1.215475	5.164969	1.545108

1	0.874483	4.735041	1.904335	1	-7.318681	-4.456459	-2.412377
1	-0.232714	3.574167	2.616211	1	2.086586	-0.635702	4.691881
6	-0.832356	5.163936	-0.949257	6	-2.587658	0.525606	0.085125
1	1.257508	4.760886	-0.625324	1	-2.576394	-0.295851	0.800633
1	0.470834	3.590774	-1.662798	1	-2.100406	1.359440	0.583500
6	-1.035819	6.034093	0.295850	6	0.733742	1.555830	-1.987406
1	-1.313319	5.792219	2.439153	6	-0.675798	2.120592	-2.215743
1	-2.151224	4.594983	1.455983	1	1.479634	2.303869	-2.274556
1	-0.654624	5.789877	-1.831671	6	-0.907287	3.114978	-1.069562
1	-1.745052	4.586707	-1.146411	6	-0.118227	2.638648	0.163098
1	-1.896039	6.702088	0.169620	1	-1.960476	3.285263	-0.814493
1	-0.156432	6.679664	0.429852	1	-0.489992	4.097683	-1.330754
IM3_{dppb}				8	-0.090876	3.350682	1.163985
				1	0.918658	0.654565	-2.586605
				6	-1.733024	0.995417	-2.251961
15	0.861592	0.434155	2.171682	1	-1.519569	0.367718	-3.117703
6	-0.820503	0.368784	2.915475	1	-2.732201	1.429082	-2.382042
6	-1.474812	-0.862564	3.072714	6	-0.781769	2.834428	-3.578063
6	-2.795880	-0.908638	3.518509	1	-0.557111	2.145582	-4.400040
6	-3.481066	0.270853	3.815447	1	-0.065033	3.659879	-3.628508
6	-2.830997	1.497744	3.674284	1	-1.784166	3.248369	-3.748875
6	-1.510293	1.550526	3.228549	6	-4.009303	0.901708	-0.266975
6	1.545179	-1.193849	2.673597	6	-4.483148	2.094145	-0.008454
6	1.518093	-2.242169	1.745162	6	-4.887731	3.300649	0.304338
6	2.085449	-1.425646	3.948111	6	-4.789985	4.453495	-0.669623
1	-1.033182	2.510483	3.076650	1	-5.779546	4.890027	-0.854894
1	1.067817	-2.083738	0.775357	1	-4.365031	4.139212	-1.625070
8	-1.078957	-2.060896	0.008594	1	-4.158169	5.249171	-0.256022
16	-1.554443	-1.513980	-1.269290	6	2.048325	-3.491159	2.070479
7	-1.757382	0.124483	-1.067489	6	2.610231	-3.704565	3.328595
8	-0.783899	-1.716802	-2.503929	1	3.034454	-4.672281	3.580233
6	-3.193305	-2.179167	-1.527309	6	2.620979	-2.671699	4.270377
6	-3.921722	-2.650468	-0.435086	6	-5.463181	3.606397	1.669500
6	-3.769013	-2.101308	-2.796895	1	-6.486152	3.994299	1.584167
1	-3.450132	-2.704669	0.539415	1	-4.866136	4.380352	2.168047
6	-5.246397	-3.039344	-0.621611	1	-5.477208	2.718292	2.304181
6	-5.092854	-2.495576	-2.964670	1	-4.638267	0.137727	-0.722503
1	-3.181052	-1.744752	-3.635114	1	-4.511594	0.233834	4.156322
1	-5.820426	-3.404289	0.225516	1	-0.961342	-1.783307	2.824223
6	-5.852200	-2.965545	-1.882747	28	0.994781	1.088469	-0.067706
1	-5.547102	-2.438328	-3.950000	1	-3.354581	2.421303	3.902369
6	-7.278762	-3.411289	-2.082164	1	-3.289387	-1.869887	3.632020
1	-7.781651	-2.810004	-2.845062	1	2.032397	-4.283792	1.329706
1	-7.853318	-3.338510	-1.154809	1	3.045060	-2.837949	5.256449

15	3.069864	0.150320	-0.423472	6	2.089999	4.304822	-0.143575
6	4.060198	1.042855	-1.692607	6	1.392600	1.008757	2.400534
6	4.870035	0.380513	-2.623564	6	0.514055	-0.078811	2.464175
6	4.012713	2.446245	-1.712129	6	2.001306	1.465899	3.581766
6	5.623103	1.106051	-3.548508	1	2.599054	3.858069	-0.988822
1	4.910988	-0.703140	-2.628463	1	0.055143	-0.457075	1.560543
6	4.775546	3.169046	-2.626959	8	-2.169037	-1.721604	1.851666
1	3.359053	2.969661	-1.022319	16	-2.540309	-2.004308	0.458642
6	5.582271	2.500115	-3.550081	7	-1.898300	-0.771275	-0.483739
1	6.242175	0.578418	-4.268389	8	-2.153500	-3.274156	-0.169160
1	4.729049	4.254168	-2.628172	6	-4.318856	-1.863179	0.350013
1	6.168947	3.062754	-4.270216	6	-5.003686	-1.115494	1.309267
6	4.126331	0.393045	1.088761	6	-4.988945	-2.420329	-0.740093
6	3.308149	-1.610710	-0.861580	1	-4.462653	-0.704715	2.153837
6	4.393152	-2.380513	-0.420815	6	-6.374345	-0.919715	1.163701
6	2.304740	-2.217759	-1.630712	6	-6.359745	-2.212666	-0.869936
6	4.466941	-3.737392	-0.735799	1	-4.443939	-3.017388	-1.461877
1	5.177097	-1.929662	0.178231	1	-6.913161	-0.339361	1.907482
6	2.380117	-3.573663	-1.944697	6	-7.071527	-1.459568	0.073681
1	1.445582	-1.644222	-1.959448	1	-6.887208	-2.643532	-1.716341
6	3.459744	-4.337132	-1.495104	6	-8.560401	-1.263547	-0.061236
1	5.307634	-4.327599	-0.382732	1	-8.871868	-1.279606	-1.109309
1	1.584239	-4.027957	-2.526467	1	-8.879116	-0.313566	0.376770
1	3.515956	-5.395677	-1.732030	1	-9.107211	-2.061852	0.455256
6	1.734648	1.670531	3.247897	1	2.683142	2.310796	3.549265
1	1.405737	1.548788	4.285569	6	-2.002010	0.591094	0.080919
1	1.340520	2.624587	2.884069	1	-2.007911	0.479594	1.166939
6	3.271925	1.684256	3.181040	1	-1.073895	1.105864	-0.176482
1	3.597488	2.558886	3.756823	6	0.484577	-0.953655	-2.334132
1	3.680287	0.810046	3.700087	6	-0.887649	-0.491369	-2.854716
6	3.894169	1.767051	1.773396	1	1.212757	-0.929561	-3.155939
1	3.260962	2.410265	1.151953	6	-0.807050	1.036094	-3.014499
1	4.858884	2.277445	1.851228	6	0.305903	1.588843	-2.110314
1	3.883112	-0.424423	1.772297	1	-1.749675	1.541063	-2.787505
1	5.177709	0.279075	0.809421	1	-0.543495	1.316847	-4.042462
IM3_{dppc}				8	0.720414	2.726722	-2.280112
				1	0.450463	-1.986221	-1.966068
				6	-2.056407	-0.947350	-1.941248
15	1.822654	1.681799	0.751237	1	-2.176984	-2.018906	-2.098241
6	1.584127	3.487595	0.879775	1	-2.979186	-0.448461	-2.270330
6	0.852274	4.072853	1.922834	6	-1.198708	-1.134032	-4.225460
6	0.657844	5.453871	1.959162	1	-1.172561	-2.227225	-4.159340
6	1.184562	6.263135	0.952042	1	-0.451659	-0.823930	-4.962348
6	1.896215	5.683915	-0.101067	1	-2.186214	-0.840208	-4.604597

6	-3.175517	1.443247	-0.360372	1	-0.435270	-4.420017	1.512878
6	-2.966188	2.667862	-0.780152	1	1.066014	-5.357239	3.283146
6	-2.598410	3.871362	-1.147522	6	3.677900	1.433865	0.764085
6	-2.331450	4.238824	-2.590551	1	4.158348	2.025632	1.549296
1	-2.748362	5.226825	-2.818007	1	4.054599	1.784163	-0.202137
1	-2.762791	3.514125	-3.283525	6	3.954682	-0.068222	0.952615
1	-1.249086	4.270923	-2.762833	1	3.772481	-0.340717	1.994690
6	0.242174	-0.706054	3.680872	1	4.991267	-0.316185	0.710110
6	0.852521	-0.247373	4.846496				
1	0.649839	-0.735025	5.795602	IM3_{dppp}			
6	1.730590	0.841203	4.797012				
6	-2.344010	4.956148	-0.124850	15	1.423179	2.077714	0.773963
1	-2.983701	5.827756	-0.313045	6	0.298566	3.498878	1.065353
1	-1.302913	5.290476	-0.194627	6	0.288263	4.572821	0.160277
1	-2.520697	4.604028	0.893383	6	-0.579105	5.646173	0.354529
1	-4.181867	1.046564	-0.233404	6	-1.456591	5.657422	1.440788
1	1.033053	7.338094	0.981285	6	-1.472142	4.580191	2.326736
1	0.437349	3.451426	2.708279	6	-0.600104	3.506761	2.142005
28	1.169472	0.315144	-0.946775	6	1.398806	1.197658	2.385057
1	2.292320	6.305827	-0.898120	6	0.752265	-0.042997	2.434237
1	0.091456	5.895305	2.773863	6	1.988368	1.703731	3.554537
1	-0.441075	-1.547250	3.692606	1	-0.611447	2.679658	2.843067
1	2.205773	1.198987	5.705876	1	0.294683	-0.448713	1.541753
15	2.775992	-1.093028	-0.103168	8	-1.636846	-1.972517	1.830980
6	3.866537	-1.770075	-1.408320	16	-1.979034	-2.302057	0.441207
6	4.481512	-3.025150	-1.324381	7	-1.653840	-0.937080	-0.482297
6	4.088251	-0.968335	-2.538906	8	-1.342937	-3.438870	-0.236875
6	5.317450	-3.465286	-2.351412	6	-3.746375	-2.576014	0.395797
1	4.299188	-3.659774	-0.463385	6	-4.536286	-2.103866	1.445001
6	4.933337	-1.406107	-3.557143	6	-4.322935	-3.187337	-0.718533
1	3.574441	-0.014531	-2.622934	1	-4.061840	-1.645211	2.304849
6	5.548965	-2.656296	-3.465000	6	-5.919917	-2.236933	1.365046
1	5.785842	-4.442760	-2.282319	6	-5.708551	-3.308530	-0.782894
1	5.098622	-0.779164	-4.428336	1	-3.693698	-3.573156	-1.511899
1	6.198696	-3.002821	-4.263132	1	-6.539926	-1.871730	2.179060
6	2.320660	-2.505502	0.959742	6	-6.526852	-2.834520	0.251525
6	3.162119	-3.032764	1.950395	1	-6.163355	-3.781524	-1.648723
6	1.027318	-3.025735	0.810568	6	-8.024456	-2.995939	0.185089
6	2.709805	-4.057962	2.780571	1	-8.379711	-3.004076	-0.849036
1	4.166307	-2.640976	2.081633	1	-8.536687	-2.189610	0.717435
6	0.576601	-4.051460	1.639365	1	-8.335564	-3.941419	0.645873
1	0.360844	-2.609954	0.065356	1	2.469299	2.676907	3.549544
6	1.417027	-4.565466	2.627793	6	-2.059365	0.360354	0.105942
1	3.364562	-4.457130	3.549782	1	-1.935874	0.269420	1.186855

1	-1.331939	1.098051	-0.234543	6	5.673882	-2.704012	-2.515291
6	0.678255	-0.707129	-2.367501	1	4.839992	-2.906931	-0.540088
6	-0.758733	-0.434287	-2.851741	6	4.920161	-0.796716	-3.793187
1	1.373788	-0.572248	-3.204928	1	3.458386	0.459668	-2.825872
6	-0.912395	1.099146	-2.941269	6	5.706635	-1.945110	-3.686703
6	0.205426	1.748084	-2.116527	1	6.277301	-3.603335	-2.432472
1	-1.876086	1.458864	-2.568003	1	4.933423	-0.208560	-4.706039
1	-0.824206	1.463721	-3.972560	1	6.336498	-2.252366	-4.516313
8	0.568287	2.892215	-2.353456	6	2.828716	-1.996896	0.938505
1	0.796775	-1.739052	-2.015068	6	3.692495	-2.286092	2.003679
6	-1.814014	-1.109624	-1.940588	6	1.693539	-2.796518	0.741319
1	-1.745878	-2.180996	-2.126973	6	3.416385	-3.351618	2.860968
1	-2.817384	-0.773085	-2.236446	1	4.573528	-1.677506	2.177503
6	-0.995899	-1.053942	-4.246954	6	1.421281	-3.862930	1.594487
1	-0.797743	-2.131365	-4.234343	1	0.999701	-2.566918	-0.057831
1	-0.322377	-0.597256	-4.978433	6	2.281188	-4.139080	2.659421
1	-2.025193	-0.901558	-4.597479	1	4.085846	-3.562433	3.689927
6	-3.464389	0.814716	-0.230281	1	0.523688	-4.448947	1.430817
6	-3.716351	1.947866	-0.836585	1	2.065000	-4.961433	3.335216
6	-3.927363	3.096725	-1.430877	6	4.247938	0.550227	0.728507
6	-4.034681	3.212370	-2.935195	1	3.991829	0.558547	1.791527
1	-4.979118	3.694984	-3.215765	1	5.248699	0.120507	0.627230
1	-3.984908	2.237327	-3.423395	6	4.212433	1.979549	0.151018
1	-3.221220	3.835323	-3.326697	1	5.175343	2.466639	0.342745
6	0.705433	-0.779055	3.618389	1	4.108774	1.930838	-0.938516
6	1.316149	-0.280100	4.766859	6	3.102661	2.882752	0.721304
1	1.296205	-0.854516	5.688427	1	3.367843	3.232427	1.723871
6	1.953333	0.964929	4.735436	1	2.997011	3.770897	0.092345
6	-4.054519	4.381226	-0.644079				
1	-5.025833	4.855670	-0.833769	(R)-IM3			
1	-3.276221	5.088754	-0.951530				
1	-3.945120	4.209770	0.427570	8	5.594738	-2.032842	-1.642227
1	-4.286202	0.172666	0.083566	16	5.620464	-1.319755	-0.359364
1	-2.130976	6.495658	1.588867	7	4.090839	-1.590389	0.368116
1	0.928242	4.546849	-0.713345	8	6.707886	-1.562565	0.601964
28	1.192392	0.613926	-0.939794	6	5.576198	0.431362	-0.693404
1	-2.157788	4.575814	3.169159	6	4.873585	0.887371	-1.806774
1	-0.572512	6.473420	-0.349222	6	6.291030	1.309000	0.118725
1	0.201434	-1.738151	3.616887	1	4.376621	0.174770	-2.452138
1	2.420073	1.360506	5.632983	6	4.851546	2.250037	-2.080437
15	3.031617	-0.555381	-0.164410	6	6.266741	2.670443	-0.175096
6	4.073764	-1.161366	-1.548044	1	6.866906	0.920135	0.950788
6	4.864912	-2.313124	-1.448216	1	4.301899	2.614885	-2.943392
6	4.100159	-0.411158	-2.733230	6	5.535870	3.162117	-1.263989

1	6.820717	3.362525	0.452575	1	-6.587501	0.393812	2.449248
6	5.461391	4.642550	-1.535454	1	-6.336381	-0.615550	1.001300
1	5.331622	4.849182	-2.601380	6	-3.966420	0.207241	3.411327
1	6.361314	5.159533	-1.191392	1	-4.439009	1.096674	3.833974
1	4.606955	5.087289	-1.009739	1	-4.156315	-0.645681	4.068756
6	3.955894	-0.922484	1.677463	1	-2.890748	0.381969	3.362224
1	4.099742	-1.656979	2.479841	8	-3.818931	-1.152631	1.411732
1	4.760926	-0.190399	1.788535	8	-4.332111	1.051636	1.162432
6	1.404333	-2.519875	-0.443973	6	-2.236973	1.918447	0.233139
6	2.272003	-3.422159	0.439709	6	-2.575873	-1.496676	-0.653648
1	0.451316	-2.992228	-0.672096	8	-1.572822	-0.831458	-1.458901
6	1.650215	-3.278032	1.843187	8	-1.047597	1.483877	-0.456851
6	0.860029	-1.982150	1.797772	15	-0.300967	0.107550	-0.947294
1	2.377163	-3.249129	2.664504	7	0.259587	0.615982	-2.432171
1	0.946064	-4.086927	2.067473	6	1.622229	0.308072	-2.828472
8	-0.042591	-1.664009	2.536669	1	1.671568	-0.517829	-3.551807
1	1.898860	-2.230025	-1.379472	1	2.086247	1.194257	-3.278448
6	3.766874	-3.034816	0.364684	1	2.202626	0.036793	-1.944467
1	4.149319	-3.421155	-0.580333	6	-0.620874	1.161828	-3.454321
1	4.310628	-3.541568	1.177208	1	-1.530647	1.545409	-2.990584
6	2.209260	-4.895403	-0.015442	1	-0.123021	1.999176	-3.957314
1	2.534232	-4.990913	-1.056341	1	-0.888950	0.410156	-4.208826
1	1.186858	-5.270924	0.056500	6	-3.849721	-1.556737	-1.502472
1	2.855375	-5.534612	0.598529	6	-4.943122	-2.307310	-1.048900
6	2.624492	-0.210465	1.845012	6	-3.954472	-0.872169	-2.716489
6	2.226038	0.863817	1.048876	6	-6.124524	-2.348469	-1.785848
6	2.449109	2.163506	0.867578	1	-4.862813	-2.855208	-0.118756
6	1.779685	3.025949	-0.165270	6	-5.136724	-0.922371	-3.458492
1	1.111913	3.750913	0.318552	1	-3.107641	-0.304066	-3.077791
1	1.195023	2.442814	-0.872020	6	-6.227297	-1.654740	-2.993915
1	2.530989	3.601154	-0.720326	1	-6.964382	-2.931173	-1.419084
6	3.374930	2.911902	1.804225	1	-5.200823	-0.385267	-4.400246
1	2.785944	3.589539	2.437936	1	-7.147430	-1.692024	-3.569304
1	4.092111	3.527996	1.252463	6	-2.128754	-2.925080	-0.354789
1	3.931251	2.234778	2.455500	6	-2.047065	-3.451861	0.934863
1	2.206434	-0.280352	2.849519	6	-1.849455	-3.755109	-1.450453
28	1.255495	-0.741834	0.427028	6	-1.694618	-4.791652	1.123859
6	-2.786642	-0.618693	0.603933	1	-2.266211	-2.833679	1.793587
6	-3.296128	0.783176	0.229311	6	-1.496543	-5.086822	-1.262084
6	-4.529852	-0.078013	2.023535	1	-1.918391	-3.344941	-2.452541
1	-1.845381	-0.585084	1.169597	6	-1.424094	-5.612984	0.031486
1	-3.732889	0.755669	-0.771228	1	-1.640391	-5.189672	2.132808
6	-6.007898	-0.430281	2.025769	1	-1.282448	-5.716225	-2.120416
1	-6.180691	-1.326599	2.627217	1	-1.159565	-6.655327	0.182651

6	-1.857166	2.327719	1.654237	1	4.183898	-0.871613	-2.989731
6	-2.636977	3.250109	2.363009	1	4.927940	0.221191	-1.843830
6	-0.756703	1.746281	2.286291	6	1.347152	-2.340078	-0.454742
6	-2.322730	3.574302	3.681111	6	2.124731	-3.034361	-1.579723
1	-3.491279	3.712373	1.883735	1	0.351832	-2.771235	-0.332371
6	-0.440388	2.071657	3.605776	6	1.550530	-2.404226	-2.869656
1	-0.126102	1.054411	1.750160	6	0.768328	-1.207436	-2.361708
6	-1.224092	2.984156	4.310201	1	2.315920	-2.075957	-3.582296
1	-2.937178	4.291451	4.217504	1	0.870648	-3.070604	-3.413468
1	0.421342	1.606155	4.074345	8	-0.238044	-0.755649	-2.848143
1	-0.980458	3.238908	5.337411	1	1.870559	-2.354974	0.510187
6	-2.747068	3.119485	-0.571506	6	3.648831	-2.837074	-1.424335
6	-1.818623	3.990114	-1.155921	1	3.991134	-3.537536	-0.662506
6	-4.112869	3.385714	-0.722431	1	4.146623	-3.102553	-2.369940
6	-2.245759	5.098354	-1.883384	6	1.877702	-4.556435	-1.580533
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6	-4.538648	4.500531	-1.448748	1	0.815825	-4.768003	-1.740883
1	-4.847399	2.734758	-0.262618	1	2.447368	-5.061334	-2.369810
6	-3.609579	5.358720	-2.033628	6	2.796742	0.420286	-1.950202
1	-1.511768	5.760141	-2.334131	6	2.462251	1.246262	-0.878631
1	-5.602136	4.691879	-1.557313	6	2.789876	2.371301	-0.248415
1	-3.943073	6.222360	-2.601185	6	2.123662	2.888679	0.997971
(S)-IM3				1	1.760408	3.914610	0.848866
				1	1.284316	2.267971	1.306963
				1	2.844510	2.929492	1.824405
8	5.486686	-2.720300	0.776142	6	3.866863	3.276715	-0.808574
16	5.599909	-1.599412	-0.165461	1	3.422461	4.220385	-1.156000
7	4.095618	-1.500315	-0.975104	1	4.606863	3.536087	-0.044448
8	6.719307	-1.545803	-1.119092	1	4.387667	2.815514	-1.650029
6	5.623536	-0.086563	0.777709	1	2.386643	0.679068	-2.927982
6	4.836181	0.006578	1.924501	28	1.359773	-0.369674	-0.770163
6	6.486852	0.941347	0.408631	6	-3.100889	0.550729	-0.745480
1	4.210232	-0.828480	2.213515	6	-3.513178	-0.084863	0.584890
6	4.895002	1.164194	2.690854	6	-5.409515	0.223073	-0.749374
6	6.537412	2.093518	1.191321	1	-2.567396	-0.163057	-1.377132
1	7.115499	0.822773	-0.466457	1	-3.357044	0.620493	1.405695
1	4.286159	1.245637	3.586615	6	-6.488931	1.238240	-0.404442
6	5.736476	2.228009	2.331467	1	-6.855505	1.721443	-1.313899
1	7.207948	2.900839	0.911168	1	-7.326112	0.741690	0.093228
6	5.749735	3.500416	3.138757	1	-6.073460	2.001710	0.256057
1	5.581123	3.303263	4.201264	6	-5.888213	-0.898117	-1.663355
1	6.698907	4.032586	3.033926	1	-6.662682	-1.486054	-1.164574
1	4.954233	4.177199	2.802204	1	-6.300153	-0.476599	-2.584421
6	4.060098	-0.427949	-1.993681	1	-5.057594	-1.560040	-1.913373

8	-4.320637	0.918169	-1.361305	1	-1.731146	-2.238642	-1.538459
8	-4.898035	-0.341802	0.467975	6	-4.184131	-4.590154	-1.620038
6	-2.694261	-1.376943	0.878449	1	-5.640979	-4.897718	-0.059969
6	-2.172669	1.784486	-0.528244	1	-2.604892	-4.040909	-2.982069
8	-1.243277	1.443439	0.534805	1	-4.570094	-5.384374	-2.252059
8	-1.335771	-1.136816	0.451559	6	-2.694644	-1.750021	2.354607
15	-0.280507	0.108749	0.667887	6	-1.652127	-2.541649	2.851725
7	0.092266	0.287855	2.289976	6	-3.713603	-1.339953	3.218842
6	-0.805272	0.719833	3.352034	6	-1.614355	-2.894093	4.198211
1	-0.955642	-0.078975	4.086528	1	-0.866049	-2.861933	2.177009
1	-0.386317	1.598622	3.860350	6	-3.678077	-1.699200	4.568859
1	-1.775190	0.990621	2.942816	1	-4.540907	-0.749634	2.838975
6	1.388115	-0.193101	2.739757	6	-2.627048	-2.469455	5.063869
1	2.040817	-0.343267	1.877692	1	-0.796177	-3.501759	4.573465
1	1.857622	0.554399	3.390991	1	-4.473496	-1.371998	5.231744
1	1.301941	-1.137292	3.295170	1	-2.597482	-2.742910	6.114251
6	-2.973046	2.977954	-0.003590				
6	-3.785902	3.704536	-0.884415	IM4			
6	-2.942271	3.347907	1.343701				
6	-4.567796	4.758516	-0.420457	15	0.912797	1.868772	0.266310
1	-3.805515	3.439393	-1.933817	6	1.002772	1.209825	1.979502
6	-3.724458	4.408259	1.808258	6	1.733965	1.829303	3.001758
1	-2.289305	2.820442	2.024855	6	1.813912	1.236970	4.261734
6	-4.545253	5.112866	0.930727	6	1.174975	0.018241	4.508585
1	-5.194659	5.307046	-1.117192	6	0.431970	-0.595811	3.499154
1	-3.684685	4.682309	2.858516	6	0.336371	0.005218	2.244145
1	-5.154469	5.936470	1.290950	6	-0.504614	3.030746	0.357487
6	-1.416670	2.164214	-1.795954	6	-1.398859	3.010978	1.434756
6	-1.888979	1.820378	-3.065982	6	-0.742893	3.911988	-0.708423
6	-0.245982	2.917056	-1.683616	6	3.554211	2.478285	-0.378901
6	-1.184203	2.207700	-4.205305	6	2.361296	2.985280	0.150566
1	-2.804064	1.249313	-3.171252	1	2.260216	2.756574	2.804675
6	0.467011	3.289823	-2.820087	1	-1.216680	2.351279	2.275233
1	0.110417	3.192504	-0.700705	1	-0.050785	3.955261	-1.538638
6	0.000622	2.933832	-4.086639	1	3.587150	1.461795	-0.748801
1	-1.556876	1.927481	-5.185835	8	-6.561400	0.214881	-0.494972
1	1.389047	3.852598	-2.713916	16	-5.236987	0.729234	-0.128672
1	0.554102	3.225240	-4.974587	7	-4.198483	0.388568	-1.384940
6	-3.189432	-2.536954	0.015276	8	-5.027783	2.136187	0.227152
6	-4.290746	-3.298220	0.422465	6	-4.654363	-0.248554	1.252318
6	-2.585247	-2.817617	-1.215436	6	-2.848275	0.994037	-1.299615
6	-4.784784	-4.316655	-0.389505	6	-3.668226	0.272078	2.089604
1	-4.764248	-3.090274	1.374518	6	-5.092469	-1.565458	1.399001
6	-3.082927	-3.838543	-2.028062	1	-2.443323	0.880095	-0.287280

1	-2.927452	2.065585	-1.491283	1	-3.235721	3.778707	2.252288
1	-3.364672	1.303607	1.973089	1	-0.050989	-1.551265	3.671249
6	-3.099061	-0.544271	3.064284	1	2.388228	1.718689	5.047549
6	-4.511681	-2.370026	2.375518	6	-0.102118	1.924142	-3.189768
1	-5.879631	-1.941884	0.755928	6	1.330166	2.401419	-3.262450
1	-2.330642	-0.140649	3.716066	6	-0.998164	2.564656	-4.227900
6	-3.497514	-1.879136	3.210919	1	1.732136	2.238439	-4.271350
1	-4.850604	-3.395596	2.494000	1	1.971313	1.868105	-2.559452
6	-2.836060	-2.769467	4.232470	1	-1.025167	3.653809	-4.079614
1	-2.540254	-2.205106	5.121719	1	-0.614340	2.397979	-5.243068
1	-1.929357	-3.226139	3.817922	1	-2.320403	0.469941	-3.290421
1	-3.498691	-3.580554	4.547138	6	-1.597031	-1.173123	-2.046641
6	-2.385474	-2.020744	-3.084438	8	-0.227378	-1.395284	-1.911232
1	-2.542662	-1.605364	-4.086803	1	1.427034	3.479269	-3.063791
1	-1.948690	-3.020670	-3.164641	1	-2.028504	2.208081	-4.189170
6	-3.580724	-2.017997	-2.082018	15	2.340916	-1.456634	-0.292972
6	-2.522798	-1.812809	-0.969159	6	3.912414	-0.845296	0.429912
1	-2.112980	-2.786117	-0.687802	6	5.059372	-0.697718	-0.365999
6	-4.430813	-3.281768	-2.025912	6	3.935749	-0.355060	1.745471
1	-5.105145	-3.265343	-1.162018	6	6.196702	-0.068162	0.141043
1	-3.799622	-4.172704	-1.946349	1	5.061945	-1.073961	-1.383022
1	-5.047641	-3.388258	-2.926569	6	5.073127	0.273187	2.247733
6	-4.485204	-0.761674	-2.256920	1	3.066056	-0.462272	2.379566
1	-5.527024	-1.020607	-2.068696	6	6.206178	0.423636	1.447050
1	-4.442782	-0.414388	-3.295554	1	7.076678	0.035511	-0.487125
1	-2.780361	-1.265763	-0.064565	1	5.066012	0.651206	3.265508
6	-1.880233	0.351133	-2.294162	1	7.089751	0.919023	1.837760
6	-0.523209	1.026933	-2.284081	6	2.907440	-2.498347	-1.691211
6	4.699868	3.269787	-0.424274	6	3.806704	-3.554716	-1.479634
6	4.660140	4.582584	0.047420	6	2.439975	-2.231936	-2.984105
1	5.550467	5.203050	0.007352	6	4.248929	-4.324041	-2.552555
6	3.471200	5.100476	0.565564	1	4.160075	-3.771105	-0.475907
6	2.325402	4.306905	0.619126	6	2.888032	-3.006828	-4.056494
1	1.402002	4.713405	1.017489	1	1.692157	-1.461008	-3.130694
6	-2.533169	3.823770	1.426659	6	3.792534	-4.046556	-3.844681
6	-2.778412	4.675014	0.351427	1	4.945272	-5.140035	-2.383145
1	-3.674651	5.285957	0.336557	1	2.518963	-2.800563	-5.056710
6	-1.869343	4.730994	-0.706761	1	4.137002	-4.647520	-4.681280
1	-0.234306	-0.477262	1.457918	6	1.704305	-2.678678	0.920589
1	1.260762	-0.452377	5.483395	6	2.436743	-3.202657	1.991634
28	0.642935	0.101254	-1.090485	6	0.369659	-3.069007	0.736437
1	3.434688	6.123589	0.927716	6	1.829835	-4.088320	2.884341
1	5.618819	2.856256	-0.826470	1	3.470229	-2.911214	2.142448
1	-2.045268	5.401616	-1.542380	6	-0.231637	-3.953979	1.628182

1	-0.165458	-2.662029	-0.116178	6	2.271532	-1.590458	2.061499
6	0.495545	-4.460710	2.709792	1	1.498137	-3.236239	3.259169
1	2.401269	-4.487233	3.717405	1	1.644090	-1.696309	4.086138
1	-1.269019	-4.241178	1.481143	8	3.471082	-1.468852	2.175129
1	0.027506	-5.148255	3.408467	1	-0.665715	-0.412166	1.061747
IM4 _{dppp}				6	-0.906200	-2.848802	2.036624
				1	-1.934800	-2.483451	1.978584
				1	-0.920626	-3.740802	2.679726
15	-1.488706	1.867290	-0.006365	6	-0.890138	-1.328764	3.973490
6	-2.505100	1.542465	1.496017	1	-1.862894	-0.919571	3.690227
6	-3.436396	0.494034	1.412381	1	-0.354734	-0.558527	4.537658
6	-2.377509	2.226797	2.712580	1	-1.057849	-2.180644	4.643313
6	-2.579129	3.015748	-0.955604	6	1.848917	-2.951500	-0.060798
6	-3.717958	3.637759	-0.422973	6	1.666587	-2.137220	-1.160751
6	-2.271502	3.228746	-2.309501	6	1.384789	-2.111589	-2.460119
1	-3.533709	-0.061570	0.489034	6	1.036985	-0.871835	-3.238876
1	-1.661848	3.034900	2.815098	1	1.795770	-0.654620	-3.999568
1	-3.978212	3.477556	0.618009	1	0.937854	-0.005518	-2.586538
8	-2.695347	-4.675871	0.663310	1	0.084113	-1.012399	-3.766079
16	-1.795523	-3.917049	-0.219112	6	-4.230573	0.152378	2.504514
7	-0.519804	-3.222250	0.664024	6	-4.096580	0.843796	3.711066
8	-1.187155	-4.577740	-1.381788	1	-4.706627	0.573336	4.567595
6	-2.703215	-2.497608	-0.809910	6	-3.165371	1.877589	3.811865
6	-4.092967	-2.492647	-0.689427	6	-4.524147	4.448837	-1.223025
6	-2.034742	-1.501534	-1.520478	6	-4.201317	4.659387	-2.565021
1	-4.583031	-3.286467	-0.137517	1	-4.831560	5.289011	-3.185728
6	-4.818865	-1.465165	-1.291054	6	-3.067481	4.051404	-3.106164
6	-2.777960	-0.490613	-2.121796	6	1.348211	-3.395975	-3.260946
1	-0.954009	-1.518582	-1.580577	1	0.318521	-3.627041	-3.559067
1	-5.901014	-1.448907	-1.196410	1	1.723652	-4.241242	-2.682605
6	-4.175979	-0.451455	-2.015949	1	1.947151	-3.300790	-4.175829
1	-2.264686	0.293062	-2.667645	1	2.868510	-3.215956	0.220904
6	-4.958352	0.688433	-2.614905	1	-5.406067	4.918443	-0.796772
1	-5.979964	0.386234	-2.861607	1	-2.811261	4.206021	-4.150247
1	-4.479243	1.069846	-3.520022	1	-3.050213	2.416214	4.748018
1	-5.015797	1.526253	-1.910640	1	-4.943705	-0.661708	2.414013
1	-1.407041	2.734767	-2.746237	28	1.498573	-0.968211	0.452612
6	0.782351	-3.884242	0.487335	15	2.291426	1.039365	-0.353122
1	1.101622	-4.305498	1.446619	6	3.707423	0.577013	-1.435185
1	0.661164	-4.721230	-0.205535	6	4.665257	-0.284027	-0.871412
6	0.141019	-0.542295	1.789957	6	3.850550	0.973169	-2.768266
6	-0.078678	-1.734847	2.725367	6	5.745992	-0.724182	-1.628754
1	0.254991	0.385478	2.355303	1	4.548873	-0.617026	0.156663
6	1.346938	-2.156819	3.134972	6	4.932712	0.520678	-3.528956

1	3.117196	1.620912	-3.235518	1	3.977106	5.566850	0.240833
6	5.882538	-0.325927	-2.962305	1	2.231399	5.305631	0.342621
1	6.480880	-1.385905	-1.179860	1	3.034472	5.350543	-1.234258
1	5.027762	0.832691	-4.565028	6	2.432630	-2.828770	0.697493
1	6.722585	-0.677139	-3.553953	1	2.491563	-3.780520	0.157286
6	3.181812	2.010558	0.939209	1	3.108277	-2.903572	1.553437
6	4.145961	2.961122	0.568457	6	0.549640	-0.993745	-1.844513
6	2.889957	1.833294	2.295137	6	1.492884	-2.113748	-2.301801
6	4.789903	3.728969	1.535893	1	-0.234115	-0.826747	-2.589622
1	4.401536	3.088433	-0.479278	6	0.737115	-3.408880	-1.955213
6	3.536316	2.601566	3.265161	6	-0.258294	-3.032759	-0.864134
1	2.167571	1.083282	2.587310	1	1.370705	-4.246429	-1.638881
6	4.483890	3.551728	2.888016	1	0.148718	-3.772451	-2.807069
1	5.534651	4.460810	1.237217	8	-1.225257	-3.691553	-0.554882
1	3.303714	2.449684	4.315001	1	1.079660	-0.050155	-1.660505
1	4.989464	4.147268	3.642289	6	2.883422	-1.998376	-1.633057
6	-0.196453	3.043360	0.646358	1	3.393360	-1.153011	-2.101006
1	0.342832	2.497890	1.427189	1	3.475584	-2.893954	-1.873110
1	-0.654816	3.920245	1.115413	6	1.755693	-2.044215	-3.820655
6	0.786752	3.514834	-0.431775	1	2.192582	-1.078619	-4.095924
1	1.572348	4.100109	0.056595	1	0.818558	-2.159998	-4.373934
1	0.267044	4.197754	-1.114372	1	2.442575	-2.831359	-4.153394
6	1.447330	2.423402	-1.290801	6	1.019146	-2.593569	1.202502
1	2.193550	2.905272	-1.929305	6	0.617133	-1.422879	1.843765
1	0.708692	1.954783	-1.946219	6	0.877692	-0.718600	2.945806
IM4_{PCy3}				6	0.330249	0.652390	3.250936
				1	-0.400626	0.617859	4.069846
				1	-0.145081	1.104755	2.382426
				1	1.136023	1.319826	3.583908
15	-1.720033	0.269304	0.016674	6	1.816943	-1.259659	4.004551
8	5.437912	-1.230660	-0.530168	1	2.760864	-0.700880	3.999136
16	4.292250	-0.925810	0.339228	1	2.052763	-2.311377	3.834889
7	2.907658	-1.752843	-0.183208	1	1.378158	-1.157556	5.005642
8	4.386976	-1.135100	1.789387	1	0.467661	-3.506802	1.427126
6	3.864071	0.786507	0.068248	1	-0.085856	-1.347798	-0.013119
6	4.618681	1.556021	-0.814599	28	-2.857260	0.024324	-1.451109
6	2.856416	1.355162	0.846820	6	-3.501566	-1.375829	-1.431430
1	5.404501	1.085481	-1.394386	6	-3.932491	1.082045	-1.772715
6	4.357725	2.922158	-0.911774	1	-2.141854	0.030867	-2.284251
6	2.623297	2.722781	0.749817	1	-4.151750	-1.689039	-2.785719
1	2.274645	0.727916	1.509209	6	-4.271989	-1.406352	-0.650433
1	4.941379	3.530085	-1.597635	1	-2.767712	-2.140885	-1.176980
6	3.372071	3.527926	-0.121742	6	-4.567296	0.785451	-3.140775
1	1.853436	3.176834	1.366572	1	-4.714698	1.062941	-1.009817
6	3.136679	5.016020	-0.196882				

1	-3.519466	2.092974	-1.768440				
6	-5.179111	-0.620860	-3.180805	15	3.925849	-0.667636	-0.871951
1	-4.621780	-2.678449	-2.753112	6	5.057575	0.572377	-0.113159
1	-3.365817	-1.740554	-3.552569	6	6.338846	0.711869	-0.674981
1	-5.329393	1.539801	-3.369277	6	4.686955	1.442736	0.922609
1	-3.796916	0.870884	-3.920211	6	4.761586	-2.251855	-0.424165
1	-5.588073	-0.830186	-4.176037	6	5.527893	-2.414807	0.739988
1	-6.024417	-0.661105	-2.479399	6	4.574939	-3.353910	-1.270216
6	-1.066467	2.028991	-0.135738	1	6.643869	0.048886	-1.480548
6	-0.708826	2.376678	-1.597403	1	3.709337	1.362279	1.383400
6	-1.895194	3.154050	0.507758	1	5.688903	-1.566478	1.398280
1	-0.115790	1.973297	0.408440	8	0.695096	4.747910	1.071317
6	0.003734	3.731627	-1.695278	16	-0.345544	4.106378	0.255673
1	-1.617940	2.414031	-2.205193	7	-1.219291	3.007226	1.223996
1	-0.076466	1.597612	-2.027667	8	-1.332570	4.912911	-0.473241
6	-1.156120	4.497583	0.417620	6	0.489376	3.094137	-0.955203
1	-2.862681	3.244182	0.000398	6	1.877916	2.969206	-0.909030
1	-2.108906	2.922034	1.555874	6	-0.249480	2.559913	-2.011428
6	-0.806978	4.850942	-1.032876	1	2.433841	3.417227	-0.093766
1	0.193306	3.970094	-2.748454	6	2.530719	2.300005	-1.942529
1	0.981348	3.650546	-1.211501	6	0.420298	1.893156	-3.032971
1	-1.765303	5.288597	0.869980	1	-1.325701	2.668170	-2.024533
1	-0.232271	4.437492	1.009951	1	3.611493	2.210337	-1.916375
1	-0.253784	5.796564	-1.072249	6	1.815260	1.757429	-3.019317
1	-1.737556	5.008614	-1.596168	1	-0.149723	1.473923	-3.857279
6	-2.761296	0.190749	1.577427	6	2.540163	1.027417	-4.118684
6	-4.177151	0.795204	1.545850	1	3.292375	1.669485	-4.589622
6	-2.824375	-1.252101	2.121794	1	1.851691	0.685540	-4.895876
1	-2.173129	0.773565	2.295570	1	3.067721	0.159059	-3.707875
6	-4.799254	0.784780	2.950818	1	3.997316	-3.232562	-2.182868
1	-4.809760	0.196817	0.881104	6	-2.666696	3.247309	1.317599
1	-4.170352	1.812471	1.148670	1	-2.915911	3.487381	2.357873
6	-3.459317	-1.282298	3.517795	1	-2.912409	4.128359	0.720369
1	-3.408425	-1.878189	1.436828	6	-0.801219	0.141052	1.946404
1	-1.818973	-1.674430	2.157046	6	-0.846239	1.213668	3.038364
6	-4.848750	-0.634469	3.528417	1	-0.674083	-0.855768	2.378289
1	-5.805009	1.219706	2.914222	6	-2.261491	1.076881	3.631416
1	-4.202555	1.428257	3.612861	6	-3.082978	0.386280	2.549988
1	-3.516155	-2.316339	3.876476	1	-2.729945	2.020382	3.935678
1	-2.803420	-0.744368	4.217195	1	-2.272860	0.425543	4.513868
1	-5.259125	-0.619305	4.544725	8	-4.099172	-0.245274	2.737949
1	-5.533644	-1.242938	2.921339	1	-0.003175	0.323194	1.219290
				6	-0.528021	2.615890	2.465129
				1	0.541206	2.639279	2.249346

IM4_{dppb}

1	-0.706160	3.371820	3.244686	6	-2.588930	-3.060364	1.889566
6	0.217322	0.956101	4.125579	6	-0.782112	-5.118410	1.366710
1	1.220359	0.930491	3.686355	1	-0.273157	-4.037278	-0.407286
1	0.038970	-0.008817	4.609765	6	-2.477585	-4.133706	2.771301
1	0.209077	1.731181	4.901093	1	-3.292444	-2.263434	2.100802
6	-3.499911	2.070463	0.838375	6	-1.569819	-5.163581	2.516270
6	-3.401346	1.510641	-0.436362	1	-0.073891	-5.914808	1.157870
6	-3.685055	1.790820	-1.707772	1	-3.099465	-4.161230	3.661145
6	-3.376975	0.900403	-2.881113	1	-1.478403	-5.995778	3.207793
1	-4.297563	0.494267	-3.318982	6	2.523659	-0.715925	0.361955
1	-2.746349	0.062428	-2.598735	1	2.141182	0.304825	0.462282
1	-2.871374	1.467342	-3.674239	1	2.906889	-1.029238	1.338736
6	7.223040	1.682068	-0.210243	6	1.378898	-1.625868	-0.101583
6	6.838275	2.547232	0.817326	1	0.716968	-1.804091	0.748471
1	7.522701	3.310927	1.173698	1	1.768389	-2.610097	-0.391299
6	5.568791	2.424951	1.379919	6	-0.702199	-1.694117	-1.665723
6	6.089696	-3.651903	1.049709	1	-0.527547	-2.738442	-1.943665
6	5.888358	-4.746336	0.204302	1	-1.103197	-1.199210	-2.555154
1	6.326963	-5.709514	0.447665	6	0.599123	-0.992950	-1.258690
6	5.128444	-4.596638	-0.955479	1	0.359576	0.042137	-0.999632
6	-4.359703	3.097829	-2.073161	1	1.249040	-0.934862	-2.137653
1	-3.686677	3.728026	-2.669647				
1	-4.653606	3.664125	-1.187877	IM4_{dppe}			
1	-5.253139	2.917594	-2.685213				
1	-4.451956	1.960120	1.357793	15	-1.081125	1.910800	-0.014342
1	6.684263	-3.764705	1.951744	6	-2.010361	1.997790	1.570683
1	4.974120	-5.442319	-1.619321	6	-2.962096	0.991921	1.804040
1	5.260212	3.091425	2.179993	6	-1.799121	2.965431	2.563630
1	8.210428	1.768880	-0.654168	6	-2.020672	3.091272	-1.082071
28	-2.383883	0.347949	0.787302	6	-2.985194	3.989861	-0.605333
15	-2.045362	-1.563022	-0.390361	6	-1.767593	3.048724	-2.463451
6	-3.568026	-2.086275	-1.276193	1	-3.122713	0.224758	1.056438
6	-4.800034	-1.644458	-0.773586	1	-1.071529	3.755799	2.409640
6	-3.543345	-2.904178	-2.412494	1	-3.202275	4.031042	0.456880
6	-5.986977	-2.009978	-1.406240	8	-2.983273	-4.686324	0.322860
1	-4.822008	-1.008557	0.105870	16	-2.147822	-3.789482	-0.490253
6	-4.732083	-3.256082	-3.052231	7	-0.769111	-3.299031	0.372022
1	-2.599860	-3.265707	-2.808463	8	-1.676763	-4.218519	-1.813195
6	-5.955342	-2.808125	-2.551534	6	-3.047528	-2.262016	-0.692674
1	-6.936106	-1.661206	-1.010462	6	-4.317661	-2.128917	-0.131379
1	-4.702182	-3.881294	-3.939786	6	-2.509060	-1.269777	-1.510665
1	-6.880042	-3.081235	-3.051060	1	-4.715927	-2.930611	0.480005
6	-1.795233	-3.004552	0.732821	6	-5.049854	-0.970379	-0.387103
6	-0.897939	-4.048766	0.477510	6	-3.262790	-0.129693	-1.768978

1	-1.514278	-1.391025	-1.920226	1	-0.337686	-2.770374	-4.050466
1	-6.036127	-0.852661	0.053348	1	1.020152	-3.691525	-3.396130
6	-4.534563	0.044789	-1.205942	1	1.295229	-2.473413	-4.665044
1	-2.855733	0.648336	-2.403492	1	2.550887	-3.297469	-0.421182
6	-5.300959	1.322892	-1.425780	1	-4.427293	5.507475	-1.101291
1	-6.371502	1.133146	-1.549439	1	-2.240636	3.842112	-4.407815
1	-4.935595	1.865249	-2.300841	1	-2.342561	3.681347	4.519757
1	-5.178888	1.988682	-0.563709	1	-4.425434	0.175405	3.149255
1	-1.043418	2.337838	-2.853358	28	1.304142	-1.071980	0.312709
6	0.482684	-3.947582	-0.040759	15	2.316947	0.941729	-0.189769
1	0.890007	-4.504372	0.810417	6	3.591518	0.675491	-1.481183
1	0.264372	-4.676654	-0.826203	6	4.421603	-0.447916	-1.327102
6	0.029495	-0.828875	1.776621	6	3.747515	1.490062	-2.608095
6	-0.123478	-2.126956	2.573531	6	5.387797	-0.742917	-2.284112
1	0.177679	0.029519	2.436461	1	4.302181	-1.082825	-0.453145
6	1.320986	-2.608514	2.811668	6	4.710198	1.182843	-3.573784
6	2.174278	-1.961359	1.725001	1	3.123183	2.366178	-2.745666
1	1.455657	-3.697864	2.823418	6	5.530427	0.067500	-3.414603
1	1.710742	-2.242604	3.770841	1	6.026560	-1.611285	-2.152748
8	3.384772	-1.949441	1.711508	1	4.817805	1.819530	-4.447155
1	-0.829982	-0.622963	1.130884	1	6.277909	-0.170527	-4.165420
6	-1.011365	-3.146516	1.816046	6	3.347691	1.503692	1.234151
1	-2.043168	-2.801643	1.919713	6	4.543440	2.208026	1.028832
1	-0.954915	-4.125217	2.314976	6	2.910227	1.277387	2.544498
6	-0.831506	-1.877562	3.922167	6	5.280990	2.678411	2.113509
1	-1.807050	-1.407087	3.764880	1	4.902006	2.377755	0.018528
1	-0.234384	-1.203368	4.544276	6	3.645150	1.755456	3.630191
1	-0.984786	-2.807052	4.483547	1	2.002888	0.711734	2.709831
6	1.520687	-2.967594	-0.559007	6	4.832364	2.454874	3.417374
6	1.287609	-1.969926	-1.476395	1	6.208617	3.216532	1.941660
6	0.914588	-1.638972	-2.707851	1	3.293903	1.570873	4.641191
6	0.638117	-0.229591	-3.163979	1	5.409847	2.819532	4.261648
1	1.422913	0.128076	-3.841378	6	0.440049	2.947707	0.348361
1	0.563150	0.450840	-2.316278	1	0.764580	2.738425	1.372633
1	-0.308893	-0.187303	-3.718234	1	0.208288	4.015407	0.290816
6	-3.691806	0.960496	2.990833	6	1.556761	2.586665	-0.641336
6	-3.468894	1.926359	3.974560	1	2.348282	3.343106	-0.629760
1	-4.028007	1.897642	4.904981	1	1.164725	2.536325	-1.661828
6	-2.520537	2.927166	3.758660				
6	-3.677530	4.822039	-1.486065	(R)-IM4			
6	-3.412687	4.775162	-2.855791				
1	-3.955302	5.421160	-3.539305	8	6.705264	-1.971229	-0.350176
6	-2.450185	3.888838	-3.343154	16	6.066755	-1.100909	0.644028
6	0.718646	-2.709005	-3.761031	7	4.425792	-1.526463	0.670598

8	6.618743	-1.011762	2.005192	1	2.662462	1.920591	1.847864
6	5.993264	0.555606	-0.014467	1	1.859030	0.075502	2.212665
6	5.469441	0.757878	-1.292627	28	0.994226	-1.099366	-1.090258
6	6.547482	1.603562	0.714672	6	-2.902086	-0.533555	0.806960
1	5.033869	-0.071530	-1.836622	6	-3.342519	0.909987	0.522096
6	5.513419	2.033036	-1.841335	6	-4.463012	0.102651	2.411911
6	6.570693	2.880828	0.153027	1	-1.886259	-0.588016	1.211177
1	6.955045	1.408498	1.699983	1	-3.894981	0.945683	-0.419180
1	5.115578	2.199370	-2.838107	6	-5.958283	-0.170770	2.456805
6	6.055871	3.113650	-1.126811	1	-6.158675	-1.069115	3.046654
1	6.997391	3.705662	0.716384	1	-6.479856	0.673933	2.914273
6	6.052143	4.497711	-1.724322	1	-6.331201	-0.323020	1.442195
1	6.372133	4.480441	-2.770895	6	-3.839734	0.338485	3.781927
1	6.713425	5.173143	-1.175733	1	-4.257943	1.241035	4.234107
1	5.043642	4.928171	-1.701011	1	-4.043590	-0.514712	4.434801
6	3.682859	-0.886804	1.756968	1	-2.760378	0.465392	3.689964
1	3.775603	-1.471289	2.685688	8	-3.828329	-1.004442	1.766073
1	4.144009	0.083455	1.947731	8	-4.229168	1.244096	1.572312
6	2.353364	-2.393688	-1.198822	6	-2.159721	1.920361	0.423809
6	2.753110	-3.284613	-0.010398	6	-2.958619	-1.372556	-0.505289
1	1.709748	-2.974911	-1.900003	8	-2.376563	-0.546427	-1.533180
6	1.716424	-3.198931	1.130514	8	-1.051371	1.281567	-0.265081
6	1.271875	-1.821615	1.581193	15	-0.883000	0.171360	-1.445378
1	2.104483	-3.713821	2.023247	7	-0.943553	0.980931	-2.913956
1	0.806639	-3.730637	0.849058	6	-0.050784	0.535540	-3.977465
8	0.168093	-1.670436	2.091402	1	-0.584471	-0.074399	-4.720920
1	3.231956	-2.044998	-1.749571	1	0.390076	1.398852	-4.490244
6	4.176891	-2.957212	0.479186	1	0.760523	-0.065238	-3.557906
1	4.890754	-3.302765	-0.268204	6	-2.129001	1.685851	-3.390110
1	4.372633	-3.512950	1.411356	1	-2.764846	1.977000	-2.557143
6	2.808042	-4.763295	-0.455625	1	-1.830063	2.599772	-3.915300
1	3.497530	-4.887569	-1.296676	1	-2.713233	1.058653	-4.078104
1	1.817311	-5.100485	-0.770749	6	-4.407586	-1.614092	-0.937156
1	3.144497	-5.415436	0.359947	6	-5.189052	-2.572485	-0.279297
6	2.199762	-0.618667	1.435864	6	-4.987555	-0.859360	-1.962178
6	1.974450	0.003100	0.069347	6	-6.524521	-2.757661	-0.627956
6	2.272700	1.281509	-0.211288	1	-4.752793	-3.171663	0.509363
6	2.110512	1.877536	-1.588110	6	-6.326136	-1.047744	-2.312874
1	1.144388	2.387263	-1.692749	1	-4.386607	-0.131114	-2.490820
1	2.172693	1.111875	-2.362864	6	-7.101131	-1.993344	-1.644712
1	2.893182	2.618033	-1.781219	1	-7.115868	-3.502667	-0.104091
6	2.739345	2.284257	0.821803	1	-6.758760	-0.452866	-3.111943
1	2.128901	3.194385	0.756902	1	-8.142279	-2.139912	-1.916074
1	3.779365	2.580354	0.641235	6	-2.204990	-2.694598	-0.413930

6	-2.142728	-3.415460	0.782521	6	7.089987	1.558553	1.405129
6	-1.647068	-3.246465	-1.574743	1	7.257176	1.087020	-0.702510
6	-1.571117	-4.688375	0.804391	1	5.482659	-0.363498	3.693147
1	-2.542968	-2.985467	1.692651	6	6.585580	1.167592	2.650341
6	-1.056193	-4.509037	-1.545391	1	7.668928	2.474399	1.326206
1	-1.704053	-2.691520	-2.504894	6	6.790630	2.023926	3.873930
6	-1.032302	-5.242135	-0.357319	1	7.665286	2.671120	3.767224
1	-1.534646	-5.240837	1.738181	1	5.921363	2.670804	4.044855
1	-0.627305	-4.924689	-2.452242	1	6.923504	1.413468	4.771993
1	-0.585828	-6.231461	-0.334885	6	3.701510	-0.774047	-2.543568
6	-1.630458	2.268210	1.812520	1	3.499869	-1.520150	-3.328348
6	-2.213572	3.299561	2.556953	1	4.475051	-0.111734	-2.924684
6	-0.603038	1.512780	2.381363	6	2.082962	-1.189532	0.700496
6	-1.774309	3.568012	3.851839	6	2.091830	-2.330900	-0.342927
1	-3.014011	3.889000	2.125589	1	1.574513	-1.531719	1.607130
6	-0.167437	1.779445	3.679831	6	1.095627	-2.084772	-1.491680
1	-0.154559	0.710972	1.816867	6	1.155154	-0.779001	-2.266365
6	-0.749369	2.808177	4.419683	1	1.182872	-2.889067	-2.238599
1	-2.235090	4.371563	4.418737	1	0.084982	-2.159533	-1.092325
1	0.622362	1.171118	4.110941	8	0.181504	-0.430368	-2.926441
1	-0.409880	3.017256	5.429814	1	3.095964	-0.887882	0.964398
6	-2.541737	3.177805	-0.345873	6	3.511758	-2.621600	-0.876272
6	-1.519749	3.967603	-0.888007	1	4.103480	-3.075363	-0.082122
6	-3.872180	3.574976	-0.510210	1	3.443712	-3.370519	-1.681553
6	-1.824242	5.114682	-1.614316	6	1.630666	-3.636285	0.342539
1	-0.489533	3.662006	-0.745819	1	2.270797	-3.874847	1.198558
6	-4.176031	4.730805	-1.235490	1	0.603104	-3.525227	0.702073
1	-4.671958	2.996062	-0.061242	1	1.654993	-4.486956	-0.348849
6	-3.156531	5.497473	-1.796259	6	2.429172	0.060514	-2.260266
1	-1.023019	5.712018	-2.039344	6	2.489927	0.801408	-0.939814
1	-5.213143	5.027584	-1.359760	6	3.353905	1.798702	-0.673328
1	-3.395030	6.390956	-2.365295	6	3.493823	2.375550	0.713537
(S)-IM4				1	3.265583	3.449188	0.725901
				1	2.824320	1.871961	1.417166
				1	4.522094	2.262785	1.074345
				6	4.261969	2.424613	-1.708533
8	6.336529	-2.748095	-0.732521	1	4.292499	3.514284	-1.585621
16	5.894650	-1.396034	-1.094070	1	5.292372	2.064239	-1.606176
7	4.237232	-1.447071	-1.361240	1	3.938293	2.213125	-2.730713
8	6.508169	-0.665928	-2.210973	1	2.310471	0.763671	-3.095035
6	6.121731	-0.382194	0.365410	1	1.098435	0.413084	0.220105
6	5.639089	-0.814045	1.602654	28	-2.883805	0.702968	-0.931343
6	6.860439	0.793136	0.261820	6	-3.740076	-0.230194	-0.065755
1	5.107978	-1.754505	1.686737	6	-4.995739	0.431872	-1.897523
6	5.862589	-0.032271	2.730560				

1	-2.037854	0.172433	-1.366879	6	1.077030	3.936258	-1.795399
1	-4.085968	0.305852	0.821802	1	0.551761	2.964419	-3.645390
6	-6.100575	1.408849	-1.510792	1	1.362088	4.730813	0.189549
1	-6.160242	2.219083	-2.241446	1	1.908124	4.487120	-2.223698
1	-7.061596	0.888019	-1.478492	6	-3.033539	-2.571761	-0.726305
1	-5.897486	1.845194	-0.531206	6	-3.860853	-3.694444	-0.617769
6	-5.238952	-0.277270	-3.219650	6	-2.298417	-2.395593	-1.906129
1	-6.167664	-0.851886	-3.172237	6	-3.947124	-4.622023	-1.656631
1	-5.315341	0.452897	-4.029447	1	-4.447290	-3.848932	0.279366
1	-4.410339	-0.958890	-3.420496	6	-2.382154	-3.323939	-2.942357
8	-3.740139	1.130706	-1.969243	1	-1.639912	-1.549515	-2.042994
8	-4.842934	-0.565157	-0.884511	6	-3.207615	-4.442552	-2.824421
6	-2.985878	-1.519882	0.387789	1	-4.594703	-5.486971	-1.547344
6	-2.307097	1.868631	-0.073472	1	-1.792372	-3.162958	-3.839838
8	-1.964795	1.289049	1.208919	1	-3.271950	-5.166230	-3.631589
8	-1.573770	-1.189444	0.569362	6	-3.536605	-2.070959	1.694529
15	-0.828395	0.088501	1.313579	6	-2.718003	-2.873518	2.497634
7	-0.868268	-0.106725	2.974910	6	-4.858276	-1.835920	2.087325
6	-2.064210	0.053140	3.796026	6	-3.201373	-3.403098	3.691410
1	-2.110065	-0.738870	4.550884	1	-1.696447	-3.058788	2.187206
1	-2.056608	1.028631	4.301737	6	-5.342521	-2.367466	3.284933
1	-2.962211	-0.015664	3.187225	1	-5.517430	-1.258075	1.448088
6	0.383018	-0.013624	3.720378	6	-4.514710	-3.145571	4.093260
1	1.231373	0.007085	3.035175	1	-2.553202	-4.017048	4.309762
1	0.408407	0.904586	4.324127	1	-6.369047	-2.174076	3.581410
1	0.494944	-0.871261	4.395645	1	-4.890754	-3.555153	5.025885
6	-3.370154	2.922942	0.205785				
6	-3.700407	3.850797	-0.789741	IM5			
6	-4.062954	2.952025	1.419725				
6	-4.715075	4.780271	-0.579195	15	-1.859163	0.149095	-0.043237
1	-3.164810	3.836063	-1.731375	6	-3.262210	-0.927202	-0.571349
6	-5.081524	3.885012	1.629225	6	-3.037031	-1.899816	-1.556241
1	-3.795803	2.252558	2.201671	6	-4.079245	-2.701806	-2.013294
6	-5.413955	4.798193	0.630088	6	-5.363340	-2.551319	-1.486773
1	-4.962090	5.491461	-1.361664	6	-5.597156	-1.589002	-0.505381
1	-5.610829	3.896770	2.577479	6	-4.554952	-0.779336	-0.050494
1	-6.206059	5.522847	0.792797	6	-1.751338	1.336462	-1.436218
6	-1.066304	2.507957	-0.690905	6	-0.498325	1.862593	-1.776748
6	-0.757878	2.379224	-2.048873	6	-2.876019	1.691738	-2.196608
6	-0.281555	3.352323	0.113628	6	-2.624420	1.092908	1.330061
6	0.314586	3.087850	-2.593716	6	-3.045375	2.421482	1.214126
1	-1.346006	1.732778	-2.687199	6	-2.760886	0.430586	2.560041
6	0.773608	4.070214	-0.438525	1	-4.751662	-0.032378	0.709203
1	-0.533973	3.463429	1.163004	1	0.376014	1.592108	-1.195723

1	-3.846444	1.275410	-1.946978	1	-0.579213	2.031117	3.422561
1	-2.943531	2.941063	0.267455	1	-0.156108	1.930410	1.707233
8	5.276312	-0.938625	-0.403865	1	1.004352	2.572162	2.883056
16	4.162233	-0.519913	0.457313	6	-0.371160	2.718982	-2.870924
7	2.895559	-1.629168	0.316846	6	-1.493573	3.070411	-3.621153
8	4.362592	-0.280460	1.891326	1	-1.390843	3.732271	-4.476021
6	3.518980	0.993315	-0.244986	6	-2.748236	2.561593	-3.277986
6	3.768450	1.311924	-1.577752	6	-3.588099	3.083960	2.317469
6	2.836070	1.877912	0.590069	6	-3.728978	2.419454	3.535536
1	4.331782	0.626828	-2.200739	1	-4.152191	2.935856	4.391861
6	3.328535	2.540827	-2.073387	6	-3.320489	1.087273	3.652495
6	2.406304	3.097358	0.081511	1	-6.174788	-3.181654	-1.837871
1	2.668974	1.608002	1.622316	1	-2.042210	-2.031394	-1.960757
1	3.533717	2.802379	-3.107631	6	1.703161	0.326386	4.161057
6	2.657650	3.454925	-1.252076	1	2.622512	0.908448	4.015627
1	1.880367	3.790370	0.731861	1	1.990147	-0.707366	4.359877
6	2.230146	4.807147	-1.764805	1	1.203425	0.729229	5.051761
1	2.430603	4.913503	-2.834220	1	0.478298	-2.739540	2.437987
1	2.766253	5.608003	-1.243492	1	-3.903222	4.118897	2.222125
1	1.160040	4.970762	-1.601618	1	-3.423998	0.566290	4.599564
1	-2.408510	-0.591512	2.658056	1	-6.592774	-1.463877	-0.090022
6	2.445605	-2.299285	1.542408	1	-3.886263	-3.451556	-2.774782
1	2.514588	-3.381242	1.379243	1	-3.624176	2.831191	-3.860482
1	3.137512	-2.050666	2.351065	1	0.608155	3.093091	-3.144370
6	0.576454	-1.397386	-1.468045	28	-0.066120	-1.159226	0.383207
6	1.456242	-2.651120	-1.549834				
1	-0.180836	-1.396537	-2.256896	IM5_{dppp}			
6	0.657978	-3.741983	-0.811003				
6	-0.310988	-3.012199	0.110207	15	-3.270142	-0.183740	-0.513624
1	1.270409	-4.451578	-0.240086	6	-3.701849	-0.731637	1.193828
1	0.051698	-4.343662	-1.500422	6	-4.064727	-2.079642	1.350345
8	-1.279455	-3.497834	0.639793	6	-3.645690	0.079727	2.336589
1	1.153888	-0.468759	-1.559523	6	-4.946050	0.124995	-1.230331
6	2.855294	-2.389797	-0.938664	6	-6.045260	0.546702	-0.466635
1	3.431212	-1.822998	-1.670773	6	-5.109920	-0.041255	-2.612506
1	3.380922	-3.347711	-0.808033	1	-4.100018	-2.725991	0.477027
6	1.706033	-3.079579	-3.010553	1	-3.366471	1.124037	2.259844
1	2.174982	-2.268922	-3.577672	1	-5.937498	0.664995	0.607391
1	0.760626	-3.330420	-3.501839	8	2.089280	-4.868971	-0.496602
1	2.360724	-3.957063	-3.073589	16	2.541851	-3.501336	-0.778017
6	1.028673	-1.931421	1.956298	7	2.328704	-2.528314	0.673885
6	0.597437	-0.630425	2.175219	8	3.896763	-3.241407	-1.266262
6	0.802201	0.436338	2.946756	6	1.373398	-2.728575	-1.871012
6	0.230628	1.811682	2.717433	6	0.064267	-3.202620	-1.939123

6	1.799263	-1.637274	-2.628842	6	-7.420683	0.647117	-2.454750
1	-0.228962	-4.072181	-1.362918	1	-8.378356	0.847557	-2.925915
6	-0.843689	-2.543903	-2.763324	6	-6.336656	0.225408	-3.223981
6	0.881417	-1.009829	-3.466028	6	5.947617	0.360910	-0.163248
1	2.827492	-1.309330	-2.567111	1	6.537225	-0.270649	-0.841079
1	-1.872217	-2.887177	-2.809321	1	6.130153	0.013798	0.855725
6	-0.450823	-1.439294	-3.531739	1	6.356495	1.377324	-0.247721
1	1.203641	-0.164992	-4.068116	1	4.634458	-0.443741	2.063363
6	-1.455319	-0.699435	-4.374866	1	-8.117259	1.125088	-0.470616
1	-2.206033	-1.376505	-4.792350	1	-6.447011	0.095120	-4.296671
1	-0.975371	-0.166079	-5.199832	1	-3.884690	0.198862	4.470705
1	-1.986913	0.040531	-3.764232	1	-4.649891	-3.645274	2.703838
1	-4.272404	-0.389467	-3.210421	28	1.570958	-0.406636	0.193228
6	3.608211	-2.226763	1.385431	15	0.804396	1.558003	-0.165042
1	3.643950	-2.808874	2.312842	6	1.954076	2.847754	-0.786175
1	4.442078	-2.527883	0.753434	6	3.030241	3.173347	0.056962
6	-0.079050	-1.056938	1.061679	6	1.814474	3.514141	-2.006862
6	0.519812	-1.902545	2.220434	6	3.952914	4.140164	-0.330190
1	-0.819994	-0.358045	1.451513	1	3.145838	2.654499	1.003080
6	1.495517	-1.115426	3.158732	6	2.745351	4.482346	-2.394038
6	2.597426	-0.198785	2.587105	1	0.981418	3.293327	-2.665723
1	1.995619	-1.848589	3.810631	6	3.817285	4.792865	-1.559736
1	0.916018	-0.470858	3.824256	1	4.784302	4.380995	0.325399
8	2.675731	0.954412	2.988846	1	2.628367	4.991361	-3.346209
1	-0.626810	-1.723461	0.383335	1	4.542949	5.542119	-1.861834
6	1.260527	-3.064092	1.555875	6	0.038115	2.540830	1.199771
1	0.552553	-3.625537	0.947147	6	-0.304172	3.883431	0.964327
1	1.694306	-3.763712	2.280620	6	-0.240943	1.987912	2.453335
6	-0.594595	-2.488720	3.107591	6	-0.964002	4.629125	1.938376
1	-1.286849	-3.085295	2.506370	1	-0.042862	4.350494	0.021118
1	-1.177841	-1.684393	3.563794	6	-0.893650	2.737144	3.432632
1	-0.197885	-3.122615	3.911195	1	0.050631	0.974199	2.662430
6	3.674104	-0.714336	1.605880	6	-1.270054	4.054325	3.173971
6	3.471105	-0.071226	0.213651	1	-1.231066	5.661964	1.735696
6	4.486420	0.349085	-0.554331	1	-1.099279	2.288037	4.399638
6	4.255448	0.850833	-1.959934	1	-1.782295	4.636593	3.934074
1	4.658276	1.862266	-2.095986	6	-2.721088	1.584730	-0.222234
1	3.193005	0.877024	-2.201302	1	-2.146748	1.597994	0.703080
1	4.765613	0.205502	-2.689994	1	-3.593756	2.227862	-0.074491
6	-4.370588	-2.600384	2.605504	6	-1.836869	2.119017	-1.356927
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6	-3.939248	-0.444900	3.597364	6	-0.511686	1.355857	-1.478959
6	-7.273057	0.803358	-1.073830	1	-0.023931	1.561422	-2.434675

1	-0.718439	0.285038	-1.471835	6	2.187225	-0.175432	-1.459140
				6	2.765093	-0.314364	-2.856197
				1	2.343724	0.431828	-3.537014
(R)-IM5				1	2.582090	-1.301859	-3.287441
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8	7.113859	-1.081146	0.719103	6	2.186796	1.255953	-0.948620
16	6.016943	-0.263651	1.249038	1	1.779761	1.936261	-1.702115
7	4.591356	-1.130920	0.958248	1	3.209459	1.589000	-0.740057
8	6.055107	0.234857	2.630882	1	1.591186	1.387182	-0.044600
6	5.785775	1.141953	0.173672	1	1.342416	-0.276793	1.091789
6	5.939831	0.970356	-1.203301	28	0.387439	-1.054324	-1.452232
6	5.460277	2.382545	0.714821	6	-3.049613	-0.634131	0.721145
1	6.214550	-0.001380	-1.597508	6	-3.406188	0.854128	0.707852
6	5.742509	2.058800	-2.044369	6	-4.792354	-0.223762	2.220056
6	5.261488	3.463621	-0.144682	1	-2.060295	-0.787126	1.148830
1	5.371710	2.489263	1.789981	1	-3.972501	1.104742	-0.193352
1	5.858458	1.934193	-3.117329	6	-6.225832	-0.322489	1.709921
6	5.389528	3.317099	-1.530364	1	-6.636209	-1.310367	1.933390
1	5.001551	4.433783	0.268679	1	-6.849345	0.439002	2.186551
6	5.127616	4.474009	-2.460513	1	-6.249754	-0.182120	0.627069
1	5.856023	4.503308	-3.276497	6	-4.655130	-0.370401	3.726596
1	5.166302	5.429948	-1.932110	1	-5.216495	0.418217	4.234600
1	4.133540	4.386323	-2.915597	1	-5.039894	-1.341858	4.047536
6	3.404051	-0.550829	1.588697	1	-3.600997	-0.288271	3.999761
1	3.380132	-0.750640	2.669860	8	-3.999740	-1.234505	1.578054
1	3.456984	0.531274	1.461264	8	-4.219145	1.034287	1.850947
6	3.082703	-2.539084	-0.934887	6	-2.128994	1.750059	0.777773
6	3.561545	-3.329923	0.305438	6	-3.033085	-1.231692	-0.729840
1	2.516829	-3.227621	-1.568036	8	-2.673432	-0.158506	-1.620513
6	2.387465	-3.555873	1.274527	8	-1.099196	1.134903	-0.039200
6	1.601286	-2.300298	1.588946	15	-1.136706	0.484844	-1.574807
1	2.732496	-3.995418	2.218459	7	-1.444425	1.672757	-2.722867
1	1.676548	-4.267738	0.848625	6	-0.342125	2.174063	-3.526161
8	0.638920	-2.311471	2.338939	1	-0.645300	2.239748	-4.578940
1	3.973276	-2.249027	-1.505559	1	-0.019794	3.173946	-3.200215
6	4.729029	-2.590785	1.008935	1	0.504301	1.490146	-3.457619
1	5.663456	-2.827862	0.500277	6	-2.690831	2.413380	-2.885066
1	4.816516	-2.951134	2.046331	1	-3.461039	2.003863	-2.236401
6	4.104609	-4.699804	-0.130224	1	-2.555894	3.472623	-2.638630
1	4.891734	-4.586896	-0.882962	1	-3.035449	2.332097	-3.924333
1	3.307624	-5.314389	-0.561083	6	-4.428458	-1.680497	-1.154542
1	4.526841	-5.247263	0.719991	6	-4.974568	-2.867934	-0.653359
6	2.093224	-1.042817	0.908280	6	-5.208850	-0.879492	-1.994452
6	2.256276	-1.288771	-0.589447	6	-6.277521	-3.239197	-0.975166

1	-4.381679	-3.501110	-0.005489	16	6.159736	-1.010008	-1.675826
6	-6.515759	-1.252439	-2.316518	7	4.493332	-1.122841	-1.658993
1	-4.787177	0.029292	-2.403082	8	6.547666	-0.186435	-2.824983
6	-7.056800	-2.430335	-1.804754	6	6.561585	-0.068646	-0.208866
1	-6.685446	-4.162682	-0.575160	6	6.707428	-0.732477	1.010414
1	-7.107198	-0.619346	-2.971520	6	6.731701	1.311898	-0.297727
1	-8.073239	-2.720183	-2.053667	1	6.610821	-1.811565	1.049586
6	-1.995208	-2.347291	-0.830472	6	7.013809	0.003461	2.151175
6	-1.769471	-3.227633	0.222743	6	7.034418	2.034121	0.855298
6	-1.232684	-2.471314	-2.022145	1	6.656300	1.800547	-1.262224
6	-0.837563	-4.269501	0.093622	1	7.136541	-0.509160	3.101095
1	-2.320005	-3.113769	1.150583	6	7.174064	1.395539	2.094294
6	-0.218601	-3.444335	-2.094687	1	7.173679	3.109541	0.790369
1	-1.543039	-1.938674	-2.913019	6	7.457350	2.189077	3.344169
6	-0.054319	-4.367843	-1.047760	1	8.001257	3.110434	3.119049
1	-0.705576	-4.967788	0.913320	1	6.521258	2.473228	3.840780
1	0.348112	-3.556192	-3.013701	1	8.044905	1.609739	4.061839
1	0.688359	-5.154394	-1.138771	6	3.726979	-0.024094	-2.237873
6	-1.580460	1.746214	2.206690	1	3.476008	-0.224975	-3.288793
6	-1.978853	2.718006	3.130961	1	4.347341	0.872287	-2.217546
6	-0.732074	0.719615	2.634036	6	2.943846	-1.163063	0.652120
6	-1.535573	2.662451	4.451494	6	2.679946	-2.303619	-0.347753
1	-2.640439	3.517972	2.820025	1	2.322241	-1.338107	1.536242
6	-0.292562	0.658591	3.956072	6	1.341294	-2.041345	-1.054484
1	-0.411099	-0.049112	1.947895	6	1.348153	-0.739168	-1.824934
6	-0.691517	1.632198	4.871169	1	1.073078	-2.853302	-1.737902
1	-1.853483	3.426640	5.154792	1	0.533218	-1.972075	-0.316570
1	0.354398	-0.160877	4.252686	8	0.566141	-0.503147	-2.732039
1	-0.349885	1.590868	5.901255	1	3.987412	-1.212782	0.988039
6	-2.378963	3.165530	0.279433	6	3.840254	-2.400230	-1.381827
6	-1.294944	3.921247	-0.183380	1	4.613272	-3.069490	-1.005651
6	-3.653192	3.739494	0.296172	1	3.464850	-2.842214	-2.317076
6	-1.486521	5.220055	-0.647447	6	2.598657	-3.647307	0.388941
1	-0.308029	3.472596	-0.190837	1	3.495510	-3.816089	0.995069
6	-3.844442	5.044106	-0.166205	1	1.727035	-3.674025	1.051215
1	-4.493911	3.174592	0.684988	1	2.506302	-4.480159	-0.316924
6	-2.765237	5.785416	-0.644937	6	2.431853	0.259228	-1.432480
1	-0.638721	5.793430	-1.011118	6	2.653880	0.225649	0.072389
1	-4.839835	5.477946	-0.151444	6	2.920092	1.391313	0.804412
1	-2.915826	6.797379	-1.008658	6	3.423974	1.312318	2.231822
				1	3.022802	2.143372	2.824236
(S)-IM5				1	3.148950	0.382365	2.732205
				1	4.518468	1.391981	2.259167
8	6.683851	-2.365571	-1.480083	6	3.209372	2.733431	0.164461

1	2.794507	3.548681	0.767496	1	-7.027181	5.082261	0.351942
1	4.296453	2.891911	0.115271	6	-1.581759	2.517240	-0.938433
1	2.806524	2.835360	-0.842458	6	-1.271574	2.268047	-2.275660
1	2.061454	1.229600	-1.766012	6	-0.821568	3.454689	-0.222338
28	0.929352	0.960906	0.803207	6	-0.209057	2.938005	-2.890084
6	-3.205517	0.531904	-0.967712	1	-1.850436	1.555401	-2.851095
6	-3.855883	-0.453821	0.004363	6	0.227858	4.128823	-0.837299
6	-5.285132	-0.126763	-1.804416	1	-1.068972	3.651511	0.815395
1	-2.328511	0.082949	-1.430116	6	0.540611	3.868913	-2.176126
1	-4.192783	0.059968	0.907777	1	0.029424	2.719818	-3.925869
6	-6.535353	0.689760	-1.500140	1	0.807148	4.853048	-0.273502
1	-6.740909	1.382834	-2.319757	1	1.362782	4.392486	-2.655098
1	-7.395024	0.026263	-1.371657	6	-2.767532	-2.601929	-0.739132
1	-6.388365	1.270320	-0.587081	6	-3.615099	-3.715741	-0.765149
6	-5.402629	-1.006268	-3.040012	6	-1.904584	-2.389454	-1.818160
1	-6.210720	-1.730876	-2.909904	6	-3.597975	-4.595560	-1.845766
1	-5.614736	-0.393330	-3.920068	1	-4.295549	-3.894184	0.058847
1	-4.465537	-1.546036	-3.190730	6	-1.885698	-3.270670	-2.899962
8	-4.174900	0.767794	-1.967398	1	-1.229949	-1.547153	-1.830692
8	-4.973375	-0.969964	-0.689034	6	-2.733146	-4.377546	-2.920046
6	-2.854342	-1.584573	0.400992	1	-4.263404	-5.453899	-1.847167
6	-2.739462	1.824219	-0.225592	1	-1.200857	-3.076850	-3.720079
8	-2.321585	1.414427	1.096725	1	-2.720591	-5.064998	-3.760741
8	-1.532318	-0.988253	0.519861	6	-3.221409	-2.259647	1.713767
15	-1.034928	0.384845	1.334732	6	-2.226646	-2.929809	2.435369
7	-1.278459	0.216244	2.990245	6	-4.532929	-2.264473	2.196763
6	-2.554509	0.241438	3.693592	6	-2.531065	-3.568828	3.634361
1	-2.788261	-0.739890	4.121572	1	-1.211992	-2.930523	2.053193
1	-2.514422	0.979012	4.505940	6	-4.840278	-2.910929	3.396933
1	-3.355152	0.522952	3.014695	1	-5.319501	-1.779630	1.628137
6	-0.163997	-0.253037	3.800857	6	-3.841296	-3.557981	4.122458
1	0.760913	-0.181352	3.221886	1	-1.747917	-4.078257	4.188235
1	-0.060271	0.370293	4.698188	1	-5.862760	-2.905322	3.762527
1	-0.311155	-1.295165	4.118697	1	-4.079740	-4.055282	5.057734
6	-3.911302	2.778850	-0.027528				
6	-4.362223	3.549468	-1.106641	IM6_{dppp}			
6	-4.587404	2.860145	1.192608				
6	-5.476624	4.372221	-0.970974	15	1.479340	-1.457832	-0.915610
1	-3.841062	3.495230	-2.054913	6	3.045944	-2.353885	-0.544605
6	-5.705905	3.686567	1.328309	6	4.106426	-1.647469	0.036241
1	-4.228757	2.288981	2.038558	6	5.340691	-2.261387	0.242981
6	-6.157355	4.440752	0.246982	6	5.530116	-3.594218	-0.122739
1	-5.815500	4.960718	-1.818345	6	4.480505	-4.306042	-0.706368
1	-6.219342	3.740454	2.283866	6	3.248062	-3.689728	-0.921879

6	0.284288	-2.835189	-1.117895	6	0.218022	-1.141579	1.855460
6	-0.533599	-2.959809	-2.246985	6	1.062932	-1.672460	2.766049
6	0.119428	-3.744462	-0.057384	6	2.490789	-1.202695	2.897453
1	2.440379	-4.251650	-1.377351	1	2.681438	-0.836220	3.917259
1	-0.443214	-2.264694	-3.071007	1	2.698401	-0.389198	2.201004
8	-2.130374	-0.505349	-2.128798	1	3.211409	-2.010131	2.713772
16	-2.650415	0.544342	-1.245080	6	-1.511055	-3.955135	-2.308086
7	-2.007213	0.276477	0.287724	6	-1.677078	-4.843583	-1.246613
8	-2.429962	1.958575	-1.578838	1	-2.439944	-5.615049	-1.293566
6	-4.407731	0.283458	-1.088523	6	-0.851829	-4.739889	-0.123324
6	-4.920927	-1.006011	-1.245938	1	6.488596	-4.076595	0.045205
6	-5.232591	1.348400	-0.723563	1	3.965955	-0.618838	0.334258
1	-4.263674	-1.813531	-1.548346	6	0.697357	-2.734221	3.785866
6	-6.279297	-1.222016	-1.031508	1	1.445337	-3.538887	3.783064
6	-6.588799	1.111899	-0.514820	1	-0.284283	-3.182446	3.626782
1	-4.815904	2.344638	-0.630729	1	0.697553	-2.319163	4.803999
1	-6.687549	-2.220601	-1.159201	1	-1.395653	-2.600417	1.992026
6	-7.130498	-0.172925	-0.657093	1	-2.144213	-4.027986	-3.187255
1	-7.239121	1.937894	-0.241176	1	-0.968399	-5.431163	0.705975
6	-8.592637	-0.426932	-0.391456	1	4.620468	-5.343215	-0.996902
1	-9.193158	0.469285	-0.569371	1	6.147737	-1.693810	0.695963
1	-8.751109	-0.726760	0.651569	28	0.743099	0.204913	0.527449
1	-8.979800	-1.230822	-1.023838	15	1.555790	1.815876	-0.861008
1	0.742777	-3.652571	0.823998	6	1.188628	3.603519	-0.620053
6	-2.136321	-1.129514	0.717575	6	2.172842	4.559928	-0.342140
1	-3.182958	-1.353683	0.976553	6	-0.155163	4.005362	-0.686012
1	-1.852395	-1.748982	-0.129682	6	1.819801	5.894418	-0.131120
6	0.130357	1.539423	1.949312	1	3.215585	4.269267	-0.288721
6	-1.332227	1.509646	2.434441	6	-0.501801	5.339349	-0.480881
1	0.796232	1.399115	2.807801	1	-0.927233	3.276017	-0.903722
6	-1.590719	0.484954	3.566395	6	0.483678	6.287581	-0.197117
6	-1.873032	-0.958032	3.195051	1	2.593490	6.625993	0.083164
1	-2.442948	0.799464	4.178387	1	-1.545179	5.635676	-0.537928
1	-0.718688	0.475612	4.231347	1	0.211501	7.325484	-0.029613
8	-2.568415	-1.656058	3.915060	6	3.370460	1.749490	-0.581912
1	0.323635	2.533830	1.539224	6	3.794228	1.849905	0.756497
6	-2.342754	1.326252	1.271000	6	4.329621	1.532594	-1.576295
1	-2.376862	2.261722	0.714283	6	5.142578	1.735897	1.085434
1	-3.347749	1.143616	1.685877	1	3.054490	2.000885	1.536560
6	-1.670287	2.895214	3.038698	6	5.680148	1.398755	-1.243760
1	-1.460962	3.692285	2.318270	1	4.034721	1.453866	-2.616511
1	-1.058417	3.075862	3.927988	6	6.090010	1.500019	0.084614
1	-2.724581	2.964461	3.337657	1	5.451695	1.813293	2.123344
6	-1.256897	-1.516274	1.918790	1	6.409814	1.213457	-2.026165

1	7.139777	1.394772	0.340950	6	0.796263	5.253140	-0.282044
6	1.849602	-0.917203	-2.666561	1	1.261925	5.916050	-1.015874
1	2.897654	-0.603743	-2.666554	1	0.763272	5.775143	0.679131
1	1.789891	-1.795539	-3.316772	1	-0.237670	5.077280	-0.599531
6	0.933502	0.209016	-3.173927	1	-2.363243	-1.408291	2.270974
1	0.960893	0.216771	-4.270476	6	2.705414	-2.441553	0.627201
1	-0.100621	-0.002354	-2.894906	1	3.204273	-3.259993	0.097015
6	1.288311	1.627373	-2.693498	1	3.264844	-2.224535	1.535246
1	2.152540	2.032759	-3.230657	6	0.646583	-0.646952	-2.103650
1	0.447558	2.290856	-2.916115	6	1.532741	-1.902160	-2.299642
IM6				1	-0.278912	-0.725493	-2.681091
				6	0.947183	-3.194852	-1.651007
				6	0.407278	-3.206062	-0.206327
15	-1.532452	0.039173	-0.101465	1	1.717692	-3.979920	-1.704855
6	-2.823304	-1.158283	-0.644667	1	0.110850	-3.552111	-2.257262
6	-2.539504	-2.076494	-1.662250	8	-0.689941	-3.697588	0.006965
6	-3.529327	-2.928524	-2.147563	1	1.182963	0.219960	-2.511757
6	-4.819160	-2.878913	-1.620848	6	2.888891	-1.546124	-1.688444
6	-5.114389	-1.968330	-0.605839	1	3.277437	-0.662536	-2.195068
6	-4.125515	-1.113750	-0.120595	1	3.633789	-2.342676	-1.802689
6	-1.862281	1.482790	-1.198121	6	1.753810	-2.203850	-3.794878
6	-0.786247	2.198468	-1.731484	1	2.198971	-1.339098	-4.297765
6	-3.171035	1.888383	-1.500689	1	0.797568	-2.417177	-4.281956
6	-2.188553	0.603592	1.513404	1	2.412573	-3.067462	-3.950875
6	-2.323961	1.963210	1.816822	6	1.252630	-2.741919	0.995630
6	-2.498274	-0.355055	2.490721	6	0.700566	-1.430755	1.614072
1	-4.369229	-0.417593	0.672922	6	0.766220	-1.217536	2.939550
1	0.221819	1.880645	-1.505450	6	0.453457	0.118691	3.571852
1	-4.015140	1.335442	-1.103411	1	-0.238044	0.013159	4.415197
1	-2.090276	2.710377	1.066227	1	0.008719	0.816823	2.865325
8	4.977504	0.049312	-0.613793	1	1.373320	0.564150	3.979127
16	3.826981	0.023431	0.297485	6	-1.010382	3.300981	-2.557637
7	2.709207	-1.228223	-0.248827	6	-2.313329	3.700464	-2.853678
8	4.009942	-0.179147	1.735587	1	-2.488971	4.555080	-3.500354
6	2.888924	1.517368	0.055299	6	-3.393928	2.992103	-2.321133
6	3.156874	2.344087	-1.032802	6	-2.765207	2.360888	3.080762
6	1.958118	1.874997	1.032992	6	-3.090103	1.404041	4.041682
1	3.905554	2.055101	-1.761277	1	-3.440565	1.713571	5.021660
6	2.473936	3.557030	-1.134180	6	-2.960832	0.045299	3.740933
6	1.285568	3.085388	0.910904	1	-5.588583	-3.547675	-1.994828
1	1.794784	1.223919	1.877255	1	-1.543457	-2.129974	-2.071271
1	2.684299	4.217922	-1.970059	6	1.257937	-2.216698	3.968249
6	1.538075	3.947369	-0.166683	1	2.205892	-1.875733	4.406697
1	0.559781	3.365925	1.668583	1	1.419584	-3.220329	3.571625

1	0.543023	-2.299481	4.797222	1	-2.833974	-1.323172	0.624134
1	1.212962	-3.581365	1.699792	1	-1.377476	-0.879730	-0.291007
1	-2.864676	3.418147	3.308410	6	-0.519776	1.477329	2.474359
1	-3.205696	-0.703628	4.488022	6	-2.009510	1.440349	2.900681
1	-6.115131	-1.922262	-0.186686	1	0.048256	1.840863	3.338608
1	-3.285231	-3.640866	-2.929619	6	-2.229215	0.215866	3.805848
1	-4.410774	3.295730	-2.551393	6	-1.950170	-1.083121	3.071411
1	-0.163388	3.840573	-2.970163	1	-3.242757	0.178320	4.218899
28	0.527958	-0.567329	-0.127098	1	-1.540519	0.266708	4.660574
IM7_{dppp}				8	-2.382408	-2.157028	3.445771
				1	-0.398745	2.222315	1.687268
				6	-2.969698	1.384874	1.672646
15	1.949619	-1.598172	-0.848846	1	-3.224591	2.401504	1.375036
6	3.532606	-2.488518	-0.562854	1	-3.905259	0.878748	1.964535
6	4.435798	-1.936659	0.354563	6	-2.355101	2.717823	3.679720
6	5.671170	-2.544476	0.585591	1	-2.097090	3.607744	3.095764
6	6.010054	-3.713874	-0.095450	1	-1.803848	2.758488	4.624446
6	5.112470	-4.275299	-1.008456	1	-3.424988	2.763944	3.914130
6	3.880891	-3.665771	-1.241520	6	-1.083995	-0.935877	1.823895
6	0.707967	-2.956595	-0.777239	6	0.014005	0.096094	2.060036
6	-0.453370	-2.918869	-1.567054	6	1.295378	-0.374627	2.429809
6	0.830014	-3.976998	0.180683	6	2.314668	0.607243	2.979726
1	3.180307	-4.111698	-1.941564	1	2.245840	0.666593	4.078238
1	-0.580179	-2.145812	-2.316355	1	2.192436	1.613235	2.577910
8	-2.145712	0.664619	-2.029642	1	3.333958	0.284440	2.743433
16	-3.081756	1.117164	-0.993696	6	-1.468085	-3.859869	-1.387960
7	-2.369712	0.754411	0.490390	6	-1.344068	-4.855403	-0.418767
8	-3.528984	2.512415	-0.923347	1	-2.138171	-5.580991	-0.273078
6	-4.531801	0.079273	-1.085956	6	-0.185854	-4.914425	0.359071
6	-4.424452	-1.207341	-1.616693	1	6.968987	-4.190760	0.085087
6	-5.734268	0.536642	-0.544912	1	4.162787	-1.024804	0.874712
1	-3.484187	-1.533799	-2.044669	6	1.596191	-1.795868	2.860922
6	-5.538192	-2.042011	-1.598899	1	2.616158	-2.078017	2.580826
6	-6.838227	-0.312203	-0.537316	1	0.921750	-2.538817	2.439527
1	-5.800750	1.548822	-0.162542	1	1.529610	-1.878662	3.957812
1	-5.463082	-3.042632	-2.015443	1	-0.668373	-1.922848	1.626536
6	-6.756447	-1.612389	-1.054612	1	-2.357690	-3.813998	-2.010051
1	-7.780651	0.040517	-0.128011	1	-0.073502	-5.691180	1.109555
6	-7.945880	-2.537499	-1.006379	1	5.373739	-5.188091	-1.536065
1	-8.886601	-1.980365	-1.017487	1	6.364188	-2.105980	1.297604
1	-7.931869	-3.139954	-0.089974	28	1.216587	0.015184	0.394734
1	-7.947494	-3.230650	-1.852258	15	1.449756	1.700532	-0.985118
1	1.727143	-4.036463	0.786843	6	0.773674	3.414005	-1.075834
6	-1.962524	-0.651287	0.596757	6	1.492653	4.487117	-1.627193

6	-0.534926	3.630281	-0.635671	6	0.832808	-3.812346	0.471039
6	0.907359	5.747491	-1.727536	1	-1.484042	-4.627241	1.286168
1	2.512805	4.336304	-1.967569	1	-3.521997	-2.421686	2.225762
6	-1.129324	4.888118	-0.749398	1	-0.222347	0.299698	2.658784
1	-1.091197	2.803531	-0.218767	1	0.738110	-1.716978	3.146648
6	-0.406268	5.949581	-1.290742	8	1.879457	0.388313	1.825425
1	1.471957	6.573191	-2.151590	16	2.615420	1.116286	0.783496
1	-2.157721	5.020865	-0.429587	7	2.288405	0.367142	-0.677682
1	-0.861714	6.931710	-1.379455	8	2.386665	2.557699	0.597737
6	3.188898	2.034673	-0.468011	6	4.352700	0.865852	1.096576
6	3.449566	2.988376	0.530928	6	4.767809	-0.288264	1.764585
6	4.254340	1.246971	-0.928090	6	5.277225	1.774240	0.578950
6	4.731048	3.141326	1.055024	1	4.031482	-0.980493	2.157628
1	2.641297	3.613869	0.896040	6	6.131332	-0.524242	1.915219
6	5.538035	1.397339	-0.402214	6	6.636403	1.520541	0.742469
1	4.085316	0.498163	-1.692727	1	4.929533	2.668171	0.073816
6	5.780821	2.342036	0.594577	1	6.463276	-1.420124	2.432426
1	4.910964	3.885183	1.825860	6	7.083707	0.371655	1.409456
1	6.343319	0.767302	-0.768302	1	7.362786	2.224786	0.346895
1	6.778799	2.459647	1.006085	6	8.557079	0.118255	1.604431
6	2.043845	-1.263854	-2.692535	1	8.900076	0.529819	2.561530
1	3.086913	-1.018887	-2.921573	1	9.150875	0.586865	0.814990
1	1.816923	-2.191319	-3.229233	1	8.779888	-0.952396	1.611300
6	1.122273	-0.128540	-3.173155	1	0.307481	-4.027875	-0.451487
1	1.050032	-0.192857	-4.266178	6	2.606807	-1.070454	-0.676101
1	0.105422	-0.259382	-2.790362	1	3.691879	-1.221396	-0.778263
6	1.581056	1.291725	-2.813045	1	2.293362	-1.470429	0.285380
1	2.604425	1.475110	-3.160253	6	0.181756	0.801827	-2.660275
1	0.935184	2.008692	-3.326819	6	1.662093	0.876419	-3.091076
IM7				1	-0.402231	0.383781	-3.486436
				6	2.140740	-0.354097	-3.900593
				6	2.591492	-1.569770	-3.118037
15	-1.014419	-1.705952	0.723704	1	2.985036	-0.085598	-4.544368
6	-2.263513	-2.943067	0.181308	1	1.328479	-0.674512	-4.563736
6	-3.324706	-2.493022	-0.610753	8	3.477606	-2.295008	-3.537942
6	-4.373201	-3.347045	-0.949539	1	-0.161065	1.826124	-2.515229
6	-4.371082	-4.668692	-0.504481	6	2.607656	1.143906	-1.888435
6	-3.321597	-5.125861	0.295436	1	2.516327	2.192524	-1.612265
6	-2.280110	-4.267132	0.645277	1	3.653021	0.962500	-2.187293
6	-1.787362	-1.135223	2.301521	6	1.837016	2.092601	-4.031631
6	-3.014096	-1.633822	2.767430	1	1.466050	3.006541	-3.558416
6	-1.160378	-0.105604	3.017412	1	1.269281	1.938113	-4.954648
6	0.377147	-2.772552	1.299509	1	2.888815	2.245074	-4.307481
6	1.071294	-2.506662	2.487120	6	1.902024	-1.861897	-1.788330

6	0.399165	-1.659453	-1.930559	1	-3.526815	3.502480	-1.778855
6	-0.275241	-2.449031	-2.795954	6	-0.008033	5.119199	-1.884384
6	-1.672921	-2.131609	-3.260525	1	0.637405	3.453987	-0.688663
1	-1.666415	-1.937980	-4.344390	6	-1.077208	5.729574	-2.545148
1	-2.061194	-1.242412	-2.763592	1	-3.179195	5.614155	-3.004462
1	-2.367610	-2.963001	-3.094233	1	0.977286	5.575698	-1.901474
6	-3.599054	-1.106875	3.918270	1	-0.927064	6.661221	-3.082432
6	-2.966350	-0.081769	4.624636	6	-3.301448	1.153536	-0.478445
1	-3.427775	0.333388	5.515784	6	-3.700137	0.949566	-1.811697
6	-1.742035	0.410733	4.175345	6	-4.142657	0.709601	0.552289
6	2.207621	-3.243507	2.824747	6	-4.935042	0.371601	-2.102409
6	2.664021	-4.261455	1.986459	1	-3.037309	1.238053	-2.620852
1	3.550081	-4.831733	2.248941	6	-5.373035	0.121223	0.256962
6	1.965293	-4.549699	0.812693	1	-3.835963	0.805978	1.585762
1	-5.182868	-5.338103	-0.773675	6	-5.780561	-0.036167	-1.067343
1	-3.329883	-1.472446	-0.963508	1	-5.230464	0.230049	-3.137611
6	0.311571	-3.662396	-3.492680	1	-6.006242	-0.222694	1.068986
1	-0.405374	-4.493280	-3.472056	1	-6.741168	-0.488805	-1.293634
1	1.247727	-4.013109	-3.055108				
1	0.513775	-3.454062	-4.553560	IM8			
1	2.158185	-2.901877	-1.566536				
1	2.731753	-3.021034	3.749893	15	-1.359687	-1.909026	0.237245
1	2.304506	-5.345042	0.155690	6	-2.696537	-2.900309	-0.540453
1	-3.316818	-6.150441	0.655713	6	-3.687255	-2.184379	-1.227906
1	-5.185376	-2.973294	-1.564829	6	-4.774881	-2.846258	-1.794743
1	-1.251511	1.222840	4.700475	6	-4.876811	-4.235246	-1.696142
1	-4.552655	-1.498034	4.261540	6	-3.893455	-4.956598	-1.015765
28	-0.349663	-0.156720	-0.983012	6	-2.813247	-4.292659	-0.432558
15	-1.604495	1.772717	-0.159138	6	-2.005073	-1.726187	1.956948
6	-1.703592	2.644031	1.469816	6	-3.198256	-2.312875	2.399597
6	-2.884959	3.230835	1.943791	6	-1.325334	-0.843115	2.809155
6	-0.510831	2.862905	2.170035	6	0.024171	-3.114291	0.452643
6	-2.881597	3.970658	3.125470	6	0.806854	-3.130384	1.616874
1	-3.810340	3.118428	1.391081	6	0.423708	-3.918678	-0.629266
6	-0.504840	3.622799	3.338998	1	-2.060511	-4.856893	0.108022
1	0.416600	2.445335	1.806357	1	-3.743946	-2.988355	1.751266
6	-1.692307	4.166442	3.829606	1	-0.415581	-0.366000	2.464950
1	-3.808014	4.406889	3.487632	1	0.524511	-2.524813	2.468258
1	0.431336	3.782114	3.865740	8	1.887578	-0.097114	1.820772
1	-1.690787	4.749171	4.746111	16	2.828971	0.766351	1.097870
6	-1.465406	3.315085	-1.169635	7	2.535866	0.547701	-0.536443
6	-2.536174	3.940944	-1.814564	8	2.850156	2.215354	1.334886
6	-0.197827	3.919440	-1.203236	6	4.469066	0.127081	1.382557
6	-2.339625	5.139975	-2.504363	6	4.637625	-1.245360	1.582671

6	5.565549	0.985478	1.295822	6	2.358314	-4.690433	0.599484
1	3.772434	-1.894926	1.649544	1	3.259555	-5.293579	0.654808
6	5.927590	-1.754155	1.699815	6	1.578236	-4.695873	-0.559046
6	6.848170	0.456297	1.419899	1	-5.718097	-4.754169	-2.146192
1	5.405679	2.047915	1.151358	1	-3.600370	-1.107441	-1.315302
1	6.067451	-2.820418	1.854513	6	-1.027464	-1.754936	-3.426825
6	7.049108	-0.915854	1.621709	1	-2.075930	-2.004926	-3.251690
1	7.707424	1.118300	1.360193	1	-0.423583	-2.536056	-2.971536
6	8.439428	-1.476868	1.781132	1	-0.857379	-1.803313	-4.513852
1	8.715266	-1.538505	2.840854	1	1.251702	-2.003621	-2.275275
1	9.183671	-0.848232	1.284932	1	2.544761	-3.917171	2.604346
1	8.511797	-2.486473	1.366791	1	1.868080	-5.303542	-1.410971
1	-0.179525	-3.944611	-1.529650	1	-3.970782	-6.036859	-0.932433
6	2.420830	-0.852802	-0.948355	1	-5.537123	-2.274443	-2.315246
1	3.411721	-1.327204	-1.031104	1	-1.303984	0.164692	4.703772
1	1.857625	-1.373368	-0.177611	1	-4.640516	-2.457656	3.988750
6	1.080708	1.459562	-2.775953	28	-0.721727	-0.090331	-0.850979
6	2.618163	1.556440	-2.846667	15	-1.513053	1.762541	0.164450
1	0.703815	1.785177	-3.754731	6	-1.487203	2.359651	1.925500
6	3.138900	0.459411	-3.791106	6	-2.576132	3.026397	2.505614
6	2.629202	-0.931195	-3.445250	6	-0.301715	2.243106	2.657775
1	4.234820	0.432645	-3.821610	6	-2.491296	3.524682	3.804351
1	2.811403	0.671587	-4.817057	1	-3.496239	3.152063	1.945455
8	2.972622	-1.918616	-4.067968	6	-0.208930	2.759097	3.950973
1	0.716859	2.189222	-2.054569	1	0.550645	1.740177	2.227770
6	3.258565	1.452037	-1.437460	6	-1.307154	3.391113	4.533407
1	3.234531	2.435196	-0.968311	1	-3.348164	4.027171	4.244190
1	4.314936	1.150203	-1.535991	1	0.723329	2.658503	4.498899
6	3.017598	2.931747	-3.405549	1	-1.241478	3.784390	5.543773
1	2.556417	3.734186	-2.821017	6	-1.205919	3.436595	-0.573596
1	2.688190	3.038344	-4.443642	6	-2.162208	4.280767	-1.149298
1	4.104921	3.070110	-3.383621	6	0.125628	3.884264	-0.491715
6	1.654081	-0.994302	-2.278481	6	-1.790778	5.523848	-1.669179
6	0.556786	0.048642	-2.475690	1	-3.204340	3.986401	-1.177213
6	-0.709058	-0.360882	-2.926454	6	0.490185	5.130481	-0.995210
6	-1.628760	0.667833	-3.554153	1	0.875952	3.261857	-0.011271
1	-1.417233	0.756931	-4.632380	6	-0.465321	5.950449	-1.601295
1	-1.519000	1.659748	-3.113677	1	-2.546208	6.163997	-2.116283
1	-2.673297	0.361047	-3.458448	1	1.521170	5.462445	-0.910480
6	-3.707373	-2.006681	3.662507	1	-0.180681	6.918128	-2.003482
6	-3.028864	-1.119412	4.500388	6	-3.306084	1.388746	-0.071287
1	-3.435649	-0.871265	5.476329	6	-3.963779	1.579686	-1.296951
6	-1.829832	-0.545157	4.073866	6	-3.998952	0.715690	0.951924
6	1.960165	-3.913786	1.688324	6	-5.271787	1.130965	-1.489161

1	-3.452965	2.068771	-2.114461	1	-0.449980	4.499778	-0.297486
6	-5.299535	0.257868	0.754997	6	-3.167468	-1.469366	1.698376
1	-3.517907	0.540248	1.905043	1	-3.645008	-0.563183	2.069522
6	-5.945887	0.466262	-0.464474	1	-3.654581	-2.319177	2.193786
1	-5.758816	1.298778	-2.445568	6	-1.031515	-2.762976	1.443895
1	-5.799985	-0.272438	1.559172	6	-1.457485	-3.095429	-0.029234
1	-6.959856	0.108942	-0.616355	1	0.060069	-2.687228	1.519118
IM9				6	-0.246327	-3.272225	-0.982493
				6	0.413082	-1.937238	-1.460401
				1	-0.543754	-3.815461	-1.886653
	15	1.996048	0.003790	0.005104	1	0.536377	-3.861247
6	3.293067	-1.107998	-0.665866	8	0.882929	-1.873812	-2.579942
6	4.180353	-0.735869	-1.678848	1	-1.323240	-3.604311	2.082387
6	5.148887	-1.637349	-2.126041	6	-2.291481	-1.932380	-0.593461
6	5.239603	-2.909097	-1.562713	1	-2.649925	-2.171233	-1.596766
6	4.358167	-3.282901	-0.544535	1	-1.653504	-1.010884	-0.746953
6	3.388946	-2.388091	-0.101256	6	-2.310081	-4.373824	-0.049473
6	2.795184	0.517129	1.573320	1	-3.190972	-4.264870	0.589062
6	4.098056	1.042212	1.548931	1	-1.725351	-5.226373	0.310771
6	2.156294	0.313778	2.799991	1	-2.656712	-4.599001	-1.063092
6	1.631206	1.278439	-2.433381	6	-1.662752	-1.463594	2.018802
6	2.003165	1.469295	-1.090742	6	-0.944029	-0.184551	1.552718
6	2.278865	2.760362	-0.624312	6	-1.110804	0.974218	2.219186
1	4.110124	0.248150	-2.128600	6	-1.988064	1.170603	3.439165
1	4.612096	1.173030	0.601832	1	-1.449441	1.729746	4.215865
1	1.405976	0.276944	-2.790437	1	-2.337935	0.236983	3.885296
1	2.552219	2.916341	0.412961	1	-2.874650	1.769393	3.189127
8	-5.597426	-0.351560	0.521959	6	2.195534	3.850257	-1.492725
16	-4.533683	-0.542094	-0.465270	6	1.837772	3.659162	-2.827341
7	-3.416360	-1.590126	0.241949	1	1.776956	4.508575	-3.501126
8	-4.792956	-1.079376	-1.803161	6	1.558055	2.371859	-3.294583
6	-3.666392	1.004597	-0.657823	6	2.804343	0.652145	3.989878
6	-3.892056	2.032695	0.256492	6	4.089329	1.192039	3.960900
6	-2.724105	1.146838	-1.680333	6	4.736488	1.386961	2.737127
1	-4.643970	1.906127	1.026617	1	2.696763	-2.683105	0.683094
6	-3.164344	3.212954	0.139346	1	4.590432	1.456947	4.887183
6	-1.980130	2.320978	-1.759768	1	1.145335	-0.078316	2.806128
1	-2.593163	0.362502	-2.416377	1	5.990918	-3.608885	-1.915543
1	-3.348792	4.024976	0.837157	6	-0.377825	2.233437	1.825712
6	-2.186672	3.367482	-0.852398	1	-1.047787	3.100467	1.831809
1	-1.228663	2.426971	-2.535552	1	0.050283	2.146093	0.827538
6	-1.347245	4.616046	-0.916072	1	0.431773	2.454169	2.535767
1	-1.896216	5.487596	-0.548186	1	-1.593260	-1.545210	3.112284
1	-1.008924	4.820182	-1.935026	1	4.423532	-4.272557	-0.102463

1	5.829337	-1.343626	-2.919667	6	1.521788	0.355403	0.222871
1	5.740759	1.798929	2.710483	1	1.103374	-0.541719	-0.247735
1	2.299660	0.495710	4.938559	1	2.176405	0.018081	1.036935
1	2.409732	4.848526	-1.123124	6	1.805515	3.245927	0.819515
1	1.279607	2.217529	-4.332879	6	1.639597	3.478066	-0.705941
28	0.007161	-0.756753	-0.037673	1	1.906322	4.228723	1.282493
IM10				6	0.246532	4.071845	-1.012108
				6	-0.847934	3.035757	-0.968936
				1	0.223227	4.545520	-2.002091
15	-2.220424	-0.644708	-0.183357	1	-0.004896	4.851937	-0.282150
6	-3.905989	-0.677835	-0.901434	8	-1.943166	3.137205	-1.526300
6	-4.717263	-1.821842	-0.866710	1	2.761377	2.730698	0.968029
6	-5.996581	-1.790551	-1.415101	6	1.817453	2.163884	-1.530870
6	-6.477905	-0.616806	-2.002969	1	2.500259	2.357286	-2.360007
6	-5.676342	0.523163	-2.042395	1	0.863455	1.836949	-1.960205
6	-4.391864	0.495813	-1.494312	6	2.725277	4.475045	-1.144231
6	-2.475833	-1.078065	1.577638	1	3.719160	4.060503	-0.946849
6	-3.648005	-0.696202	2.243754	1	2.635638	5.424712	-0.605739
6	-1.423820	-1.641825	2.316676	1	2.658563	4.686201	-2.216857
6	-0.422574	-1.892254	-1.891377	6	0.363086	1.160508	0.807855
6	-1.360583	-2.107145	-0.873210	6	0.683961	2.462084	1.456956
6	-1.595019	-3.415818	-0.421114	6	-0.070113	2.931889	2.480326
1	-4.347233	-2.735238	-0.413227	6	-1.264194	2.146913	2.983995
1	-4.467470	-0.257269	1.684035	1	-1.783861	2.683957	3.782567
1	-0.205322	-0.883316	-2.225567	1	-0.995272	1.159311	3.375031
1	-2.292895	-3.592103	0.390845	1	-1.986812	1.970297	2.175191
8	4.377080	0.850795	-2.331000	6	-0.908610	-4.487102	-0.988334
16	3.320430	0.037608	-1.716678	6	0.021834	-4.263638	-2.007875
7	2.407957	1.075277	-0.737264	1	0.560601	-5.100399	-2.442751
8	2.455157	-0.783382	-2.585664	6	0.266686	-2.966387	-2.457884
6	4.040520	-1.043713	-0.495872	6	-1.547260	-1.824975	3.693121
6	5.081170	-0.567610	0.302339	6	-2.717483	-1.439800	4.349956
6	3.546605	-2.338179	-0.350905	6	-3.766593	-0.877339	3.621514
1	5.450219	0.442030	0.161026	1	-3.765463	1.383441	-1.529506
6	5.624413	-1.407311	1.269000	1	-2.811223	-1.578298	5.422645
6	4.105138	-3.165432	0.621531	1	-0.510603	-1.943771	1.813987
1	2.734362	-2.677690	-0.983723	1	-7.475835	-0.595257	-2.430693
1	6.432429	-1.046493	1.899331	6	0.109882	4.267589	3.155818
6	5.146926	-2.715620	1.442490	1	0.984576	4.826226	2.820993
1	3.724488	-4.175285	0.746544	1	0.200290	4.139898	4.242852
6	5.764900	-3.624099	2.475195	1	-0.773292	4.904161	2.997485
1	6.029434	-3.074074	3.383188	1	-0.105629	0.486115	1.529625
1	6.685711	-4.080130	2.091875	1	-6.045292	1.435608	-2.500671
1	5.086514	-4.435756	2.751241	1	-6.619151	-2.679812	-1.386095

1	-4.680529	-0.577986	4.125660	6	2.555101	-0.933691	1.231859
1	-0.727604	-2.266156	4.252297	1	3.024659	-1.823922	1.669635
1	-1.093809	-5.495912	-0.631177	1	2.602987	-0.168526	2.010197
1	1.010381	-2.770164	-3.221407	6	1.721132	-1.538713	-1.890707
28	-1.154547	1.361221	-0.401411	6	2.891017	-2.397246	-1.425823
IM11				1	1.032028	-2.144984	-2.510711
				6	2.419384	-3.550747	-0.464409
				6	0.957328	-3.512699	-0.039068
				1	3.053891	-3.576909	0.427742
15	-1.702339	0.105863	-0.301627	1	2.535188	-4.510645	-0.972592
6	-3.060242	-1.099401	-0.531425	8	0.148125	-4.243842	-0.603511
6	-2.741575	-2.465558	-0.527750	1	2.101073	-0.704900	-2.503449
6	-3.752608	-3.416769	-0.675415	6	3.951689	-1.482680	-0.765086
6	-5.079003	-3.014184	-0.833118	1	4.491155	-0.948421	-1.547289
6	-5.398439	-1.653693	-0.854871	1	4.680423	-2.100833	-0.217167
6	-4.393627	-0.698817	-0.709833	6	3.595064	-3.060288	-2.629228
6	-2.168136	1.497872	-1.401168	1	3.917908	-2.304863	-3.353074
6	-1.751251	1.428865	-2.739730	1	2.912908	-3.749914	-3.135261
6	-2.871952	2.624787	-0.962029	1	4.478535	-3.629141	-2.312818
6	-1.932715	0.790658	1.378356	6	1.070998	-1.190284	0.907250
6	-0.886775	1.574932	1.890277	6	0.544279	-2.578177	1.058896
6	-3.059960	0.546639	2.171623	6	-0.335520	-2.970363	2.019828
1	-4.640979	0.357856	-0.743363	6	-0.785916	-2.074002	3.145617
1	-1.196318	0.560224	-3.087337	1	-1.872459	-1.928967	3.101918
1	-3.187473	2.692080	0.073899	1	-0.321647	-1.089142	3.148243
1	-0.005058	1.753545	1.287653	1	-0.575839	-2.552875	4.110333
8	4.925552	1.197935	-0.939973	6	-2.033283	2.468332	-3.623407
16	4.127617	0.999069	0.275631	6	-2.731854	3.593435	-3.175924
7	3.369716	-0.474359	0.111022	1	-2.945056	4.408396	-3.860700
8	4.753919	1.139539	1.599351	6	-3.152404	3.667228	-1.847627
6	2.746292	2.140069	0.251463	6	-0.975483	2.120129	3.168846
6	1.891335	2.177763	-0.852356	6	-2.102487	1.873406	3.956789
6	2.596529	3.042075	1.303625	1	-2.168485	2.288162	4.958038
1	2.025678	1.471909	-1.662442	6	-3.141171	1.086765	3.456665
6	0.877349	3.132346	-0.895482	6	-0.961067	-4.341507	2.090871
6	1.575880	3.990015	1.246731	1	-0.916147	-4.722311	3.118255
1	3.282151	2.994271	2.141800	1	-0.508609	-5.063254	1.415097
1	0.206097	3.161935	-1.747007	1	-2.025831	-4.272860	1.828457
6	0.701865	4.047111	0.153142	1	0.483031	-0.501654	1.510107
1	1.455689	4.696552	2.063572	1	-5.863167	-3.756231	-0.950636
6	-0.436440	5.033115	0.136918	1	-1.714271	-2.796100	-0.420553
1	-0.794392	5.215682	-0.878614	1	-4.016486	0.889032	4.068105
1	-0.144686	5.987635	0.584844	1	-0.158936	2.727090	3.547216
1	-1.282396	4.641539	0.714726	1	-3.492249	-4.470594	-0.676093
1	-3.866811	-0.070229	1.791624				

1	-6.428366	-1.337717	-0.991704	1	-2.363312	-0.220251	-1.944822
1	-3.694659	4.540123	-1.496656	6	-1.777871	2.320968	-0.047543
1	-1.702050	2.406324	-4.655439	6	-1.492791	1.694752	1.340148
28	0.373693	-0.739617	-0.832290	1	-1.979493	3.386005	0.078513
IM12				6	-0.277615	2.340666	2.053574
				6	1.124259	2.416213	1.337859
				1	-0.087386	1.786513	2.984092
15	2.391862	-0.326549	-0.026643	1	-0.518414	3.366346	2.358442
6	3.708850	-0.301548	1.243091	8	1.969494	3.121174	1.854061
6	4.290577	-1.481968	1.731223	1	-2.701572	1.874396	-0.429472
6	5.341527	-1.418112	2.643947	6	-1.207452	0.177816	1.184857
6	5.822235	-0.177603	3.071649	1	-1.472679	-0.347028	2.102301
6	5.247328	0.997594	2.587342	1	-0.135602	0.015353	1.042611
6	4.191418	0.941036	1.675869	6	-2.741002	1.899089	2.212954
6	3.335994	-0.541405	-1.592702	1	-3.610636	1.416361	1.758919
6	4.735590	-0.609767	-1.607921	1	-2.970144	2.963955	2.328770
6	2.643050	-0.598620	-2.812930	1	-2.597941	1.473500	3.211759
6	1.033430	-2.177683	1.546012	6	-0.490736	0.781618	-1.596930
6	1.548013	-1.932275	0.262209	6	-0.676160	2.095783	-1.069064
6	1.255615	-2.833887	-0.768313	6	0.350361	3.068114	-1.240123
1	3.918241	-2.444793	1.397332	6	1.339247	2.985724	-2.388927
1	5.289881	-0.562377	-0.678254	1	0.914381	3.463101	-3.285079
1	1.263405	-1.494976	2.358760	1	1.623191	1.968508	-2.660021
1	1.658289	-2.674608	-1.761717	1	2.254440	3.527236	-2.133987
8	-2.948229	-1.992872	1.824273	6	0.440144	-3.939719	-0.525704
16	-2.987527	-1.705181	0.385105	6	-0.090938	-4.159054	0.743879
7	-1.908484	-0.469738	0.080999	1	-0.754653	-4.998596	0.919649
8	-2.774636	-2.757986	-0.614334	6	0.217147	-3.280672	1.783375
6	-4.588397	-0.986957	0.033518	6	3.330964	-0.738370	-4.016627
6	-5.343368	-0.448083	1.075817	6	4.725566	-0.803562	-4.021842
6	-5.050686	-0.941382	-1.282504	6	5.423030	-0.736186	-2.816075
1	-4.979066	-0.526333	2.093458	1	3.723764	1.855325	1.327821
6	-6.560495	0.163778	0.787711	1	5.263795	-0.903332	-4.959499
6	-6.267931	-0.320124	-1.553446	1	1.561917	-0.537400	-2.814357
1	-4.473313	-1.406960	-2.072758	1	6.639824	-0.129889	3.785027
1	-7.152248	0.582934	1.596863	6	0.260477	4.466491	-0.676246
6	-7.038296	0.243270	-0.527737	1	-0.380483	4.551474	0.199282
1	-6.630527	-0.279439	-2.576867	1	-0.119787	5.157921	-1.442069
6	-8.370584	0.884049	-0.825443	1	1.255968	4.812027	-0.384913
1	-8.583761	1.702337	-0.131716	1	-0.027078	0.687996	-2.572795
1	-9.184751	0.155258	-0.730320	1	5.610512	1.963235	2.925543
1	-8.404522	1.280836	-1.843859	1	5.785703	-2.334646	3.020882
6	-1.458431	-0.345902	-1.329580	1	6.507917	-0.783724	-2.811357
1	-0.995723	-1.288317	-1.636748	1	2.777759	-0.789185	-4.949744

1	0.205792	-4.621244	-1.337339	1	4.295246	2.188583	-2.520343
1	-0.199995	-3.439675	2.772098	6	2.803553	-1.716390	-1.996972
28	0.992312	1.359801	-0.201347	6	2.103415	-1.093899	-3.228624
IM13				1	2.831685	-1.101363	-4.050747
				1	1.313655	-1.782743	-3.531553
				6	4.149428	-1.031185	-1.670148
15	-1.782999	-1.805556	-0.174452	1	4.559086	-1.513734	-0.779653
6	-0.937768	-2.598150	1.248508	1	4.854074	-1.224394	-2.493431
6	-0.455183	-1.759491	2.265393	6	3.160844	-3.176753	-2.342167
6	0.190300	-2.301757	3.373408	1	3.650487	-3.674551	-1.498032
6	0.383836	-3.681397	3.468952	1	2.259452	-3.746712	-2.589235
6	-0.076912	-4.518967	2.451850	1	3.837200	-3.224430	-3.201939
6	-0.740469	-3.982311	1.347363	6	2.385298	1.355340	-2.955380
6	-3.454090	-1.428065	0.482462	6	1.537642	0.312182	-3.094256
6	-4.251640	-0.550311	-0.265159	6	0.063637	0.488945	-3.045050
6	-3.929648	-1.907061	1.709397	6	-0.787690	-0.420200	-3.942464
6	-2.110350	-3.221399	-1.301943	1	-0.514626	-1.473795	-3.921544
6	-3.271377	-4.001787	-1.217818	1	-1.845966	-0.365518	-3.648129
6	-1.137540	-3.549459	-2.256510	1	-0.743421	-0.084809	-4.992659
1	-1.105838	-4.639477	0.565946	6	-5.493109	-0.135829	0.211490
1	-3.878829	-0.161432	-1.206621	6	-5.954793	-0.605685	1.443781
1	-3.315676	-2.577347	2.300755	1	-6.914916	-0.273633	1.826952
1	-4.032447	-3.758365	-0.484274	6	-5.176228	-1.497210	2.185039
8	6.596653	0.529964	-0.750391	6	-3.450788	-5.089923	-2.073080
16	5.254699	1.019718	-0.392730	6	-2.472072	-5.414278	-3.014119
7	4.057802	0.409438	-1.426790	1	-2.614945	-6.261479	-3.678050
8	5.007844	2.466971	-0.307422	6	-1.311964	-4.642326	-3.103076
6	4.789268	0.250444	1.147563	1	0.890419	-4.102954	4.332430
6	5.554472	-0.805433	1.645425	1	-0.574588	-0.688240	2.185780
6	3.648989	0.694956	1.812536	6	-0.387822	1.926975	-3.301175
1	6.447993	-1.112261	1.113483	1	-0.071474	2.250553	-4.306176
6	5.152386	-1.433269	2.820701	1	-1.478533	2.001364	-3.273666
6	3.258731	0.051529	2.983742	1	1.995977	2.360928	-2.868311
1	3.073052	1.517474	1.411555	1	-4.355948	-5.685797	-2.002409
1	5.741793	-2.255066	3.218066	1	-0.548912	-4.884029	-3.837077
6	3.996016	-1.021082	3.499472	1	0.072880	-5.592491	2.519503
1	2.354246	0.375201	3.488503	1	0.544752	-1.639905	4.156133
6	3.544288	-1.744308	4.742758	1	-5.534541	-1.866129	3.141705
1	4.394436	-2.046859	5.361486	1	-6.078707	0.575151	-0.362213
1	2.883968	-1.119988	5.351046	28	-0.662293	-0.097598	-1.219476
1	2.989706	-2.651982	4.478139	15	-1.501577	1.988082	-0.011523
1	-0.250394	-2.933587	-2.335719	6	-3.160864	2.742471	-0.282986
6	3.848081	1.206538	-2.671689	6	-3.845918	3.482421	0.692655
1	4.399199	0.714952	-3.488575	6	-3.777352	2.539144	-1.525482

6	-5.117240	3.993691	0.433242	6	-1.110626	-4.960833	1.924553
1	-3.389062	3.644248	1.662874	6	-1.743979	-4.113302	1.014590
6	-5.044384	3.057691	-1.791391	6	-3.638657	-0.990531	0.849343
1	-3.264121	1.957228	-2.284216	6	-4.333558	0.170910	0.481488
6	-5.720262	3.782513	-0.808398	6	-3.994706	-1.642103	2.040209
1	-5.637025	4.558690	1.201416	6	-2.980685	-2.603524	-1.473370
1	-5.504704	2.889406	-2.760486	6	-4.281435	-2.350443	-1.927694
1	-6.710607	4.180633	-1.008130	6	-2.215176	-3.580914	-2.130503
6	-1.502722	1.690116	1.810176	1	-2.508566	-4.509105	0.355307
6	-0.348953	1.916743	2.576148	1	-4.039170	0.692755	-0.419699
6	-2.620947	1.113784	2.433440	1	-3.467120	-2.536758	2.348761
6	-0.314982	1.568934	3.926495	1	-4.889506	-1.602303	-1.431344
1	0.524102	2.361110	2.115445	8	6.358416	-0.210896	-1.037236
6	-2.581700	0.762494	3.782255	16	5.130210	0.413390	-0.516674
1	-3.527332	0.939251	1.868765	7	3.788648	0.038764	-1.492865
6	-1.427845	0.983690	4.534438	8	5.090177	1.869187	-0.314481
1	0.582768	1.765280	4.506037	6	4.710976	-0.407841	1.011384
1	-3.456556	0.308753	4.237410	6	5.361215	-1.600270	1.338880
1	-1.397172	0.708954	5.584544	6	3.730039	0.130513	1.839534
6	-0.342052	3.417691	-0.151472	1	6.134376	-1.982423	0.681977
6	-0.764646	4.752274	-0.101235	6	4.999782	-2.269065	2.503680
6	1.028181	3.142846	-0.302124	6	3.379485	-0.552908	3.001514
6	0.167854	5.787946	-0.183464	1	3.238581	1.056110	1.577893
1	-1.818445	4.987824	-0.003368	1	5.498410	-3.198747	2.764341
6	1.960829	4.178268	-0.365677	6	3.998038	-1.760068	3.344539
1	1.363003	2.117731	-0.376007	1	2.597976	-0.145766	3.634975
6	1.529177	5.505004	-0.306850	6	3.599336	-2.508076	4.592353
1	-0.173000	6.818810	-0.147855	1	4.456519	-2.656854	5.258222
1	3.015054	3.934985	-0.462926	1	2.828783	-1.969803	5.150561
1	2.250131	6.315252	-0.363507	1	3.207508	-3.501988	4.346919
1	0.006216	2.646817	-2.587615	1	-1.209168	-3.799847	-1.788288
6	1.881418	-1.752843	-0.755295	6	3.656409	0.915572	-2.686039
1	2.483668	-1.909053	0.147182	1	4.149466	0.437787	-3.547663
1	1.206487	-2.608427	-0.849764	1	4.186111	1.843868	-2.475535
6	0.985858	-0.551277	-0.487671	6	2.292217	-1.916798	-2.215721
8	1.186122	0.155457	0.485712	6	1.775219	-1.164237	-3.458544
IM14				1	2.586812	-1.139640	-4.197577
				1	0.980399	-1.755819	-3.916261
				6	3.678167	-1.399679	-1.767810
15	-2.210900	-1.548743	-0.180754	1	3.944946	-1.937223	-0.855913
6	-1.397375	-2.755420	0.949762	1	4.413237	-1.680574	-2.538313
6	-0.421059	-2.261006	1.827884	6	2.527637	-3.386606	-2.623439
6	0.203897	-3.107531	2.741558	1	2.934871	-3.967769	-1.789403
6	-0.134272	-4.460637	2.788607	1	1.586858	-3.854096	-2.930876

1	3.229321	-3.458110	-3.461590	6	0.871471	1.915298	3.927201
6	2.207616	1.213764	-2.959188	1	1.329902	2.861099	2.055443
6	1.301311	0.256255	-3.224737	6	-1.147248	0.598615	3.989779
6	-0.149370	0.557500	-3.285540	1	-2.273753	0.522978	2.171201
6	-1.096312	-0.441378	-3.265593	6	-0.012742	1.096727	4.632575
1	-0.832046	-1.489261	-3.228977	1	1.749360	2.322561	4.420624
1	-2.408260	0.584192	-1.464922	1	-1.852462	-0.032105	4.522629
1	-2.127240	-0.228511	-3.513092	1	0.175059	0.859861	5.675793
6	-5.349044	0.681525	1.288123	6	0.354013	3.312717	-0.325639
6	-5.684999	0.036592	2.478781	6	-0.046963	4.613879	-0.664981
1	-6.462966	0.441293	3.119383	6	1.722580	2.991806	-0.371020
6	-5.009576	-1.128406	2.847935	6	0.898662	5.571713	-1.034121
6	-4.803664	-3.056963	-3.011560	1	-1.095723	4.884487	-0.637953
6	-4.036612	-4.027211	-3.657271	6	2.667170	3.961135	-0.709873
1	-4.445378	-4.576566	-4.499784	1	2.041580	1.981610	-0.148114
6	-2.740492	-4.289522	-3.209691	6	2.256453	5.251772	-1.048390
1	0.358317	-5.123220	3.494445	1	0.570077	6.572867	-1.298140
1	-0.137591	-1.218488	1.789383	1	3.716421	3.686714	-0.708233
6	-0.564116	1.978024	-3.600873	1	2.991224	6.003655	-1.321157
1	-0.176598	2.268781	-4.585250	1	-0.179784	2.698384	-2.876671
1	-1.652247	2.061337	-3.615081	6	1.237613	-1.927302	-1.085465
1	1.890480	2.234837	-2.796755	1	1.654523	-2.464575	-0.225590
1	-5.815506	-2.850470	-3.347914	1	0.383388	-2.503850	-1.449228
1	-2.136152	-5.046862	-3.700444	6	0.713977	-0.577126	-0.543280
1	-1.383747	-6.011459	1.960335	8	1.399458	-0.028718	0.311756
1	0.960791	-2.704394	3.406067				
1	-5.267554	-1.637630	3.772009	IM15			
1	-5.849641	1.598831	0.994870				
28	-1.026613	0.097747	-1.099897	15	2.871028	0.936680	-0.176164
15	-0.866633	2.013698	0.146762	6	3.882024	0.237158	1.203466
6	-2.421946	2.999667	0.280434	6	3.784228	-1.138806	1.442195
6	-2.808374	3.636555	1.467024	6	4.555982	-1.751845	2.426008
6	-3.233091	3.140107	-0.854743	6	5.444960	-0.994553	3.190512
6	-3.993490	4.371227	1.524362	6	5.561173	0.374335	2.949178
1	-2.189374	3.549805	2.352254	6	4.790701	0.987198	1.959053
6	-4.409944	3.885362	-0.802451	6	3.912325	0.430022	-1.622597
1	-2.947283	2.632816	-1.769401	6	3.348920	0.325788	-2.900962
6	-4.798728	4.496652	0.391986	6	5.280224	0.158772	-1.470545
1	-4.285570	4.846629	2.456109	6	3.251545	2.735763	-0.071113
1	-5.027908	3.980202	-1.690634	6	3.833154	3.430389	-1.138432
1	-5.721004	5.068362	0.437900	6	2.916141	3.439861	1.097797
6	-0.487779	1.707420	1.927779	1	4.898882	2.050332	1.783598
6	0.636222	2.220316	2.585226	1	2.286178	0.499408	-3.021825
6	-1.382509	0.904573	2.650775	1	5.738632	0.232629	-0.491449

1	4.100252	2.903548	-2.047244	6	4.124946	-0.047160	-3.998376
8	-4.099093	-1.780907	-0.378812	6	5.482310	-0.326897	-3.832936
16	-4.403927	-0.694554	0.557253	1	6.086869	-0.626475	-4.684015
7	-3.084513	0.368080	0.522741	6	6.056340	-0.221056	-2.565163
8	-4.695223	-0.964789	1.967797	6	4.081324	4.800970	-1.039976
6	-5.770751	0.230404	-0.125736	6	3.765768	5.490234	0.130089
6	-6.002086	0.191241	-1.501898	1	3.969858	6.553987	0.210057
6	-6.545999	1.033754	0.712334	6	3.184667	4.802814	1.198422
1	-5.405538	-0.463842	-2.126742	1	6.045963	-1.466832	3.962069
6	-7.021509	0.974007	-2.038555	1	3.112349	-1.738302	0.848073
6	-7.560364	1.809035	0.157308	6	0.565552	2.979557	-2.565983
1	-6.368832	1.024408	1.781653	1	-0.281491	3.017647	-3.262465
1	-7.214483	0.940485	-3.107134	1	1.329313	3.670897	-2.926209
6	-7.808841	1.797542	-1.222521	1	-1.054578	1.269730	-2.095569
1	-8.175293	2.427542	0.805046	1	4.533834	5.325088	-1.877030
6	-8.888438	2.666327	-1.816719	1	2.932761	5.331616	2.113348
1	-8.496242	3.660425	-2.063853	1	6.255755	0.972876	3.531724
1	-9.287290	2.233978	-2.738400	1	4.459291	-2.821625	2.586920
1	-9.717264	2.807752	-1.117472	1	7.111334	-0.437577	-2.424794
1	2.455729	2.906912	1.921812	1	3.665193	-0.130053	-4.978944
6	-2.657635	0.706653	-0.834102	28	0.669881	0.328964	-0.171847
1	-3.402112	1.382910	-1.299669	15	0.138692	-1.845211	-0.071776
1	-2.668281	-0.218870	-1.405811	6	-1.004329	-2.554437	-1.332207
6	-0.915052	0.675003	2.351810	6	-1.549210	-3.838867	-1.195744
6	-1.775222	1.920508	1.994569	6	-1.246024	-1.837705	-2.509155
1	-0.799651	0.602062	3.437439	6	-2.369678	-4.365802	-2.189916
6	-1.092519	2.877569	0.999340	1	-1.336555	-4.426183	-0.309397
1	-1.754175	3.748479	0.877320	6	-2.061152	-2.369134	-3.509274
1	-0.188769	3.258487	1.482687	1	-0.770330	-0.870802	-2.632801
1	-1.427023	-0.216976	2.003720	6	-2.636761	-3.628454	-3.345129
6	-3.160476	1.466293	1.489747	1	-2.799301	-5.355117	-2.064094
1	-3.724408	1.091934	2.344388	1	-2.243564	-1.798927	-4.415960
1	-3.706963	2.323863	1.063601	1	-3.279121	-4.040795	-4.117624
6	-2.020017	2.746659	3.272514	6	1.599972	-2.919229	-0.422612
1	-2.507329	2.138473	4.040499	6	1.960916	-4.024234	0.359412
1	-1.068427	3.102221	3.678561	6	2.386651	-2.586649	-1.533890
1	-2.653031	3.619860	3.071960	6	3.116690	-4.747815	0.058440
6	-1.323450	1.376458	-1.051573	1	1.357382	-4.305963	1.214247
6	-0.707781	2.408297	-0.384888	6	3.540194	-3.306756	-1.831731
6	0.146141	3.349549	-1.162344	1	2.106544	-1.735779	-2.139542
6	0.461975	4.568684	-0.695052	6	3.915067	-4.384824	-1.027410
1	0.181079	4.925017	0.286211	1	3.394315	-5.595163	0.678926
1	0.850500	0.002760	-1.645671	1	4.152381	-3.006475	-2.676521
1	1.054433	5.248810	-1.295686	1	4.822349	-4.940212	-1.245736

6	-0.459129	-2.451408	1.552017	1	-5.548997	2.136235	1.131787
6	-1.797751	-2.787268	1.790133	1	-6.752589	-2.661610	1.484798
6	0.422017	-2.349608	2.643766	6	-6.273388	-0.873565	2.585871
6	-2.246446	-3.021320	3.091130	1	-5.820306	1.081937	3.369407
1	-2.504712	-2.829020	0.972505	6	-6.394852	-1.522681	3.941311
6	-0.024674	-2.605103	3.936784	1	-7.051854	-2.396124	3.909347
1	1.448275	-2.034325	2.489267	1	-6.789263	-0.824272	4.685086
6	-1.362874	-2.937484	4.165629	1	-5.414739	-1.861171	4.298964
1	-3.295915	-3.242223	3.254732	6	-2.969383	1.774439	-1.481057
1	0.668512	-2.520015	4.768357	1	-2.145411	1.625436	-2.180780
1	-1.714713	-3.114649	5.177678	1	-3.400596	2.756757	-1.677854
1	0.971060	1.967460	-2.597007	6	-2.582320	-0.855070	0.134720
6	0.489902	0.718411	1.738424	6	-2.611051	-1.380569	-1.326251
8	1.405125	1.067049	2.478090	1	-2.156320	-1.660736	0.737052
IM16				6	-1.179978	-1.500687	-1.900895
				6	-0.307562	-0.265657	-1.666270
				1	-1.225578	-1.705420	-2.977023
				1	-0.691507	-2.344306	-1.415107
15	1.710368	-1.916228	0.072400	1	-0.691507	-2.344306	-1.415107
6	2.294335	-2.546878	-1.547851	8	-0.055886	0.492545	-2.594591
6	2.640688	-3.890086	-1.767250	1	-3.624512	-0.755073	0.464610
6	3.148008	-4.293590	-3.001420	6	-3.499747	-0.530787	-2.300651
6	3.324749	-3.359831	-4.025567	1	-4.382883	-1.100206	-2.591522
6	2.995401	-2.022146	-3.809282	1	-2.938609	-0.342522	-3.223155
6	2.481051	-1.615682	-2.578436	6	-3.213954	-2.799657	-1.281394
6	0.942744	-3.389583	0.877472	1	-4.222216	-2.771140	-0.855337
6	1.066284	-3.578386	2.262220	1	-2.604282	-3.466472	-0.664106
6	0.110280	-4.261824	0.156983	1	-3.282637	-3.231892	-2.285680
6	4.505712	-2.251465	0.571599	6	-2.471179	1.728822	-0.040270
6	3.284966	-1.720406	1.009173	6	-1.845326	0.436972	0.462116
6	3.263181	-0.924710	2.162105	6	-1.223407	0.546242	1.779944
1	2.515936	-4.618463	-0.973395	6	-0.577191	-0.500937	2.410167
1	1.711772	-2.926215	2.839682	1	-0.118637	-0.350190	3.382173
1	4.544572	-2.852670	-0.328945	1	-1.766868	2.554297	0.070014
1	2.323605	-0.487352	2.478120	6	4.437212	-0.653507	2.863543
8	-6.334569	0.226596	-2.508308	6	5.651151	-1.174293	2.413746
16	-5.583015	1.021890	-1.531208	1	6.571021	-0.948695	2.944861
7	-3.968100	0.757618	-1.812279	6	5.680758	-1.977279	1.271075
8	-5.752824	2.473220	-1.410620	6	-0.584821	-5.283346	0.803928
6	-5.949587	0.312357	0.071865	6	-0.463348	-5.452775	2.183547
6	-6.312923	-1.031311	0.158249	6	0.369275	-4.598984	2.908087
6	-5.785497	1.082486	1.223391	1	2.227718	-0.576248	-2.421440
1	-6.478217	-1.599470	-0.749856	1	-1.006135	-6.246534	2.687451
6	-6.470534	-1.614835	1.413498	1	0.017330	-4.160154	-0.917816
6	-5.946187	0.485068	2.470221	1	3.719519	-3.676393	-4.986539

6	-1.196609	1.901478	2.462515	28	0.394814	-0.104329	0.071893
1	-2.216663	2.275271	2.602912	1	-0.655178	-1.526673	2.075766
1	-0.730520	1.831379	3.447450	1	-0.658928	2.656140	1.882493
1	-3.328630	1.975448	0.603888				
1	3.137413	-1.285205	-4.592780	IM17			
1	3.408412	-5.335663	-3.162079				
1	6.623598	-2.383292	0.916108	15	2.837849	1.254992	-0.303625
1	4.404100	-0.006846	3.734073	6	3.666679	1.472365	1.322732
1	0.481432	-4.727740	3.980600	6	4.765243	2.328656	1.495699
1	-1.218540	-5.948556	0.224899	6	5.384113	2.436641	2.739745
15	1.827383	1.866499	0.114708	6	4.906280	1.697692	3.825890
6	2.811321	2.390423	1.583457	6	3.799058	0.864535	3.667631
6	4.028450	3.080261	1.486114	6	3.178010	0.760868	2.423179
6	2.294343	2.113964	2.855117	6	2.805152	3.002560	-0.889286
6	4.716757	3.466918	2.635645	6	3.480759	3.456713	-2.026478
1	4.440785	3.306823	0.508965	6	1.993281	3.900140	-0.173554
6	2.972470	2.513476	4.006485	6	5.428166	0.193781	-0.953609
1	1.364850	1.564448	2.934645	6	4.123067	0.482727	-1.372185
6	4.190584	3.186392	3.898727	6	3.718869	0.074886	-2.654381
1	5.662423	3.993292	2.545224	1	5.129297	2.911586	0.654984
1	2.555230	2.291233	4.984491	1	4.115512	2.778515	-2.586482
1	4.727143	3.491193	4.792333	1	5.752814	0.483359	0.038832
6	1.005730	3.449734	-0.355944	1	2.704292	0.283559	-2.978661
6	1.145114	4.630404	0.388120	8	-7.067874	1.714140	0.615185
6	0.130417	3.440853	-1.455889	16	-6.083708	0.718977	1.054125
6	0.428819	5.776010	0.036347	7	-4.642267	1.531067	1.270103
1	1.808498	4.659038	1.244543	8	-6.309168	-0.120098	2.235849
6	-0.566530	4.593536	-1.814783	6	-5.786792	-0.401967	-0.308201
1	-0.009019	2.521177	-2.013560	6	-5.910277	0.061082	-1.618163
6	-0.425046	5.763867	-1.066598	6	-5.319939	-1.689641	-0.044769
1	0.543446	6.680735	0.626485	1	-6.308235	1.052955	-1.801673
1	-1.235636	4.569149	-2.669933	6	-5.521393	-0.765579	-2.669536
1	-0.980234	6.656780	-1.337800	6	-4.931590	-2.501335	-1.107098
6	3.137861	1.626978	-1.159092	1	-5.246235	-2.033391	0.979975
6	2.963574	2.021690	-2.492328	1	-5.610278	-0.408678	-3.691694
6	4.280661	0.882255	-0.820186	6	-5.005479	-2.047123	-2.430398
6	3.906698	1.675973	-3.461636	1	-4.551090	-3.498700	-0.906269
1	2.091352	2.593436	-2.781317	6	-4.500437	-2.900607	-3.564825
6	5.218072	0.537357	-1.790644	1	-5.007795	-2.663170	-4.503839
1	4.441286	0.570901	0.203873	1	-4.638827	-3.965619	-3.358290
6	5.033915	0.929376	-3.117403	1	-3.427234	-2.732603	-3.717648
1	3.754824	1.992535	-4.489447	6	-3.495261	0.781590	1.787002
1	6.087279	-0.047128	-1.504854	1	-2.947963	1.445489	2.467297
1	5.761087	0.654662	-3.875545	1	-3.869481	-0.036765	2.404398

6	-2.964060	2.124121	-0.984023	6	1.093710	-3.032996	-0.908299
6	-3.317773	3.294889	-0.035165	6	1.126921	-4.412132	-0.652973
1	-2.498900	2.526822	-1.889568	6	1.244642	-2.580042	-2.223016
6	-1.990232	3.531153	0.727836	6	1.277176	-5.318487	-1.700259
6	-1.215957	2.226933	0.679563	1	1.042876	-4.771578	0.368141
1	-2.102358	3.894931	1.754159	6	1.408020	-3.486334	-3.271985
1	-1.371773	4.268169	0.195975	1	1.243949	-1.510496	-2.402875
8	-0.207621	1.987552	1.322210	6	1.417248	-4.856527	-3.012574
1	-3.847693	1.561392	-1.288760	1	1.296953	-6.384678	-1.494158
6	-4.500647	2.939004	0.912314	1	1.529904	-3.121846	-4.287906
1	-5.438562	3.232162	0.440818	1	1.542196	-5.564671	-3.826511
1	-4.409208	3.534044	1.832991	6	-0.432493	-2.348788	1.470795
6	-3.731200	4.552325	-0.812570	6	-1.435875	-3.193609	0.977625
1	-4.595043	4.346394	-1.453643	6	-0.622675	-1.745782	2.728149
1	-2.912190	4.904010	-1.448000	6	-2.591819	-3.435029	1.723212
1	-4.005547	5.368468	-0.134172	1	-1.321010	-3.655475	0.003669
6	-2.577434	0.216357	0.700962	6	-1.767539	-2.002498	3.478915
6	-1.919478	1.238193	-0.252057	1	0.113421	-1.041143	3.103445
6	-0.968227	0.548598	-1.238208	6	-2.762337	-2.845721	2.975793
6	0.035433	1.350434	-1.823039	1	-3.359536	-4.091856	1.324337
1	0.434438	1.083689	-2.801388	1	-1.894291	-1.528264	4.447488
1	-1.774931	-0.324654	1.193535	1	-3.662807	-3.033279	3.552360
6	4.598651	-0.598416	-3.499099	6	2.462045	-2.328268	1.421863
6	5.894810	-0.890978	-3.068310	6	2.437983	-2.783890	2.744343
1	6.577784	-1.428617	-3.719049	6	3.702564	-2.190908	0.778861
6	6.304932	-0.493179	-1.795600	6	3.631041	-3.055724	3.420371
6	1.867942	5.222919	-0.590079	1	1.493911	-2.929905	3.255549
6	2.542153	5.669517	-1.730889	6	4.888857	-2.468740	1.449403
6	3.346861	4.783829	-2.445292	1	3.738996	-1.855141	-0.250808
1	2.311013	0.127561	2.293206	6	4.858459	-2.891061	2.780812
1	2.440443	6.700287	-2.057259	1	3.595472	-3.401337	4.449718
1	1.454866	3.551622	0.702395	1	5.835388	-2.343891	0.932270
1	5.392277	1.780339	4.793723	1	5.783324	-3.095647	3.311677
6	-1.583992	-0.599835	-2.016152	28	0.897532	0.234215	-0.400561
1	-2.533032	-0.298709	-2.483762	1	0.131498	2.406304	-1.579995
1	-0.912955	-0.929018	-2.812162	1	-1.801943	-1.470101	-1.390367
1	-3.135026	-0.503879	0.105201				
1	3.418285	0.292039	4.507720	IM18			
1	6.236159	3.098644	2.864444				
1	7.311022	-0.718554	-1.453441	6	-3.974628	0.893938	1.462806
1	4.269496	-0.906372	-4.487212	7	-4.030897	1.199645	0.003825
1	3.878696	5.123515	-3.329565	1	-5.028063	0.881722	1.767174
1	1.243137	5.908488	-0.024027	1	-3.514911	1.736777	1.989031
15	0.984606	-1.783796	0.442970	6	-5.310787	1.152796	-0.719885

16	-2.636894	1.363883	-0.881757	28	-1.380875	-0.286291	1.335329
1	-5.181961	1.716705	-1.643512	6	1.886777	-1.371674	-1.126290
1	-6.043694	1.690684	-0.106750	6	3.027167	-0.414476	-0.768193
6	-5.832801	-0.252607	-1.051693	6	3.554503	-1.518350	-2.757155
8	-3.022360	1.612012	-2.277410	1	0.993451	-0.816134	-1.415725
8	-1.715647	0.211088	-0.662217	1	3.566837	-0.772261	0.112030
6	-1.796153	2.822910	-0.279180	6	4.661115	-2.564061	-2.718214
6	-6.813519	-0.293094	-2.277136	1	4.385491	-3.426823	-3.330019
6	-1.264867	2.876464	1.010262	1	5.593222	-2.140275	-3.101898
6	-1.597909	3.867538	-1.181815	1	4.812643	-2.901207	-1.690651
1	-7.872347	-0.488838	-2.086066	6	3.280403	-0.952605	-4.143531
1	-6.724044	0.585488	-2.927043	1	4.170027	-0.445056	-4.525506
1	-1.381720	2.035104	1.687784	1	3.009050	-1.758140	-4.831215
6	-0.528342	3.993416	1.390325	1	2.461927	-0.232031	-4.089883
6	-0.837113	4.965843	-0.789597	8	2.355183	-2.106507	-2.238317
1	-2.008512	3.798243	-2.181227	8	3.893684	-0.432866	-1.884166
1	-0.114086	4.036669	2.393282	6	2.485176	1.018544	-0.476709
6	-0.282359	5.042220	0.493527	6	1.508828	-2.282748	0.088532
1	-0.656335	5.767229	-1.499749	8	1.667752	-1.473456	1.277505
6	0.610830	6.190642	0.885499	8	1.245032	0.880296	0.251922
1	1.660512	5.935382	0.693932	15	0.761417	-0.102483	1.504118
1	0.518697	6.425384	1.949979	7	1.524941	0.380944	2.921707
1	0.382339	7.093124	0.312467	6	2.950898	0.248851	3.201037
6	-3.263159	-0.394796	1.802401	1	3.462641	1.215993	3.137883
6	-2.389891	-0.573901	2.893710	1	3.088532	-0.158677	4.210601
6	-2.319309	-0.958675	4.168562	1	3.411220	-0.433798	2.490516
6	-3.566134	-1.165325	5.000091	6	0.844777	1.363457	3.753398
1	-4.469644	-0.960911	4.420658	1	-0.231864	1.313325	3.576202
1	-3.568059	-0.513167	5.884503	1	1.023172	1.137720	4.810959
1	-3.621251	-2.196593	5.375953	1	1.206263	2.382873	3.553626
6	-6.447176	-0.975321	0.149411	6	2.505260	-3.430522	0.221661
1	-7.260953	-0.385023	0.585937	6	2.398592	-4.546573	-0.617636
1	-5.708728	-1.174741	0.928472	6	3.570684	-3.363868	1.124240
1	-6.865899	-1.940042	-0.157275	6	3.346123	-5.565074	-0.565266
6	-4.840672	-1.174013	-1.836915	1	1.573749	-4.613097	-1.316348
1	-4.044962	-0.610990	-2.334751	6	4.521261	-4.386151	1.176708
1	-4.390798	-2.016262	-1.307769	1	3.646064	-2.520221	1.797290
6	-5.976425	-1.462499	-2.816058	6	4.415919	-5.487373	0.329258
8	-6.184243	-2.326900	-3.629145	1	3.248937	-6.421801	-1.225399
6	-1.017638	-1.258150	4.867586	1	5.340925	-4.319244	1.886140
1	-0.867819	-0.609103	5.741721	1	5.154796	-6.282137	0.369157
1	-0.166956	-1.141356	4.195019	6	0.073682	-2.793921	-0.011364
1	-1.017486	-2.289152	5.247874	6	-0.561217	-2.950040	-1.248223
1	-3.690461	-1.286573	1.339065	6	-0.616088	-3.140480	1.158602

6	-1.862168	-3.451474	-1.314258	6	-1.140668	3.529249	-0.613513
1	-0.039706	-2.689593	-2.162967	6	-6.544226	1.358783	0.767984
6	-1.918072	-3.633311	1.091268	6	0.154495	3.583323	-0.097586
1	-0.130298	-3.020089	2.119340	6	-1.820270	4.691061	-0.981744
6	-2.544004	-3.793178	-0.145817	1	-7.237099	1.327723	1.613816
1	-2.344266	-3.567299	-2.280146	1	-6.650547	2.324213	0.258324
1	-2.444981	-3.871961	2.009574	1	0.669142	2.666627	0.151678
1	-3.556692	-4.182271	-0.199246	6	0.775203	4.818767	0.051208
6	2.119196	1.715068	-1.788374	6	-1.182383	5.919201	-0.826861
6	3.086483	2.407082	-2.525928	1	-2.816209	4.624414	-1.404832
6	0.821756	1.614527	-2.297058	1	1.787458	4.855885	0.443010
6	2.759116	2.982699	-3.751972	6	0.119340	6.002597	-0.310639
1	4.096849	2.491121	-2.142907	1	-1.698590	6.829239	-1.119651
6	0.493316	2.189088	-3.526085	6	0.815556	7.334107	-0.186232
1	0.069657	1.095026	-1.723007	1	1.417397	7.542170	-1.079300
6	1.461442	2.874653	-4.258673	1	1.492465	7.351114	0.672713
1	3.520441	3.515587	-4.314224	1	0.099318	8.152887	-0.075728
1	-0.523670	2.097137	-3.895936	6	-1.158523	0.160366	2.090803
1	1.210057	3.323580	-5.215252	6	0.116417	0.005438	2.650944
6	3.451686	1.863529	0.339333	6	0.743345	-0.210478	3.810794
6	2.944166	2.967101	1.036367	6	0.008881	-0.069272	5.127552
6	4.820384	1.591244	0.395444	1	-1.036437	0.209805	4.974348
6	3.786846	3.768677	1.801100	1	0.479131	0.692344	5.765510
1	1.882324	3.173251	0.981292	1	0.035355	-1.008838	5.697734
6	5.667448	2.399539	1.159813	6	-4.893908	0.167807	2.322633
1	5.230888	0.759339	-0.167218	1	-5.026420	0.817969	3.195449
6	5.154658	3.484167	1.869217	1	-3.910830	-0.302886	2.383126
1	3.378245	4.614235	2.347523	1	-5.639816	-0.631653	2.382522
1	6.729416	2.176155	1.199560	6	-5.104374	0.011703	-0.227289
1	5.813457	4.106433	2.467382	1	-4.644198	0.465005	-1.111724
IM19				1	-4.726965	-1.004768	-0.115512
				6	-6.619049	0.191296	-0.230256
				8	-7.536521	-0.404111	-0.737406
				6	2.182769	-0.639595	3.934292
6	-1.785929	1.519098	1.902537	1	2.783177	0.096008	4.485170
7	-2.675221	1.640536	0.716048	1	2.646930	-0.784380	2.960425
1	-2.430647	1.762066	2.755698	1	2.250470	-1.584161	4.492987
1	-1.010388	2.294251	1.875449	1	-1.883389	-0.646053	2.182776
6	-4.058362	2.109757	0.896841	1	0.270898	-0.222941	0.767972
16	-1.944288	1.944981	-0.749497	28	2.345844	0.228633	0.101407
1	-4.336958	2.718029	0.034663	15	2.421859	1.391110	-1.328747
1	-4.102058	2.754136	1.784317	6	3.213461	2.548016	-1.333408
6	-5.051399	0.951708	1.021465	6	1.618037	1.113097	-2.443481
8	-3.003481	2.049854	-1.761309	6	3.182120	3.419356	-2.423313
8	-0.872604	0.952290	-0.919077				

1	3.847074	2.775943	-0.484172	6	1.581078	-2.457103	-3.952387
6	1.597824	1.977550	-3.534693	1	1.847487	-3.197165	-1.958926
1	0.997864	0.229548	-2.451216	6	-0.423843	-1.182652	-4.362583
6	2.372211	3.139441	-3.524217	1	-1.703323	-0.866844	-2.672036
1	3.792894	4.317624	-2.409976	6	0.772789	-1.732767	-4.828265
1	0.966255	1.742162	-4.385746	1	2.527062	-2.867681	-4.291731
1	2.345559	3.821504	-4.369060	1	-1.052790	-0.597897	-5.027426
6	3.426231	1.106623	1.308633	1	1.077875	-1.584714	-5.859774
6	4.810287	0.908438	1.377936	6	0.388849	-3.595269	0.350279
6	2.828530	2.051945	2.154630	6	0.535097	-4.808811	-0.334132
6	5.582969	1.640785	2.281288	6	0.806360	-3.509480	1.686064
1	5.282587	0.180923	0.726192	6	1.132598	-5.902195	0.291152
6	3.602272	2.794344	3.044161	1	0.187305	-4.896053	-1.358248
1	1.750288	2.165411	2.138739	6	1.386074	-4.610652	2.317680
6	4.982453	2.587363	3.112326	1	0.688235	-2.567901	2.216059
1	6.654918	1.473362	2.332701	6	1.562641	-5.804834	1.617233
1	3.126646	3.520086	3.697642	1	1.254598	-6.834351	-0.252897
1	5.585024	3.156063	3.814448	1	1.709285	-4.530114	3.351609
6	3.417504	-1.157931	-0.466957	1	2.023442	-6.659839	2.103426
6	3.495167	-2.295761	0.349275				
6	4.080661	-1.163033	-1.700446				
6	4.193227	-3.426491	-0.066962				
1	2.981797	-2.307318	1.301736	15	-2.503944	-1.026183	-0.596945
6	4.786969	-2.293517	-2.115761	6	-2.268530	-2.853601	-0.657637
1	4.027054	-0.294003	-2.345679	6	-1.311111	-3.351157	-1.561262
6	4.835997	-3.430293	-1.307747	6	-0.945486	-4.694194	-1.540590
1	4.212033	-4.306762	0.567676	6	-1.524560	-5.564768	-0.612091
1	5.290844	-2.287269	-3.078097	6	-2.481936	-5.082269	0.279852
1	5.371474	-4.314101	-1.641824	6	-2.857214	-3.737015	0.255803
15	-0.422224	-2.104516	-0.366119	6	-3.046802	-0.603120	-2.302677
6	-2.171758	-2.703209	-0.269153	6	-2.927549	0.740248	-2.694982
6	-2.981041	-3.027020	-1.365458	6	-3.562787	-1.534873	-3.211752
6	-2.696094	-2.879009	1.023425	6	-4.056415	-0.817570	0.376438
6	-4.283866	-3.493735	-1.175090	6	-5.263762	-0.429455	-0.219663
1	-2.596098	-2.931769	-2.373254	6	-4.009392	-0.959347	1.773790
6	-3.992751	-3.351881	1.212867	1	-3.591967	-3.377364	0.965904
1	-2.071313	-2.675433	1.886757	1	-2.527295	1.459384	-1.986175
6	-4.797157	-3.654421	0.111570	1	-3.661658	-2.574591	-2.918339
1	-4.898107	-3.731949	-2.038246	1	-5.320227	-0.309151	-1.295350
1	-4.375399	-3.481876	2.220928	1	-3.089682	-1.252015	2.266490
1	-5.813150	-4.008581	0.254476	8	-1.790914	-2.904399	3.354528
6	-0.016395	-2.118438	-2.151821	8	0.542804	-0.744081	-1.851235
6	1.192368	-2.651318	-2.626884	6	-0.792644	-2.521496	2.788955
6	-0.808162	-1.358043	-3.034554	16	1.786326	-1.540847	-1.804095

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6	-0.083477	-1.181846	2.695779	6	6.188657	-2.201029	2.759449
7	1.853753	-2.242034	-0.280106	1	5.720331	-1.795518	3.665332
8	2.009835	-2.618698	-2.772032	1	7.249950	-1.926044	2.794386
6	3.113038	-0.355138	-1.934772	1	6.110485	-3.289549	2.789149
6	1.166740	-1.941060	2.128622	1	4.776169	-3.505120	-1.072938
1	0.030144	-0.584981	3.604156	6	5.594158	-0.124280	1.355876
1	-0.565298	-0.558356	1.916470	1	5.125008	0.374029	2.213840
6	2.753545	-3.404733	-0.141886	1	5.091299	0.204741	0.446465
6	4.332405	-0.711565	-2.508751	1	6.636963	0.215041	1.320768
6	2.898464	0.926957	-1.431178	1	-1.231139	-6.610189	-0.585553
1	2.482533	-4.114939	-0.921434	1	-0.846282	-2.680008	-2.272425
1	2.494606	-3.857175	0.816358	1	-2.937807	-5.749234	1.005461
1	4.467074	-1.705558	-2.917987	1	-0.198610	-5.051716	-2.243356
6	5.349698	0.237549	-2.564155	1	-3.221127	2.184336	-4.262125
6	3.924862	1.864738	-1.494166	1	-4.336072	-1.864635	-5.192778
1	1.930187	1.189231	-1.029138	1	-7.320648	0.120395	0.081740
1	6.301248	-0.026819	-3.016710	1	-5.088125	-0.858300	3.626847
6	5.166104	1.531562	-2.053306	28	-0.737084	0.179532	-0.243357
1	3.745400	2.867552	-1.119645	15	-0.411626	2.121836	0.486275
6	6.286893	2.539026	-2.084212	6	-1.949492	3.094153	0.813576
1	6.892930	2.472958	-1.172183	6	-2.067016	4.474044	0.599953
1	5.900335	3.559985	-2.146076	6	-3.058418	2.384538	1.295118
1	6.955172	2.370597	-2.933255	6	-3.274964	5.123966	0.859232
6	1.764641	-1.309686	0.852230	1	-1.221507	5.040234	0.224720
1	2.747445	-0.877162	1.069931	6	-4.260833	3.034613	1.567185
1	1.110775	-0.483805	0.533751	1	-2.973013	1.316024	1.442148
6	0.265884	-3.208632	1.932945	6	-4.372253	4.408347	1.343023
1	-0.080991	-3.323979	0.902401	1	-3.358875	6.192528	0.681719
1	0.643623	-4.169590	2.294641	1	-5.105844	2.459899	1.933483
6	-3.942354	-1.132697	-4.493352	1	-5.310653	4.919299	1.538655
6	-3.820403	0.204203	-4.875812	6	0.469070	2.204301	2.108334
1	-4.116082	0.513707	-5.874015	6	-0.213982	2.419459	3.312420
6	-3.316737	1.142044	-3.971453	6	1.833322	1.869478	2.161265
6	-6.395251	-0.186430	0.560805	6	0.444057	2.290294	4.537467
6	-6.341439	-0.337380	1.946600	1	-1.266766	2.679423	3.293007
1	-7.223526	-0.150500	2.552092	6	2.492219	1.755360	3.383189
6	-5.144612	-0.731674	2.549834	1	2.384203	1.697807	1.242153
6	4.243618	-3.105251	-0.210641	6	1.797613	1.956077	4.579313
6	4.896037	-2.380411	0.662921	1	-0.104303	2.455414	5.460452
6	2.229942	-2.143584	3.210227	1	3.550329	1.510256	3.403641
1	1.788369	-2.577633	4.113753	1	2.308672	1.856661	5.532119
1	2.678715	-1.183387	3.484909	6	0.548455	3.316721	-0.550250
1	3.031898	-2.806116	2.870168	6	1.372181	4.327231	-0.034704
6	5.528129	-1.625288	1.527904	6	0.438078	3.177820	-1.942877

6	2.070236	5.179639	-0.893757	6	2.990518	4.865109	1.359416
1	1.469209	4.445190	1.039622	1	2.207006	4.899972	2.120954
6	1.127762	4.032992	-2.800164	1	2.576572	5.257620	0.424850
1	-0.169797	2.371427	-2.344888	1	3.788040	5.549241	1.672134
6	1.948342	5.035437	-2.277251	6	1.561068	-1.342044	-2.849881
1	2.705677	5.958568	-0.481455	1	1.755251	-2.356609	-3.216024
1	1.037369	3.907876	-3.875107	1	0.922083	-0.810105	-3.560606
1	2.493441	5.696916	-2.944171	6	2.770994	-0.467135	-2.416121
IM21				6	1.835861	0.137993	-1.333594
15	-2.856809	0.042212	0.037414	1	1.239929	0.950526	-1.756833
6	-3.873556	-0.022150	-1.481756	6	3.350327	0.481149	-3.458485
6	-5.226430	0.341068	-1.505397	1	4.055018	1.184140	-2.999855
6	-5.939709	0.293928	-2.703948	1	2.557083	1.062978	-3.938396
6	-5.306570	-0.113870	-3.879020	1	3.887242	-0.066053	-4.242826
6	-3.958400	-0.478904	-3.855552	6	3.890245	-1.360998	-1.806400
6	-3.238474	-0.440250	-2.662308	1	4.873253	-0.964755	-2.061606
6	-2.071276	1.693125	-0.025210	1	3.843498	-2.360253	-2.255488
6	-2.707171	2.809032	-0.587126	1	2.259441	0.469214	-0.385952
6	-0.770215	1.823890	0.478070	6	1.481251	-2.296923	-0.446889
6	-4.685391	-1.065966	1.797923	6	0.314595	-2.569236	0.472578
6	-4.081867	0.136470	1.395015	6	-5.625083	-1.076000	2.826147
1	-5.720108	0.654615	-0.591142	6	-5.962198	0.114562	3.474743
1	-3.703920	2.707870	-1.005112	1	-6.688971	0.107262	4.281313
1	-0.261178	0.951443	0.875580	6	-5.359132	1.311384	3.087400
1	-4.420720	-1.994158	1.297364	6	-4.423969	1.325462	2.050804
8	6.288001	-0.711732	-0.305894	1	-3.959171	2.258752	1.752184
16	5.097042	-0.795646	0.545266	6	-2.054667	4.041120	-0.626052
7	3.892591	-1.524037	-0.347423	6	-0.759359	4.164233	-0.117122
8	5.116383	-1.469543	1.846312	1	-0.248809	5.122058	-0.158468
6	4.545342	0.882611	0.835812	6	-0.116542	3.053923	0.431579
6	2.693875	-1.923086	0.418747	1	-2.189938	-0.725784	-2.626714
6	3.777547	1.175389	1.962271	1	-5.864018	-0.151323	-4.810324
6	4.818400	1.865183	-0.119091	28	-1.161606	-1.513683	0.208283
1	2.382088	-1.104089	1.079080	1	-5.616344	2.238083	3.591703
1	2.960390	-2.761711	1.062612	1	-6.089148	-2.010868	3.125569
1	3.603778	0.406512	2.706060	1	0.898480	3.130635	0.802649
6	3.270006	2.465383	2.122728	1	-2.552529	4.901673	-1.062946
6	4.303973	3.144792	0.054740	1	-3.466968	-0.801627	-4.768679
1	5.437807	1.621499	-0.974473	1	-6.988870	0.574239	-2.718763
1	2.674554	2.700031	3.000745	6	0.105149	-3.442663	1.460998
6	3.521671	3.465029	1.175090	6	-1.225137	-3.307577	2.189902
1	4.514910	3.911603	-0.685655	6	1.014973	-4.546204	1.934559
				1	-1.852524	-4.200837	2.082178
				1	-1.853597	-2.454695	1.841021

1	0.469151	-5.497132	1.995526	1	-4.114089	3.758310	0.569972
1	1.863786	-4.689507	1.262159	1	-4.270016	3.085855	2.205935
1	1.720487	-3.200190	-1.026325	1	-7.408334	1.352669	2.018868
6	0.995904	-1.172554	-1.417443	6	-2.432610	0.925837	-0.049568
8	-0.392180	-1.030147	-1.344943	6	-2.183727	-0.008568	-1.051763
1	-1.083506	-3.120160	3.261705	6	-2.500174	-0.615099	-2.189521
1	1.409801	-4.341846	2.938812	6	-3.846476	-0.410986	-2.845173
IM22				1	-4.496949	0.231203	-2.251146
				1	-4.356231	-1.369565	-2.989824
				1	-3.724653	0.043631	-3.838321
8	-6.735754	-0.809674	1.694508	6	-1.559033	-1.529828	-2.927962
6	-7.949455	3.304575	1.159580	1	-1.371897	-1.153325	-3.943001
16	-5.285195	-1.013361	1.583846	1	-2.001411	-2.528685	-3.041093
8	-8.996314	3.860992	1.376548	1	-0.601409	-1.629983	-2.417121
7	-4.628053	0.455437	1.143501	1	-2.359808	1.982364	-0.321108
8	-4.484601	-1.507395	2.707809	28	-0.622087	0.161239	-0.004954
6	-5.045512	-2.163272	0.231953	6	3.364546	1.327474	-0.069338
6	-3.151191	0.615485	1.247959	6	4.203447	0.120234	0.353994
6	-3.820789	-2.819665	0.094781	6	5.515314	2.051756	0.474892
6	-6.088929	-2.403565	-0.661047	1	2.600555	1.538766	0.682096
1	-2.774350	-0.301090	1.700305	1	4.395618	-0.531492	-0.500673
1	-2.949542	1.414446	1.967568	6	6.625235	2.253751	-0.547146
1	-3.030552	-2.644431	0.814560	1	6.662994	3.300238	-0.860297
6	-3.643846	-3.712987	-0.955380	1	7.590073	1.979345	-0.112277
6	-5.895047	-3.303400	-1.708148	1	6.434479	1.633272	-1.425040
1	-7.043416	-1.912823	-0.510974	6	5.699944	2.850161	1.757860
1	-2.694344	-4.228729	-1.062834	1	6.616042	2.539276	2.266390
6	-4.671139	-3.962142	-1.877127	1	5.766679	3.917092	1.528440
1	-6.707872	-3.499672	-2.401660	1	4.854544	2.676636	2.426370
6	-4.446293	-4.898974	-3.036641	8	4.266162	2.409941	-0.132522
1	-5.391512	-5.259466	-3.450774	8	5.427303	0.659026	0.807457
1	-3.849225	-5.766494	-2.739799	6	3.473402	-0.712141	1.456840
1	-3.903573	-4.392435	-3.844571	6	2.650062	1.054636	-1.430157
6	-6.970730	3.333415	-0.024208	8	2.257311	-0.341925	-1.415036
1	-7.328433	2.727293	-0.865377	8	2.058329	-0.712139	1.149653
1	-6.701195	4.325251	-0.399639	15	1.208548	-0.909362	-0.263837
6	-5.931804	2.597385	0.892175	7	1.238619	-2.508957	-0.752895
6	-7.043305	2.383748	1.973787	6	2.405799	-3.219387	-1.265225
1	-6.819430	2.715666	2.992123	1	2.788930	-3.933381	-0.527467
6	-5.394123	1.318894	0.242213	1	2.133004	-3.762506	-2.178535
1	-4.751960	1.586659	-0.604002	1	3.197297	-2.513946	-1.507702
1	-6.235269	0.747032	-0.156783	6	0.150001	-3.368044	-0.305379
6	-4.822929	3.530970	1.374624	1	-0.703807	-2.750240	-0.016498
1	-5.243010	4.478223	1.729812	1	-0.160557	-4.027179	-1.125120

1	0.449769	-3.991074	0.548514	1	5.122339	-5.858654	1.742348
6	3.633200	1.209979	-2.584215				
6	3.963424	2.492863	-3.039161	IM23			
6	4.261844	0.103562	-3.161685				
6	4.914679	2.664777	-4.040556	8	-0.010474	-3.920323	-2.454406
1	3.477424	3.355829	-2.600077	8	-2.026418	1.520235	-1.329016
6	5.216403	0.276593	-4.166985	6	-0.924527	-3.190035	-2.151870
1	3.992175	-0.892718	-2.836835	16	-2.597707	1.203397	0.011265
6	5.549667	1.556454	-4.606127	6	-2.084875	-2.572429	-2.935269
1	5.161566	3.666202	-4.379930	7	-3.091278	-0.383324	-0.057493
1	5.693996	-0.593524	-4.607611	8	-1.836014	1.371860	1.249013
1	6.291788	1.691145	-5.387211	6	-4.044545	2.234455	0.126776
6	1.418594	1.932189	-1.635122	6	-2.809040	-2.373166	-1.555782
6	1.192141	3.091483	-0.885632	1	-2.567406	-3.183765	-3.703008
6	0.505265	1.578573	-2.637241	1	-1.759528	-1.614683	-3.359975
6	0.059757	3.875024	-1.126757	6	-3.690762	-0.947893	1.165041
1	1.908311	3.405145	-0.133964	6	-4.416333	2.742247	1.370820
6	-0.622533	2.357170	-2.874490	6	-4.831474	2.445938	-1.007798
1	0.679588	0.677853	-3.214687	1	-3.248149	-0.419688	2.011865
6	-0.850799	3.508841	-2.116718	1	-3.369862	-1.988820	1.237202
1	-0.103559	4.774220	-0.540479	1	-3.779777	2.571337	2.231178
1	-1.331270	2.057608	-3.639287	6	-5.600688	3.468851	1.475665
1	-1.730409	4.118006	-2.301724	6	-6.009712	3.173660	-0.882117
6	3.601495	-0.012003	2.808789	1	-4.515718	2.057745	-1.969259
6	4.773510	-0.152666	3.561428	1	-5.896795	3.869897	2.440640
6	2.587374	0.826080	3.282972	6	-6.414033	3.693248	0.357371
6	4.934137	0.543266	4.756665	1	-6.626929	3.345288	-1.759373
1	5.563362	-0.803092	3.205245	6	-7.680162	4.503057	0.471995
6	2.749992	1.525283	4.481125	1	-8.062990	4.503993	1.495813
1	1.665962	0.916049	2.721108	1	-8.462295	4.115642	-0.187246
6	3.924574	1.390092	5.219460	1	-7.500670	5.546438	0.186097
1	5.850152	0.424833	5.327643	6	-3.447353	-0.979599	-1.352081
1	1.952019	2.170026	4.837349	1	-4.539769	-1.042070	-1.436275
1	4.050413	1.932420	6.151665	1	-3.077702	-0.303628	-2.120414
6	3.966583	-2.150338	1.525065	6	-1.434284	-2.603461	-0.849666
6	3.143731	-3.116432	2.117585	1	-0.913891	-1.649859	-0.690698
6	5.218946	-2.529145	1.033849	1	-1.381063	-3.205782	0.060389
6	3.554862	-4.444432	2.193312	6	-5.201373	-0.849715	1.202330
1	2.175893	-2.816351	2.503801	6	-5.994669	-1.891048	1.177521
6	5.632774	-3.861684	1.113440	6	-3.795721	-3.512801	-1.291281
1	5.881173	-1.785528	0.603028	1	-3.316863	-4.484847	-1.450615
6	4.801453	-4.822981	1.685480	1	-4.653629	-3.449609	-1.969868
1	2.904764	-5.184999	2.649663	1	-4.180009	-3.491778	-0.267720
1	6.606820	-4.144488	0.725698	6	-6.774536	-2.944586	1.166410

6	-7.190834	-3.636087	2.445864	6	6.353971	2.671238	-0.798123
1	-6.870860	-4.685242	2.434450	1	5.043607	1.110588	-1.503189
1	-8.283344	-3.634795	2.544714	6	6.453858	3.850569	-0.061804
1	-6.761779	-3.152432	3.325384	1	5.377311	5.299782	1.118395
1	-5.622614	0.153978	1.253501	1	7.231046	2.257031	-1.287061
6	-7.303946	-3.529888	-0.123733	1	7.408887	4.359338	0.031192
1	-6.957785	-4.563392	-0.247091	6	1.491901	2.731474	-0.629576
1	-6.982432	-2.952722	-0.992229	6	0.701839	3.248086	0.401415
1	-8.400364	-3.556698	-0.108927	6	1.234796	3.132788	-1.950887
28	-0.298240	0.720519	-1.754493	6	-0.334580	4.141936	0.118034
6	2.432129	0.973693	0.967024	1	0.884315	2.947615	1.426738
6	3.278301	-0.300292	0.974054	6	0.201651	4.025264	-2.230123
6	3.630896	0.859862	2.970554	1	1.859651	2.747433	-2.748335
1	1.368292	0.737277	1.026206	6	-0.590987	4.529173	-1.194943
1	4.102997	-0.217119	0.262877	1	-0.948017	4.520739	0.929931
6	4.986380	1.534649	3.143658	1	0.009626	4.318927	-3.257861
1	4.862290	2.520090	3.600272	1	-1.402680	5.216626	-1.414264
1	5.630308	0.925090	3.783811	6	1.559590	-1.932700	1.820954
1	5.462374	1.661696	2.169349	6	2.039945	-2.769947	2.833693
6	2.899935	0.592951	4.279546	6	0.289106	-1.361872	1.963782
1	3.484612	-0.086044	4.905877	6	1.272098	-3.027630	3.967915
1	2.744245	1.529855	4.821599	1	3.022120	-3.216615	2.735280
1	1.933198	0.131493	4.068728	6	-0.474020	-1.610334	3.105666
8	2.811486	1.682272	2.132149	1	-0.106406	-0.724871	1.183924
8	3.800190	-0.385685	2.289459	6	0.012208	-2.444130	4.112386
6	2.440877	-1.569106	0.620249	1	1.662123	-3.681563	4.742530
6	2.656956	1.780631	-0.348068	1	-1.446677	-1.139451	3.206918
8	2.782958	0.804666	-1.395825	1	-0.583038	-2.638625	5.000003
8	1.529398	-1.263941	-0.447739	6	3.327159	-2.737501	0.201441
15	1.487606	-0.208627	-1.750417	6	2.771543	-3.758377	-0.579912
7	2.238553	-0.992194	-3.029162	6	4.668166	-2.827329	0.590246
6	3.597183	-1.511964	-2.993542	6	3.551786	-4.840860	-0.979577
1	3.603585	-2.608799	-2.992744	1	1.739536	-3.690790	-0.903231
1	4.160975	-1.155971	-3.866508	6	5.447461	-3.915556	0.188715
1	4.109052	-1.172206	-2.094450	1	5.102680	-2.058657	1.220224
6	1.440599	-1.427345	-4.164109	6	4.894104	-4.923000	-0.599933
1	0.463997	-0.938309	-4.118451	1	3.107812	-5.617332	-1.595739
1	1.929182	-1.135319	-5.103620	1	6.488466	-3.970780	0.494145
1	1.290885	-2.514783	-4.164185	1	5.502272	-5.765725	-0.915943
6	3.983702	2.532775	-0.296258				
6	4.088847	3.725013	0.430985	IM24			
6	5.125662	2.016706	-0.916800				
6	5.313240	4.377721	0.547969	8	4.963140	-1.736472	-0.267965
1	3.208976	4.137352	0.909424	16	5.116822	-0.591387	0.636153

7	4.319602	0.686949	-0.054022	6	1.681425	1.492499	-1.084833
8	4.692208	-0.664130	2.039395	8	0.434666	1.331910	-1.697114
6	6.848747	-0.144853	0.631419	1	1.347627	-3.603442	-2.715971
6	4.177500	0.778873	-1.505383	1	4.231859	-2.690060	-2.434976
6	7.382946	0.558904	1.711235	6	-2.338724	-0.256876	1.379174
6	7.627200	-0.437139	-0.489816	6	-3.707997	0.276303	0.942754
1	4.723041	-0.044272	-1.960390	6	-3.402011	0.657096	3.230919
1	4.659567	1.713190	-1.825083	1	-1.529957	0.384686	1.013664
1	6.767664	0.754558	2.581971	1	-4.345619	-0.552870	0.628450
6	8.710448	0.977000	1.658457	6	-4.188044	-0.032113	4.334885
6	8.952213	-0.011396	-0.525155	1	-3.536299	-0.239938	5.187519
1	7.199234	-1.005958	-1.307450	1	-5.008899	0.608898	4.666770
1	9.132573	1.522153	2.498194	1	-4.590402	-0.974622	3.958725
6	9.513360	0.701379	0.543578	6	-2.783335	1.984426	3.653740
1	9.563829	-0.239561	-1.393778	1	-3.565727	2.703275	3.907507
6	10.958995	1.129281	0.509115	1	-2.143202	1.830750	4.526984
1	11.124842	2.025780	1.112945	1	-2.184897	2.401112	2.842146
1	11.289466	1.338176	-0.512331	8	-2.377339	-0.237380	2.791000
1	11.609206	0.341067	0.907883	8	-4.271436	0.853378	2.104856
6	2.140508	2.924868	-0.690742	6	-3.602631	1.283194	-0.245718
1	2.884120	3.414159	-1.331788	6	-2.106035	-1.698858	0.832136
1	1.283102	3.591381	-0.573439	8	-2.584494	-1.698222	-0.537080
6	2.605048	2.355218	0.686814	8	-2.550529	0.828270	-1.125218
6	1.699247	1.130829	0.424877	15	-2.057093	-0.628654	-1.679050
1	0.693686	1.290983	0.822237	7	-3.044751	-1.167947	-2.920696
6	2.297903	3.218649	1.905082	6	-4.451202	-1.530585	-2.770274
1	2.462652	2.660584	2.834371	1	-5.107491	-0.741715	-3.155719
1	1.254055	3.545705	1.891385	1	-4.652826	-2.460479	-3.315664
1	2.930564	4.114951	1.934301	1	-4.685621	-1.688912	-1.719718
6	4.080234	1.901120	0.729877	6	-2.658058	-0.797863	-4.278464
1	4.333729	1.670514	1.765396	1	-1.595436	-0.539006	-4.305610
1	4.748408	2.704062	0.382157	1	-2.829709	-1.640240	-4.958981
1	2.060668	0.150703	0.722591	1	-3.233618	0.065187	-4.641699
6	2.708909	0.774990	-1.986387	6	-2.979484	-2.707613	1.578297
6	2.033403	-0.524391	-2.321934	6	-2.618094	-3.117908	2.868492
28	0.203308	-0.449772	-2.064289	6	-4.159117	-3.206953	1.018761
6	2.375986	-1.681487	-2.890905	6	-3.431094	-3.989409	3.587970
6	1.231708	-2.633121	-3.210481	1	-1.699535	-2.751230	3.308474
6	3.753243	-2.171288	-3.272531	6	-4.972347	-4.084648	1.739375
1	1.153232	-2.807882	-4.290800	1	-4.432176	-2.923377	0.011451
1	0.226018	-2.276563	-2.894032	6	-4.615619	-4.474209	3.028335
1	3.694397	-2.867665	-4.117748	1	-3.136336	-4.293430	4.587910
1	4.411182	-1.350119	-3.570364	1	-5.883612	-4.463860	1.286202
1	2.702004	1.364946	-2.916598	1	-5.247677	-5.155510	3.590058

6	-0.639277	-2.111607	0.881833	6	-1.438789	3.506852	0.562502
6	0.237309	-1.574812	1.829199	6	-0.794110	3.494433	-1.768776
6	-0.174217	-3.104728	0.009165	6	3.478202	2.324153	-0.837297
6	1.567832	-1.996706	1.880717	6	2.264724	2.945145	-0.517327
1	-0.112369	-0.817456	2.521602	1	2.114672	3.502429	2.058684
6	1.152602	-3.525561	0.067172	1	-1.266667	3.199736	1.588377
1	-0.860544	-3.544156	-0.707116	1	-0.138698	3.147020	-2.560568
6	2.034021	-2.961504	0.990782	1	3.524267	1.246746	-0.910873
1	2.256325	-1.544951	2.586766	8	-6.401110	0.107691	-0.710115
1	1.503953	-4.294734	-0.613111	16	-5.102031	0.727246	-0.423108
1	3.078218	-3.251967	1.004273	7	-4.005609	0.130602	-1.524186
6	-3.153780	2.660706	0.236028	8	-4.941964	2.184173	-0.383833
6	-4.072457	3.509985	0.864521	6	-4.561463	0.115418	1.170376
6	-1.823859	3.070205	0.084185	6	-2.639961	0.705491	-1.451176
6	-3.664561	4.744559	1.362737	6	-3.640602	0.856537	1.911096
1	-5.104925	3.198887	0.970807	6	-5.005312	-1.128576	1.620116
6	-1.423309	4.312101	0.586498	1	-2.185417	0.524402	-0.467011
1	-1.118100	2.436896	-0.446627	1	-2.756864	1.785541	-1.551488
6	-2.333950	5.147611	1.232040	1	-3.325596	1.827965	1.550842
1	-4.385972	5.392047	1.852529	6	-3.161493	0.340717	3.112867
1	-0.393293	4.630868	0.458781	6	-4.509216	-1.634505	2.819164
1	-2.014218	6.110585	1.619451	1	-5.738649	-1.676767	1.039640
6	-4.898050	1.378456	-1.041518	1	-2.452870	0.920239	3.695325
6	-4.844929	1.889100	-2.345038	6	-3.578212	-0.912721	3.580077
6	-6.132023	0.997331	-0.508115	1	-4.858558	-2.598911	3.177831
6	-6.002273	1.989704	-3.112056	6	-3.027358	-1.470977	4.868066
1	-3.885862	2.193765	-2.749833	1	-2.894547	-0.685058	5.617552
6	-7.294111	1.101325	-1.277959	1	-2.047552	-1.934174	4.703220
1	-6.195501	0.634352	0.512270	1	-3.687076	-2.235160	5.288102
6	-7.232757	1.589548	-2.581672	6	-2.351481	-2.706488	-2.763210
1	-5.946622	2.381699	-4.123381	1	-2.392035	-2.342218	-3.792260
1	-8.246690	0.798563	-0.853500	1	-2.127452	-3.782677	-2.782508
1	-8.135821	1.665471	-3.179765	6	-3.569920	-2.388808	-1.832119
TS1				6	-2.564533	-2.126886	-0.676353
				1	-2.391182	-3.048443	-0.103481
				6	-4.556860	-3.532139	-1.621040
				1	-5.271281	-3.290219	-0.825949
15	0.799374	1.900961	-0.134374	1	-4.038743	-4.455940	-1.343212
6	0.850899	1.789979	1.700751	1	-5.132806	-3.732261	-2.532216
6	1.584850	2.670240	2.508112	6	-4.317368	-1.097135	-2.262587
6	1.667502	2.455473	3.883674	1	-5.392851	-1.237026	-2.156172
6	1.026608	1.357534	4.464717	1	-4.136212	-0.902552	-3.324151
6	0.277923	0.488648	3.669376	1	-2.766356	-1.326984	0.032339
6	0.183014	0.712504	2.296188	6	-1.748499	0.156689	-2.532920
6	-0.577069	3.069427	-0.449343				

6	-0.366069	0.373605	-2.552898	6	2.803717	-2.796523	-0.912006
6	4.625578	3.082820	-1.061274	6	3.509959	-3.869882	-0.352144
6	4.569973	4.474434	-0.978685	6	2.588200	-2.754336	-2.293847
1	5.461917	5.067764	-1.156899	6	4.005383	-4.883677	-1.169525
6	3.361295	5.104052	-0.673459	1	3.668568	-3.913364	0.720859
6	2.213612	4.345668	-0.443872	6	3.090226	-3.768439	-3.110499
1	1.276615	4.840160	-0.211803	1	1.998979	-1.944008	-2.705214
6	-2.528084	4.323780	0.253996	6	3.799403	-4.831482	-2.551008
6	-2.748961	4.728837	-1.060751	1	4.549955	-5.714663	-0.730875
1	-3.609082	5.344655	-1.301599	1	2.916150	-3.732325	-4.181862
6	-1.868507	4.326855	-2.069073	1	4.185958	-5.622704	-3.186778
1	-0.382205	0.027481	1.675816	6	1.500058	-2.227881	1.602988
1	1.115822	1.178178	5.531986	6	2.241019	-2.525605	2.753606
28	0.706967	-0.082902	-1.061021	6	0.136701	-2.553137	1.566561
1	3.310475	6.187329	-0.615731	6	1.621906	-3.121832	3.853815
1	5.558345	2.580823	-1.296587	1	3.295278	-2.276938	2.801904
1	-2.035190	4.641518	-3.094745	6	-0.480456	-3.148174	2.664084
1	-3.212911	4.629234	1.038419	1	-0.417728	-2.335879	0.664034
1	-0.207452	-0.378415	4.103527	6	0.261077	-3.430728	3.814721
1	2.246415	3.136368	4.500755	1	2.204954	-3.343962	4.742791
6	0.568771	0.094989	-3.512140	1	-1.540441	-3.381170	2.620451
6	1.876081	0.840709	-3.657573	1	-0.216684	-3.893932	4.673241
6	0.282639	-0.860377	-4.648540				
1	2.740776	0.162936	-3.686338	TS1 _{dppp}			
1	2.038166	1.562928	-2.859104				
1	0.221712	-0.319511	-5.605080	15	1.166376	2.092830	0.689707
1	1.091296	-1.595114	-4.759396	6	-0.018472	3.496243	0.671511
1	-2.228975	0.208387	-3.516295	6	-0.102337	4.252431	-0.512196
6	-1.449428	-2.006605	-1.727986	6	-1.002940	5.310948	-0.607931
8	-0.207769	-2.074914	-1.536763	6	-1.837179	5.624914	0.467856
1	1.888013	1.391082	-4.611527	6	-1.779419	4.860336	1.633261
1	-0.645907	-1.408234	-4.500334	6	-0.879449	3.798689	1.734914
15	2.198019	-1.400893	0.113357	6	1.109860	1.442674	2.405987
6	3.767079	-0.665371	0.725722	6	0.737172	0.102187	2.568766
6	4.946005	-0.770194	-0.027951	6	1.473982	2.189679	3.537487
6	3.765076	0.152003	1.867251	1	-0.839830	3.212092	2.646239
6	6.089700	-0.062499	0.344770	1	0.459641	-0.487293	1.704915
1	4.967736	-1.402202	-0.909050	8	-1.151544	-2.179292	1.456285
6	4.908742	0.855959	2.236824	16	-1.588465	-2.308411	0.060916
1	2.870553	0.239897	2.469128	7	-1.721069	-0.757628	-0.560270
6	6.073673	0.756646	1.474503	8	-0.804205	-3.085642	-0.907163
1	6.994610	-0.155247	-0.248771	6	-3.234612	-3.005824	0.089766
1	4.881748	1.488666	3.118742	6	-4.053331	-2.769198	1.196765
1	6.962435	1.311343	1.759598	6	-3.708528	-3.712759	-1.015277

1	-3.656808	-2.239862	2.055648	1	-4.512093	4.931871	0.631709
6	-5.364370	-3.234846	1.181369	1	-4.869242	3.556255	1.693385
6	-5.024182	-4.171819	-1.012534	1	-4.372627	-0.213066	0.209583
1	-3.046583	-3.914418	-1.849416	1	-2.529382	6.458805	0.395516
1	-6.005337	-3.054775	2.039932	1	0.525532	3.997328	-1.361618
6	-5.871109	-3.938013	0.078229	28	1.209065	0.542684	-0.797768
1	-5.398326	-4.724160	-1.869874	1	-2.434292	5.090963	2.468384
6	-7.285127	-4.461167	0.085727	1	-1.051735	5.892353	-1.524130
1	-7.661334	-4.610751	-0.929755	1	0.465225	-1.537573	3.921125
1	-7.961168	-3.775372	0.604544	1	1.760023	2.183030	5.669987
1	-7.340707	-5.426716	0.602905	15	3.030957	-0.496300	-0.046991
1	1.752787	3.234449	3.435140	6	4.104758	-1.025796	-1.439410
6	-2.211331	0.294328	0.361795	6	5.053358	-2.050507	-1.323832
1	-2.012465	-0.056518	1.375941	6	3.965124	-0.346442	-2.660924
1	-1.597615	1.182567	0.212696	6	5.854540	-2.391262	-2.413535
6	0.377194	-0.291991	-2.609940	1	5.156318	-2.585881	-0.384809
6	-1.100624	0.101482	-2.878079	6	4.780279	-0.681720	-3.742712
1	0.970661	-0.495166	-3.501953	1	3.218007	0.437888	-2.761819
6	-0.959006	1.614615	-2.554292	6	5.721915	-1.705393	-3.622834
6	0.545062	1.476759	-2.293147	1	6.581648	-3.192891	-2.319317
1	-1.527773	1.974098	-1.694527	1	4.670236	-0.148298	-4.682419
1	-1.172355	2.272773	-3.403929	1	6.346689	-1.972825	-4.470174
8	1.424339	2.187931	-2.808785	6	3.022449	-1.916729	1.107052
1	0.480283	-1.145878	-1.926852	6	3.860939	-2.019735	2.225467
6	-2.088436	-0.670320	-1.989052	6	2.045845	-2.901230	0.894024
1	-2.152773	-1.687511	-2.378248	6	3.717037	-3.082013	3.118969
1	-3.084550	-0.221006	-2.068462	1	4.621600	-1.269355	2.411194
6	-1.504146	-0.128902	-4.337193	6	1.906277	-3.963084	1.784220
1	-1.427202	-1.189242	-4.603774	1	1.374166	-2.825262	0.046166
1	-0.846398	0.435002	-5.005445	6	2.738135	-4.053051	2.902457
1	-2.533921	0.198252	-4.525227	1	4.367312	-3.147535	3.986613
6	-3.672756	0.621795	0.158249	1	1.132312	-4.704166	1.611739
6	-4.112331	1.825255	-0.110527	1	2.621645	-4.873472	3.604671
6	-4.540532	3.032800	-0.383698	6	4.120414	0.764940	0.798329
6	-4.581806	3.552093	-1.803441	1	3.820211	0.825538	1.849305
1	-5.594238	3.878518	-2.071967	1	5.158129	0.419108	0.765155
1	-4.255030	2.795754	-2.519829	6	3.984144	2.142373	0.118935
1	-3.920596	4.422027	-1.897191	1	4.903573	2.715412	0.287352
6	0.740931	-0.492149	3.830533	1	3.895510	2.013534	-0.964467
6	1.113782	0.254886	4.947310	6	2.802512	2.996747	0.611933
1	1.127135	-0.203846	5.931813	1	3.015147	3.419394	1.599713
6	1.474331	1.598361	4.800203	1	2.654831	3.835996	-0.073032
6	-5.029920	3.970300	0.696165				
1	-6.102458	4.165389	0.567827				

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				1	-3.021058	6.038340	0.711260
8	-5.535247	-0.878994	-1.070383	6	-0.939008	5.025278	-0.862899
16	-5.225094	-0.406700	0.283785	1	-0.160126	5.663078	-0.425927
7	-4.102443	0.839171	0.087653	1	-1.581699	5.687693	-1.458694
8	-6.308633	-0.010514	1.195809	1	-0.455495	4.313695	-1.527623
6	-4.268602	-1.664849	1.124358	1	-1.799322	2.023482	2.291010
6	-3.237811	-2.323182	0.451769	28	-1.367473	1.254996	-0.217236
6	-4.605634	-2.010455	2.432871	6	2.397015	-0.328622	-1.193207
1	-3.011537	-2.082661	-0.579176	6	3.147412	-0.222274	0.142323
6	-2.510824	-3.303930	1.118330	6	4.656744	0.015378	-1.629312
6	-3.883692	-3.013222	3.076731	1	1.792607	0.561497	-1.393977
1	-5.425682	-1.497889	2.922518	1	3.091741	-1.177032	0.671977
1	-1.686338	-3.794810	0.610747	6	5.745872	-0.980137	-1.997125
6	-2.822100	-3.666033	2.435594	1	5.848197	-1.041130	-3.083862
1	-4.142723	-3.286957	4.095907	1	6.701217	-0.661583	-1.572066
6	-2.044617	-4.747775	3.141921	1	5.485667	-1.966118	-1.608447
1	-1.099958	-4.955070	2.632646	6	4.936503	1.429796	-2.123589
1	-2.615798	-5.683111	3.175019	1	5.830056	1.828729	-1.638010
1	-1.822021	-4.468638	4.176559	1	5.094230	1.417295	-3.205699
6	-3.741900	1.544571	1.334173	1	4.097581	2.087977	-1.895383
1	-4.464010	2.351329	1.531070	8	3.417613	-0.454514	-2.166398
1	-3.842646	0.830856	2.154019	8	4.499311	0.009390	-0.202108
6	-2.197405	0.381370	-1.904673	6	2.562076	0.881556	1.074116
6	-3.342077	1.310269	-2.324985	6	1.460064	-1.570967	-1.190254
1	-1.690863	-0.049338	-2.762874	8	0.729431	-1.551242	0.058159
6	-2.440564	2.511782	-2.715885	8	1.130032	0.893865	0.891967
6	-1.190290	1.997926	-2.005636	15	-0.042662	-0.268223	0.778829
1	-2.769880	3.491513	-2.360258	7	-0.224696	-1.032541	2.262030
1	-2.253977	2.577974	-3.793651	6	-1.292998	-0.603422	3.149379
8	-0.026097	2.168747	-2.323952	1	-1.661434	-1.463538	3.714626
1	-2.441490	-0.415256	-1.207350	1	-0.955275	0.162840	3.862873
6	-4.283639	1.667427	-1.127793	1	-2.123639	-0.215037	2.566438
1	-5.322532	1.609728	-1.463667	6	0.777289	-1.867986	2.914345
1	-4.103780	2.695487	-0.811121	1	1.641412	-2.006598	2.271515
6	-4.149302	0.752160	-3.502989	1	1.120881	-1.404839	3.845761
1	-4.694306	-0.143362	-3.197536	1	0.350121	-2.852924	3.144610
1	-3.485075	0.495825	-4.334784	6	2.263995	-2.876460	-1.183352
1	-4.877384	1.487365	-3.865306	6	2.956591	-3.268122	-2.338202
6	-2.319269	2.108844	1.337575	6	2.312561	-3.703837	-0.058302
6	-1.889136	3.061799	0.434965	6	3.706839	-4.440856	-2.350148
6	-1.723911	4.368417	0.242548	1	2.907974	-2.649709	-3.224766
6	-2.344139	5.343099	1.225662	6	3.060811	-4.883688	-0.073193
1	-1.567640	5.956261	1.701906	1	1.748939	-3.433408	0.822911
1	-2.906444	4.828827	2.007776	6	3.767233	-5.253139	-1.215045

1	4.241497	-4.724287	-3.251858	6	3.343556	2.871250	0.004822
1	3.085562	-5.512584	0.812082	6	3.961744	2.547971	-2.320049
1	4.350695	-6.168857	-1.227543	1	3.454122	2.595613	1.046772
6	0.492662	-1.612016	-2.367983	6	2.524578	3.929324	-0.367302
6	0.677669	-0.840629	-3.517049	6	3.138436	3.617197	-2.674733
6	-0.559524	-2.536835	-2.326604	1	4.551056	2.018588	-3.059926
6	-0.183495	-0.992730	-4.608663	1	1.976242	4.473904	0.395143
1	1.493129	-0.130635	-3.572120	6	2.410862	4.321711	-1.710365
6	-1.422329	-2.681256	-3.408233	1	3.072490	3.917252	-3.716905
1	-0.685215	-3.146870	-1.438652	6	1.535750	5.487847	-2.091963
6	-1.233405	-1.908523	-4.558741	1	1.874814	6.408750	-1.604204
1	-0.031599	-0.385415	-5.495665	1	1.545877	5.658161	-3.171624
1	-2.238659	-3.395432	-3.358734	1	0.499950	5.321892	-1.780123
1	-1.902917	-2.019989	-5.405977	6	3.775259	-1.237520	-1.315485
6	3.044876	2.269673	0.657585	1	4.604914	-1.911210	-1.581293
6	4.307566	2.720747	1.060663	1	3.655942	-0.548549	-2.152822
6	2.260322	3.081319	-0.167256	6	2.149475	-0.054602	1.806570
6	4.784343	3.958034	0.634804	6	3.441912	-0.718933	2.307553
1	4.920262	2.100011	1.703571	1	1.599240	0.443580	2.607423
6	2.743591	4.319967	-0.595988	6	2.768688	-1.980719	2.899358
1	1.284846	2.743941	-0.486552	6	1.457246	-1.816451	2.138610
6	4.004826	4.762045	-0.199661	1	3.278525	-2.930486	2.721926
1	5.766605	4.293776	0.954219	1	2.567458	-1.894712	3.973501
1	2.126670	4.932524	-1.245701	8	0.341458	-2.185248	2.471573
1	4.378039	5.725627	-0.534036	1	2.260767	0.642168	0.975218
6	2.868799	0.624860	2.544239	6	4.396704	-1.119501	1.135261
6	2.052034	1.219792	3.513687	1	5.428657	-0.952810	1.451089
6	3.949391	-0.161772	2.951996	1	4.288633	-2.182066	0.920418
6	2.293788	1.007597	4.868196	6	4.183711	0.126604	3.348751
1	1.220293	1.836310	3.190968	1	4.589982	1.033019	2.893834
6	4.194083	-0.371483	4.311968	1	3.513051	0.408208	4.167702
1	4.610074	-0.602241	2.212513	1	5.025255	-0.429064	3.778044
6	3.364872	0.204743	5.272680	6	2.498303	-2.065684	-1.168826
1	1.648559	1.468990	5.610129	6	2.296161	-2.988935	-0.162307
1	5.034727	-0.987819	4.616418	6	2.487017	-4.253850	0.201877
1	3.553363	0.037035	6.328783	6	3.319821	-5.157527	-0.685478
(S)-TS1				1	2.706451	-5.983156	-1.070709
				1	3.741729	-4.617773	-1.535717
				1	4.142990	-5.613888	-0.119725
8	5.802897	1.267104	0.761184	6	1.935587	-4.929440	1.429791
16	5.171390	0.871614	-0.503512	1	1.450262	-5.870333	1.145832
7	4.146365	-0.423455	-0.140883	1	2.744788	-5.199095	2.122841
8	5.988199	0.551853	-1.682806	1	1.204409	-4.320326	1.955857
6	4.052036	2.179398	-0.981512	1	1.952957	-2.210830	-2.101536

28	1.337828	-1.299495	0.279847	6	-1.181295	-4.851279	0.092405
6	-2.659232	-0.780814	0.339746	1	-2.300665	-3.245467	0.984122
6	-2.977461	0.718636	0.228734	6	-0.262202	-4.418824	-2.096341
6	-4.750571	-0.378940	1.299861	1	-0.688889	-2.473245	-2.917355
1	-1.846928	-0.973748	1.047787	6	-0.452860	-5.280932	-1.013651
1	-3.112408	0.992946	-0.819292	1	-1.321286	-5.510471	0.943198
6	-6.096413	-0.562784	0.613364	1	0.314325	-4.744099	-2.957139
1	-6.500827	-1.553436	0.837053	1	-0.027284	-6.279669	-1.032238
1	-6.802035	0.193863	0.966729	6	-1.881832	1.522452	2.356753
1	-5.974472	-0.468316	-0.467011	6	-2.701155	2.343415	3.141173
6	-4.822624	-0.458189	2.819017	6	-1.122979	0.531047	2.979757
1	-5.435629	0.357495	3.210354	6	-2.752908	2.173273	4.523403
1	-5.266727	-1.411162	3.119556	1	-3.305231	3.108999	2.669263
1	-3.822194	-0.380704	3.246481	6	-1.179634	0.353860	4.362663
8	-3.848348	-1.377049	0.811230	1	-0.491651	-0.113403	2.390688
8	-4.204080	0.889348	0.912235	6	-1.993488	1.176770	5.140646
6	-1.888867	1.648386	0.834954	1	-3.392405	2.818168	5.118793
6	-2.227423	-1.344876	-1.040994	1	-0.588560	-0.434978	4.817501
8	-1.306836	-0.369254	-1.570234	1	-2.038584	1.044076	6.217521
8	-0.568475	1.241389	0.363602	6	-2.077272	3.105947	0.428644
15	0.030109	0.204684	-0.763429	6	-1.058808	4.010590	0.762229
7	0.566734	1.259213	-1.980352	6	-3.212388	3.576372	-0.234731
6	1.141984	0.576231	-3.140521	6	-1.160642	5.353390	0.414292
1	0.364810	0.216573	-3.831684	1	-0.184066	3.641208	1.285581
1	1.799416	1.267338	-3.674492	6	-3.313234	4.926162	-0.587030
1	1.731718	-0.278550	-2.818552	1	-4.034097	2.905569	-0.455858
6	-0.290307	2.372815	-2.386351	6	-2.289136	5.815755	-0.271330
1	-0.577444	2.961443	-1.519953	1	-0.364834	6.043009	0.679728
1	0.279963	3.013499	-3.063200	1	-4.200110	5.278396	-1.105060
1	-1.196939	2.036481	-2.910704	1	-2.370464	6.863268	-0.545092
6	-3.410115	-1.392203	-2.004999				
6	-4.344196	-2.431270	-1.905219	TS2			
6	-3.606313	-0.394940	-2.964956				
6	-5.460254	-2.460321	-2.737222	15	1.078746	1.664486	0.650112
1	-4.194914	-3.213077	-1.170666	6	0.127960	3.241094	0.529174
6	-4.725234	-0.425699	-3.800421	6	-0.869290	3.602334	1.445864
1	-2.874450	0.396666	-3.064742	6	-1.576065	4.795716	1.290889
6	-5.658188	-1.454692	-3.686502	6	-1.308172	5.637212	0.212255
1	-6.177065	-3.270740	-2.644743	6	-0.345158	5.264989	-0.728220
1	-4.861980	0.355655	-4.542296	6	0.364997	4.076798	-0.575749
1	-6.528390	-1.479201	-4.335568	6	2.819102	2.274789	0.637366
6	-1.554956	-2.708476	-0.965718	6	3.384573	2.480512	-0.633504
6	-1.727620	-3.566151	0.122345	6	3.593091	2.524492	1.775006
6	-0.816479	-3.143998	-2.074149	6	0.691016	1.058903	2.335132

6	0.133498	-0.224595	2.421179	6	-4.061348	1.156771	0.261796
6	0.870723	1.800306	3.514058	6	-4.291109	2.277687	-0.375645
1	1.091929	3.790155	-1.326577	6	-4.527275	3.373163	-1.054687
1	2.811411	2.241786	-1.524706	6	-4.700100	3.335524	-2.557897
1	3.203370	2.312708	2.761652	1	-5.671455	3.754633	-2.848428
1	-0.036889	-0.797384	1.516606	1	-4.628593	2.319155	-2.950088
8	-2.119447	-2.181714	1.431296	1	-3.925818	3.944338	-3.040571
16	-2.788176	-2.122574	0.126776	6	4.683861	2.970575	-0.753271
7	-2.469776	-0.604992	-0.520367	6	5.441225	3.243167	0.386625
8	-2.481393	-3.101116	-0.924145	1	6.455645	3.619932	0.292792
6	-4.545650	-2.195463	0.442147	6	4.895915	3.006740	1.647729
6	-5.020263	-1.924189	1.725439	6	-0.213554	-0.772225	3.656375
6	-5.425412	-2.427523	-0.616747	6	0.005546	-0.041934	4.824810
1	-4.314721	-1.760025	2.531683	1	-0.253697	-0.466133	5.790568
6	-6.395316	-1.872590	1.942049	6	0.542652	1.246619	4.751173
6	-6.795776	-2.369692	-0.382140	6	-4.646673	4.728353	-0.399435
1	-5.038833	-2.661169	-1.601961	1	-5.641168	5.151897	-0.589252
1	-6.771758	-1.661422	2.938992	1	-3.908639	5.421338	-0.816763
6	-7.301744	-2.088127	0.895221	1	-4.490489	4.670831	0.678476
1	-7.486160	-2.547858	-1.201831	1	-4.901457	0.578914	0.645034
6	-8.788666	-2.053986	1.141895	1	-1.848868	6.572321	0.101081
1	-9.328895	-1.672871	0.270619	1	-1.089861	2.960134	2.290361
1	-9.036700	-1.425418	2.001361	28	0.865225	0.145819	-0.868808
1	-9.172295	-3.060353	1.349114	1	-0.142226	5.902895	-1.583462
1	1.247004	2.816408	3.464824	1	-2.332600	5.067971	2.020982
6	-2.687298	0.539771	0.404982	1	5.488940	3.183604	2.540084
1	-2.514259	0.168884	1.415992	1	5.105806	3.128991	-1.741581
1	-1.909475	1.273418	0.205272	1	-0.658341	-1.761104	3.686900
6	-0.292898	-0.501977	-2.568675	1	0.695854	1.824999	5.657639
6	-1.664717	0.190775	-2.805697	15	2.395550	-1.439650	-0.357697
1	0.203637	-0.883453	-3.461427	6	3.352126	-1.806677	-1.886879
6	-1.218948	1.636461	-2.450805	6	4.144450	-2.955567	-2.021400
6	0.240195	1.202608	-2.304842	6	3.293172	-0.881750	-2.940300
1	-1.648821	2.064451	-1.546197	6	4.872908	-3.174381	-3.189086
1	-1.355557	2.357464	-3.263515	1	4.184245	-3.681862	-1.216419
8	1.184729	1.721839	-2.928176	6	4.031647	-1.102596	-4.104999
1	-0.370349	-1.312481	-1.834600	1	2.667129	0.003980	-2.860178
6	-2.791003	-0.416558	-1.949217	6	4.820639	-2.245886	-4.231986
1	-3.006408	-1.402699	-2.361107	1	5.480283	-4.069673	-3.286522
1	-3.694992	0.196227	-2.037745	1	3.979968	-0.380312	-4.914486
6	-2.096310	0.096589	-4.272600	1	5.388696	-2.418636	-5.141648
1	-2.236045	-0.946911	-4.576570	6	3.717230	-0.986082	0.840283
1	-1.332085	0.537868	-4.919338	6	4.969033	-0.527126	0.412849
1	-3.035707	0.634622	-4.447710	6	3.447115	-1.036114	2.217249

6	5.934715	-0.142093	1.342556	6	-4.013395	-0.533721	-2.273039
1	5.189428	-0.469253	-0.646842	1	-2.121928	0.327243	-2.828776
6	4.415035	-0.654381	3.143452	6	-4.836085	0.566402	-2.892179
1	2.483403	-1.385269	2.568128	1	-5.808632	0.195750	-3.228337
6	5.664772	-0.209737	2.708945	1	-4.322600	1.018534	-3.744151
1	6.897943	0.217908	0.994473	1	-5.014449	1.367863	-2.166330
1	4.189078	-0.704843	4.204661	1	-1.615604	2.861938	-2.578180
1	6.419637	0.089696	3.430117	6	0.988881	-3.804857	0.430954
6	1.889303	-3.097794	0.254775	1	1.194047	-4.383942	1.338906
6	2.724533	-3.933583	1.013060	1	0.958657	-4.506979	-0.403304
6	0.602083	-3.541340	-0.068718	6	0.205111	-0.481108	1.958775
6	2.274104	-5.185076	1.431225	6	0.055958	-1.816164	2.709273
1	3.718711	-3.598857	1.288508	1	0.427923	0.321391	2.668197
6	0.149849	-4.791741	0.349985	6	1.495243	-2.287120	2.980626
1	-0.062245	-2.911142	-0.643379	6	2.383240	-1.808120	1.833028
6	0.986436	-5.616336	1.101626	1	1.598478	-3.367164	3.145185
1	2.928285	-5.822818	2.019014	1	1.892407	-1.796993	3.876524
1	-0.859371	-5.097287	0.095799	8	3.537513	-1.453276	1.976495
1	0.637197	-6.588692	1.436912	1	-0.727338	-0.221352	1.451922
TS_{2dppp}				6	-0.786496	-2.833466	1.904833
				1	-1.790337	-2.410970	1.807990
				1	-0.879337	-3.764674	2.481366
15	-1.727945	1.728601	0.067210	6	-0.697891	-1.631884	4.042823
6	-2.726983	1.267157	1.543071	1	-1.698394	-1.226329	3.865977
6	-3.586379	0.165450	1.399617	1	-0.159552	-0.924939	4.681735
6	-2.627659	1.880227	2.799294	1	-0.801368	-2.574707	4.594079
6	-2.859644	2.891752	-0.813235	6	2.081756	-2.780196	0.160927
6	-4.059449	3.377817	-0.272985	6	1.920631	-1.908616	-0.989967
6	-2.525824	3.252025	-2.129895	6	1.827136	-2.099789	-2.305643
1	-3.661538	-0.332185	0.440865	6	1.465699	-1.005630	-3.276742
1	-1.966525	2.727172	2.944966	1	2.281171	-0.809019	-3.982545
1	-4.341072	3.103577	0.738140	1	1.224702	-0.074600	-2.762627
8	-2.425003	-4.698988	0.431522	1	0.589978	-1.303412	-3.869229
16	-1.535269	-3.886725	-0.411924	6	-4.328858	-0.307903	2.479039
7	-0.320132	-3.143786	0.537346	6	-4.217287	0.307543	3.728273
8	-0.853035	-4.507655	-1.555876	1	-4.785296	-0.066319	4.574805
6	-2.482125	-2.509023	-1.027626	6	-3.365482	1.401723	3.883853
6	-3.874441	-2.587367	-0.972863	6	-4.897305	4.200832	-1.027243
6	-1.838585	-1.469452	-1.696828	6	-4.546539	4.560962	-2.329697
1	-4.342083	-3.415385	-0.452853	1	-5.200683	5.200476	-2.914531
6	-4.629848	-1.595013	-1.594139	6	-3.353055	4.088670	-2.878183
6	-2.612747	-0.492958	-2.316389	6	2.018951	-3.463165	-2.935422
1	-0.756369	-1.422536	-1.709955	1	1.055273	-3.881037	-3.249002
1	-5.714303	-1.642290	-1.550482	1	2.480136	-4.171207	-2.243192

1	2.658148	-3.389989	-3.824173	6	-3.754501	-0.934415	0.459405
1	3.089491	-3.175194	0.288367	6	-2.962889	-0.294298	2.647368
1	-5.825507	4.563727	-0.595027	6	-2.977269	2.521066	0.112557
1	-3.074610	4.358429	-3.892800	6	-4.251877	2.637487	0.686280
1	-3.271075	1.883601	4.852680	6	-2.551227	3.520592	-0.778391
1	-4.983088	-1.164587	2.346160	1	-3.756544	-0.806097	-0.615217
28	1.386708	-0.784230	0.419475	1	-2.360732	0.332916	3.294066
15	2.193503	1.142579	-0.304632	1	-4.607545	1.872032	1.367052
6	3.638088	0.859997	-1.415482	8	-2.247340	-4.605478	-2.804047
6	4.643940	0.016686	-0.913486	16	-1.343927	-3.458619	-2.972195
6	3.783619	1.403903	-2.694502	7	-0.263885	-3.346645	-1.646683
6	5.774786	-0.257975	-1.675279	8	-0.525979	-3.343378	-4.186857
1	4.525130	-0.434821	0.067806	6	-2.324510	-1.975150	-2.842366
6	4.916798	1.117206	-3.461947	6	-3.708954	-2.083602	-2.981412
1	3.013478	2.036279	-3.121632	6	-1.695684	-0.732207	-2.792608
6	5.914996	0.289572	-2.954437	1	-4.164977	-3.065694	-3.030758
1	6.546148	-0.908508	-1.273759	6	-4.471830	-0.919876	-3.063464
1	5.011616	1.541699	-4.457190	6	-2.475363	0.416992	-2.883882
1	6.794990	0.067226	-3.550546	1	-0.621032	-0.675013	-2.671236
6	3.021065	2.133275	1.011070	1	-5.550545	-0.994231	-3.167612
6	3.768638	3.268899	0.659392	6	-3.869359	0.346213	-3.017197
6	2.932320	1.764604	2.355870	1	-1.995473	1.388673	-2.839679
6	4.390642	4.035608	1.641159	6	-4.704131	1.600311	-3.057461
1	3.875725	3.543465	-0.385979	1	-5.614442	1.455293	-3.645530
6	3.562574	2.530351	3.339172	1	-4.146525	2.438203	-3.482928
1	2.386602	0.871056	2.621900	1	-5.004830	1.896103	-2.045795
6	4.285415	3.668237	2.985891	1	-1.581352	3.434195	-1.260257
1	4.963588	4.913925	1.358918	6	1.091124	-3.828680	-1.954918
1	3.491958	2.230145	4.380396	1	1.262265	-4.800695	-1.478769
1	4.775008	4.263268	3.751087	1	1.176218	-3.974270	-3.032727
6	-0.469791	2.903371	0.784753	6	-0.072754	-1.868667	1.005411
1	0.100098	2.324536	1.518422	6	-0.167137	-3.403177	0.918199
1	-0.947504	3.734743	1.313408	1	0.009564	-1.557421	2.051323
6	0.470470	3.469065	-0.285090	6	1.280801	-3.906705	1.051579
1	1.225436	4.086195	0.211284	6	2.214821	-2.865593	0.440300
1	-0.096481	4.140203	-0.941065	1	1.457077	-4.902554	0.626032
6	1.182809	2.443992	-1.184094	1	1.566714	-3.966579	2.107680
1	1.845427	2.996053	-1.855681	8	3.319770	-2.609818	0.877663
1	0.460889	1.904014	-1.803273	1	-0.977457	-1.409179	0.600080
TS_{2dppp}-CF₃				6	-0.859238	-3.847550	-0.390481
				1	-1.884779	-3.470449	-0.353424
				1	-0.918092	-4.944373	-0.421124
15	-1.855083	1.079318	0.375570	6	-1.025722	-3.995156	2.055027
6	-2.957051	-0.099762	1.259862	1	-2.054750	-3.631247	2.002951

1	-0.615603	-3.701691	3.026348	1	4.564333	2.937543	3.855997
1	-1.055635	-5.090695	2.019621	1	2.761368	-0.830019	4.853767
6	2.128261	-2.801807	-1.522218	6	-0.755871	1.699288	1.747061
6	1.994239	-1.455180	-2.042485	1	-0.233852	0.815946	2.129179
6	2.024268	-0.905608	-3.256237	1	-1.335198	2.127472	2.571396
6	1.652840	0.529585	-3.525452	6	0.258721	2.737792	1.256081
1	2.497799	1.093013	-3.937734	1	0.927412	2.982841	2.086854
1	1.307856	1.033146	-2.621115	1	-0.269061	3.664453	1.001732
1	0.844359	0.574877	-4.267300	6	1.108911	2.343899	0.036010
6	-4.519927	-1.947674	1.024342	1	1.830899	3.145975	-0.138483
6	-4.495060	-2.144846	2.407708	1	0.487938	2.260361	-0.860488
6	-3.723198	-1.313028	3.219045	6	4.291256	1.163519	5.879654
6	-5.074739	3.719639	0.380323	6	7.349585	1.500681	-2.828296
6	-4.630442	4.707789	-0.500566	6	-5.496626	5.901045	-0.792396
6	-3.361744	4.612098	-1.075909	6	-5.221166	-3.314797	3.007220
6	2.376084	-1.708177	-4.490605	9	-5.258511	6.910317	0.076389
1	1.478042	-1.907677	-5.086447	9	-6.810451	5.602527	-0.699685
1	2.829392	-2.668894	-4.237040	9	-5.274262	6.389412	-2.032687
1	3.081765	-1.153965	-5.121556	9	-6.345710	-3.615038	2.322753
1	3.148567	-3.184848	-1.510032	9	-4.445993	-4.426564	2.997615
1	-6.063874	3.795480	0.818529	9	-5.570650	-3.090229	4.292129
1	-3.025474	5.374408	-1.769966	9	4.352481	2.445109	6.305654
1	-3.714694	-1.465876	4.292488	9	3.565367	0.468216	6.781485
1	-5.123063	-2.592280	0.394420	9	5.550697	0.674739	5.921183
28	1.251218	-1.268575	-0.320869	9	8.283042	2.019960	-1.997053
15	2.046476	0.733442	0.175676	9	7.262934	2.329810	-3.891767
6	3.606874	1.052076	-0.756164	9	7.833973	0.319368	-3.270147
6	4.607081	0.070378	-0.645428				
6	3.833844	2.165486	-1.568737	TS2_{dppp}-OCH₃			
6	5.810189	0.214602	-1.322420				
1	4.425908	-0.816977	-0.045441	15	-1.819883	1.308942	-0.241651
6	5.039801	2.306956	-2.258437	6	-2.939442	0.856201	1.142170
1	3.072931	2.925845	-1.699248	6	-3.732552	-0.294669	0.971004
6	6.027458	1.333921	-2.134282	6	-2.988346	1.502399	2.380606
1	6.577012	-0.547755	-1.237797	6	-2.898618	2.381179	-1.282672
1	5.205311	3.166542	-2.897901	6	-4.162207	2.838999	-0.894354
6	2.712129	0.851488	1.893163	6	-2.462214	2.694364	-2.584398
6	3.485501	1.961836	2.268625	1	-3.701804	-0.829270	0.030057
6	2.461704	-0.154079	2.829556	1	-2.386763	2.386309	2.561488
6	3.976944	2.074066	3.563998	1	-4.532884	2.604080	0.098057
1	3.713431	2.736078	1.542598	8	-2.257979	-5.171979	0.297521
6	2.958278	-0.048528	4.128602	16	-1.332023	-4.330950	-0.476063
1	1.890560	-1.021276	2.531923	7	-0.260309	-3.499165	0.565545
6	3.708554	1.066790	4.496475	8	-0.506261	-4.940119	-1.528138

6	-2.283433	-3.022054	-1.221503	6	-4.969999	3.581463	-1.759992
6	-3.669696	-3.167682	-1.288980	6	-4.509327	3.890670	-3.044978
6	-1.630790	-1.971563	-1.864561	6	-3.242557	3.446435	-3.450977
1	-4.143427	-4.001966	-0.784772	6	2.435405	-3.811420	-2.639325
6	-4.410802	-2.232989	-2.009148	1	1.529788	-4.290400	-3.029269
6	-2.389994	-1.053287	-2.583688	1	2.859088	-4.469500	-1.877291
1	-0.555285	-1.870736	-1.781605	1	3.156705	-3.735542	-3.462740
1	-5.491398	-2.332479	-2.060780	1	3.153867	-3.355727	0.663864
6	-3.785248	-1.162747	-2.665275	1	-5.945420	3.911268	-1.423216
1	-1.893879	-0.224187	-3.075887	1	-2.905159	3.689456	-4.453058
6	-4.598351	-0.122140	-3.390965	1	-3.790086	1.549367	4.371603
1	-5.517059	-0.549807	-3.802667	1	-5.144000	-1.666145	1.857188
1	-4.030431	0.333497	-4.205588	28	1.332687	-1.053902	0.524249
1	-4.880315	0.688286	-2.709115	15	2.136107	0.883698	-0.185109
1	-1.497065	2.331110	-2.928256	6	3.688856	0.625659	-1.135345
6	1.084110	-4.091992	0.617677	6	4.676092	-0.164213	-0.511857
1	1.223194	-4.626711	1.564655	6	3.945974	1.118758	-2.412830
1	1.174918	-4.823919	-0.186042	6	5.876568	-0.429881	-1.145860
6	-0.025157	-0.766226	1.912378	1	4.483694	-0.583241	0.472180
6	-0.179638	-2.076180	2.705049	6	5.152439	0.847956	-3.070559
1	0.062965	0.078672	2.601635	1	3.204747	1.707261	-2.941897
6	1.246474	-2.454161	3.141650	6	6.123601	0.072331	-2.434812
6	2.224094	-1.971968	2.070236	1	6.641345	-1.035432	-0.671127
1	1.388218	-3.519409	3.364870	1	5.312036	1.242106	-4.066624
1	1.522644	-1.907185	4.050121	6	2.771368	1.941286	1.176536
8	3.340390	-1.555736	2.315814	6	3.540317	3.074370	0.882007
1	-0.905964	-0.589029	1.290332	6	2.517911	1.638854	2.521303
6	-0.879952	-3.169785	1.865605	6	4.022576	3.907005	1.890120
1	-1.890525	-2.810603	1.652730	1	3.782877	3.308410	-0.150605
1	-0.979437	-4.084109	2.467700	6	2.995987	2.455763	3.537307
6	-1.076354	-1.881942	3.945507	1	1.957013	0.747866	2.763735
1	-2.071627	-1.539520	3.647555	6	3.745654	3.598209	3.229329
1	-0.644155	-1.121358	4.603305	1	4.613002	4.775842	1.626631
1	-1.189802	-2.806542	4.525023	1	2.810336	2.223648	4.580567
6	2.146408	-3.019743	0.419104	6	-0.690396	2.559851	0.556100
6	2.062817	-2.198274	-0.776180	1	-0.174095	2.032732	1.364561
6	2.114405	-2.439224	-2.085944	1	-1.253670	3.386414	1.002283
6	1.801820	-1.398599	-3.130192	6	0.330368	3.131353	-0.433620
1	2.675496	-1.182642	-3.756455	1	1.005676	3.797064	0.112732
1	1.463611	-0.465266	-2.678968	1	-0.193458	3.754269	-1.168638
1	1.007754	-1.761968	-3.796675	6	1.173621	2.109481	-1.215136
6	-4.539942	-0.774814	1.990046	1	1.885047	2.668171	-1.829329
6	-4.568768	-0.118925	3.230684	1	0.545414	1.521287	-1.890235
6	-3.789130	1.026470	3.423058	8	7.331173	-0.254392	-2.975853

8	4.166233	4.338158	4.292315	6	2.150067	-3.606424	0.403276
8	-5.376125	-0.674189	4.177187	1	0.107262	-3.186686	-0.135596
8	-5.211564	4.604408	-3.969785	6	1.857547	-3.428071	1.905801
6	7.617349	0.206758	-4.285061	6	1.258398	-2.043322	2.085519
1	8.613049	-0.166995	-4.527283	1	2.736805	-3.555966	2.549538
1	6.896742	-0.181902	-5.016149	1	1.099358	-4.141661	2.242545
1	7.620349	1.303335	-4.335736	8	0.354737	-1.745524	2.834487
6	4.953336	5.489495	4.034472	1	1.256815	-2.737159	-1.391425
1	4.406258	6.226512	3.432723	6	3.565645	-3.164409	-0.009115
1	5.184359	5.921504	5.008955	1	3.692245	-3.431232	-1.059715
1	5.888631	5.232051	3.521651	1	4.320215	-3.712805	0.574070
6	-5.386817	-0.087111	5.467994	6	2.044783	-5.098152	0.028979
1	-6.064243	-0.693639	6.070316	1	2.181667	-5.232518	-1.048990
1	-4.388039	-0.098025	5.922504	1	1.055550	-5.479973	0.291797
1	-5.755579	0.946309	5.439540	1	2.798959	-5.706366	0.543972
6	-6.506836	5.059197	-3.613753	6	2.659027	-0.622748	1.945769
1	-6.890014	5.592260	-4.484747	6	2.149481	0.548350	1.259171
1	-7.176908	4.222869	-3.377023	6	2.458224	1.841221	1.365503
1	-6.473256	5.743600	-2.756515	6	1.785336	2.931058	0.576033
(R)-TS2				1	1.015944	3.426581	1.180746
				1	1.306885	2.529159	-0.314938
				1	2.509893	3.697856	0.280261
8	4.655607	-1.646640	-2.311874	6	3.521129	2.333379	2.323783
16	5.121244	-1.295190	-0.964108	1	3.119240	3.128226	2.965999
7	3.827787	-1.707103	0.085377	1	4.367245	2.763646	1.773472
8	6.387249	-1.849864	-0.458607	1	3.903837	1.537458	2.967342
6	5.223862	0.481682	-0.837711	1	2.561176	-0.608591	3.031355
6	4.224835	1.282797	-1.392359	28	1.257775	-0.914030	0.420432
6	6.378738	1.040238	-0.292702	6	-2.837922	-0.426553	0.586733
1	3.325902	0.840981	-1.796218	6	-3.169941	0.977085	0.066935
6	4.401349	2.660450	-1.407192	6	-4.669152	0.372140	1.767742
6	6.527516	2.426397	-0.296644	1	-1.935963	-0.421704	1.211158
1	7.146665	0.389013	0.108546	1	-3.506195	0.921290	-0.971061
1	3.632065	3.287974	-1.845701	6	-6.155773	0.125564	1.564866
6	5.545632	3.254177	-0.853503	1	-6.487175	-0.708541	2.189060
1	7.423111	2.869329	0.129187	1	-6.723156	1.017914	1.841375
6	5.691121	4.754209	-0.837767	1	-6.345160	-0.114567	0.517150
1	5.408437	5.191482	-1.800351	6	-4.304127	0.734961	3.202352
1	6.716829	5.056308	-0.611959	1	-4.766874	1.685155	3.479089
1	5.037787	5.197797	-0.076634	1	-4.658958	-0.044989	3.881712
6	3.978705	-1.210209	1.463039	1	-3.223415	0.833687	3.309438
1	4.337321	-2.012511	2.119444	8	-3.960772	-0.798370	1.359873
1	4.733478	-0.419107	1.487568	8	-4.251113	1.414199	0.875457
6	1.089045	-2.758682	-0.308944	6	-2.001959	1.996844	0.124282

6	-2.619816	-1.432026	-0.564747	1	0.124301	1.281306	4.231344
8	-1.522333	-0.910383	-1.360716	1	-1.038306	3.209755	5.317733
8	-0.816445	1.422571	-0.475535	6	-2.325015	3.228314	-0.729142
15	-0.194492	-0.027406	-0.898401	6	-1.273117	4.032408	-1.187531
7	0.426246	0.390644	-2.400748	6	-3.638796	3.589480	-1.050091
6	1.458316	-0.467663	-2.982191	6	-1.526511	5.163414	-1.959233
1	1.027816	-1.296582	-3.562139	1	-0.255507	3.758388	-0.944498
1	2.087716	0.126705	-3.652610	6	-3.890910	4.727425	-1.820592
1	2.092991	-0.888396	-2.203016	1	-4.470532	3.000192	-0.683750
6	-0.425534	1.048916	-3.387958	6	-2.838867	5.516207	-2.280892
1	-1.143578	1.699537	-2.888888	1	-0.697029	5.770619	-2.309844
1	0.198654	1.667959	-4.041616	1	-4.916601	4.991827	-2.060115
1	-0.963649	0.322587	-4.013341	1	-3.037421	6.397886	-2.882865
6	-3.840654	-1.481573	-1.484747				
6	-4.999728	-2.140316	-1.051975	(S)-TS2			
6	-3.840094	-0.866069	-2.739423				
6	-6.139302	-2.163051	-1.852931	8	4.451439	-2.465486	1.535506
1	-5.002733	-2.630331	-0.086571	16	5.068201	-1.759100	0.405743
6	-4.980848	-0.896502	-3.544754	7	3.802696	-1.531882	-0.738757
1	-2.943461	-0.367435	-3.082402	8	6.249603	-2.329158	-0.262130
6	-6.135273	-1.539926	-3.103148	6	5.511361	-0.114229	0.944617
1	-7.030607	-2.674655	-1.501932	6	4.726065	0.540257	1.892571
1	-4.962162	-0.415006	-4.518019	6	6.726433	0.422363	0.519567
1	-7.022930	-1.562818	-3.728180	1	3.796678	0.099855	2.222627
6	-2.294739	-2.837762	-0.071824	6	5.170485	1.749270	2.415964
6	-2.108662	-3.145307	1.277265	6	7.148589	1.642497	1.043454
6	-2.176350	-3.858145	-1.026051	1	7.333032	-0.128373	-0.190072
6	-1.801231	-4.451891	1.664599	1	4.572010	2.257082	3.166576
1	-2.197150	-2.382506	2.038021	6	6.380823	2.322009	1.997284
6	-1.870483	-5.159029	-0.641358	1	8.093948	2.065956	0.717089
1	-2.322348	-3.620190	-2.074376	6	6.825146	3.653852	2.544925
6	-1.683338	-5.461007	0.710890	1	6.593722	3.744262	3.610300
1	-1.654793	-4.672598	2.717369	1	7.899635	3.803808	2.412540
1	-1.776630	-5.937053	-1.392715	1	6.310101	4.473809	2.029723
1	-1.449849	-6.476911	1.015700	6	4.093420	-0.530397	-1.780539
6	-1.685300	2.375660	1.568718	1	4.459057	-1.017201	-2.693020
6	-2.331698	3.457571	2.178014	1	4.889946	0.132722	-1.434398
6	-0.801814	1.601944	2.326983	6	0.935883	-2.408973	-1.068243
6	-2.098493	3.755813	3.519572	6	2.054338	-2.978312	-1.951797
1	-3.020403	4.064397	1.602548	1	-0.041367	-2.646550	-1.497095
6	-0.569148	1.899017	3.669538	6	1.989713	-2.175485	-3.263584
1	-0.256196	0.785310	1.877319	6	1.487852	-0.779790	-2.924772
6	-1.218263	2.975963	4.272559	1	2.944025	-2.131856	-3.802434
1	-2.606668	4.599692	3.976804	1	1.252978	-2.604442	-3.950452

8	0.688975	-0.148625	-3.571426	1	-0.854959	-0.614819	3.841036
1	0.966865	-2.843829	-0.060470	1	0.042305	0.926237	3.864582
6	3.425053	-2.874885	-1.256663	1	-1.459194	0.784143	2.937953
1	3.397979	-3.536110	-0.388247	6	1.374732	-0.977761	2.386723
1	4.210967	-3.238090	-1.934753	1	1.983119	-1.139967	1.495257
6	1.847199	-4.476896	-2.250995	1	1.985469	-0.472194	3.143561
1	1.836290	-5.055693	-1.321760	1	1.076992	-1.953996	2.790097
1	0.886348	-4.628507	-2.751709	6	-2.700498	3.066246	0.277365
1	2.635569	-4.885581	-2.895194	6	-3.479777	3.946252	-0.485307
6	2.853490	0.320647	-2.038685	6	-2.505073	3.341230	1.633459
6	2.331004	1.091644	-0.913941	6	-4.068041	5.062233	0.102551
6	2.748924	2.209114	-0.318128	1	-3.626631	3.749801	-1.540041
6	2.066546	2.812981	0.882841	6	-3.095207	4.462249	2.223085
1	1.691930	3.822213	0.661352	1	-1.873254	2.691607	2.222993
1	1.233518	2.201845	1.228027	6	-3.883839	5.322839	1.462464
1	2.779095	2.927644	1.708968	1	-4.671492	5.731428	-0.503487
6	3.948342	2.986862	-0.815687	1	-2.930080	4.661279	3.277967
1	3.668316	4.027453	-1.030123	1	-4.343206	6.193823	1.920182
1	4.739863	3.021846	-0.058545	6	-1.500489	2.149757	-1.725148
1	4.370087	2.557770	-1.727738	6	-2.137175	1.859413	-2.936445
1	2.884178	0.863067	-2.983713	6	-0.287933	2.842691	-1.742411
28	1.268656	-0.459983	-0.926929	6	-1.556260	2.247480	-4.144845
6	-3.231081	0.714644	-0.521536	1	-3.098185	1.357151	-2.946693
6	-3.488412	-0.033873	0.785148	6	0.299731	3.212507	-2.947492
6	-5.515940	0.768193	-0.021915	1	0.193062	3.078734	-0.805186
1	-2.904113	0.016147	-1.292110	6	-0.334635	2.917001	-4.154651
1	-3.128464	0.540095	1.643931	1	-2.058931	2.015241	-5.078705
6	-6.076847	1.935873	0.781199	1	1.255544	3.727864	-2.940191
1	-6.487300	2.692986	0.108776	1	0.121902	3.204010	-5.097183
1	-6.869585	1.584062	1.447279	6	-3.496152	-2.365443	-0.197538
1	-5.286623	2.397928	1.375960	6	-4.651932	-3.036546	0.218728
6	-6.558910	0.025407	-0.842328	6	-3.049249	-2.533201	-1.512681
1	-7.327897	-0.391413	-0.186558	6	-5.355154	-3.849000	-0.667376
1	-7.032628	0.707900	-1.552730	1	-5.003387	-2.917863	1.236505
1	-6.078646	-0.790145	-1.386458	6	-3.755368	-3.348594	-2.399594
8	-4.487496	1.243803	-0.900306	1	-2.144413	-2.034882	-1.836540
8	-4.892034	-0.171937	0.860431	6	-4.911534	-4.005855	-1.982444
6	-2.775030	-1.416380	0.760854	1	-6.251325	-4.360966	-0.329660
6	-2.129390	1.810411	-0.379022	1	-3.394604	-3.468419	-3.416859
8	-1.122844	1.315380	0.550525	1	-5.460009	-4.640421	-2.672186
8	-1.465531	-1.210759	0.185213	6	-2.626568	-2.034881	2.142680
15	-0.287145	-0.100005	0.480918	6	-1.617525	-2.982540	2.352114
7	0.213545	-0.150290	2.074438	6	-3.478723	-1.696681	3.197471
6	-0.560379	0.252987	3.241156	6	-1.444208	-3.561258	3.606607

1	-0.963844	-3.246634	1.528151	1	-0.231484	4.788752	-1.595326
6	-3.309940	-2.285551	4.453532	1	-2.845445	-0.288620	2.595097
1	-4.278756	-0.981523	3.038374	6	2.839880	-2.092137	1.146562
6	-2.289224	-3.211262	4.664255	1	3.250055	-3.079261	0.901938
1	-0.650819	-4.286761	3.759766	1	3.471325	-1.666023	1.927545
1	-3.975834	-2.013543	5.267067	6	0.381254	-1.667771	-1.605195
1	-2.153786	-3.662039	5.642699	6	1.572718	-2.629506	-1.717298
TS3				1	-0.485872	-2.082291	-2.132436
				6	1.223076	-3.806592	-0.791416
				6	0.332672	-3.262447	0.320200
15	-1.683399	-0.038995	-0.049663	1	2.092274	-4.332931	-0.379376
6	-3.174861	-1.110160	-0.197659	1	0.623698	-4.556161	-1.319894
6	-3.035249	-2.441354	-0.608033	8	-0.590328	-3.860793	0.822959
6	-4.159478	-3.249021	-0.780730	1	0.608902	-0.704913	-2.071614
6	-5.435410	-2.737103	-0.548907	6	2.892845	-1.917570	-1.345788
6	-5.584971	-1.410643	-0.139070	1	3.082255	-1.161961	-2.109762
6	-4.463669	-0.602086	0.037772	1	3.723533	-2.637147	-1.396629
6	-1.689970	0.906903	-1.628729	6	1.763458	-3.137709	-3.160564
6	-0.503738	1.526993	-2.043642	1	1.935947	-2.300216	-3.844427
6	-2.843865	1.051565	-2.410969	1	0.865587	-3.664939	-3.496764
6	-2.264369	1.215195	1.160357	1	2.613152	-3.825752	-3.247824
6	-2.158419	2.588809	0.915061	6	1.413100	-2.198109	1.667959
6	-2.774513	0.775334	2.391802	6	0.748994	-0.993762	2.115569
1	-4.590531	0.424254	0.363057	6	0.980294	-0.232660	3.190555
1	0.396225	1.410224	-1.454494	6	0.310963	1.085351	3.483194
1	-3.766405	0.568188	-2.111876	1	-0.350860	1.012937	4.354840
1	-1.777663	2.940071	-0.037115	1	-0.276062	1.444715	2.642823
8	4.973970	-0.009402	-1.028325	1	1.067361	1.842746	3.730959
16	3.982376	0.091139	0.050699	6	-0.475656	2.288893	-3.211584
7	2.912362	-1.232768	-0.041322	6	-1.629149	2.431274	-3.983695
8	4.404113	0.203622	1.452606	1	-1.604772	3.017503	-4.897478
6	2.962561	1.514845	-0.303414	6	-2.811828	1.809073	-3.581623
6	3.169926	2.243383	-1.472919	6	-2.540819	3.509267	1.893639
6	2.048747	1.939478	0.661111	6	-3.050554	3.065896	3.113600
1	3.910701	1.907330	-2.189234	1	-3.352093	3.782683	3.871248
6	2.434253	3.411142	-1.676605	6	-3.175397	1.695097	3.356155
6	1.321163	3.103330	0.439366	1	-6.309395	-3.368043	-0.680351
1	1.910858	1.356106	1.558879	1	-2.050220	-2.852098	-0.768937
1	2.594667	3.991142	-2.581397	6	2.041103	-0.610038	4.207736
6	1.495779	3.851660	-0.733814	1	2.939349	0.006362	4.069963
1	0.600914	3.427809	1.183531	1	2.337577	-1.658586	4.129590
6	0.648244	5.067544	-1.001487	1	1.681679	-0.433080	5.228939
1	1.197185	5.826203	-1.566751	1	1.237192	-3.081113	2.281676
1	0.292377	5.520415	-0.072169	1	-2.448988	4.573206	1.695275

1	-3.572318	1.343255	4.303560	1	-2.727088	-0.593140	2.590675
1	-6.574887	-1.004491	0.046472	6	2.896567	-2.119870	0.592044
1	-4.032211	-4.282731	-1.087062	1	3.302501	-3.064908	0.211694
1	-3.711874	1.909575	-4.180817	1	3.574296	-1.769428	1.371725
1	0.452950	2.758894	-3.516855	6	0.253684	-1.440953	-1.926900
28	0.110179	-1.274198	0.326903	6	1.445926	-2.361374	-2.223856
TS3a				1	-0.642384	-1.811455	-2.438227
				6	1.173809	-3.640112	-1.413828
				6	0.356724	-3.239741	-0.190279
15	-1.720578	-0.037461	-0.073161	1	2.075055	-4.193245	-1.123675
6	-3.205730	-1.113268	-0.248001	1	0.546944	-4.336920	-1.981169
6	-3.076816	-2.391763	-0.803679	8	-0.524775	-3.906711	0.301080
6	-4.200999	-3.195340	-0.995262	1	0.437755	-0.428277	-2.297154
6	-5.466266	-2.731501	-0.637953	6	2.779214	-1.669266	-1.862508
6	-5.605151	-1.457570	-0.083237	1	2.908137	-0.830623	-2.548365
6	-4.483751	-0.653698	0.112913	1	3.613384	-2.362564	-2.046715
6	-1.835545	1.074814	-1.535241	6	1.545036	-2.703515	-3.724086
6	-0.686693	1.767848	-1.940040	1	1.661384	-1.792508	-4.320199
6	-3.032745	1.272253	-2.236347	1	0.632700	-3.207314	-4.057270
6	-2.241229	1.067108	1.300101	1	2.394822	-3.361509	-3.943012
6	-2.160466	2.460805	1.202655	6	1.509834	-2.314483	1.191069
6	-2.675366	0.487563	2.502411	6	0.860203	-1.182226	1.816416
1	-4.601792	0.331032	0.550675	6	1.136446	-0.543901	2.958880
1	0.246419	1.610168	-1.415271	6	0.455325	0.720371	3.419490
1	-3.927178	0.734115	-1.945626	1	-0.216054	0.542178	4.266169
1	-1.838791	2.919941	0.274956	1	-0.129930	1.174188	2.624809
8	4.849824	0.233985	-1.475447	1	1.204395	1.447449	3.761903
16	3.938817	0.191952	-0.323929	6	-0.738266	2.653521	-3.016170
7	2.876903	-1.132184	-0.493827	6	-1.934755	2.848063	-3.707396
8	4.459859	0.149545	1.047984	1	-1.972403	3.531114	-4.550768
6	2.882571	1.628469	-0.436479	6	-3.080204	2.153535	-3.316460
6	2.995148	2.488241	-1.527222	6	-2.491816	3.262676	2.297240
6	2.039162	1.924292	0.634353	6	-2.925709	2.680808	3.487996
1	3.684156	2.249033	-2.328990	1	-3.187811	3.305592	4.336344
6	2.234130	3.657241	-1.542765	6	-3.025986	1.290061	3.583985
6	1.283268	3.090907	0.598847	1	-6.339918	-3.359571	-0.784510
1	1.976983	1.241964	1.468805	1	-2.099082	-2.767601	-1.063654
1	2.321193	4.338874	-2.384539	6	2.248671	-1.027539	3.879094
6	1.361823	3.969482	-0.491405	1	3.058324	-0.283181	3.873350
1	0.616379	3.315959	1.424921	1	2.678432	-1.954283	3.488971
6	0.481817	5.189912	-0.559043	1	1.388389	-3.264609	1.709816
1	0.984460	6.023247	-1.058470	1	-2.419969	4.343161	2.212665
1	0.175924	5.519271	0.437573	1	-3.364518	0.830640	4.507744
1	-0.427718	4.965752	-1.130763	1	-6.586568	-1.089167	0.200354

1	-4.081336	-4.189180	-1.415452	1	0.342358	5.341306	-0.946472
1	-4.013233	2.294058	-3.853984	1	-0.200879	4.446033	-2.372631
1	0.162169	3.178870	-3.315391	1	-2.894564	0.207922	2.556366
28	0.110911	-1.267860	0.051161	6	2.816081	-2.006115	1.300651
6	1.790281	-1.261918	5.326217	1	3.202785	-3.029463	1.221822
1	2.616060	-1.639386	5.937823	1	3.482015	-1.461419	1.971761
1	1.429215	-0.340021	5.791800	6	0.253562	-1.992482	-1.381488
1	0.977916	-1.995796	5.362694	6	1.413650	-2.997637	-1.373539
TS3a'				1	-0.645650	-2.460827	-1.798326
				6	1.076139	-3.987992	-0.246508
				6	0.243382	-3.234865	0.783818
15	-1.708796	-0.058583	-0.084491	1	1.949793	-4.458187	0.220518
6	-3.232446	-1.092172	-0.016805	1	0.441154	-4.801286	-0.614995
6	-3.137852	-2.481512	-0.159688	8	-0.672586	-3.708503	1.415900
6	-4.288047	-3.271166	-0.166368	1	0.487341	-1.129909	-2.011798
6	-5.545313	-2.683612	-0.033966	6	2.766521	-2.276571	-1.182505
6	-5.650209	-1.298502	0.109414	1	2.945515	-1.675205	-2.074860
6	-4.503065	-0.507360	0.120374	1	3.574193	-3.022152	-1.133509
6	-1.722942	0.598068	-1.805460	6	1.526631	-3.750079	-2.714755
6	-0.532381	1.113293	-2.336048	1	1.688088	-3.047226	-3.538575
6	-2.886109	0.631638	-2.586348	1	0.602182	-4.298647	-2.918882
6	-2.233049	1.409865	0.890364	1	2.354847	-4.469151	-2.716752
6	-2.056021	2.714165	0.415056	6	1.409888	-1.992221	1.885147
6	-2.764244	1.215760	2.174817	6	0.780831	-0.721973	2.168140
1	-4.595296	0.566179	0.240020	6	1.028525	0.169795	3.134414
1	0.375574	1.077080	-1.749049	6	0.309886	1.496195	3.260908
1	-3.812452	0.224558	-2.198904	1	-0.457107	1.413202	4.043931
1	-1.663675	2.877053	-0.581929	1	-0.226197	1.695872	2.335160
8	4.878323	-0.386881	-1.314213	6	-0.509848	1.668146	-3.615439
16	3.959869	-0.085341	-0.208294	6	-1.673182	1.702553	-4.385158
7	2.859145	-1.372961	-0.022534	1	-1.653657	2.126848	-5.384578
8	4.472557	0.237635	1.129018	6	-2.859469	1.179898	-3.868662
6	2.948973	1.294155	-0.724637	6	-2.381245	3.807566	1.220803
6	3.145928	1.866842	-1.979346	6	-2.906643	3.607555	2.497125
6	2.061291	1.852798	0.194659	1	-3.163456	4.458293	3.120840
1	3.864056	1.427277	-2.661881	6	-3.108210	2.306965	2.967288
6	2.426317	3.014253	-2.314580	1	-6.439428	-3.299863	-0.036065
6	1.355960	2.998711	-0.154737	1	-2.167924	-2.947577	-0.241142
1	1.921524	1.382407	1.156840	6	2.084825	-0.101052	4.189700
1	2.575346	3.471211	-3.289158	1	2.991453	0.487945	4.004088
6	1.518386	3.590045	-1.415928	1	2.371852	-1.154586	4.215241
1	0.661070	3.430500	0.557709	1	1.247742	-2.764474	2.636938
6	0.686219	4.779011	-1.818793	1	-2.232826	4.815298	0.843642
1	1.241772	5.459369	-2.470689	1	-3.520030	2.143620	3.958551

1	-6.625296	-0.832530	0.216125	6	-1.238180	4.617081	2.496274
1	-4.195260	-4.348298	-0.265226	1	-1.116050	5.704134	2.513376
1	-3.767214	1.195458	-4.464470	1	-1.040555	4.232334	3.500239
1	0.422019	2.061458	-4.007084	1	-2.289729	4.410632	2.259404
28	0.068000	-1.267977	0.465306	1	-2.006431	-2.529436	2.510817
1	1.721130	0.175120	5.187312	6	2.115895	-0.754782	-1.917519
6	1.208342	2.695477	3.601934	1	2.397537	-1.202779	-2.877996
1	0.611872	3.613344	3.619996	1	3.035181	-0.567073	-1.368195
1	1.680183	2.588536	4.582986	6	-1.502711	-0.141359	-2.417764
1	2.008348	2.830512	2.867592	6	-0.537068	-0.306608	-3.599780
TS3b				1	-2.481177	-0.566046	-2.671039
				6	-0.184901	-1.803614	-3.626396
				6	-0.292779	-2.320011	-2.196832
15	-2.406508	-0.516439	0.452202	1	0.799470	-2.028364	-4.053874
6	-3.658952	-1.851404	0.247783	1	-0.918742	-2.369694	-4.210646
6	-3.637331	-2.661390	-0.893463	8	-0.706888	-3.414282	-1.886659
6	-4.612011	-3.642250	-1.081529	1	-1.661201	0.916095	-2.186952
6	-5.619929	-3.822898	-0.135680	6	0.691023	0.617456	-3.442608
6	-5.649025	-3.020481	1.007155	1	0.340594	1.646023	-3.533692
6	-4.674623	-2.043460	1.200332	1	1.386936	0.441856	-4.276617
6	-3.337702	1.012024	0.020737	6	-1.195022	0.098668	-4.934305
6	-2.607708	2.177072	-0.253264	1	-1.523266	1.142655	-4.900853
6	-4.737121	1.060148	-0.019545	1	-2.074805	-0.523223	-5.125183
6	-2.315450	-0.404908	2.286237	1	-0.510113	-0.013396	-5.783670
6	-2.403959	0.819124	2.959178	6	1.279595	-1.720045	-1.089472
6	-2.085530	-1.576468	3.024488	6	0.916050	-1.357085	0.258961
1	-4.700138	-1.431733	2.095199	6	1.621229	-1.290516	1.390310
1	-1.525851	2.144295	-0.247459	6	-3.265993	3.372312	-0.540253
1	-5.317562	0.165801	0.172697	6	-4.660595	3.414320	-0.572786
1	-2.596214	1.728976	2.402865	1	-5.172868	4.343092	-0.805606
8	2.321653	2.841433	-2.854263	6	-5.393232	2.255160	-0.316151
16	2.245292	1.931168	-1.704300	6	-2.245481	0.873704	4.345639
7	1.420054	0.514097	-2.164994	6	-2.016652	-0.294026	5.072874
8	3.464260	1.520482	-0.994663	1	-1.897874	-0.250727	6.151196
6	1.181761	2.702024	-0.492909	6	-1.947016	-1.521492	4.408315
6	0.620112	3.947974	-0.765650	1	-6.375972	-4.588512	-0.282303
6	1.017301	2.090152	0.749745	1	-2.847629	-2.544801	-1.619878
1	0.790946	4.411891	-1.730129	1	1.577421	-2.758232	-1.211667
6	-0.133590	4.577272	0.224607	1	-2.311976	1.830236	4.856015
6	0.253115	2.727920	1.721455	1	-1.772667	-2.435220	4.968424
1	1.466298	1.125486	0.938115	1	-6.428309	-3.157143	1.751040
1	-0.570117	5.551986	0.024174	1	-4.572712	-4.270575	-1.965992
6	-0.342228	3.972477	1.471303	1	-6.478451	2.277437	-0.348913
1	0.107595	2.245951	2.682530	1	-2.683402	4.262634	-0.749814

28	-0.627206	-0.918717	-0.807960	16	2.034887	2.786333	0.721324
6	1.093054	-0.779857	2.707292	7	0.710330	2.927804	-0.329968
1	0.132510	-0.289564	2.585517	8	3.148883	2.246948	-0.073009
1	0.970614	-1.587126	3.439393	6	1.546924	1.511768	1.874558
6	3.082433	-1.677303	1.504709	6	1.497577	1.799777	3.236408
1	3.185247	-2.440330	2.298670	6	1.375135	0.208776	1.404717
1	3.657965	-0.801209	1.843496	1	1.653383	2.817889	3.574141
1	1.796753	-0.060319	3.148012	6	1.275604	0.757068	4.138259
8	3.618334	-2.176726	0.294557	6	1.188145	-0.820378	2.318854
6	4.942301	-2.669512	0.424864	1	1.377462	0.017041	0.341136
1	4.973670	-3.483211	1.167317	1	1.233976	0.972815	5.202261
1	5.175683	-3.108019	-0.552250	6	1.129788	-0.563756	3.696928
6	5.969281	-1.614154	0.784371	1	1.064134	-1.834676	1.954713
6	7.045677	-1.933954	1.617115	6	0.849374	-1.681148	4.666678
6	5.865792	-0.315632	0.271763	1	1.225229	-1.451567	5.667327
6	8.016900	-0.978901	1.921570	1	1.302316	-2.619767	4.335033
1	7.123938	-2.936491	2.031579	1	-0.232416	-1.846055	4.747529
6	6.827246	0.643193	0.587426	1	-1.378004	-2.556376	-2.324655
1	5.025316	-0.041219	-0.354780	6	0.983290	2.814747	-1.768483
6	7.908287	0.314026	1.408047	1	0.766206	3.776396	-2.248500
1	8.849701	-1.241442	2.567670	1	2.046340	2.611746	-1.909908
1	6.724719	1.648692	0.190570	6	-2.130307	2.190195	0.134623
1	8.657618	1.061717	1.651155	6	-1.751248	3.604100	-0.325278
TS3b'				1	-3.219426	2.072971	0.137609
				6	-1.995983	3.608081	-1.843839
				6	-1.829063	2.172615	-2.327077
15	-2.138884	-0.870484	-0.104913	1	-1.344829	4.287607	-2.406515
6	-3.712765	-1.166803	-1.021720	1	-3.027205	3.894965	-2.078329
6	-4.437423	-0.074147	-1.514481	8	-2.466155	1.653257	-3.211168
6	-5.661781	-0.265966	-2.152993	1	-1.787625	2.006569	1.156192
6	-6.180364	-1.551182	-2.307463	6	-0.293899	3.926209	0.071644
6	-5.467502	-2.646627	-1.818082	1	-0.259866	3.999845	1.160002
6	-4.242285	-2.458001	-1.179838	1	-0.010431	4.913207	-0.322718
6	-2.719272	-0.765483	1.642045	6	-2.623156	4.680716	0.350735
6	-1.965401	-0.055230	2.584593	1	-2.521292	4.632171	1.439776
6	-3.883674	-1.425241	2.064012	1	-3.677706	4.522667	0.105463
6	-1.366949	-2.535105	-0.167529	1	-2.349501	5.693342	0.030630
6	-1.010652	-3.241539	0.986750	6	0.177591	1.686730	-2.399397
6	-1.118502	-3.106266	-1.425022	6	0.455543	0.335334	-1.979328
1	-3.698626	-3.317830	-0.806737	6	1.513618	-0.429592	-2.273875
1	-1.068023	0.459955	2.276564	6	-2.357818	-0.013171	3.922923
1	-4.486408	-1.971377	1.347591	6	-3.514437	-0.675074	4.334412
1	-1.220119	-2.820724	1.963662	1	-3.824120	-0.638281	5.374579
8	2.201623	4.027214	1.488916	6	-4.277068	-1.379600	3.400536

6	-0.393804	-4.490883	0.884566	6	-5.503580	-1.463752	0.151823
6	-0.156808	-5.055986	-0.367968	6	-4.375725	-0.653271	0.273333
1	0.316480	-6.029761	-0.445971	6	-1.693462	0.908201	-1.565146
6	-0.532632	-4.365044	-1.522978	6	-0.540173	1.587551	-1.980619
1	-7.131614	-1.699989	-2.809494	6	-2.869525	1.034801	-2.315853
1	-4.036721	0.923033	-1.415767	6	-2.091718	1.148382	1.259236
1	-0.014342	1.824455	-3.462820	6	-2.232498	2.513101	0.981306
1	-0.111264	-5.025966	1.786340	6	-2.339038	0.686316	2.561273
1	-0.351382	-4.799971	-2.501116	1	-4.475825	0.354056	0.662375
1	-5.862746	-3.651489	-1.933480	1	0.375494	1.484347	-1.413413
1	-6.203302	0.592163	-2.538910	1	-3.766839	0.508982	-2.010046
1	-5.181755	-1.893200	3.711727	1	-2.059459	2.880647	-0.023373
1	-1.756173	0.542500	4.635123	8	4.975711	0.322733	-0.643394
28	-1.111137	0.892651	-0.981265	16	3.881054	0.287252	0.335584
6	1.784757	-1.812197	-1.713768	7	2.916428	-1.092069	0.056471
1	1.214636	-1.986249	-0.793448	8	4.160162	0.325848	1.776514
1	1.483561	-2.578865	-2.435293	6	2.804467	1.665094	-0.028265
8	3.174569	-2.041334	-1.508324	6	3.032783	2.432611	-1.169500
6	3.720368	-1.258849	-0.454936	6	1.826848	2.023302	0.901456
1	3.365665	-0.223599	-0.505718	1	3.824746	2.151108	-1.853815
1	3.385476	-1.666008	0.514497	6	2.253407	3.568958	-1.384763
6	5.223977	-1.262719	-0.531722	6	1.063194	3.162397	0.671459
6	5.922965	-2.394694	-0.963620	1	1.669810	1.415752	1.782430
6	5.936117	-0.123752	-0.140001	1	2.427859	4.175917	-2.268987
6	7.316982	-2.389653	-0.996090	6	1.255362	3.944794	-0.476099
1	5.364267	-3.266765	-1.286540	1	0.298124	3.440619	1.387861
6	7.331399	-0.122741	-0.165014	6	0.366413	5.128190	-0.754350
1	5.391174	0.763918	0.170921	1	0.907927	5.929184	-1.265906
6	8.025382	-1.255676	-0.592332	1	-0.060802	5.533524	0.166673
1	7.852388	-3.271041	-1.338093	1	-0.465248	4.827262	-1.403927
1	7.875335	0.767288	0.138196	1	-2.230900	-0.370603	2.782540
1	9.111301	-1.253254	-0.617962	6	2.867352	-2.067061	1.152914
6	2.585905	0.045530	-3.239489	1	3.367827	-2.991232	0.841343
1	3.494266	0.361288	-2.714829	1	3.421406	-1.669121	2.004310
1	2.885561	-0.767477	-3.909237	6	0.508627	-1.587405	-1.710060
1	2.233114	0.883984	-3.844140	6	1.790339	-2.427419	-1.821444
TS3c				1	-0.301786	-2.068644	-2.272068
				6	1.501822	-3.704805	-1.013665
				6	0.530066	-3.331527	0.099858
				1	2.396032	-4.195345	-0.610985
15	-1.612418	-0.080492	-0.019579	1	0.984867	-4.447701	-1.630526
6	-3.112956	-1.137526	-0.102458	8	-0.385299	-4.023553	0.482519
6	-2.998237	-2.443641	-0.595599	1	0.653261	-0.594403	-2.145043
6	-4.128941	-3.251320	-0.713815	6	3.017924	-1.639159	-1.309334
6	-5.382178	-2.764140	-0.342164				

1	3.164304	-0.793215	-1.983479	6	2.618303	0.985958	2.524200
1	3.916651	-2.268441	-1.387639	6	2.246049	1.274975	-1.074353
6	2.111634	-2.795946	-3.283664	6	2.104739	2.636439	-0.784020
1	2.252261	-1.892504	-3.886235	6	2.832261	0.889112	-2.289848
1	1.283356	-3.362583	-3.719381	1	4.541071	0.510932	-0.150944
1	3.020737	-3.403858	-3.368678	1	-0.565106	1.315904	1.382056
6	1.428529	-2.326108	1.577466	1	3.568122	0.533505	2.264700
6	0.641666	-1.205949	2.049320	1	1.665450	2.945595	0.157443
6	0.696717	-0.444418	3.138343	8	-5.036273	-0.123275	0.696263
6	-0.566795	2.392649	-3.118310	16	-4.021354	0.038417	-0.353197
6	-1.742314	2.517009	-3.861101	7	-2.928717	-1.272694	-0.281033
1	-1.760948	3.137434	-4.752153	8	-4.410924	0.199149	-1.758701
6	-2.891228	1.834346	-3.459226	6	-3.036108	1.463665	0.084211
6	-2.599931	3.404015	1.992292	6	-3.305449	2.153120	1.265013
6	-2.839774	2.938959	3.285135	6	-2.084911	1.928156	-0.824248
1	-3.127434	3.632199	4.069694	1	-4.073401	1.785956	1.935952
6	-2.714573	1.575791	3.565691	6	-2.593164	3.320517	1.539286
1	-6.260833	-3.396167	-0.430362	6	-1.378983	3.089726	-0.530136
1	-2.025144	-2.832670	-0.862563	1	-1.901306	1.378601	-1.735787
1	1.289977	-3.248579	2.140522	1	-2.801729	3.870086	2.453226
1	-2.705045	4.460781	1.764274	6	-1.614092	3.797342	0.657360
1	-2.904086	1.205606	4.568645	1	-0.628697	3.444986	-1.229008
1	-6.476019	-1.080248	0.446162	6	-0.789572	5.008390	1.006574
1	-4.024999	-4.265748	-1.086207	1	-1.379820	5.758790	1.540574
1	-3.807126	1.922308	-4.035927	1	-0.364963	5.475360	0.113888
1	0.335505	2.912078	-3.423884	1	0.042620	4.719882	1.661267
28	0.145672	-1.356030	0.228894	1	2.931381	-0.165233	-2.528216
6	1.689780	-0.610041	4.262254	6	-2.772485	-2.056015	-1.514147
1	2.461874	0.168808	4.215908	1	-3.205508	-3.052949	-1.365727
1	1.201012	-0.528678	5.240277	1	-3.340211	-1.572008	-2.311745
1	2.195796	-1.578232	4.213268	6	-0.492109	-1.780540	1.408481
1	0.008968	0.393945	3.236856	6	-1.678102	-2.755944	1.395393
TS3c'				1	0.345490	-2.216540	1.965241
				6	-1.260614	-3.881715	0.434419
				6	-0.304234	-3.274064	-0.583479
15	1.628605	-0.033660	0.056703	1	-2.098425	-4.383591	-0.064282
6	3.132355	-1.079112	0.248781	1	-0.694659	-4.659236	0.959327
6	2.999881	-2.431918	0.583934	8	0.657332	-3.833912	-1.056190
6	4.130925	-3.223161	0.786084	1	-0.757207	-0.844817	1.909341
6	5.405713	-2.673111	0.658733	6	-2.981231	-2.039026	0.977445
6	5.547928	-1.324953	0.323632	1	-3.235781	-1.335746	1.771204
6	4.420216	-0.532591	0.117268	1	-3.800031	-2.772352	0.927807
6	1.518115	0.849620	1.666683	6	-1.953170	-3.339400	2.796009
6	0.294345	1.427757	2.030193	1	-2.175198	-2.539504	3.509863

1	-1.073289	-3.878468	3.159913	1	-4.475119	0.378975	0.890945
1	-2.800505	-4.035796	2.794503	1	0.179642	1.539086	-1.595674
6	-1.314317	-2.145068	-1.940878	1	-4.035782	0.721770	-1.768571
6	-0.623594	-0.922634	-2.289461	1	-2.054172	2.918313	0.151284
6	-0.787470	-0.126354	-3.346759	8	4.737283	0.328389	-1.553186
6	0.177533	2.141311	3.222929	16	3.828115	0.257504	-0.402082
6	1.277922	2.276167	4.070237	7	2.807077	-1.100566	-0.572148
1	1.183895	2.824633	5.002754	8	4.358087	0.227255	0.967593
6	2.497124	1.695010	3.719033	6	2.729795	1.661340	-0.508458
6	2.528411	3.598705	-1.703720	6	2.822111	2.520778	-1.602252
6	3.114614	3.209097	-2.907645	6	1.878260	1.939322	0.561781
1	3.448435	3.958347	-3.618922	1	3.517701	2.295281	-2.402239
6	3.274210	1.850415	-3.193915	6	2.031779	3.669471	-1.624659
1	6.285139	-3.291192	0.812949	6	1.100609	3.091310	0.522034
1	2.016864	-2.870960	0.663074	1	1.820875	1.261289	1.402151
1	-1.096983	-2.997805	-2.582605	1	2.099377	4.347177	-2.471313
1	2.408834	4.652958	-1.471308	6	1.154728	3.965335	-0.572861
1	3.730129	1.540417	-4.129273	1	0.431744	3.306713	1.347862
1	6.537226	-0.889490	0.218975	6	0.243894	5.162515	-0.644834
1	4.010669	-4.273434	1.033136	1	0.731521	6.013124	-1.129964
1	3.356026	1.789728	4.376689	1	-0.086703	5.474771	0.349233
1	-0.778234	2.579992	3.487912	1	-0.649736	4.917877	-1.232990
28	-0.106646	-1.286322	-0.479759	1	-2.089490	-0.504841	2.750047
6	-0.161316	1.210968	-3.621825	6	2.868068	-2.089630	0.512488
1	0.363236	1.601793	-2.752765	1	3.327500	-3.011853	0.137004
1	0.554041	1.161754	-4.451760	1	3.514305	-1.705353	1.303025
1	-0.933433	1.933106	-3.917559	6	0.198620	-1.521985	-2.046665
1	-1.503857	-0.447870	-4.110558	6	1.439931	-2.384222	-2.325935
TS3d				1	-0.680796	-1.971493	-2.524718
				6	1.225855	-3.674792	-1.516032
				6	0.400502	-3.311966	-0.288189
15	-1.693998	-0.044812	-0.071916	1	2.153895	-4.184892	-1.230873
6	-3.207990	-1.086556	-0.065386	1	0.628451	-4.397734	-2.081827
6	-3.156527	-2.369932	-0.624175	8	-0.479119	-3.994512	0.185107
6	-4.303651	-3.161672	-0.672397	1	0.314853	-0.519730	-2.469828
6	-5.510909	-2.681096	-0.165093	6	2.735921	-1.632512	-1.947420
6	-5.569261	-1.403582	0.395612	1	2.827904	-0.782049	-2.624449
6	-4.424553	-0.609668	0.448063	1	3.603246	-2.283106	-2.133295
6	-1.912644	1.034485	-1.541518	6	1.579416	-2.725710	-3.823078
6	-0.789822	1.702933	-2.047813	1	1.664158	-1.811529	-4.419769
6	-3.160647	1.239342	-2.144638	1	0.695228	-3.269699	-4.168466
6	-2.032552	1.106785	1.318932	1	2.460830	-3.345898	-4.027601
6	-2.151099	2.490290	1.142142	6	1.484257	-2.358970	1.089182
6	-2.181256	0.566798	2.606026	6	0.755952	-1.260356	1.689479

6	0.870780	-0.579045	2.824041	6	2.008709	2.648795	0.237069
6	-0.915940	2.574281	-3.128856	6	3.001206	1.411683	-1.584907
6	-2.162357	2.776719	-3.723869	1	4.499662	0.435640	0.551284
1	-2.258985	3.448957	-4.571231	1	-0.633830	0.891345	1.759065
6	-3.282585	2.105333	-3.231638	1	3.363347	-0.380060	2.697368
6	-2.398813	3.322157	2.236411	1	1.456091	2.673153	1.168189
6	-2.539847	2.779450	3.513535	8	-4.987799	-0.376489	0.933204
1	-2.733938	3.427093	4.363084	16	-4.039156	0.019504	-0.115593
6	-2.436978	1.397747	3.694663	7	-2.941803	-1.261272	-0.386936
1	-6.402032	-3.300756	-0.199474	8	-4.516028	0.472245	-1.427673
1	-2.217474	-2.754864	-0.996934	6	-3.030614	1.332771	0.554039
6	1.878710	-0.834971	3.924766	6	-3.306631	1.830463	1.825966
1	2.486534	-1.705017	3.645295	6	-2.057496	1.916273	-0.256957
1	1.410321	-3.302128	1.629421	1	-4.086341	1.371098	2.422370
1	-2.488151	4.394188	2.086195	6	-2.578280	2.924886	2.292049
1	-2.549232	0.967031	4.685012	6	-1.341689	3.007016	0.224505
1	-6.505194	-1.025409	0.796055	1	-1.854795	1.509574	-1.238127
1	-4.247488	-4.159146	-1.097197	1	-2.787206	3.322517	3.281525
1	-4.253779	2.253703	-3.694194	6	-1.581142	3.519430	1.507699
1	-0.036128	3.084679	-3.506325	1	-0.577832	3.456226	-0.400802
28	0.070487	-1.334615	-0.073354	6	-0.743834	4.645665	2.055269
1	0.191707	0.250680	3.021234	1	-1.337372	5.327611	2.671207
6	1.144248	-1.157453	5.236671	1	-0.276852	5.223592	1.253525
1	1.853759	-1.344139	6.050303	1	0.057361	4.246854	2.690685
1	0.506830	-0.316591	5.535907	1	3.199011	0.469455	-2.085510
1	0.505325	-2.039224	5.126192	6	-2.797205	-1.704085	-1.779137
6	2.812280	0.374737	4.097935	1	-3.256442	-2.694303	-1.892464
1	3.396441	0.555951	3.192325	1	-3.351086	-1.018605	-2.424036
1	2.231686	1.278385	4.321729	6	-0.486871	-2.205522	1.068741
1	3.507608	0.214592	4.929556	6	-1.684827	-3.135902	0.833619
TS3d'				1	0.354897	-2.773741	1.482361
				6	-1.296239	-3.992779	-0.382390
				6	-0.335400	-3.164936	-1.222692
				1	-2.146428	-4.336321	-0.983859
15	1.608154	-0.164633	0.268990	1	-0.743654	-4.887824	-0.076299
6	3.126819	-1.204020	0.233706	8	0.616535	-3.599638	-1.828767
6	3.020015	-2.588207	0.056179	1	-0.736332	-1.424800	1.791873
6	4.161239	-3.391595	0.072984	6	-2.985451	-2.327020	0.631768
6	5.418535	-2.823066	0.270660	1	-3.226172	-1.851750	1.582841
6	5.535015	-1.442169	0.446439	1	-3.809867	-3.019380	0.403538
6	4.398623	-0.636574	0.424886	6	-1.945828	-4.045258	2.051541
6	1.396685	0.234671	2.054561	1	-2.142447	-3.444493	2.945401
6	0.169979	0.769942	2.473440	1	-1.068893	-4.668020	2.252420
6	2.415251	0.049360	2.997638	1	-2.804549	-4.709370	1.894809
6	2.258284	1.425074	-0.394738				

6	-1.344605	-1.725001	-2.233238	6	-0.303137	-3.752494	-0.020500
6	-0.599107	-0.488359	-2.327598	1	2.089173	-4.403999	-1.487694
6	-0.689301	0.493229	-3.224544	1	-0.911775	-2.194692	-2.985260
6	-0.023758	1.137265	3.804223	8	-2.070539	-0.031343	-2.108824
6	0.998624	0.956839	4.737150	16	-2.659128	0.936638	-1.177811
1	0.844621	1.234339	5.775641	7	-2.022144	0.610539	0.346383
6	2.214848	0.407473	4.331436	8	-2.511710	2.380305	-1.404601
6	2.474013	3.839959	-0.323287	6	-4.398489	0.562995	-1.054680
6	3.211977	3.818772	-1.506477	6	-4.829941	-0.748397	-1.269336
1	3.579780	4.744894	-1.937418	6	-5.289263	1.560927	-0.657405
6	3.484111	2.598498	-2.129647	1	-4.122478	-1.505241	-1.589902
1	6.305660	-3.449262	0.281013	6	-6.174629	-1.053677	-1.079748
1	2.052977	-3.035121	-0.120355	6	-6.631020	1.234990	-0.475643
1	-1.169436	-2.413246	-3.059584	1	-4.933502	2.575609	-0.519587
1	2.268899	4.782708	0.175554	1	-6.519739	-2.069592	-1.249993
1	4.060955	2.571651	-3.048577	6	-7.092010	-0.073285	-0.675768
1	6.511354	-0.990963	0.596192	1	-7.333188	2.008562	-0.178005
1	4.062352	-4.461957	-0.079030	6	-8.538655	-0.425909	-0.439594
1	3.011586	0.253730	5.053114	1	-9.189321	0.442297	-0.574491
1	-0.979177	1.551714	4.106764	1	-8.686716	-0.792009	0.583612
28	-0.092693	-1.264370	-0.644129	1	-8.873421	-1.214770	-1.119100
6	0.116074	1.764429	-3.308384	1	0.400689	-3.753796	0.805876
1	0.639399	1.904755	-2.360641	6	-2.133831	-0.801693	0.740256
6	-0.787528	2.982589	-3.560877	1	-3.176702	-1.057480	0.983105
1	-0.191438	3.900121	-3.613485	1	-1.824020	-1.400825	-0.110735
1	-1.323914	2.878009	-4.511459	6	0.091902	1.341336	1.992781
1	-1.536737	3.110482	-2.774852	6	-1.316621	1.625960	2.541944
6	1.159893	1.643277	-4.432295	1	0.837725	1.528553	2.763548
1	1.756447	2.558030	-4.515401	6	-1.728224	0.673626	3.679685
1	1.835937	0.803762	-4.248715	6	-1.967963	-0.752776	3.231626
1	0.667298	1.471946	-5.396698	1	-2.632444	1.024466	4.187908
1	-1.420847	0.382569	-4.035130	1	-0.929540	0.651041	4.431802
TS3_{dppp}				8	-2.686541	-1.517906	3.849418
				1	0.242895	2.092266	1.210066
				6	-2.347437	1.603462	1.381664
15	1.202759	-1.590016	-0.958589	1	-2.336271	2.575129	0.889784
6	2.659694	-2.595611	-0.455944	1	-3.361270	1.435361	1.780450
6	3.649536	-1.986683	0.324275	6	-1.329121	3.059587	3.112014
6	4.809505	-2.680636	0.669112	1	-0.963366	3.774758	2.368375
6	4.989408	-3.996051	0.241586	1	-0.686425	3.127313	3.995324
6	4.007655	-4.612925	-0.538238	1	-2.341479	3.357738	3.411499
6	2.851231	-3.916885	-0.887670	6	-1.253940	-1.161179	1.949269
6	-0.103907	-2.868879	-1.097612	6	0.167871	-0.607597	1.948256
6	-1.023616	-2.882541	-2.156460	6	1.049974	-1.107926	2.870695

6	2.408800	-0.501047	3.102567	1	2.742892	-1.145079	-2.767522
1	2.500687	-0.118805	4.132251	1	1.382619	-2.078645	-3.358825
1	2.617895	0.314152	2.409284	6	0.998344	0.067144	-3.280621
1	3.206022	-1.245653	2.980564	1	1.011095	0.030798	-4.377296
6	-2.118204	-3.748889	-2.134770	1	-0.051555	0.094364	-2.982225
6	-2.312180	-4.613834	-1.056903	6	1.659930	1.391425	-2.856161
1	-3.166131	-5.284246	-1.039508	1	2.613589	1.549365	-3.371721
6	-1.395768	-4.615991	-0.001374	1	1.008364	2.217940	-3.155207
1	5.889111	-4.540605	0.513361				
1	3.509782	-0.967158	0.655464				
6	0.791097	-2.307041	3.753916				
1	1.513176	-3.108767	3.538259	8	6.656507	-2.470081	0.159900
1	-0.210219	-2.728546	3.663456	16	5.987943	-1.482933	1.014757
1	0.936684	-2.050685	4.814615	7	4.328780	-1.616046	0.695094
1	-1.235981	-2.251896	1.946739	8	6.242361	-1.456791	2.462296
1	-2.819468	-3.744870	-2.964600	6	6.344325	0.145597	0.377192
1	-1.534666	-5.288884	0.839703	6	6.308656	0.355093	-1.002852
1	4.143571	-5.636838	-0.874665	6	6.708588	1.163937	1.252987
1	5.568021	-2.187406	1.268998	1	6.035714	-0.457143	-1.666506
28	0.794351	0.178876	0.311743	6	6.637300	1.609302	-1.501828
15	1.896248	1.604621	-1.015011	6	7.029415	2.419621	0.735050
6	1.674095	3.416433	-0.799046	1	6.746368	0.962613	2.317476
6	2.719277	4.337568	-0.647862	1	6.619528	1.780162	-2.574606
6	0.346630	3.874202	-0.731333	6	6.995181	2.661706	-0.642423
6	2.442949	5.688266	-0.431274	1	7.312288	3.220603	1.411779
1	3.749056	4.001116	-0.699382	6	7.311217	4.025670	-1.200756
6	0.075015	5.226705	-0.526560	1	7.963642	3.955724	-2.076694
1	-0.476519	3.177859	-0.856543	1	7.802805	4.658565	-0.457806
6	1.122104	6.136486	-0.368478	1	6.394643	4.536470	-1.519146
1	3.262146	6.392663	-0.317820	6	3.496941	-0.844350	1.620766
1	-0.956567	5.564430	-0.487315	1	3.384201	-1.362152	2.584442
1	0.911388	7.188364	-0.199235	1	4.012321	0.097083	1.817392
6	3.689028	1.354270	-0.713047	6	2.448465	-1.888542	-1.481792
6	4.169388	1.649484	0.576641	6	2.543986	-3.007902	-0.433857
6	4.560928	0.741037	-1.621019	1	1.831626	-2.245287	-2.353865
6	5.475718	1.339304	0.942968	6	1.333953	-2.945807	0.514289
1	3.507053	2.122347	1.295297	6	1.137334	-1.652744	1.278439
6	5.868344	0.418424	-1.250735	1	1.373787	-3.757588	1.250962
1	4.226574	0.497139	-2.622502	1	0.416104	-3.113009	-0.055804
6	6.330216	0.713019	0.030273	8	0.252048	-1.560037	2.116215
1	5.824471	1.576637	1.943673	1	3.416693	-1.581799	-1.871541
1	6.522720	-0.069639	-1.966787	6	3.877779	-2.967254	0.347894
1	7.345329	0.457472	0.318244	1	4.663396	-3.402954	-0.269012
6	1.651730	-1.216973	-2.739711	1	3.777253	-3.595294	1.247756

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6	2.504566	-4.381044	-1.136437	1	-2.572442	2.761868	-3.334453
1	3.289698	-4.453778	-1.895697	1	-3.042180	1.295225	-4.234633
1	1.535657	-4.530735	-1.620852	6	-4.624181	-1.576108	-0.746565
1	2.650212	-5.195492	-0.416696	6	-5.383335	-2.480651	0.008223
6	2.102843	-0.499987	1.029683	6	-5.238345	-0.904258	-1.806882
6	2.159406	-0.112403	-0.431852	6	-6.729869	-2.687370	-0.277529
6	2.755248	1.016982	-0.872086	1	-4.919269	-3.019197	0.824392
6	2.978121	1.307984	-2.332822	6	-6.589629	-1.112760	-2.094128
1	2.388925	2.174166	-2.662172	1	-4.653838	-0.233041	-2.419998
1	2.711694	0.455680	-2.961795	6	-7.342387	-1.999434	-1.327660
1	4.030654	1.558561	-2.515651	1	-7.302523	-3.388772	0.321938
6	3.214265	2.126145	0.047151	1	-7.048119	-0.581501	-2.923115
1	2.830892	3.090039	-0.312261	1	-8.392904	-2.161691	-1.549659
1	4.306652	2.209214	0.063559	6	-2.429744	-2.646355	-0.226151
1	2.867293	2.005271	1.075070	6	-2.255258	-3.248897	1.022745
1	1.714560	0.333632	1.621431	6	-2.024292	-3.331432	-1.379531
28	0.784202	-0.878524	-1.492410	6	-1.710759	-4.532028	1.113703
6	-3.068276	-0.414128	0.893531	1	-2.552805	-2.725831	1.923832
6	-3.402195	1.041544	0.543386	6	-1.471154	-4.606935	-1.285826
6	-4.648126	0.393960	2.412857	1	-2.161640	-2.861314	-2.346863
1	-2.061823	-0.508445	1.305574	6	-1.322627	-5.216552	-0.036664
1	-3.946312	1.083318	-0.403534	1	-1.581715	-4.988397	2.090169
6	-6.156002	0.209397	2.317174	1	-1.165172	-5.129099	-2.187621
1	-6.467229	-0.659441	2.903118	1	-0.897060	-6.212742	0.036747
1	-6.667243	1.095981	2.701720	6	-1.604872	2.296889	1.809061
1	-6.440334	0.049282	1.275408	6	-2.071536	3.449083	2.451944
6	-4.146834	0.651289	3.827793	6	-0.719053	1.456588	2.487840
1	-4.569321	1.583630	4.211065	6	-1.656891	3.753409	3.747275
1	-4.443594	-0.170177	4.485694	1	-2.762888	4.109095	1.941796
1	-3.059031	0.736203	3.827601	6	-0.304274	1.760935	3.785411
8	-4.016714	-0.775211	1.878512	1	-0.362388	0.551206	2.022118
8	-4.256894	1.490356	1.574911	6	-0.770031	2.911153	4.420973
6	-2.117335	1.917254	0.419220	1	-2.029311	4.651609	4.231166
6	-3.159883	-1.316236	-0.378030	1	0.376819	1.084060	4.292918
8	-2.604006	-0.563796	-1.474590	1	-0.449002	3.150063	5.430625
8	-1.086550	1.095833	-0.181593	6	-2.328568	3.159759	-0.433979
15	-1.099985	0.139558	-1.536894	6	-1.219390	3.752400	-1.049370
7	-1.424698	1.041425	-2.915748	6	-3.588971	3.742879	-0.588474
6	-0.322084	1.403623	-3.790722	6	-1.373307	4.894681	-1.830424
1	-0.591178	1.206521	-4.836547	1	-0.243610	3.296894	-0.920924
1	-0.065568	2.468533	-3.695197	6	-3.741887	4.893017	-1.367467
1	0.556731	0.807407	-3.540854	1	-4.450068	3.308271	-0.091215
6	-2.688617	1.674535	-3.266420	6	-2.638158	5.467842	-1.995577
1	-3.445055	1.461159	-2.517198	1	-0.506864	5.340815	-2.310050

1	-4.726706	5.335727	-1.483010	6	3.252601	1.743347	-0.053016
1	-2.758840	6.358024	-2.605531	6	3.421656	2.058920	1.411662
(S)-TS3				1	2.977053	3.034196	1.649791
				1	2.943543	1.308068	2.044989
				1	4.485479	2.117601	1.672258
8	6.591024	-2.529013	-1.218727	6	3.943822	2.716889	-0.975388
16	6.091485	-1.164581	-1.417352	1	3.669300	3.746523	-0.718912
7	4.424119	-1.251474	-1.546885	1	5.032067	2.642300	-0.860419
8	6.575986	-0.314757	-2.510640	1	3.701127	2.558181	-2.026966
6	6.407342	-0.279115	0.106151	1	2.182848	1.093164	-2.557139
6	6.172035	-0.902867	1.333702	28	1.039719	0.353813	0.531797
6	6.930537	1.009735	0.050358	6	-3.066241	0.706338	-0.892841
1	5.815439	-1.925985	1.366633	6	-3.847486	-0.260370	0.001039
6	6.430049	-0.206958	2.510044	6	-5.199006	0.371231	-1.789442
6	7.194216	1.690137	1.238866	1	-2.242309	0.192424	-1.386203
1	7.141420	1.454868	-0.914821	1	-4.121821	0.225413	0.940478
1	6.247228	-0.688592	3.466562	6	-6.354012	1.307040	-1.454639
6	6.938108	1.100558	2.482505	1	-6.453239	2.074268	-2.226644
1	7.607515	2.693971	1.198410	1	-7.288162	0.741856	-1.393789
6	7.176788	1.858809	3.763248	1	-6.168710	1.800542	-0.498518
1	7.926375	2.643380	3.630133	6	-5.387047	-0.407261	-3.083116
1	6.252789	2.340889	4.105580	1	-6.276171	-1.039541	-3.014831
1	7.513519	1.194836	4.564595	1	-5.506000	0.281955	-3.923424
6	3.737291	-0.388797	-2.501381	1	-4.515709	-1.042102	-3.255280
1	3.509439	-0.947440	-3.421883	8	-3.988767	1.137982	-1.871371
1	4.421255	0.412645	-2.773858	8	-5.018838	-0.570293	-0.725053
6	2.560549	-1.028000	0.646120	6	-3.013451	-1.541767	0.315939
6	2.430777	-2.216722	-0.322049	6	-2.464089	1.872589	-0.049686
1	2.025508	-1.246072	1.579301	8	-2.065327	1.303104	1.217807
6	1.250489	-2.012721	-1.288050	8	-1.625299	-1.144063	0.471340
6	1.253110	-0.722298	-2.088557	15	-0.925754	0.100104	1.343194
1	1.191034	-2.840943	-2.007618	7	-1.147554	-0.135325	2.992706
1	0.314101	-2.034909	-0.723990	6	-2.408265	-0.031623	3.717895
8	0.355844	-0.481895	-2.884348	1	-2.707015	-1.003086	4.127333
1	3.596053	-0.825401	0.906944	1	-2.303870	0.683815	4.544324
6	3.749294	-2.466527	-1.097277	1	-3.196983	0.319063	3.058164
1	4.446373	-3.009048	-0.459616	6	-0.065760	-0.719315	3.769338
1	3.542278	-3.119868	-1.958661	1	0.873982	-0.631612	3.221070
6	2.145730	-3.501595	0.480289	1	0.043707	-0.181704	4.719635
1	2.922331	-3.674004	1.233085	1	-0.251489	-1.779680	3.995030
1	1.182343	-3.419421	0.993398	6	-3.536633	2.910041	0.266184
1	2.104461	-4.380661	-0.173615	6	-3.923614	3.823063	-0.723229
6	2.434220	0.233011	-1.929655	6	-4.184413	2.937921	1.503949
6	2.551845	0.668141	-0.487228	6	-4.949196	4.732917	-0.483603

1	-3.422805	3.811724	-1.683746	6	3.584264	-0.951321	-0.297687
6	-5.214143	3.851466	1.743909	6	3.537860	-2.295977	-0.684403
1	-3.871145	2.256596	2.283758	6	4.703208	-2.972008	-1.044518
6	-5.603582	4.747786	0.750552	6	5.931919	-2.313734	-1.025963
1	-5.239549	5.431479	-1.262649	6	5.989264	-0.970092	-0.652149
1	-5.706468	3.861542	2.711966	6	4.825092	-0.290883	-0.298129
1	-6.404280	5.457341	0.936518	6	2.095485	-0.108562	2.048774
6	-1.262100	2.531139	-0.717828	6	0.874740	-0.102590	2.738839
6	-0.986959	2.378715	-2.077972	6	3.295638	-0.191976	2.769805
6	-0.445402	3.366997	0.058475	6	2.535315	1.656175	-0.247697
6	0.089502	3.056292	-2.656543	6	2.850745	2.648865	0.683650
1	-1.607133	1.742382	-2.697357	6	2.614879	1.935934	-1.619639
6	0.624821	4.040141	-0.518958	1	4.879471	0.758427	-0.031062
1	-0.663775	3.482377	1.114721	1	-0.058640	-0.041073	2.188977
6	0.893173	3.889011	-1.882591	1	4.242958	-0.216250	2.242913
1	0.294661	2.923346	-3.714029	1	2.785412	2.436792	1.745428
1	1.251921	4.682353	0.092251	8	-4.583053	-2.517358	0.605973
1	1.726571	4.416720	-2.335201	16	-3.908908	-1.323452	0.081965
6	-3.058740	-2.483866	-0.889509	7	-2.492576	-1.827550	-0.754974
6	-4.042265	-3.475693	-0.980226	8	-4.609517	-0.375085	-0.788488
6	-2.175969	-2.312801	-1.960587	6	-3.282836	-0.410664	1.479298
6	-4.138882	-4.278273	-2.115438	6	-3.095546	-1.057251	2.699717
1	-4.739842	-3.618394	-0.163576	6	-3.056552	0.958627	1.340460
6	-2.271510	-3.117254	-3.096786	1	-3.318100	-2.113867	2.792829
1	-1.403806	-1.558712	-1.932316	6	-2.671159	-0.309425	3.797458
6	-3.253560	-4.103316	-3.180696	6	-2.620203	1.683767	2.443235
1	-4.909195	-5.042222	-2.166454	1	-3.243798	1.446002	0.393683
1	-1.570137	-2.958476	-3.910416	1	-2.545902	-0.799894	4.758745
1	-3.329651	-4.730363	-4.064204	6	-2.426381	1.065888	3.686510
6	-3.476834	-2.244356	1.583602	1	-2.431847	2.746216	2.332139
6	-2.584803	-3.087512	2.256637	6	-1.955412	1.875050	4.868099
6	-4.777793	-2.099297	2.073439	1	-2.038810	1.310818	5.800895
6	-2.976539	-3.751370	3.416233	1	-2.538059	2.795361	4.973623
1	-1.579225	-3.203636	1.868175	1	-0.905862	2.165792	4.744976
6	-5.172747	-2.768576	3.234735	1	2.355723	1.165938	-2.341092
1	-5.489643	-1.478050	1.539985	6	-2.365192	-1.349411	-2.136300
6	-4.273408	-3.589756	3.913072	1	-2.490399	-2.191162	-2.828862
1	-2.271990	-4.396684	3.932774	1	-3.166472	-0.640285	-2.346319
1	-6.185412	-2.645071	3.606841	6	0.203312	-2.580968	0.247155
1	-4.579741	-4.105458	4.818154	6	-0.620124	-3.563647	-0.606035
				1	1.142526	-3.034251	0.571895
TS3_{CF3}				6	-0.083660	-3.469937	-2.047562
				6	0.429493	-2.059676	-2.296644
15	2.061834	-0.047133	0.221401	1	-0.824343	-3.749501	-2.808126

1	0.778636	-4.130244	-2.195869	6	3.335422	-1.016840	0.738616
8	1.364778	-1.769138	-3.002669	6	4.519210	-1.741417	0.604539
1	-0.337332	-2.279790	1.155948	6	5.410918	-1.451179	-0.430633
6	-2.125314	-3.234144	-0.513776	6	5.123983	-0.415852	-1.320749
1	-2.454568	-3.484136	0.494114	6	3.946304	0.320115	-1.183610
1	-2.685615	-3.886806	-1.200107	6	1.955907	2.313304	1.195305
6	-0.471114	-5.014251	-0.104125	6	1.058986	3.370722	1.424380
1	-0.788941	-5.094323	0.940087	6	3.169316	2.292656	1.892955
1	0.575050	-5.330228	-0.161972	6	1.282932	1.789615	-1.568270
1	-1.069357	-5.717890	-0.695242	6	1.338746	3.174132	-1.767419
6	-1.020313	-0.673444	-2.371417	6	1.061013	0.948470	-2.669011
6	-0.670097	0.507917	-1.600776	1	3.732095	1.122426	-1.880340
6	-1.192234	1.734510	-1.551585	1	0.105594	3.390923	0.907901
6	-0.764152	2.767813	-0.542449	1	3.869597	1.480931	1.735731
6	0.861336	-0.184925	4.131029	1	1.539373	3.839804	-0.937322
6	2.058310	-0.262783	4.843696	8	-4.980938	-1.716423	0.122309
1	2.041867	-0.331997	5.927287	16	-3.584998	-1.499553	-0.285904
6	3.276098	-0.261921	4.161755	7	-2.563205	-1.332216	1.063107
6	3.246277	3.913879	0.244892	8	-2.933210	-2.467194	-1.178491
6	3.336369	4.186694	-1.119595	6	-3.467359	0.139881	-0.977171
1	3.644457	5.171405	-1.457599	6	-4.611740	0.935215	-1.025790
6	3.021967	3.194441	-2.051663	6	-2.237510	0.604919	-1.443409
1	6.838245	-2.840042	-1.309728	1	-5.550298	0.539600	-0.654754
1	2.590052	-2.809887	-0.718363	6	-4.516198	2.225183	-1.543092
6	-2.288500	2.206747	-2.475946	6	-2.163305	1.894718	-1.960274
1	-0.746251	-0.600140	-3.421632	1	-1.352561	-0.019447	-1.378479
1	3.483874	4.685087	0.971520	1	-5.401478	2.854266	-1.578286
1	3.082521	3.405917	-3.114799	6	-3.293790	2.720849	-2.015866
1	6.939898	-0.445399	-0.644009	1	-1.215252	2.269258	-2.321757
1	4.645967	-4.012596	-1.349228	6	-3.192505	4.110740	-2.592173
1	4.210263	-0.327335	4.711316	1	-3.646965	4.155021	-3.589176
1	-0.086589	-0.203391	4.654146	1	-2.148970	4.420990	-2.689281
28	0.244311	-0.867495	-0.697826	1	-3.714560	4.841834	-1.966659
9	0.111880	3.666456	-1.032602	1	1.042959	-0.122017	-2.494584
9	-1.837352	3.485138	-0.103176	6	-1.855774	-2.551714	1.488499
9	-0.204831	2.214926	0.556011	1	-2.229972	-2.867666	2.469721
9	-2.051631	3.462466	-2.916598	1	-2.065221	-3.350477	0.773475
9	-2.407411	1.416735	-3.567764	6	-1.172357	1.104885	1.932260
9	-3.503774	2.222057	-1.878252	6	-2.091168	0.345253	2.901991
				1	-0.552137	1.801518	2.500850
TS3 _{NCH3}				6	-1.133786	-0.524680	3.738497
				6	0.070263	-0.844080	2.860740
15	1.470116	0.953170	0.060669	1	-1.589693	-1.447083	4.119718
6	3.037116	0.015935	-0.162722	1	-0.753013	0.026766	4.604886

8	1.216928	-0.888931	3.253425	6	1.566354	-4.562372	0.780965
1	-1.737410	1.672474	1.180416	1	0.703636	-4.843828	1.410673
6	-3.130768	-0.488157	2.128757	1	2.207409	-5.446807	0.690136
1	-3.820167	0.213618	1.654483	1	2.123668	-3.776046	1.292701
1	-3.724452	-1.105357	2.818435				
6	-2.884416	1.292576	3.822022				
1	-3.516188	1.963070	3.229633	TS3 _{PPh3-CF3}			
1	-2.198279	1.909826	4.409558				
1	-3.531950	0.747232	4.520103	15	0.894275	-0.075201	0.011324
6	-0.352307	-2.292706	1.515867	6	2.619887	-0.703975	0.194492
6	0.272341	-2.003258	0.248578	6	2.849209	-2.078774	0.321191
6	0.802540	-2.765519	-0.723703	6	4.141224	-2.567297	0.503092
6	1.380773	4.393538	2.313459	6	5.218169	-1.683891	0.562309
6	2.594127	4.364518	3.004839	6	5.005048	-0.309662	0.432685
1	2.841707	5.156996	3.704640	6	3.714494	0.175685	0.246837
6	3.482756	3.311095	2.794804	6	0.467088	0.480150	1.714022
6	1.141711	3.707532	-3.044277	6	-0.880640	0.481683	2.095993
6	0.907126	2.866698	-4.132658	6	1.433171	0.949806	2.614604
1	0.753417	3.285656	-5.122514	6	1.203110	1.516840	-0.848453
6	0.879296	1.482405	-3.942116	6	0.709577	2.734724	-0.370110
1	6.325705	-2.026190	-0.540199	6	1.888400	1.483311	-2.073729
1	2.646637	-1.237609	1.546214	1	3.561968	1.242962	0.135369
1	0.179787	-2.907303	2.240954	1	-1.636249	0.123549	1.410543
1	1.182339	4.783581	-3.186202	1	2.482297	0.937497	2.344287
1	0.706716	0.819501	-4.784776	1	0.189527	2.775835	0.579912
1	5.815190	-0.179205	-2.124243	8	-5.492939	-2.201232	-0.148426
1	4.741123	-2.539142	1.307313	16	-4.479639	-1.500725	-0.947682
1	4.426313	3.278856	3.331281	7	-3.055769	-2.443340	-1.008116
1	0.679667	5.207189	2.473855	8	-4.764083	-1.076165	-2.323632
28	-0.141028	-0.269004	0.944005	6	-4.010871	-0.036511	-0.035537
7	1.038523	-2.242501	-2.027954	6	-4.557599	0.197501	1.226028
7	1.202668	-4.107129	-0.542091	6	-3.205969	0.914884	-0.660761
6	2.304745	-2.584543	-2.660995	1	-5.207005	-0.545380	1.674719
1	2.541241	-1.823633	-3.414864	6	-4.282186	1.405714	1.865024
1	3.099474	-2.583921	-1.915462	6	-2.936611	2.112542	-0.004661
1	2.295227	-3.564551	-3.166122	1	-2.800270	0.708707	-1.639538
6	-0.098797	-2.247704	-2.947109	1	-4.714331	1.601418	2.842857
1	-0.028078	-1.412762	-3.655351	6	-3.467378	2.377735	1.265506
1	-0.150627	-3.170592	-3.549017	1	-2.304908	2.850782	-0.489117
1	-1.026669	-2.155613	-2.384126	6	-3.150915	3.660722	1.990066
6	0.590368	-5.133545	-1.374403	1	-4.063734	4.155758	2.336858
1	0.482846	-4.777541	-2.397779	1	-2.611390	4.359129	1.345306
1	1.226361	-6.025432	-1.387781	1	-2.531052	3.471516	2.874125
1	-0.408118	-5.426724	-1.010423	1	2.262360	0.539749	-2.457657

6	-2.631337	-2.878821	-2.345589	1	-2.048073	-1.478753	-5.001669
1	-2.725956	-3.968391	-2.417915	6	-0.741922	2.048318	5.525948
1	-3.303164	-2.446208	-3.088401	6	1.664387	5.086496	-3.191656
6	-0.675408	-2.594764	0.805946	6	6.620935	-2.209765	0.698768
6	-1.504013	-3.841940	0.464804	9	0.275983	2.247294	6.385607
1	0.231801	-2.888938	1.345907	9	-1.330864	3.254487	5.315123
6	-0.718080	-4.546710	-0.654873	9	-1.659920	1.274546	6.143459
6	0.043433	-3.470571	-1.420579	9	0.740722	5.080073	-4.180437
1	-1.335067	-5.150052	-1.330781	9	1.480911	6.219598	-2.481505
1	0.040367	-5.218780	-0.238446	9	2.874559	5.166729	-3.786822
8	1.155089	-3.593845	-1.877830	9	7.411328	-1.349795	1.378863
1	-1.233080	-1.926623	1.468461	9	7.195170	-2.400833	-0.509996
6	-2.943080	-3.447268	0.064752	9	6.653178	-3.393893	1.345773
1	-3.424553	-3.029629	0.950636				
1	-3.510216	-4.348484	-0.210318	TS3_{PPh3}-OCH₃			
6	-1.646406	-4.784523	1.676502				
1	-2.137005	-4.270759	2.509591	15	1.177521	-0.108756	-0.006983
1	-0.660316	-5.112215	2.019083	6	2.731557	-1.086371	0.006493
1	-2.235511	-5.677798	1.436925	6	2.692550	-2.477705	0.195457
6	-1.210241	-2.418969	-2.637779	6	3.861217	-3.220324	0.272899
6	-0.944754	-0.999370	-2.646156	6	5.108224	-2.589669	0.164143
6	-1.332506	-0.055505	-3.511209	6	5.167737	-1.203598	-0.027820
6	-1.137838	1.429354	-3.343866	6	3.984604	-0.468787	-0.105889
6	-1.255548	0.951906	3.350181	6	1.079817	0.562924	1.697706
6	-0.289337	1.446259	4.226234	6	-0.154788	1.029132	2.179568
6	1.057866	1.440643	3.863375	6	2.197013	0.661235	2.532721
6	0.871379	3.901363	-1.118687	6	1.680332	1.358996	-0.982925
6	1.548354	3.856316	-2.335973	6	1.466548	2.668981	-0.529716
6	2.071388	2.647242	-2.807266	6	2.233530	1.174666	-2.255879
1	2.023376	-2.769828	0.254293	1	4.046446	0.602618	-0.260960
6	-2.121354	-0.416898	-4.756252	1	-1.036987	0.950097	1.558185
1	-0.702818	-2.998886	-3.408122	1	3.159570	0.296210	2.193429
1	0.481153	4.844694	-0.753986	1	1.051829	2.837402	0.457619
1	2.605319	2.621324	-3.750918	8	-5.480365	-0.699192	0.801084
1	5.844635	0.374779	0.481524	16	-4.488942	-0.354366	-0.226720
1	4.310299	-3.633947	0.596147	7	-3.326742	-1.596603	-0.327911
1	1.805301	1.815623	4.552852	8	-4.906655	-0.045855	-1.600370
1	-2.298960	0.940476	3.639842	6	-3.580076	1.061855	0.373390
28	-0.403734	-1.591044	-0.897765	6	-3.853587	1.576400	1.639238
1	-0.757928	1.690039	-2.360303	6	-2.686952	1.698077	-0.488638
1	-0.449914	1.832632	-4.096221	1	-4.575901	1.078195	2.275478
1	-2.094485	1.947686	-3.494377	6	-3.206278	2.743767	2.044492
1	-1.767809	0.158047	-5.620616	6	-2.047340	2.858267	-0.066353
1	-3.182467	-0.173101	-4.616393	1	-2.494690	1.276781	-1.463837

1	-3.417072	3.156656	3.027242	1	2.988152	1.270216	4.430859
6	-2.289958	3.393827	1.206829	1	-1.214844	1.946831	3.816077
1	-1.341799	3.346635	-0.730878	28	-0.516464	-1.386791	-0.632213
6	-1.533460	4.604214	1.687108	1	-0.292367	1.693880	-2.461189
1	-2.146934	5.231172	2.340615	1	-0.173458	1.563048	-4.220143
1	-1.182984	5.215504	0.851145	1	-1.650492	2.180916	-3.494339
1	-0.654654	4.291083	2.264920	1	-2.088987	0.146111	-5.364419
1	2.393507	0.168452	-2.630754	1	-3.386806	0.302826	-4.177429
6	-3.174116	-2.238417	-1.639197	1	-2.669355	-1.285081	-4.495226
1	-3.515938	-3.278366	-1.571910	8	0.659224	2.246993	5.492671
1	-3.823592	-1.732314	-2.354857	8	2.597683	4.690243	-3.318819
6	-0.787468	-2.107764	1.202346	8	6.195439	-3.403019	0.251632
6	-1.907819	-3.154717	1.127262	6	3.121067	4.542228	-4.629706
1	0.100033	-2.541938	1.677172	1	2.433861	3.981706	-5.275713
6	-1.461971	-4.136162	0.030334	1	3.241972	5.552624	-5.021851
6	-0.598116	-3.355588	-0.954288	1	4.095889	4.038520	-4.620607
1	-2.285401	-4.645694	-0.484302	6	1.766032	2.351597	6.374652
1	-0.817587	-4.919751	0.444148	1	1.383715	2.815425	7.284638
8	0.370743	-3.799490	-1.527031	1	2.181877	1.365726	6.617193
1	-1.089853	-1.251763	1.812461	1	2.559486	2.981370	5.952750
6	-3.271890	-2.485294	0.845801	6	7.480709	-2.814906	0.131700
1	-3.525855	-1.882347	1.718927	1	7.664660	-2.081293	0.926920
1	-4.047862	-3.260354	0.757327	1	8.196426	-3.632603	0.224101
6	-2.079164	-3.905528	2.463203	1	7.611473	-2.327315	-0.842576
1	-2.319716	-3.205858	3.270348				
1	-1.149772	-4.417705	2.729923	TS4			
1	-2.878167	-4.655598	2.416778				
6	-1.736131	-2.159453	-2.134157	15	1.003706	1.191652	0.060654
6	-1.151637	-0.855504	-2.363562	6	0.698807	3.013819	0.081744
6	-1.425110	0.053875	-3.305310	6	1.088044	3.856164	-0.968000
6	-0.846153	1.444168	-3.361719	6	0.730607	5.205405	-0.968419
6	-0.262150	1.589305	3.443985	6	-0.036189	5.730493	0.071253
6	0.867053	1.686819	4.269755	6	-0.440787	4.895632	1.115773
6	2.102387	1.215718	3.810085	6	-0.078328	3.550403	1.119296
6	1.776350	3.759052	-1.334026	6	2.435015	1.017891	-1.082958
6	2.327938	3.561701	-2.607464	6	2.377610	-0.007397	-2.035702
6	2.569742	2.258430	-3.063339	6	3.560359	1.858214	-1.064098
1	1.741000	-2.983420	0.259108	6	1.727295	0.923020	1.743782
6	-2.445925	-0.220473	-4.393885	6	3.096283	0.893006	2.041894
1	-1.491289	-2.915259	-2.879926	6	0.811125	0.641887	2.769045
1	1.609218	4.775790	-0.994307	1	-0.403447	2.915167	1.935604
1	2.996671	2.078561	-4.042100	1	1.510830	-0.661490	-2.051963
1	6.117273	-0.691023	-0.120794	1	3.609593	2.676201	-0.352932
1	3.833300	-4.296408	0.405254	1	3.828114	1.077329	1.264905

8	-1.410352	-4.247235	1.342080	1	-1.700299	3.860005	-1.542033
16	-0.766129	-2.927738	1.397069	6	3.416149	-0.192972	-2.948775
7	-1.740871	-1.785314	0.505338	6	4.533105	0.642879	-2.915125
8	-0.465350	-2.294241	2.684154	1	5.341598	0.502021	-3.626405
6	0.741392	-3.008211	0.449965	6	4.603921	1.668722	-1.969470
6	0.847566	-3.870262	-0.640889	6	3.533047	0.594453	3.333647
6	1.830461	-2.251963	0.884323	6	2.610769	0.331601	4.347764
1	0.013330	-4.501968	-0.923078	1	2.954418	0.091407	5.349238
6	2.058374	-3.935393	-1.330290	6	1.245081	0.359011	4.062293
6	3.031113	-2.339689	0.191611	1	-0.318417	6.778937	0.068654
1	1.731181	-1.620034	1.755061	1	1.662987	3.460578	-1.797196
1	2.151202	-4.602845	-2.182217	6	-3.753194	3.072862	0.036257
6	3.164469	-3.177606	-0.925135	1	-3.263859	3.952898	0.474153
1	3.874490	-1.740455	0.520584	1	-4.330112	2.571365	0.812852
6	4.482994	-3.273469	-1.647505	1	-4.470376	3.452926	-0.704327
1	4.382639	-3.803459	-2.598322	1	-3.578203	0.846318	1.570871
1	5.220405	-3.812521	-1.041409	1	4.597927	0.563253	3.546070
1	4.888055	-2.277750	-1.849696	1	0.518648	0.126964	4.834459
1	-0.246556	0.600389	2.533214	1	-1.039369	5.292578	1.930458
6	-2.637706	-1.042206	1.420297	1	1.045496	5.842665	-1.789694
1	-3.417624	-1.704778	1.823913	1	5.467135	2.327138	-1.943729
1	-2.025860	-0.707673	2.254941	1	3.351842	-0.989783	-3.683459
6	-2.117575	-0.324170	-1.840848	28	-0.746286	0.068310	-0.479042
6	-3.066351	-1.502840	-1.629164	TS5			
1	-2.485274	0.358109	-2.605463				
6	-4.474147	-1.032862	-1.214910				
6	-4.588659	-0.194381	0.049767	15	-0.942705	-1.698512	0.728680
1	-5.144398	-1.893127	-1.096676	6	-2.147937	-2.936198	0.093253
1	-4.904146	-0.429928	-2.023973	6	-3.110388	-2.493718	-0.818659
8	-5.673823	0.187240	0.448242	6	-4.108890	-3.353785	-1.275357
1	-1.125858	-0.708465	-2.207474	6	-4.154308	-4.673223	-0.826482
6	-2.442625	-2.474087	-0.604609	6	-3.204249	-5.123889	0.093318
1	-1.688541	-3.064119	-1.127805	6	-2.211383	-4.260531	0.554926
1	-3.194180	-3.170848	-0.213489	6	-1.733361	-1.226628	2.328009
6	-3.222479	-2.290674	-2.947128	6	-2.915991	-1.813113	2.803633
1	-2.247387	-2.614022	-3.325676	6	-1.171599	-0.159486	3.043581
1	-3.693017	-1.666959	-3.713098	6	0.448839	-2.780641	1.276611
1	-3.847996	-3.180501	-2.807239	6	1.177055	-2.504985	2.443311
6	-3.293184	0.182375	0.750849	6	0.894427	-3.817119	0.437756
6	-2.427729	0.924067	-0.264543	1	-1.486879	-4.616107	1.278955
6	-2.725522	2.195095	-0.638364	1	-3.374202	-2.629434	2.258808
6	-2.050451	2.857960	-1.808666	1	-0.270346	0.313144	2.673459
1	-2.760989	2.982360	-2.640278	1	0.853671	-1.714960	3.108526
1	-1.195147	2.278898	-2.160048	8	1.863595	0.465217	1.809567

16	2.622718	1.190265	0.785249	6	-3.524544	-1.333185	3.962967
7	2.293459	0.456995	-0.687843	6	-2.960042	-0.266220	4.665993
8	2.422352	2.634319	0.595500	1	-3.443127	0.114241	5.561204
6	4.352301	0.898474	1.100058	6	-1.777446	0.313512	4.207469
6	4.739342	-0.291423	1.721555	6	2.328543	-3.230758	2.750253
6	5.297797	1.811919	0.632009	6	2.774251	-4.243969	1.899060
1	3.987957	-0.987046	2.078419	1	3.672953	-4.804867	2.137386
6	6.096639	-0.558270	1.874623	6	2.046703	-4.539638	0.744907
6	6.650671	1.526859	0.798526	1	-4.926782	-5.347082	-1.185587
1	4.970697	2.733511	0.164118	1	-3.077470	-1.471391	-1.166019
1	6.406780	-1.481791	2.355399	6	-0.016318	-3.368458	-3.492655
6	7.070196	0.342041	1.418788	1	-0.768473	-4.116333	-3.202289
1	7.393667	2.235013	0.442826	1	0.957102	-3.723992	-3.153979
6	8.536406	0.053773	1.618864	1	0.007029	-3.374162	-4.593380
1	8.870744	0.401963	2.603735	1	1.828516	-2.751151	-1.587791
1	9.149284	0.558793	0.867447	1	2.874348	-3.004691	3.662181
1	8.742560	-1.018922	1.565310	1	2.376619	-5.331274	0.078672
1	0.337451	-4.054996	-0.461734	1	-3.238994	-6.147168	0.455946
6	2.528193	-0.992225	-0.702435	1	-4.847557	-2.985295	-1.980121
1	3.604131	-1.210825	-0.780931	1	-1.341369	1.158710	4.729141
1	2.166434	-1.391163	0.240801	1	-4.445148	-1.790895	4.314287
6	0.373208	0.649213	-2.661291	28	-0.394265	-0.086922	-0.773908
6	1.823400	0.871624	-3.119925	15	-1.689216	1.710016	-0.094163
1	-0.280459	0.556315	-3.526305	6	-1.794980	2.610767	1.519626
6	2.386279	-0.307246	-3.934225	6	-2.988040	3.137458	2.031032
6	2.611366	-1.570612	-3.132611	6	-0.594550	2.873464	2.192528
1	3.333011	-0.042785	-4.417274	6	-2.985653	3.869508	3.217983
1	1.680480	-0.551983	-4.738154	1	-3.922893	2.976673	1.506298
8	3.398379	-2.431384	-3.484292	6	-0.590551	3.623365	3.367775
1	0.089938	1.570910	-2.152879	1	0.338830	2.489668	1.804098
6	2.713588	1.193144	-1.888889	6	-1.787819	4.112714	3.892259
1	2.617410	2.252188	-1.655630	1	-3.920592	4.259853	3.609770
1	3.771907	0.988717	-2.118358	1	0.350323	3.816470	3.874677
6	1.862329	2.113864	-4.034602	1	-1.787709	4.687009	4.814131
1	1.395686	2.973764	-3.546337	6	-1.548999	3.225385	-1.146853
1	1.321697	1.919150	-4.966107	6	-2.617356	3.878622	-1.772363
1	2.894274	2.378688	-4.297145	6	-0.262196	3.781067	-1.246358
6	1.793019	-1.695845	-1.854563	6	-2.400637	5.046530	-2.506158
6	0.353457	-1.251014	-2.110039	1	-3.623918	3.487316	-1.679268
6	-0.404633	-2.006256	-2.964442	6	-0.050951	4.955079	-1.968495
6	-1.714763	-1.520804	-3.526837	1	0.570920	3.311715	-0.731282
1	-1.614352	-1.296937	-4.602024	6	-1.117810	5.585222	-2.611355
1	-2.072927	-0.622973	-3.023325	1	-3.239879	5.541357	-2.986615
1	-2.496715	-2.284305	-3.443767	1	0.948816	5.375646	-2.027309

1	-0.952870	6.494925	-3.181002	6	-2.175960	3.328748	-1.168396
6	-3.387541	1.080696	-0.381150	1	-1.545857	2.226064	-2.906993
6	-3.871629	0.941432	-1.693586	6	-1.295313	4.517278	-1.450629
6	-4.136609	0.528308	0.670411	1	-1.690085	5.425847	-0.987455
6	-5.086816	0.303954	-1.941973	1	-1.191562	4.693789	-2.524769
1	-3.292434	1.327594	-2.525220	1	-0.287314	4.348691	-1.055488
6	-5.344989	-0.119164	0.417658	6	-2.962704	-1.413529	1.770220
1	-3.771089	0.588706	1.687448	1	-3.562795	-0.649086	2.268954
6	-5.830502	-0.226535	-0.885838	1	-3.181158	-2.358669	2.280413
1	-5.445512	0.213733	-2.963086	6	-0.893474	-2.920225	0.965362
1	-5.900249	-0.548440	1.246040	6	-1.694866	-3.227966	-0.295588
1	-6.772559	-0.730290	-1.079347	1	0.111364	-3.351588	0.955711
TS6				6	-0.657866	-3.321750	-1.416911
				6	0.217919	-2.060057	-1.325715
				1	-1.096760	-3.395950	-2.417738
				1	-0.019728	-4.201442	-1.262693
15	1.958127	-0.043499	0.034031	8	0.725782	-1.606283	-2.339325
6	3.183931	-1.157999	-0.767401	1	-1.380560	-3.296930	1.859743
6	3.997375	-0.768419	-1.833927	6	-2.579537	-2.018094	-0.668312
6	4.927511	-1.662749	-2.369028	1	-3.208916	-2.273676	-1.522878
6	5.054006	-2.946180	-1.840033	1	-1.899621	-1.207838	-0.981593
6	4.245970	-3.337920	-0.769153	6	-2.533202	-4.502727	-0.145142
6	3.315214	-2.449328	-0.238282	1	-3.293178	-4.375218	0.632231
6	2.888690	0.369227	1.570013	1	-1.900315	-5.353257	0.128681
6	4.269996	0.621405	1.507306	1	-3.050192	-4.747223	-1.078546
6	2.250902	0.390080	2.815618	6	-1.481252	-1.094092	1.974155
6	1.419522	1.451615	-2.254120	6	-0.857961	0.121214	1.629822
6	2.037965	1.480045	-0.993550	6	-0.967884	1.382475	2.061497
6	2.673553	2.653377	-0.567035	6	-1.917956	1.762969	3.177678
1	3.898614	0.224805	-2.256787	1	-1.353188	2.170361	4.028092
1	4.783060	0.577981	0.552298	1	-2.506133	0.917355	3.539369
1	0.939969	0.536803	-2.584424	1	-2.610100	2.551353	2.860069
1	3.142339	2.693360	0.409191	6	2.696648	3.780283	-1.390270
8	-5.430903	-0.086603	1.050173	6	2.093460	3.743826	-2.647792
16	-4.612022	-0.407307	-0.122928	1	2.115932	4.620200	-3.288579
7	-3.460824	-1.529400	0.391781	6	1.457323	2.576709	-3.076242
8	-5.194651	-0.963615	-1.345606	6	2.974131	0.679372	3.974603
6	-3.710349	1.067592	-0.571214	6	4.340462	0.946027	3.901839
6	-3.757426	2.173472	0.274692	6	4.987823	0.915715	2.663944
6	-2.936702	1.089129	-1.735442	1	2.677940	-2.757080	0.586112
1	-4.387618	2.141558	1.155238	1	4.902050	1.169854	4.803936
6	-3.003799	3.300824	-0.039505	1	1.186492	0.194872	2.866379
6	-2.164399	2.212188	-2.015542	1	5.775925	-3.640261	-2.259609
1	-2.955051	0.250779	-2.421000	6	-0.113695	2.520362	1.569183
1	-3.048127	4.170414	0.610206				

1	-0.686754	3.452609	1.540609	1	-2.026030	-0.223354	4.084007
1	0.268972	2.330737	0.569805	6	-1.856455	-2.890438	3.536489
1	0.740676	2.689434	2.238611	1	-2.318578	-3.871674	3.398719
1	-1.110950	-1.548077	2.894791	1	-1.841847	-2.662392	4.606245
1	4.339015	-4.336526	-0.352492	1	-0.817745	-2.961660	3.195929
1	5.549495	-1.354191	-3.204068	6	-2.685432	1.337128	-1.885587
1	6.053835	1.112610	2.600724	1	-3.401949	0.534826	-2.063735
1	2.465882	0.694051	4.934230	1	-2.772521	2.022954	-2.734464
1	3.189137	4.685245	-1.047150	6	-0.367359	2.725424	-1.610247
1	0.988769	2.540465	-4.055504	6	-1.056882	3.561630	-0.541613
28	0.025449	-1.059371	0.358005	1	0.687405	2.977561	-1.747361
TS6_{CF3}				6	0.021285	3.828299	0.511966
				6	0.620943	2.463883	0.863799
				1	-0.353152	4.312413	1.419779
				1	0.814017	4.457882	0.089357
15	2.247052	0.112096	0.063867	8	0.996528	2.207878	1.990098
6	3.492114	1.402078	0.471529	1	-0.842506	2.827728	-2.581125
6	4.272393	1.375766	1.629280	6	-2.128345	2.715141	0.179669
6	5.183528	2.404228	1.883422	1	-2.678467	3.346817	0.879738
6	5.323771	3.458949	0.983244	1	-1.597965	1.947922	0.771692
6	4.550743	3.485092	-0.181368	6	-1.661227	4.845873	-1.121690
6	3.639210	2.464026	-0.433506	1	-2.462977	4.605721	-1.826501
6	3.038710	-0.654718	-1.405464	1	-0.900892	5.430985	-1.649059
6	4.433578	-0.818471	-1.445339	1	-2.088973	5.471388	-0.331995
6	2.274262	-1.060123	-2.505601	6	-1.268957	0.754127	-1.922320
6	1.829479	-0.794967	2.658105	6	-0.813936	-0.370725	-1.205638
6	2.404147	-1.110802	1.416343	6	-1.123644	-1.668446	-1.204727
6	3.008340	-2.358726	1.230204	6	-2.080820	-2.296637	-2.187988
1	4.162648	0.562417	2.337215	6	3.039632	-3.282664	2.275591
1	5.038519	-0.491398	-0.606104	6	2.472014	-2.967052	3.509565
1	1.353144	0.169721	2.792704	1	2.494649	-3.689584	4.319916
1	3.437069	-2.618858	0.269925	6	1.871580	-1.719407	3.699047
8	-5.308217	0.817456	-0.841222	6	2.888842	-1.626943	-3.622632
16	-4.449134	1.447984	0.163829	6	4.272657	-1.795243	-3.650703
7	-3.111768	2.067102	-0.681898	6	5.044380	-1.391065	-2.558506
8	-4.919219	2.543447	1.013547	1	3.038383	2.485459	-1.338492
6	-3.794963	0.170285	1.220986	1	4.750293	-2.236825	-4.520097
6	-3.869718	-1.157458	0.803805	1	1.198765	-0.949214	-2.478958
6	-3.145894	0.515003	2.410261	1	6.031032	4.257651	1.184781
1	-4.388481	-1.404283	-0.112839	6	-0.423662	-2.653213	-0.305483
6	-3.270117	-2.146079	1.577928	1	-0.848648	0.804444	-2.925707
6	-2.539367	-0.486252	3.163518	1	4.658699	4.301180	-0.889715
1	-3.136618	1.544926	2.747025	1	5.781150	2.378909	2.789684
1	-3.309251	-3.176939	1.243095	1	6.122786	-1.516225	-2.576297
6	-2.580412	-1.826364	2.754427				

1	2.283135	-1.939573	-4.467711	6	3.826573	-3.844537	-2.844537
1	3.503080	-4.252244	2.120433	1	4.499346	-4.620510	-2.469483
1	1.427263	-1.468479	4.657663	1	4.001724	-3.727158	-3.917714
28	0.272647	1.038904	-0.416557	1	2.799489	-4.209210	-2.719022
9	0.786612	-3.031034	-0.791818	6	2.433922	1.566179	1.930246
9	-0.206929	-2.141333	0.920700	1	3.036885	0.742145	2.317468
9	-1.140881	-3.789412	-0.141328	1	2.590942	2.414687	2.607797
9	-1.468417	-3.292705	-2.871899	6	0.309924	3.035342	1.164454
9	-3.179913	-2.842222	-1.615766	6	1.104136	3.506456	-0.049401
9	-2.524484	-1.405906	-3.104790	1	-0.717211	3.409113	1.185567
TS6 _{NCH3}				6	0.090876	3.644898	-1.184435
				6	-0.782159	2.373955	-1.217326
				1	0.551704	3.799132	-2.166762
15	-2.296288	-0.000690	-0.118238	1	-0.567226	4.502417	-0.991851
6	-3.660002	1.100804	-0.683241	8	-1.359281	2.084821	-2.255441
6	-4.489693	0.809460	-1.768921	1	0.772416	3.348670	2.096231
6	-5.526249	1.679744	-2.113570	6	2.089278	2.395342	-0.475041
6	-5.744187	2.841384	-1.374175	1	2.735031	2.776974	-1.268026
6	-4.920593	3.134014	-0.283901	1	1.506957	1.551307	-0.882818
6	-3.883683	2.269673	0.056772	6	1.859284	4.810798	0.235377
6	-3.138836	-0.808822	1.309846	1	2.616268	4.654939	1.010336
6	-4.480915	-1.209173	1.193317	1	1.170347	5.590334	0.576852
6	-2.472936	-1.021375	2.520730	1	2.372027	5.174818	-0.660879
6	-1.748752	-0.984985	-2.669866	6	0.963768	1.152900	2.003512
6	-2.248770	-1.314097	-1.399664	6	0.469079	-0.031301	1.439093
6	-2.655144	-2.629089	-1.143167	6	0.698638	-1.350254	1.572965
1	-4.320645	-0.086989	-2.354739	6	-2.558612	-3.603194	-2.138496
1	-5.019882	-1.028821	0.269280	6	-2.061047	-3.272918	-3.399558
1	-1.448571	0.038066	-2.868545	1	-1.987938	-4.031862	-4.172942
1	-3.037247	-2.898273	-0.166356	6	-1.661583	-1.960538	-3.661935
8	5.179985	1.098298	1.432730	6	-3.122904	-1.643626	3.588244
16	4.485477	1.407760	0.178532	6	-4.448844	-2.054273	3.459063
7	2.955947	1.923896	0.601074	6	-5.127579	-1.832661	2.258008
8	5.013656	2.381685	-0.779851	1	-3.232503	2.503735	0.894445
6	4.286739	-0.132117	-0.712769	1	-4.955542	-2.537087	4.289473
6	4.648781	-1.328424	-0.096619	1	-1.443239	-0.702264	2.609220
6	3.806635	-0.121066	-2.025256	1	-6.549057	3.517831	-1.645736
1	5.052608	-1.305845	0.908261	1	0.526021	1.473427	2.951735
6	4.518361	-2.523959	-0.800424	1	-5.083888	4.037879	0.295759
6	3.668922	-1.325318	-2.708431	1	-6.159853	1.449348	-2.965062
1	3.573988	0.817671	-2.513815	1	-6.163867	-2.139745	2.152552
1	4.811987	-3.456921	-0.327164	1	-2.590014	-1.803823	4.521207
6	4.018752	-2.543416	-2.108440	1	-2.874029	-4.620480	-1.925425
1	3.294671	-1.320341	-3.728219	1	-1.278439	-1.693516	-4.642495

28	-0.495728	1.197725	0.320101	6	-4.461602	-0.810721	0.658733
7	0.225514	-2.288468	0.632746	6	-4.520608	-1.062291	-1.755235
7	1.334304	-1.914720	2.701899	1	-4.170231	-1.189834	1.631211
6	-0.168002	-3.609223	1.090289	6	-5.188462	0.368427	0.546156
1	-0.670519	-3.531037	2.055041	6	-5.257599	0.117118	-1.848551
1	-0.867305	-4.032351	0.362512	1	-4.258969	-1.636849	-2.636522
1	0.672356	-4.316318	1.193240	1	-5.449294	0.923363	1.442500
6	0.807230	-2.269311	-0.701787	6	-5.582150	0.859770	-0.708275
1	0.097853	-2.670050	-1.428293	1	-5.570229	0.475250	-2.825080
1	1.046706	-1.243539	-0.977376	6	-6.292714	2.182288	-0.821008
1	1.730076	-2.867553	-0.753618	1	-5.560132	2.995578	-0.782925
6	1.296624	-1.200775	3.960259	1	-6.994815	2.332834	0.004261
1	1.504203	-1.904291	4.774342	1	-6.842524	2.265271	-1.762132
1	2.032251	-0.382589	4.036463	6	-0.986596	-1.408224	-1.151555
1	0.302046	-0.777799	4.114592	1	-0.152919	-1.963612	-1.596315
6	2.554053	-2.681406	2.488737	1	-1.739831	-1.322003	-1.941165
1	2.638410	-3.482486	3.232862	6	-1.043037	-0.425343	2.016006
1	2.542934	-3.126540	1.494446	6	-0.684671	-1.890462	2.306884
1	3.453065	-2.049142	2.561643	1	-0.903250	0.228240	2.875848
TS7 _{CF3}				6	0.709853	-1.919992	2.965066
				6	1.525430	-0.695527	2.503831
				1	1.268620	-2.829691	2.705615
				1	0.647022	-1.888813	4.058710
15	2.583070	-0.026068	-0.300945	1	0.647022	-1.888813	4.058710
6	4.240220	-0.036535	0.460954	8	2.414060	-0.234413	3.180826
6	5.276556	-0.867104	0.014842	1	-2.081417	-0.364001	1.702598
6	6.542035	-0.776331	0.595097	6	-0.671029	-2.703910	0.980376
6	6.778671	0.143580	1.617269	1	-0.920258	-3.747851	1.186161
6	5.748027	0.974080	2.061878	1	0.332967	-2.689166	0.544392
6	4.481099	0.885264	1.490296	6	-1.731676	-2.472750	3.277191
6	2.676121	1.420994	-1.420096	1	-2.714481	-2.537712	2.808390
6	3.728986	1.544510	-2.340488	1	-1.802313	-1.855972	4.179020
6	1.703054	2.425170	-1.347944	1	-1.452396	-3.488094	3.579484
6	2.642227	-2.760403	-0.781616	6	-0.551177	-0.002266	-0.804742
6	2.528463	-1.495813	-1.383675	6	-0.902606	0.746595	0.302977
6	2.217478	-1.412586	-2.746109	6	-1.344368	2.011517	0.519971
1	5.098607	-1.580917	-0.782127	6	-2.196667	2.708090	-0.486717
1	4.502634	0.784001	-2.382612	6	2.020000	-2.576044	-3.493075
1	2.881005	-2.833472	0.275606	6	2.132939	-3.828218	-2.889308
1	2.120153	-0.442483	-3.220367	1	1.970163	-4.730108	-3.470579
8	-3.361158	-3.714131	0.810953	6	2.451339	-3.918428	-1.531708
16	-3.032664	-2.925692	-0.381302	6	1.760060	3.524185	-2.206100
7	-1.570114	-2.168906	-0.048710	6	2.796173	3.631112	-3.132778
8	-2.996897	-3.559370	-1.705853	6	3.783464	2.642600	-3.195488
6	-4.112185	-1.507934	-0.500190	1	3.674615	1.509997	1.855295

1	2.841697	4.484592	-3.802444	6	-4.798581	-1.162122	-1.632101
1	0.903736	2.359107	-0.621729	1	-4.339095	-0.812440	1.724070
1	7.763855	0.211713	2.068728	6	-5.658055	0.393877	0.519317
6	-0.981177	2.782276	1.744777	6	-5.730388	-0.142121	-1.828836
1	-0.212035	0.565979	-1.668337	1	-4.458704	-1.785831	-2.451053
1	5.926453	1.684304	2.863012	1	-5.994962	0.995638	1.358718
1	7.341847	-1.422412	0.245851	6	-6.165661	0.653750	-0.763790
1	4.597558	2.730787	-3.908514	1	-6.122444	0.038378	-2.825693
1	0.987889	4.283888	-2.144057	6	-7.132502	1.788472	-0.986428
1	1.771955	-2.500915	-4.547300	1	-7.670965	1.676862	-1.931055
1	2.541203	-4.890055	-1.056052	1	-6.601714	2.747860	-1.018201
28	0.737005	-0.069950	0.878701	1	-7.867277	1.851826	-0.178187
9	-1.070768	4.114781	1.546865	6	-1.167653	-1.029787	-0.988068
9	-1.764981	2.496524	2.819886	1	-0.492053	-1.705357	-1.523632
9	0.296705	2.521722	2.141996	1	-2.015060	-0.844960	-1.657677
9	-1.525542	3.695320	-1.149140	6	-1.083296	0.185443	2.120908
9	-2.668551	1.870228	-1.433012	6	-0.767353	-1.266597	2.523057
9	-3.274299	3.313116	0.082366	1	-0.915745	0.889511	2.935607
TS7 _{NCH3}				6	0.619544	-1.280816	3.207376
				6	1.423580	-0.070331	2.679395
				1	1.181250	-2.196100	2.973917
15	2.523873	-0.132207	-0.276298	1	0.539037	-1.220592	4.299304
6	4.173097	-0.495693	0.438487	8	2.204580	0.529853	3.394760
6	5.047571	-1.443502	-0.112639	1	-2.121222	0.240239	1.811905
6	6.320471	-1.622439	0.429624	6	-0.757232	-2.154552	1.243781
6	6.731569	-0.854657	1.519958	1	-0.970617	-3.191366	1.515300
6	5.864606	0.091142	2.070246	1	0.234857	-2.137349	0.783073
6	4.590050	0.272842	1.535931	6	-1.847083	-1.762731	3.502047
6	2.903947	1.304423	-1.359568	1	-2.824076	-1.822884	3.019361
6	4.023854	1.292064	-2.204763	1	-1.915422	-1.093647	4.366424
6	2.075353	2.433539	-1.335828	1	-1.608230	-2.767790	3.866151
6	2.135478	-2.818840	-0.902275	6	-0.475388	0.290986	-0.707333
6	2.227890	-1.520933	-1.431733	6	-0.864051	1.187121	0.300506
6	1.924010	-1.315472	-2.783013	6	-1.236260	2.481936	0.411363
1	4.735504	-2.042566	-0.961096	6	1.524189	-2.385555	-3.585381
1	4.683235	0.430049	-2.213439	6	1.424847	-3.669800	-3.049749
1	2.375234	-2.992353	0.142908	1	1.100941	-4.497614	-3.672324
1	1.988934	-0.318841	-3.205308	6	1.738961	-3.885361	-1.706005
8	-3.355601	-3.370551	1.147645	6	2.354539	3.529007	-2.154588
16	-3.056122	-2.649182	-0.094927	6	3.461498	3.504725	-3.002509
7	-1.708941	-1.697588	0.212323	6	4.296320	2.384033	-3.025913
8	-2.920259	-3.386666	-1.359427	1	3.906764	0.979572	1.992205
6	-4.296497	-1.384056	-0.352913	1	3.679353	4.356956	-3.639283
6	-4.727564	-0.616721	0.731695	1	1.213179	2.453338	-0.679198

1	7.722160	-0.996329	1.941921	1	4.552763	0.609740	-2.205443
1	0.017323	0.694794	-1.589659	1	1.743115	-2.816623	-0.452583
1	6.175111	0.683793	2.925292	1	1.697840	0.564152	-3.113384
1	6.989959	-2.360947	-0.001612	8	-3.654313	-2.881995	0.795159
1	5.163517	2.364648	-3.679182	16	-3.304608	-1.984850	-0.313181
1	1.705242	4.398801	-2.125202	7	-1.989406	-1.066455	0.211239
1	1.284145	-2.212160	-4.630096	8	-3.080159	-2.543842	-1.655770
1	1.664646	-4.881789	-1.281756	6	-4.548051	-0.709257	-0.462948
28	0.737746	0.230537	0.930232	6	-4.874770	0.066685	0.651774
7	-2.075839	3.076384	-0.568005	6	-5.188458	-0.521040	-1.684023
7	-0.875876	3.376954	1.424202	1	-4.362826	-0.092821	1.593478
6	-1.481151	4.173559	-1.324632	6	-5.850350	1.048161	0.528183
1	-0.832918	3.810664	-2.141350	6	-6.168728	0.466218	-1.789295
1	-2.269428	4.793626	-1.764978	1	-4.908204	-1.136675	-2.531094
1	-0.882904	4.789971	-0.652030	1	-6.104840	1.660797	1.388697
6	-2.889273	2.191048	-1.381553	6	-6.512973	1.262250	-0.691630
1	-3.693957	2.773173	-1.844414	1	-6.670018	0.622208	-2.740251
1	-2.322460	1.696078	-2.186520	6	-7.582245	2.319641	-0.801661
1	-3.330444	1.418105	-0.753096	1	-7.254669	3.263866	-0.354919
6	0.317550	3.192550	2.225964	1	-8.492574	2.011410	-0.274101
1	0.733779	4.176003	2.480343	1	-7.850757	2.510447	-1.843717
1	0.130802	2.659256	3.168659	6	-1.451230	-0.199605	-0.861960
1	1.061943	2.615818	1.675095	1	-0.912427	-0.803796	-1.598517
6	-1.916957	4.151369	2.082583	1	-2.319944	0.224766	-1.380682
1	-2.241812	3.675572	3.023083	6	-1.033976	0.392538	2.348937
1	-1.547671	5.155035	2.325098	6	-0.911024	-1.136455	2.483597
1	-2.773807	4.240188	1.415215	1	-0.777313	0.913846	3.269556
TS7				6	0.466044	-1.446252	3.110962
				6	1.438598	-0.309597	2.718950
				1	0.878909	-2.396026	2.743329
				1	0.411748	-1.518784	4.203733
15	2.401489	0.003458	-0.273739	8	2.349579	0.027293	3.449842
6	3.978957	-0.790341	0.217240	1	-2.060232	0.629345	2.080871
6	4.630259	-1.737929	-0.585837	6	-1.020688	-1.776495	1.073319
6	5.866276	-2.255285	-0.197447	1	-1.311704	-2.824813	1.173370
6	6.462745	-1.827874	0.989479	1	-0.050824	-1.757487	0.567873
6	5.818794	-0.882566	1.789966	6	-2.048016	-1.655297	3.380679
6	4.582089	-0.363414	1.410208	1	-3.021350	-1.505601	2.908160
6	2.984545	1.555228	-1.062233	1	-2.039377	-1.141589	4.347823
6	4.051390	1.544002	-1.973440	1	-1.941066	-2.729960	3.561889
6	2.360295	2.768514	-0.746330	6	-0.563415	0.939314	-0.399895
6	1.481163	-2.372189	-1.408358	6	-0.710890	1.687370	0.774983
6	1.793906	-1.025957	-1.660524	6	-0.773212	2.974147	1.154973
6	1.462018	-0.473191	-2.903462	6	-1.345206	4.000177	0.203862
1	4.173258	-2.073163	-1.510341				

1	-2.160015	4.564920	0.677739	1	-2.519950	3.133136	-0.207791
1	-1.731940	3.535669	-0.705786	1	-0.042357	2.067112	1.114188
1	-0.582540	4.737717	-0.084412	8	4.989247	0.293306	-1.158491
6	0.813411	-1.247513	-3.867319	16	4.287278	0.223611	0.126872
6	0.488756	-2.577830	-3.601748	7	3.229669	-1.068139	0.027571
1	-0.034014	-3.171619	-4.344399	8	5.046682	0.187764	1.386776
6	0.832146	-3.141738	-2.371255	6	3.164709	1.612183	0.251414
6	2.788369	3.953913	-1.346967	6	2.328165	1.921661	-0.823370
6	3.840027	3.935056	-2.262563	6	3.195141	2.411943	1.392062
6	4.472347	2.728034	-2.574209	1	2.308702	1.284606	-1.699512
1	4.069929	0.343544	2.052623	6	1.525918	3.055695	-0.751145
1	4.172607	4.857567	-2.729025	6	2.372166	3.536439	1.455563
1	1.543709	2.782177	-0.032419	1	3.866294	2.153330	2.202915
1	7.424192	-2.232848	1.291105	1	0.881105	3.306543	-1.584748
6	-0.295258	3.507077	2.480506	6	1.531475	3.875684	0.388357
1	0.245406	2.755924	3.056931	1	2.392247	4.164640	2.342069
1	-1.127909	3.891892	3.085496	6	0.602150	5.058059	0.482085
1	0.386431	4.353154	2.320013	1	0.404221	5.488408	-0.502715
1	-0.085975	1.445180	-1.237421	1	1.009328	5.838712	1.130662
1	6.274258	-0.552795	2.718682	1	-0.363901	4.748841	0.900065
1	6.362194	-2.991002	-0.823770	1	-3.733682	-0.040962	1.769850
1	5.296799	2.711656	-3.280691	6	2.489161	-1.391133	1.242654
1	2.299736	4.890567	-1.095837	1	2.673133	-2.435121	1.507482
1	0.553497	-0.804912	-4.824218	1	2.892318	-0.800637	2.072845
1	0.581265	-4.175539	-2.156605	6	1.261471	-1.757718	-1.972028
28	0.735263	0.393349	1.100558	6	2.280713	-2.835056	-1.524880
TS8				1	0.607292	-2.178889	-2.753635
				6	1.552829	-3.803151	-0.533566
				6	0.160825	-3.237838	-0.231271
				1	2.110634	-3.981402	0.388402
15	-1.699554	0.236601	-0.398795	1	1.380832	-4.782697	-0.990674
6	-3.371994	-0.423266	-0.764463	8	-0.886707	-3.794684	-0.534988
6	-3.565266	-1.811078	-0.720187	1	1.767119	-0.882980	-2.394952
6	-4.837767	-2.345539	-0.933272	6	3.525337	-2.162066	-0.897829
6	-5.917520	-1.503860	-1.198802	1	4.122266	-1.731665	-1.701709
6	-5.726161	-0.120526	-1.255320	1	4.140911	-2.925820	-0.396256
6	-4.459981	0.418735	-1.039244	6	2.812916	-3.653079	-2.718590
6	-1.550722	1.698578	-1.494106	1	3.245166	-2.987892	-3.473379
6	-0.907361	1.504332	-2.725296	1	1.996960	-4.211309	-3.187876
6	-2.040843	2.970040	-1.167682	1	3.585052	-4.373186	-2.416926
6	-1.886587	0.956669	1.276596	6	1.003208	-1.106491	1.151356
6	-0.863751	1.786881	1.762996	6	0.022584	-2.088326	1.442334
6	-2.938240	0.601979	2.130614	6	-0.795886	-2.402511	2.456404
1	-4.315288	1.492887	-1.089003	6	-0.577824	-1.809230	3.827847
1	-0.495879	0.526274	-2.958524				

1	-1.496409	-1.315426	4.167008	1	-0.133131	-1.150067	1.705837
1	0.228127	-1.072720	3.830015	8	3.919499	0.753894	-1.089451
1	-0.341953	-2.590976	4.561289	16	3.569306	-0.663294	-1.215495
6	-0.773826	2.561748	-3.624541	7	2.001929	-0.693316	-1.993111
6	-1.266489	3.826961	-3.294091	8	4.445315	-1.592308	-1.941962
1	-1.153163	4.653220	-3.989272	6	3.233682	-1.351317	0.388530
6	-1.896616	4.029597	-2.064234	6	2.828171	-0.496413	1.410473
6	-0.897701	2.261722	3.072214	6	3.351003	-2.726525	0.595072
6	-1.951162	1.907119	3.918093	1	2.795321	0.568130	1.239636
1	-1.978443	2.273118	4.939877	6	2.467339	-1.037641	2.637962
6	-2.968334	1.077443	3.443453	6	2.973897	-3.252577	1.829086
6	-1.975300	-3.328103	2.329751	1	3.727010	-3.365851	-0.195238
1	-2.034349	-4.004037	3.190628	1	2.128695	-0.373336	3.426185
1	-1.943209	-3.907500	1.408391	6	2.505440	-2.422257	2.857347
1	-2.900614	-2.736380	2.325318	1	3.038884	-4.323712	1.994644
1	0.754396	-0.066583	1.364357	6	2.052268	-2.989092	4.177434
1	-6.905303	-1.921896	-1.368824	1	2.029042	-4.081163	4.160928
1	-2.724312	-2.471363	-0.532238	1	1.048782	-2.627202	4.425627
1	-0.096690	2.903609	3.426809	1	2.718676	-2.676458	4.989215
1	-3.792146	0.800418	4.094782	1	-2.519526	2.353431	2.388392
1	-6.563482	0.536973	-1.469714	6	1.353910	-2.039430	-1.896274
1	-4.978339	-3.421620	-0.898391	1	0.911043	-2.267929	-2.864384
1	-2.274626	5.013279	-1.802047	1	2.089520	-2.822142	-1.701627
1	-0.272889	2.403125	-4.574601	6	0.440507	1.576147	-2.438298
28	-0.010727	-1.387681	-0.509672	6	0.815954	0.725036	-3.668970
TS8CF3				1	-0.401498	2.240274	-2.639896
				6	-0.387207	-0.207895	-3.977480
				6	-1.278140	-0.263371	-2.736731
				1	-0.077483	-1.213648	-4.278329
15	-0.283527	1.500266	0.596992	1	-1.006941	0.193807	-4.785635
6	-1.301638	2.965046	0.154859	8	-2.443652	0.018929	-2.785908
6	-2.295764	2.830996	-0.826139	1	1.291343	2.169802	-2.091966
6	-3.099161	3.919050	-1.162984	6	2.094214	-0.068616	-3.340681
6	-2.916537	5.151818	-0.533695	1	2.930227	0.632989	-3.312077
6	-1.928015	5.292200	0.440741	1	2.314035	-0.827713	-4.100852
6	-1.123971	4.205043	0.785247	6	1.108417	1.608151	-4.897273
6	1.120062	2.283809	1.489305	1	1.925945	2.304127	-4.683786
6	2.156071	2.858553	0.736558	1	0.223516	2.193908	-5.161706
6	1.206041	2.296224	2.888235	1	1.390898	1.007572	-5.769869
6	-1.228225	0.684734	1.939567	6	0.311689	-1.945955	-0.805494
6	-0.922153	-0.647391	2.247836	6	-0.986253	-1.541118	-1.052628
6	-2.261035	1.328936	2.632821	6	-2.157516	-2.031066	-0.577197
1	-0.357587	4.323923	1.542851	6	-2.183305	-3.481742	-0.188340
1	2.118646	2.829852	-0.345380	6	3.260307	3.423865	1.369914
1	0.408379	1.861325	3.480185				

6	3.346023	3.420889	2.764097	8	3.203675	-1.699727	-2.385476
1	4.212598	3.850305	3.257332	16	2.555579	-2.406274	-1.273934
6	2.316535	2.859381	3.520215	7	0.886156	-1.996052	-1.338455
6	-1.631976	-1.326118	3.236040	8	2.709075	-3.864211	-1.132440
6	-2.656769	-0.678109	3.926175	6	3.138830	-1.677123	0.257721
1	-3.222751	-1.209604	4.685105	6	3.812349	-0.457155	0.203283
6	-2.967122	0.649132	3.624885	6	3.039259	-2.381436	1.460190
6	-3.414482	-1.268783	-0.293920	1	3.931402	0.048762	-0.743698
1	0.550115	-2.385886	0.158067	6	4.337742	0.082552	1.373521
1	-3.540373	5.999149	-0.802375	6	3.552536	-1.816684	2.625817
1	-2.446929	1.879311	-1.317316	1	2.601373	-3.372194	1.477868
1	-3.770097	1.153516	4.153961	1	4.853166	1.036319	1.326550
1	-1.409099	-2.369229	3.434180	6	4.199817	-0.573862	2.603049
1	-3.866713	3.800571	-1.921764	1	3.467015	-2.358808	3.563220
1	-1.779231	6.248155	0.934119	6	4.722918	0.057291	3.867623
1	2.375475	2.858049	4.604707	1	5.726648	0.468082	3.721741
1	4.061850	3.846842	0.772979	1	4.763814	-0.661965	4.689781
28	0.125241	0.146595	-1.143504	1	4.075179	0.885620	4.178638
9	-1.705685	-3.698517	1.075022	1	-1.482074	3.167146	1.758049
9	-3.426694	-4.001525	-0.223353	6	0.127647	-2.624598	-0.218614
9	-1.412879	-4.245559	-1.001370	1	-0.519105	-3.403559	-0.625844
9	-3.211648	0.062131	-0.192792	1	0.820408	-3.142699	0.443357
9	-3.938398	-1.661360	0.899093	6	-1.151310	-0.192567	-2.821655
9	-4.384449	-1.458450	-1.214156	6	-1.013212	-1.704292	-3.122291
TS8_{NCH3}				1	-2.067033	0.182243	-3.292100
				6	-2.218220	-2.384299	-2.407464
				6	-2.744067	-1.378631	-1.374583
15	0.007871	1.507505	-0.249890	1	-1.968669	-3.347931	-1.956302
6	-0.940892	2.992073	-0.791771	1	-3.036989	-2.562853	-3.111975
6	-2.162831	2.807974	-1.452234	8	-3.898717	-0.980585	-1.392677
6	-2.921743	3.910265	-1.849986	1	-0.316762	0.383099	-3.235071
6	-2.464349	5.203227	-1.598083	6	0.365313	-2.287237	-2.708617
6	-1.241338	5.394781	-0.949244	1	1.109580	-1.877293	-3.392293
6	-0.483237	4.296246	-0.550195	1	0.336665	-3.376761	-2.861056
6	1.707757	1.913995	-0.807906	6	-1.105999	-1.982085	-4.640462
6	2.130639	1.412879	-2.045783	1	-0.314571	-1.450949	-5.179779
6	2.570453	2.740350	-0.072962	1	-2.069141	-1.631377	-5.021949
6	0.094416	1.706966	1.574506	1	-1.017048	-3.050590	-4.873357
6	0.978090	0.878244	2.287493	6	-0.678744	-1.632476	0.602437
6	-0.792842	2.521284	2.290557	6	-2.060974	-1.554069	0.483968
1	0.468647	4.453023	-0.053854	6	-3.080291	-1.420434	1.401540
1	1.493412	0.730092	-2.590881	6	3.384901	1.750651	-2.553995
1	2.267386	3.104677	0.903136	6	4.233289	2.584810	-1.824092
1	1.664195	0.236398	1.749165	1	5.212869	2.842557	-2.215236

6	3.825447	3.074619	-0.580189	6	-4.297435	-0.433142	-0.108416
6	0.978083	0.871590	3.679860	6	-3.837626	-1.946369	1.717394
6	0.088063	1.686085	4.386433	6	-2.265673	-3.055045	-1.500316
1	0.082975	1.676713	5.472291	6	-3.497078	-3.722254	-1.484691
6	-0.794667	2.508703	3.687652	6	-1.312804	-3.412435	-2.465756
1	-0.190252	-1.233706	1.488055	1	-1.249719	-4.635284	0.219911
1	-3.053181	6.060658	-1.910543	1	-3.991252	0.026232	-1.039458
1	-2.504587	1.799224	-1.657135	1	-3.190850	-2.667318	2.203629
1	-1.487963	3.146690	4.228133	1	-4.243012	-3.459151	-0.742838
1	1.665855	0.220130	4.210074	8	6.556879	0.308234	-0.933914
1	-3.866995	3.754541	-2.361302	16	5.267425	0.838121	-0.459383
1	-0.877466	6.400126	-0.758340	7	3.986506	0.379807	-1.473546
1	4.486722	3.715819	-0.004196	8	5.107402	2.285337	-0.252711
1	3.706289	1.335755	-3.503470	6	4.839916	-0.029031	1.037469
28	-1.146566	-0.290534	-0.836014	6	5.548484	-1.180342	1.388198
7	-3.237750	-2.398494	2.398936	6	3.778233	0.432283	1.811236
7	-4.063392	-0.475385	1.373570	1	6.382888	-1.500086	0.774189
6	-3.325302	-1.929182	3.780173	6	5.167203	-1.885162	2.525261
1	-3.890589	-2.647777	4.382696	6	3.409003	-0.287871	2.944657
1	-2.327037	-1.807788	4.230796	1	3.246105	1.327426	1.523900
1	-3.833586	-0.966269	3.814109	1	5.712003	-2.781745	2.808115
6	-2.522369	-3.654537	2.258667	6	4.087540	-1.454950	3.312202
1	-1.455505	-3.576531	2.520121	1	2.563552	0.052420	3.533970
1	-2.983073	-4.396028	2.919708	6	3.655525	-2.257629	4.512995
1	-2.594504	-3.998145	1.225444	1	4.516379	-2.623072	5.081395
6	-3.834693	0.852815	0.839148	1	3.028807	-1.665651	5.185496
1	-4.290181	0.961744	-0.148688	1	3.073487	-3.132332	4.200539
1	-4.251845	1.598558	1.528365	1	-0.360145	-2.897257	-2.484404
1	-2.763429	1.020538	0.747479	6	3.784141	1.270250	-2.645804
6	-5.456278	-0.802737	1.639686	1	4.262843	0.808418	-3.523966
1	-5.855466	-0.201351	2.467095	1	4.298195	2.210623	-2.449015
1	-6.054036	-0.601386	0.742877	6	2.533771	-1.603169	-2.078300
1	-5.538488	-1.858083	1.895190	6	1.813637	-0.871999	-3.238275
TS9				1	2.483754	-0.906182	-4.108473
				1	0.945989	-1.471347	-3.518754
				6	3.949122	-1.042023	-1.813294
				1	4.376070	-1.612434	-0.985908
15	-1.833646	-1.733585	-0.297073	1	4.581651	-1.229743	-2.694946
6	-0.951797	-2.655343	1.027504	6	2.760536	-3.064693	-2.519423
6	-0.394624	-1.913625	2.080658	1	3.256783	-3.638400	-1.729579
6	0.268184	-2.560394	3.120218	1	1.809113	-3.558856	-2.738636
6	0.399652	-3.950519	3.113225	1	3.383148	-3.117383	-3.419258
6	-0.142371	-4.693239	2.063202	6	2.325689	1.535316	-2.856085
6	-0.821828	-4.050718	1.026857	6	1.394699	0.572420	-3.029072
6	-3.449995	-1.367567	0.501396				

6	-0.033989	0.936288	-3.056821	1	-3.305715	0.856581	2.006037
6	-1.097454	0.049002	-3.358819	6	-1.165728	0.763673	4.636336
1	-0.927970	-0.996730	-3.586254	1	0.847406	1.539125	4.613487
1	-2.132389	0.068036	-2.052546	1	-3.204551	0.117681	4.340925
1	-1.953836	0.463098	-3.883493	1	-1.119762	0.439485	5.671803
6	-5.493479	-0.054530	0.497495	6	-0.167124	3.410955	0.012651
6	-5.863192	-0.619381	1.720131	6	-0.632094	4.733828	0.002188
1	-6.786605	-0.315521	2.204023	6	1.215040	3.183492	-0.111645
6	-5.039174	-1.573280	2.320988	6	0.264176	5.797972	-0.114748
6	-3.767134	-4.724758	-2.418167	1	-1.693037	4.940618	0.077913
6	-2.810333	-5.077127	-3.370674	6	2.110596	4.247987	-0.212738
1	-3.023583	-5.857635	-4.094695	1	1.587086	2.170203	-0.136207
6	-1.578104	-4.419979	-3.390593	6	1.635610	5.560701	-0.216342
1	0.919172	-4.453935	3.923558	1	-0.114778	6.816085	-0.124667
1	-0.467144	-0.835637	2.083402	1	3.172641	4.033712	-0.293372
6	-0.360689	2.407854	-3.232809	1	2.328086	6.392918	-0.303012
1	0.039956	2.760727	-4.192315	1	0.060489	3.039056	-2.453065
1	-1.439630	2.570386	-3.237732	6	1.695086	-1.627601	-0.778325
1	2.017666	2.561998	-2.715238	1	2.352154	-1.848528	0.071056
1	-4.726925	-5.232509	-2.398033	1	0.980155	-2.451674	-0.853444
1	-0.827106	-4.687305	-4.128185	6	0.871600	-0.380292	-0.412822
1	-0.043245	-5.774698	2.051728	8	1.250884	0.270777	0.552285
1	0.683388	-1.970892	3.930383				
1	-5.325123	-2.020182	3.268677	TS10			
1	-6.114381	0.701906	0.028185				
28	-0.844828	0.013028	-1.250610	15	-2.783109	0.908873	0.244315
15	-1.307136	1.953730	0.136494	6	-4.017516	0.061608	-0.841560
6	-2.967894	2.739213	-0.051947	6	-3.642458	-1.093629	-1.528508
6	-3.602451	3.454834	0.974833	6	-4.552808	-1.789434	-2.320806
6	-3.627229	2.609815	-1.281280	6	-5.858241	-1.318765	-2.457362
6	-4.867628	4.008279	0.779809	6	-6.239190	-0.143699	-1.805962
1	-3.109773	3.567132	1.934306	6	-5.325509	0.544960	-1.009017
6	-4.887883	3.171096	-1.483913	6	-3.427746	0.543742	1.946985
1	-3.154288	2.036235	-2.070489	6	-2.506067	0.488800	3.002580
6	-5.514720	3.867800	-0.449615	6	-4.776727	0.289206	2.230451
1	-5.347777	4.551237	1.588645	6	-3.375895	2.634618	-0.017841
1	-5.382997	3.055818	-2.443766	6	-3.892332	3.439740	1.001174
1	-6.500192	4.298691	-0.599785	6	-3.307589	3.141542	-1.326344
6	-1.276259	1.593387	1.948047	1	-5.625071	1.471789	-0.531898
6	-0.112425	1.783567	2.707226	1	-1.452527	0.624171	2.779758
6	-2.389411	0.998863	2.563195	1	-5.508078	0.297333	1.431831
6	-0.059908	1.373151	4.039206	1	-3.959657	3.057063	2.013630
1	0.755089	2.245177	2.254841	8	3.876536	-1.665632	0.822149
6	-2.333083	0.585796	3.893923	16	4.254512	-0.747173	-0.254771

7	2.930574	0.307151	-0.502878	6	-5.189226	-0.003119	3.530887
8	4.654162	-1.249605	-1.572462	6	-4.330117	4.737461	0.721362
6	5.577127	0.285292	0.361301	6	-4.269950	5.232547	-0.580265
6	5.731991	0.450556	1.738601	1	-4.619416	6.237563	-0.798463
6	6.404516	0.955741	-0.541380	6	-3.761196	4.427112	-1.603755
1	5.098057	-0.106671	2.418958	1	-6.571681	-1.854628	-3.076682
6	6.724094	1.306278	2.210212	1	-2.628943	-1.443180	-1.441133
6	7.390110	1.808251	-0.051082	6	-0.696674	3.522091	1.882424
1	6.289931	0.786057	-1.605624	1	0.173384	3.672584	2.534634
1	6.857246	1.431249	3.281138	1	-1.411592	4.316714	2.097443
6	7.560238	2.002719	1.326726	1	1.039253	1.926336	1.858356
1	8.043902	2.325311	-0.747750	1	-4.729005	5.354041	1.522047
6	8.608754	2.953507	1.846117	1	-3.710405	4.806610	-2.620313
1	8.202513	3.968208	1.938026	1	-7.247766	0.242286	-1.923194
1	8.965307	2.653634	2.835334	1	-4.236510	-2.694121	-2.831040
1	9.468768	3.006407	1.172848	1	-6.238241	-0.204777	3.727957
1	-2.896851	2.518123	-2.114245	1	-2.180578	0.159676	5.103832
6	2.517803	0.954543	0.749521	28	-0.407886	0.505931	-0.119248
1	3.232073	1.759464	1.001808	15	-0.126211	-1.780878	-0.049194
1	2.587764	0.198787	1.530894	6	0.877821	-2.468003	1.342080
6	0.929699	0.574062	-2.728187	6	1.297064	-3.806645	1.325127
6	1.875462	1.732390	-2.317561	6	1.119849	-1.704632	2.486993
1	0.764489	0.581287	-3.811075	6	1.995898	-4.343316	2.402498
6	1.160284	2.790232	-1.467156	1	1.077064	-4.430466	0.465822
1	1.866766	3.619698	-1.303181	6	1.809269	-2.244090	3.573427
1	0.368810	3.197584	-2.100716	1	0.756424	-0.684146	2.526714
1	1.392803	-0.375435	-2.464735	6	2.262077	-3.560798	3.528164
6	3.152721	1.212465	-1.640994	1	2.328063	-5.376569	2.366500
1	3.714372	0.646113	-2.383664	1	1.991764	-1.633026	4.452980
1	3.766933	2.072413	-1.324859	1	2.807622	-3.981253	4.367705
6	2.355225	2.453557	-3.594495	6	-1.616554	-2.844036	0.239926
1	2.862009	1.756647	-4.269413	6	-1.979770	-3.934656	-0.559463
1	1.502837	2.881572	-4.130099	6	-2.408628	-2.527084	1.350555
1	3.049552	3.268575	-3.357104	6	-3.143607	-4.653481	-0.280046
6	1.137098	1.576404	0.833744	1	-1.368947	-4.217389	-1.408105
6	0.530736	2.444451	-0.133847	6	-3.570352	-3.241964	1.627909
6	-0.306847	3.551291	0.420108	1	-2.121001	-1.710655	1.997805
6	-0.663579	4.635390	-0.291261	6	-3.949399	-4.302243	0.803043
1	-0.420772	4.780263	-1.334811	1	-3.420062	-5.490098	-0.915410
1	0.006464	0.522992	1.335068	1	-4.179811	-2.957349	2.479878
1	-1.271158	5.409400	0.163343	1	-4.861504	-4.855152	1.006574
6	-2.915183	0.204461	4.305073	6	0.594681	-2.513267	-1.571298
6	-4.261712	-0.043550	4.573552	6	1.928449	-2.930124	-1.644846
1	-4.584661	-0.275817	5.584016	6	-0.171346	-2.487148	-2.751628

6	2.485429	-3.313303	-2.866247	6	-6.038190	-0.850445	4.274208
1	2.547415	-2.933177	-0.758315	1	-6.673203	-1.727317	4.426832
6	0.380282	-2.889801	-3.963942	1	-6.379168	-0.058779	4.947699
1	-1.188201	-2.112656	-2.737098	1	-5.020720	-1.123155	4.579891
6	1.714250	-3.301635	-4.026295	6	-3.151439	1.630342	-1.786633
1	3.531857	-3.596726	-2.901002	1	-2.404742	1.429283	-2.557178
1	-0.226835	-2.860335	-4.863724	1	-3.619878	2.587024	-2.020643
1	2.149649	-3.597472	-4.976117	6	-2.696465	-0.784703	0.150351
1	-1.159197	2.577779	2.171048	6	-2.751489	-1.458462	-1.236123
6	-0.443116	0.643838	-2.039835	1	-2.271832	-1.519145	0.836309
8	-1.440676	0.807674	-2.727803	6	-1.296205	-1.433246	-1.752852
TS11				6	-0.614464	-0.120298	-1.357619
				1	-1.238205	-1.553538	-2.839106
15	1.620605	-1.909694	0.089294	1	-0.758649	-2.260547	-1.291384
6	2.134954	-2.511569	-1.565502	8	-0.293012	0.699226	-2.221155
6	2.561063	-3.828492	-1.807480	1	-3.703621	-0.569855	0.516060
6	2.997233	-4.206187	-3.076111	6	-3.736200	-0.768376	-2.237067
6	3.016073	-3.272876	-4.116216	1	-4.640464	-1.369427	-2.334773
6	2.597137	-1.963798	-3.882396	1	-3.276326	-0.744807	-3.233182
6	2.156505	-1.583481	-2.614579	6	-3.225369	-2.913177	-1.077552
6	0.776502	-3.368058	0.850332	1	-4.224104	-2.939046	-0.627515
6	0.743756	-3.484616	2.249654	1	-2.547717	-3.481309	-0.435368
6	0.047304	-4.293983	0.088652	1	-3.280699	-3.420400	-2.047617
6	4.396304	-2.439085	0.587044	6	-2.494868	1.729455	-0.408591
6	3.205410	-1.849187	1.031659	6	-1.844475	0.483180	0.194111
6	3.225878	-1.086198	2.207630	6	-1.235906	0.756331	1.541694
1	2.549036	-4.557476	-1.003820	6	-0.764230	-0.234453	2.362650
1	1.306429	-2.788309	2.861698	1	-0.345941	0.017626	3.332254
1	4.409247	-3.010215	-0.333252	1	-1.755913	2.530004	-0.472421
1	2.316342	-0.594184	2.532052	6	4.408150	-0.909185	2.924590
8	-6.577087	-0.030042	-2.342188	6	5.591283	-1.490969	2.468434
16	-5.759860	0.894379	-1.549196	1	6.518620	-1.339365	3.012685
7	-4.166835	0.585551	-1.913515	6	5.580567	-2.258486	1.301715
8	-5.931151	2.348382	-1.624988	6	-0.692389	-5.303629	0.707305
6	-5.990212	0.423190	0.162398	6	-0.721241	-5.404736	2.097485
6	-6.329324	-0.894218	0.469836	6	0.003869	-4.491595	2.866070
6	-5.723930	1.346984	1.173485	1	1.830490	-0.566599	-2.439686
1	-6.569061	-1.585227	-0.330129	1	-1.297455	-6.189436	2.577935
6	-6.360851	-1.294918	1.803846	1	0.063354	-4.239374	-0.993667
6	-5.758088	0.930725	2.501095	1	3.356273	-3.568928	-5.104268
1	-5.504281	2.375883	0.912520	6	-1.193547	2.185069	2.049306
1	-6.622358	-2.320761	2.047881	1	-2.209637	2.569536	2.195354
6	-6.058565	-0.397509	2.836324	1	-0.684371	2.234425	3.014061
1	-5.550785	1.646656	3.291702	1	-3.264843	2.077258	0.291809

1	2.615379	-1.228981	-4.680476	TS12			
1	3.322986	-5.227050	-3.253054				
1	6.499573	-2.710190	0.939392	15	-3.060966	0.359424	0.006102
1	4.407269	-0.287495	3.813530	6	-3.477367	1.515376	-1.351489
1	-0.002495	-4.565082	3.949653	6	-4.793237	1.862291	-1.692981
1	-1.245364	-6.011106	0.096375	6	-5.033789	2.769685	-2.723475
15	1.961438	1.819548	0.058614	6	-3.963146	3.332829	-3.422536
6	2.991847	2.192690	1.540444	6	-2.652954	2.979275	-3.096835
6	4.306152	2.674794	1.476033	6	-2.405734	2.067916	-2.068952
6	2.398122	2.020661	2.798254	6	-3.298496	1.321010	1.550967
6	5.013805	2.958795	2.644431	6	-4.221707	2.367450	1.675713
1	4.778695	2.821979	0.511244	6	-2.520660	0.956069	2.659939
6	3.096635	2.321525	3.966500	6	-4.790721	-1.490912	-1.175098
1	1.389554	1.628013	2.852221	6	-4.471611	-0.814980	0.013455
6	4.411440	2.785926	3.892002	1	-5.625329	1.409728	-1.162331
1	6.035088	3.322504	2.579447	1	-4.815926	2.670072	0.820322
1	2.619793	2.183637	4.932718	1	-1.793866	0.155206	2.552234
1	4.963085	3.011978	4.799703	1	-4.268222	-1.239927	-2.093763
6	1.323547	3.504784	-0.357457	8	6.367853	-1.894362	0.519486
6	1.714449	4.659014	0.336768	16	5.196728	-1.267679	1.139279
6	0.363109	3.619923	-1.377472	7	3.856435	-1.736105	0.260124
6	1.160337	5.899108	0.015644	8	4.857099	-1.475855	2.549461
1	2.448334	4.594455	1.131297	6	5.341075	0.494170	0.882381
6	-0.176846	4.864034	-1.703187	6	2.545559	-1.477531	0.896661
1	0.036581	2.724380	-1.894809	6	4.632205	1.369453	1.705853
6	0.216185	6.007369	-1.005753	6	6.062230	0.967324	-0.215489
1	1.471095	6.782617	0.565963	1	2.396775	-0.413302	1.124189
1	-0.916305	4.935032	-2.495756	1	2.527731	-2.023458	1.841954
1	-0.213158	6.973810	-1.252680	1	4.100475	0.982989	2.567609
6	3.215550	1.493938	-1.249950	6	4.633478	2.731084	1.408497
6	3.043131	1.949911	-2.563454	6	6.054331	2.329806	-0.495967
6	4.285621	0.627767	-0.970081	1	6.623100	0.270610	-0.827909
6	3.917858	1.544074	-3.572728	1	4.079899	3.417018	2.043471
1	2.224385	2.617560	-2.803117	6	5.335785	3.230291	0.304323
6	5.157395	0.226873	-1.979042	1	6.613254	2.703516	-1.349513
1	4.437102	0.261843	0.037070	6	5.349314	4.707090	0.000405
6	4.975144	0.679854	-3.286652	1	4.464258	5.205766	0.404461
1	3.769582	1.907429	-4.585578	1	5.384500	4.891668	-1.077206
1	5.972147	-0.449949	-1.739848	1	6.229716	5.189146	0.442613
1	5.649348	0.360404	-4.075534	6	1.905019	-1.429907	-2.601163
28	0.561376	-0.002939	0.203855	1	1.641697	-2.490377	-2.655144
1	-0.862668	-1.289851	2.146075	1	1.631609	-0.945191	-3.546282
1	-0.687548	2.866295	1.362539	6	3.360469	-1.030877	-2.177089
				6	2.746013	0.180002	-1.436267

1	2.616867	1.029851	-2.115715				
6	4.326156	-0.732684	-3.318849	15	2.068549	0.330251	-0.036642
1	5.235172	-0.250171	-2.942673	6	1.739708	1.844644	-1.019954
1	3.868657	-0.063630	-4.054526	6	2.682457	2.881540	-1.093011
1	4.625474	-1.649692	-3.840353	6	2.400906	4.034567	-1.822662
6	4.007944	-2.031381	-1.176420	6	1.180185	4.159778	-2.491987
1	5.083415	-2.080600	-1.346712	6	0.242992	3.127968	-2.429588
1	3.633336	-3.043972	-1.363757	6	0.517785	1.973380	-1.695042
1	3.208767	0.546433	-0.522686	6	3.867241	0.067299	-0.276798
6	1.448419	-1.972197	-0.030227	6	4.280455	-0.508108	-1.487461
6	0.093612	-1.909744	0.359550	6	4.833847	0.438391	0.666676
6	-5.775954	-2.476136	-1.185548	6	1.910612	0.873000	1.705815
6	-6.448627	-2.808192	-0.006738	6	2.308520	0.000770	2.733094
1	-7.213191	-3.579006	-0.014131	6	1.288962	2.083023	2.038700
6	-6.133812	-2.143859	1.178445	1	-0.208573	1.170228	-1.633762
6	-5.152105	-1.150717	1.190301	1	3.540711	-0.795318	-2.226113
1	-4.916615	-0.635644	2.115533	1	4.531298	0.889007	1.604842
6	-4.369334	3.030819	2.893173	1	2.775439	-0.947327	2.487901
6	-3.600720	2.653929	3.996856	8	-4.988554	-1.022721	1.535960
1	-3.718673	3.172819	4.943467	16	-4.678332	-0.819789	0.116773
6	-2.675630	1.615661	3.879235	7	-3.342372	-1.754350	-0.238231
1	-1.389418	1.762375	-1.832641	8	-5.667576	-1.074779	-0.935210
1	-4.152340	4.037487	-4.227029	6	-4.160373	0.885865	-0.087147
28	-1.063167	-0.625522	-0.025580	6	-3.827835	1.648579	1.031667
1	-6.655326	-2.393714	2.097751	6	-4.009056	1.411775	-1.373018
1	-6.016958	-2.987041	-2.113086	1	-4.004789	1.245936	2.020827
1	-2.070148	1.324364	4.732313	6	-3.287574	2.919624	0.858601
1	-5.084083	3.843760	2.980720	6	-3.458947	2.682264	-1.529696
1	-1.820983	3.403632	-3.650901	1	-4.336942	0.839533	-2.232511
1	-6.054290	3.034391	-2.984393	1	-3.028439	3.512560	1.731359
6	-1.118958	-2.588163	0.429797	6	-3.069913	3.446782	-0.421120
6	-1.682422	-3.037367	1.766847	1	-3.343403	3.093342	-2.529071
6	-1.626023	-3.366927	-0.778161	6	-2.424453	4.796961	-0.600531
1	-2.770557	-2.911556	1.777058	1	-2.800890	5.305037	-1.493392
1	-1.264056	-2.461706	2.596181	1	-1.339430	4.692060	-0.718888
1	-2.716938	-3.305772	-0.840848	1	-2.604624	5.443996	0.262422
1	-1.207117	-2.984952	-1.712902	1	0.971790	2.761181	1.254439
1	1.718301	-2.976747	-0.382185	6	-2.919134	-1.741021	-1.667128
6	1.396958	-0.562350	-1.411014	1	-3.795084	-1.997161	-2.265147
8	0.284905	0.086274	-1.273054	1	-2.594909	-0.731828	-1.947006
1	-1.467551	-4.101102	1.943424	6	-0.934020	-0.278747	0.318149
1	-1.353140	-4.428497	-0.687006	6	-1.287179	-1.386340	1.333996
				1	-0.541499	0.599599	0.831869
TS13				6	-0.053787	-2.319473	1.674052

6	1.152158	-2.454684	0.701181	8	-5.415491	-1.008549	-1.827224
1	-0.391923	-3.340312	1.893388	16	-5.690025	-0.017017	-0.779909
1	0.422898	-1.955701	2.589001	7	-4.857734	-0.515175	0.570347
8	2.232531	-2.864791	1.046216	8	-5.440760	1.412072	-1.008334
1	-1.797547	0.041809	-0.248005	6	-7.408741	-0.165707	-0.309893
6	-2.475536	-2.278159	0.823743	6	-4.033365	-1.721583	0.538667
1	-3.128469	-2.513835	1.665106	6	-8.136469	0.973428	0.024998
1	-2.094736	-3.223876	0.440880	6	-7.990626	-1.434742	-0.254828
6	-1.703988	-0.755710	2.680883	1	-4.421412	-2.377303	-0.242503
1	-2.635736	-0.201032	2.576956	1	-4.168869	-2.228049	1.502233
1	-0.927974	-0.075749	3.045191	1	-7.666135	1.947384	-0.046324
1	-1.866799	-1.530244	3.441591	6	-9.464489	0.834684	0.429439
6	-1.787835	-2.691611	-1.931548	6	-9.315420	-1.553925	0.147303
6	-0.539792	-2.450158	-1.539422	1	-7.412695	-2.307836	-0.537366
6	0.652665	-3.219060	-1.354361	1	-10.037793	1.719325	0.691645
6	0.525528	-4.628552	-0.803106	6	-10.072079	-0.423642	0.497154
1	0.281785	-5.305867	-1.633630	1	-9.775554	-2.537415	0.188831
1	-0.275502	-4.714186	-0.065600	6	-11.514763	-0.569815	0.910588
1	1.462028	-4.968961	-0.351882	1	-11.892450	0.344566	1.375030
6	5.632974	-0.711481	-1.749181	1	-11.643525	-1.392363	1.621203
6	6.590952	-0.346898	-0.800551	1	-12.149559	-0.789075	0.043888
1	7.645351	-0.511233	-1.000590	6	-2.400548	0.041528	2.617815
6	6.188700	0.228479	0.404511	1	-2.698345	-0.930983	3.024520
6	2.090260	0.342019	4.066563	1	-1.727536	0.526166	3.334203
6	1.463812	1.547683	4.391625	6	-3.518512	1.014283	2.121234
1	1.287061	1.806612	5.431012	6	-2.652511	1.321864	0.870592
6	1.064673	2.415441	3.375652	1	-2.038174	2.213804	1.014528
1	0.964402	5.057670	-3.063460	6	-3.806437	2.191295	3.049477
1	3.635009	2.781418	-0.582494	1	-4.421339	2.946567	2.546402
6	1.839164	-3.041498	-2.278291	1	-2.874901	2.670838	3.364835
1	2.776004	-3.119092	-1.714901	1	-4.338988	1.870782	3.953616
1	1.807308	-2.078173	-2.795506	6	-4.857542	0.332412	1.762649
1	1.842630	-3.829382	-3.046832	1	-5.605955	1.112117	1.602636
1	-2.034473	-3.633882	-2.425742	1	-5.202673	-0.272366	2.613611
1	2.402964	-0.339263	4.852004	1	-3.160604	1.393541	-0.089158
1	0.575959	3.353633	3.620491	6	-2.553371	-1.427996	0.321283
1	-0.705977	3.217074	-2.948681	6	-2.051673	-1.036961	-0.925671
1	3.134227	4.833740	-1.873581	28	-0.382355	-0.446004	-1.067195
1	6.929200	0.517246	1.144399	6	-2.115115	-0.719428	-2.261319
1	5.938842	-1.159073	-2.689901	6	-2.397573	0.696041	-2.746836
28	0.537589	-1.215662	-0.584060	6	-2.427703	-1.813274	-3.266992
				1	-1.892293	0.866730	-3.702973
TS14				1	-2.055456	1.455809	-2.042753
				1	-1.868606	-1.650386	-4.195788

1	-2.172409	-2.803883	-2.881375	1	6.792303	2.852582	-2.693754
1	-1.893594	-2.076422	0.891858	1	7.077709	4.944551	-1.376594
6	-1.777845	0.092985	1.200546	6	1.481558	2.543737	-0.519192
8	-0.517297	-0.028565	0.914113	6	0.956725	3.090270	0.655989
1	-3.476712	0.828589	-2.895834	6	0.844079	2.803416	-1.737361
1	-3.498766	-1.796785	-3.503436	6	-0.174249	3.905834	0.606964
6	2.987937	0.953475	0.821676	1	1.436282	2.885792	1.606415
6	4.061612	-0.124874	0.631771	6	-0.298855	3.600469	-1.781261
6	4.518436	1.097178	2.574711	1	1.252444	2.382150	-2.648941
1	2.024294	0.527398	1.117317	6	-0.808186	4.161797	-0.609212
1	4.654510	0.094703	-0.258892	1	-0.565825	4.333855	1.525359
6	5.708208	2.036028	2.709646	1	-0.787374	3.788258	-2.732503
1	5.424320	2.925132	3.279075	1	-1.695344	4.786739	-0.643413
1	6.526474	1.531111	3.229894	6	3.020724	-2.102325	1.831054
1	6.042918	2.344359	1.717485	6	3.947922	-2.728711	2.671755
6	3.976816	0.598905	3.909377	6	1.704797	-1.924087	2.273745
1	4.733564	0.000807	4.422854	6	3.570950	-3.164253	3.940347
1	3.706280	1.449469	4.541551	1	4.968155	-2.870226	2.334642
1	3.094946	-0.022996	3.749601	6	1.333633	-2.359150	3.548416
8	3.488398	1.781236	1.855870	1	0.970955	-1.438137	1.640983
8	4.904256	-0.020877	1.764398	6	2.260746	-2.978304	4.386133
6	3.460538	-1.555058	0.472553	1	4.302186	-3.647956	4.581543
6	2.780442	1.744460	-0.507802	1	0.310663	-2.206329	3.881761
8	2.777234	0.764498	-1.566871	1	1.967460	-3.316071	5.376053
8	2.257711	-1.461541	-0.315660	6	4.426901	-2.507046	-0.222474
15	1.740424	-0.529508	-1.585097	6	3.911077	-3.658397	-0.830830
7	2.314896	-1.188430	-3.017313	6	5.805723	-2.279864	-0.255742
6	3.728303	-1.305251	-3.359981	6	4.755168	-4.553986	-1.481831
1	4.079799	-2.338245	-3.250154	1	2.840923	-3.831236	-0.799605
1	3.886564	-0.985710	-4.397592	6	6.652918	-3.179749	-0.908441
1	4.327550	-0.671368	-2.709451	1	6.224820	-1.411387	0.241110
6	1.441496	-2.104711	-3.738106	6	6.131729	-4.314158	-1.527730
1	0.406784	-1.939081	-3.430624	1	4.340610	-5.439444	-1.954979
1	1.521210	-1.926291	-4.817498	1	7.721883	-2.989263	-0.930509
1	1.704855	-3.154965	-3.542969	1	6.790868	-5.010020	-2.038119
6	3.973106	2.661126	-0.790408				
6	4.131688	3.850910	-0.067442				
6	4.940320	2.318612	-1.740245				
6	5.242404	4.664469	-0.275198				
1	3.385477	4.138579	0.661608				
6	6.053070	3.136149	-1.950266				
1	4.812333	1.419393	-2.327353				
6	6.212354	4.308658	-1.215022				
1	5.349342	5.580489	0.298278				