

## Supporting Information

### Theoretical insight into dihydrogen activation with $\beta$ -diketiminato ligand supported Group 13 and 14 elements: mechanism and activity difference

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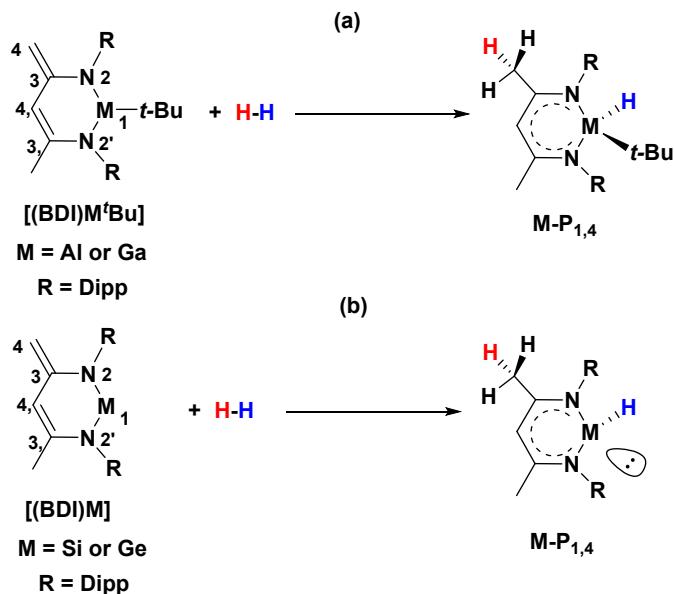
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**S1: Computational details.**



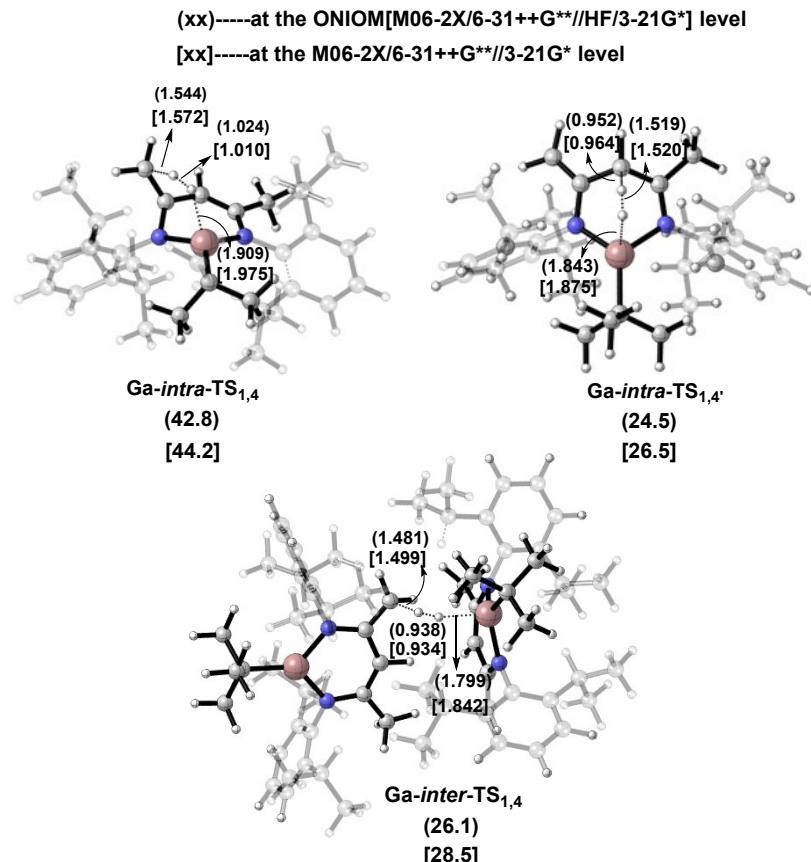
Optimization and frequency calculation in gas phase: ONIOM[M06-2X/6-31++G\*\*//HF/3-21G\*], the keyword “Int = ultrafine” was used.

Solvation Method: M06-2X/6-311++G\*\*

For single-point energy calculation, the SCRF = (benzene, SMD, ExternalIteration) keyword was used.

## S2: Testing the reliability of the present ONIOM approach

To probe the feasibility and reliability of the present ONIOM[M06-2X/6-31++G\*\*//HF/3-21G\*] the approach, the geometric optimization and free energy calculation for the bimoleualr 1,4-addition, 1,4'-addtion, termolecular 1,4-addition of H<sub>2</sub> with the [(BDI)Ga'Bu] complex were performed with a full DFT calculation using the Gen method, respetively. Similar to the ONION calculation, the core region was treated by the M06-2X functional with the 6-31++G\*\* basis set, while the rest region (two Dipp groups) was optimized at the M06-2X/3-21G\* level. Then, single-point energy in benzene solvent (experimentally used) was calculated at the M06-2X/6-311++G\*\* level on the M06-2X/Gen-optimized structures by using the continuum solvation model (SMD).



**Figure S1.** Optimized structures of the TSs for the bimolecular 1,4-addition, 1,4'-addtion, termolecular 1,4-addition of H<sub>2</sub> with the [(BDI)Ga'Bu] complex using ONIOM and Gen method, respectively. The relative free energies (in kcal mol<sup>-1</sup>) are given below.

### S3: Activation-stain model analysis

**Table S1** Activation energy  $\Delta E^\ddagger$ , strain energy  $\Delta E_{\text{strain}}^\ddagger$  and interaction energies  $\Delta E_{\text{int}}^\ddagger$  (all in kcal mol<sup>-1</sup>) for the TSs along the activation of H<sub>2</sub> with the (BDI)Ga'Bu complex .

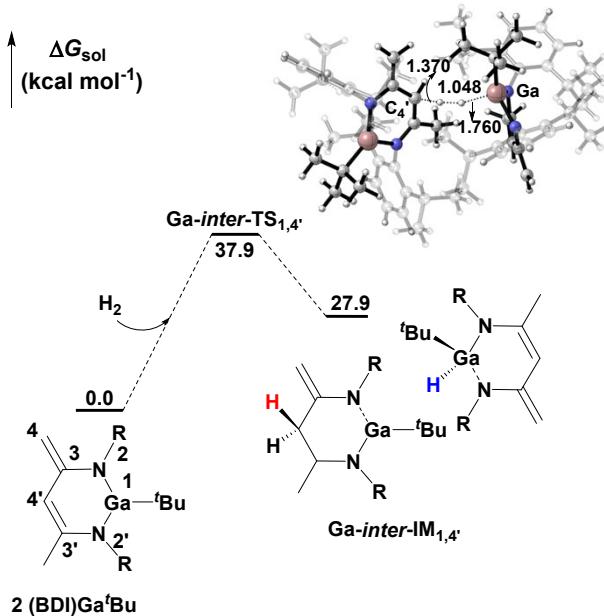
Transition States	$\Delta E_{\text{strain}}^\ddagger$ <sup>a</sup>			$\Delta E_{\text{int}}^\ddagger$ <sup>b</sup>	$\Delta E^\ddagger$ <sup>c</sup>
	(BDI)Ga'Bu	H <sub>2</sub>	total		
Ga- <i>intra</i> -TS <sub>1,4</sub>	33.1	20.3	53.4	-16.6	36.8
Ga- <i>intra</i> -TS <sub>1,2'</sub>	9.0	21.2	30.1	-2.9	27.2
Ga- <i>intra</i> -TS <sub>1,4'</sub>	20.3	12.8	33.1	-15.7	17.4
Ga- <i>inter</i> -TS <sub>1,4</sub>	7.5, 9.5	11.5	28.4	-22.6	5.9
Ga- <i>inter</i> -TS <sub>1,4'</sub>	11.1, 14.1	23.0	48.7	-32.5	16.2

is the strain energy associated with deforming the reactants from their equilibrium geometry to the geometry they adopt in the TS;

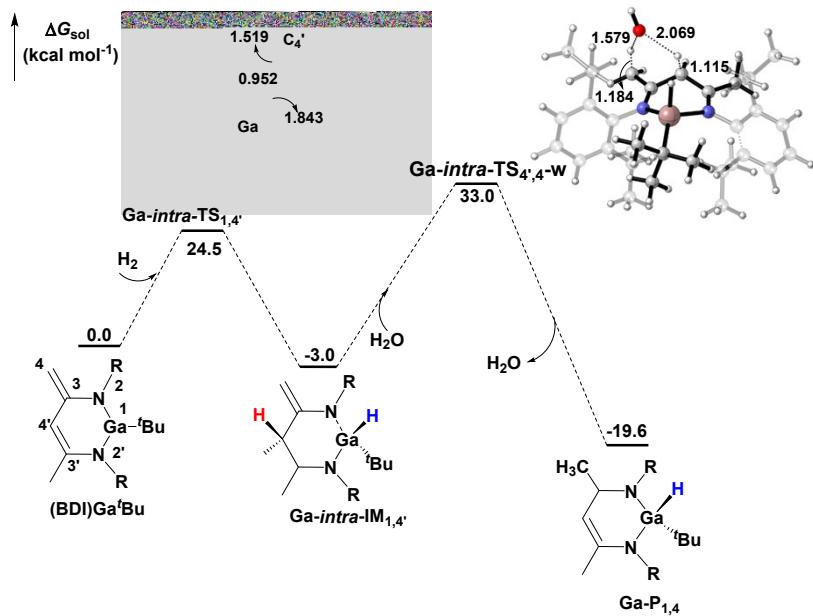
<sup>b</sup> $\Delta E_{\text{int}}^\ddagger$  is the actual interaction energy between the deformed reactants in the TS;

<sup>c</sup> $\Delta E^\ddagger$  is the relative activation energy without zero-point energy correction.

### S4: Intermolecular 1,4'-addition of dihydrogen with the [(BDI)Ga'Bu] complex.

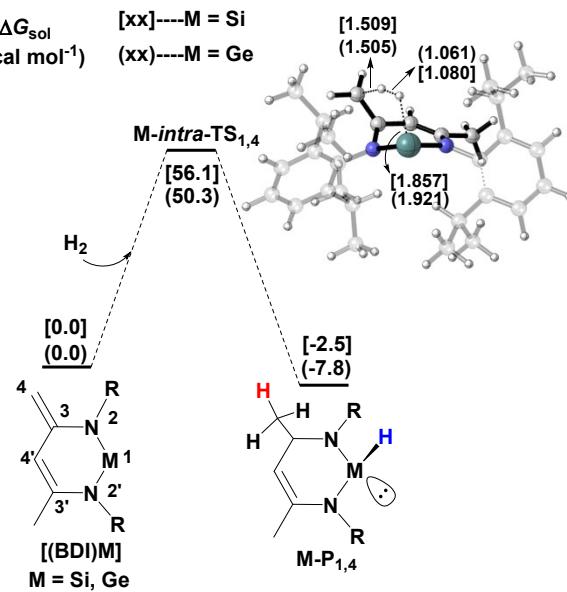


**Figure S2.** Computed free energy profile for intermolecular 1,4'-addition of H<sub>2</sub> with the [(BDI)Ga'Bu] complex. The critical bond distances in the selected key TS are labeled in Å.

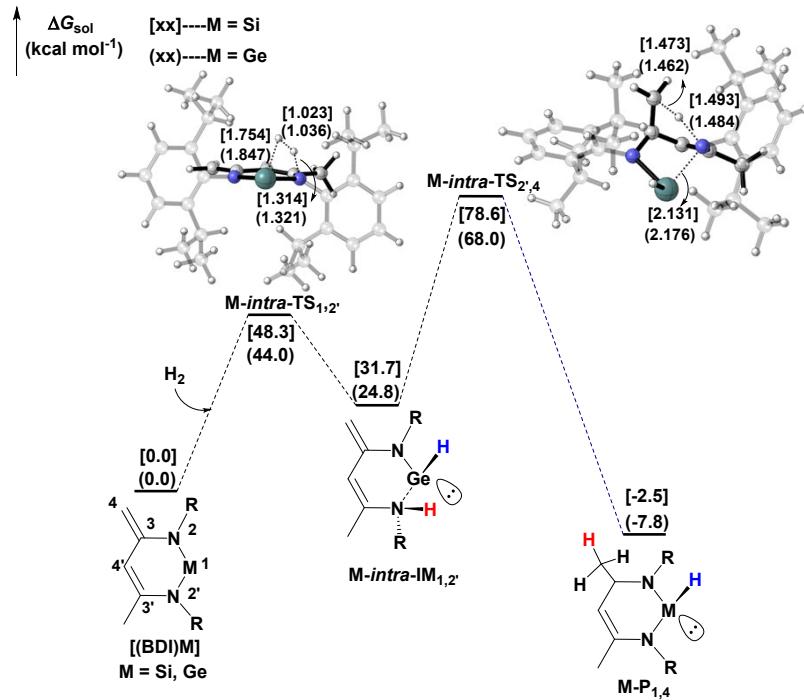


**Figure S3.** Computed free energy profile for water-assisted intermolecular 4',4-H-shift. The critical bond distances in the selected key TS are labeled in Å.

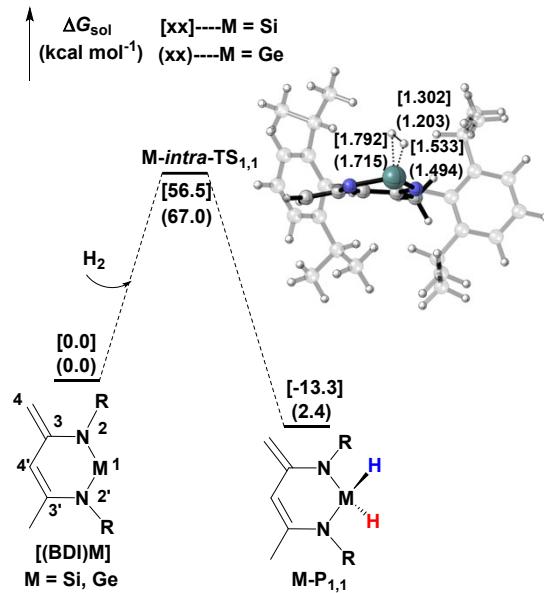
### S5: Mechanisms of dihydrogen activation with the BDI-ligated Group 14 elements.



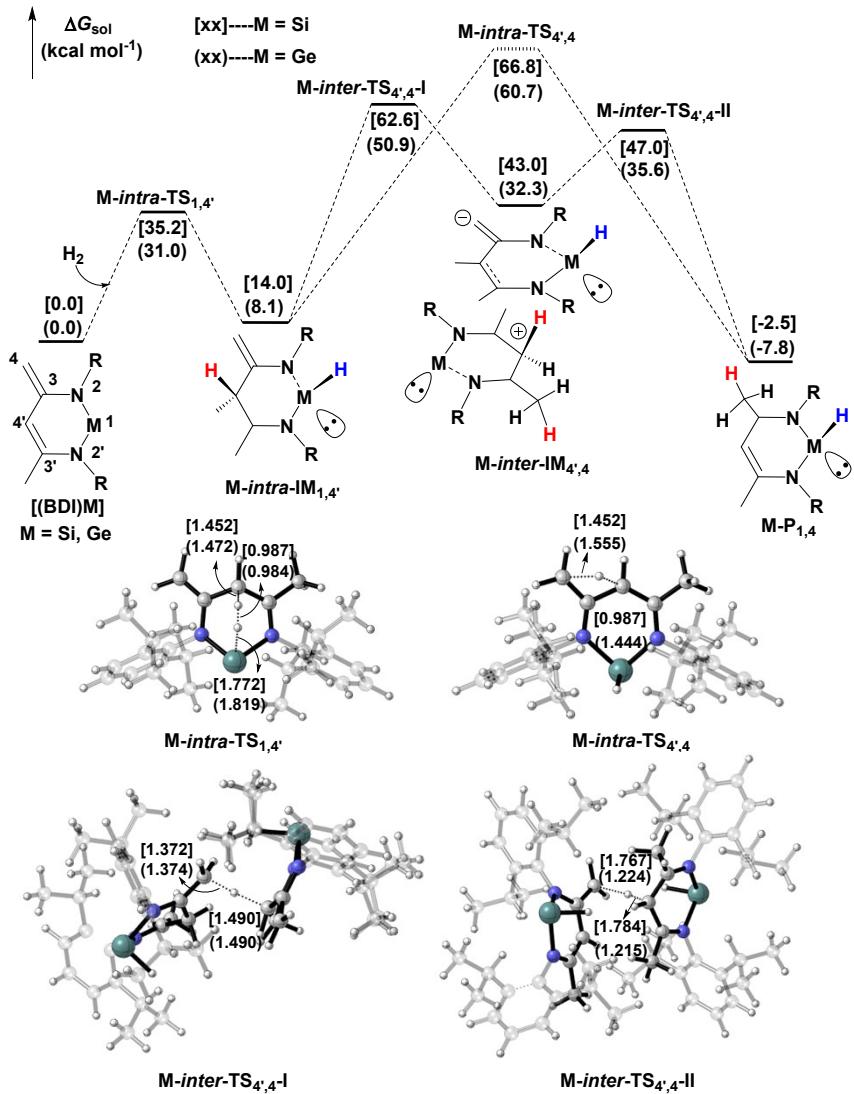
**Figure S4.** Computed free energy profile for intermolecular 1,4-addition of H<sub>2</sub> with the [(BDI)Si] and [(BDI)Ge] compounds. The critical bond distances in the selected key TS are labeled in Å.



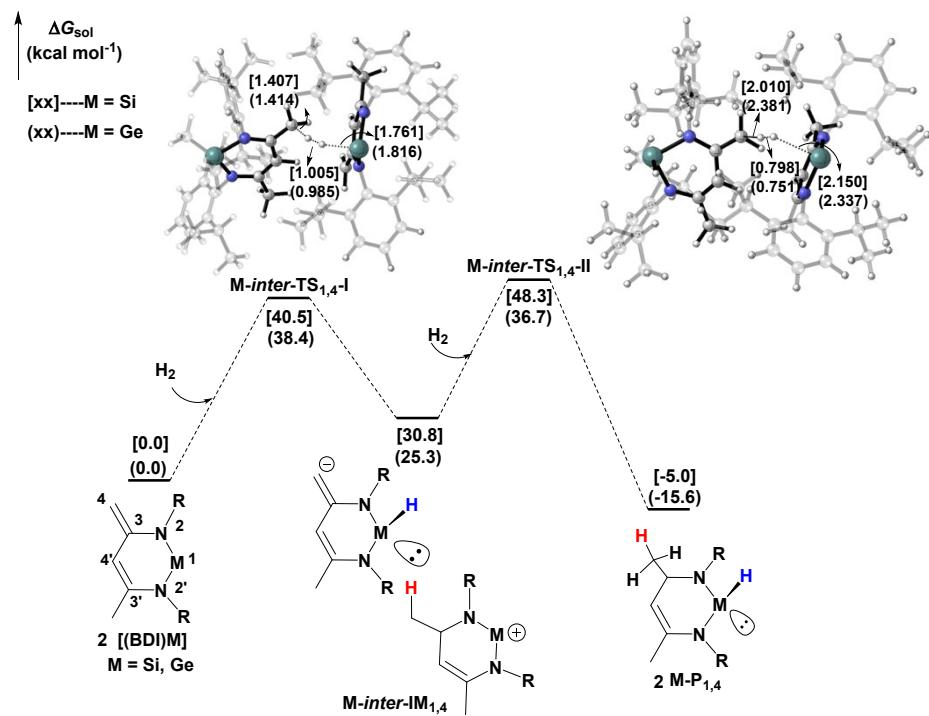
**Figure S5.** Computed free energy profile for the intramolecular 1,2'-addition of  $\text{H}_2$  with the  $[(\text{BDI})\text{Si}]$  and  $[(\text{BDI})\text{Ge}]$  compounds, followed by the 2'4-H-shift. The critical bond distances in the selected key TS are labeled in Å.



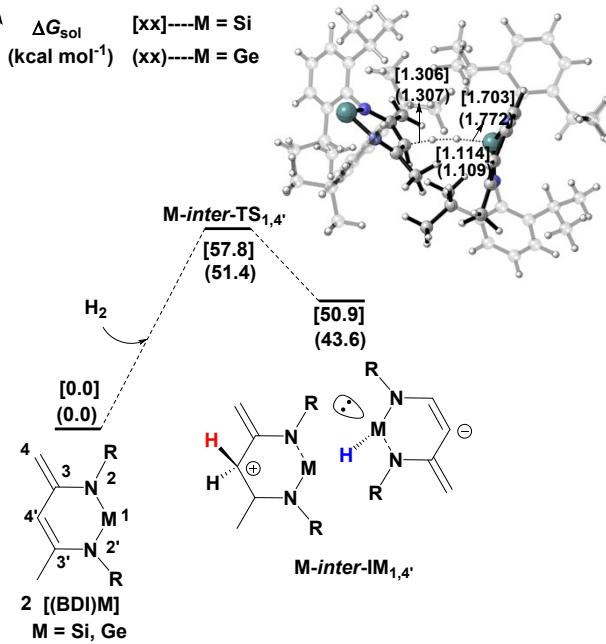
**Figure S6.** Computed free energy profile for the intramolecular 1,1'-addition of  $\text{H}_2$  with the  $[(\text{BDI})\text{Si}]$  and  $[(\text{BDI})\text{Ge}]$  compounds. The critical bond distances in the selected key TS are labeled in Å.



**Figure S7.** Computed free energy profile for the intramolecular 1,4'-addition of  $\text{H}_2$  with the  $[(\text{BDI})\text{Si}]$  and  $[(\text{BDI})\text{Ge}]$  compounds, followed by the intramolecular/intermolecular 4'4'-H-shift. The critical bond distances in the selected key TS are labeled in Å.



**Figure S8.** Computed free energy profile for the two successive intermolecular 1,4-addition of  $\text{H}_2$  with the  $[(\text{BDI})\text{Si}]$  and  $[(\text{BDI})\text{Ge}]$  compounds. The critical bond distances in the selected key TS are labeled in Å.

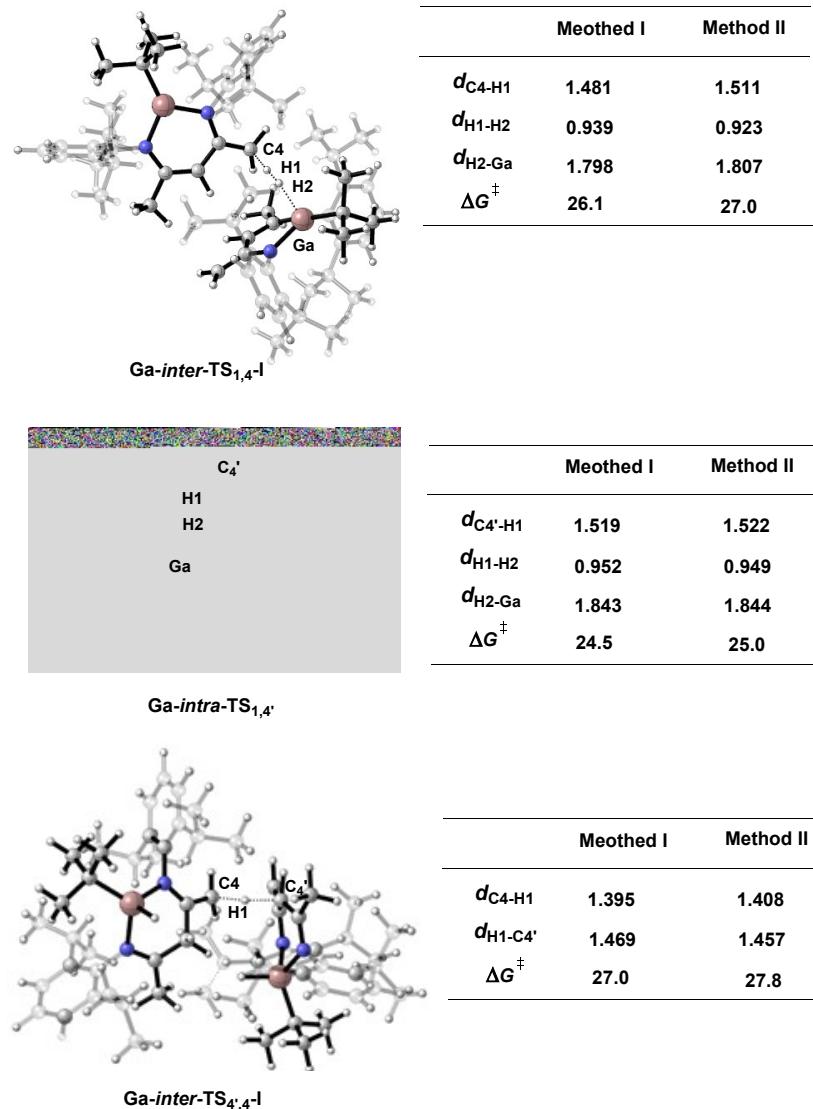


**Figure S9.** Computed free energy profile for the intermolecular 1,4'-addition of  $\text{H}_2$  with the  $[(\text{BDI})\text{Si}]$  and  $[(\text{BDI})\text{Ge}]$  compounds. The critical bond distances in the selected key TS are labeled in Å.

## S6: Solvent effect on the reaction.

**Method I:** The initial optimization and frequency calculation at the ONIOM[M06-2X/6-31++G\*\*//HF/3-21G\*] in gas phase, followed by the single-point energy calculation at the M06-2X/6-311++G\*\* level in benzene solvent with the SMD solvation model.

**Method II:** The initial optimization and frequency calculation at the ONIOM[M06-2X/6-31++G\*\*//HF/3-21G\*] in benzene solvent, followed by the single-point energy calculation at the M06-2X/6-311++G\*\* level in benzene solvent with the SMD solvation model.



**Figure S10.** Optimized-structures of the crucial TSs in dihydrogen activation with the [(BDI)GaBu] complex. The critical bond distances in the selected key TS are labeled in Å, and the free energy barriers are given in kcal mol<sup>-1</sup>.

## S7: Energy summary

**Table S2** Energies of the stationary points involved in H<sub>2</sub> activation with the [(BDI)Ga'Bu] complex.

	$H_c^a$	$G_c^b$	$E_{sol}^c$	$\Delta H_{sol}^d$	$\Delta G_{sol}^e$
H <sub>2</sub>	0.01366	-0.00112	-1.16790	-	-
(BDI)Ga'Bu	0.82963	0.72342	-3321.15598	-	-
Ga- <i>intra</i> -TS <sub>1,4</sub>	0.84220	0.73194	-3322.26529	36.1	42.8
Ga-P <sub>1,4</sub>	0.84874	0.73982	-3322.37265	-27.2	-19.6
Ga- <i>intra</i> -TS <sub>1,4'</sub>	0.84344	0.73362	-3322.29621	17.5	24.5
Ga- <i>intra</i> -IM <sub>1,4'</sub>	0.84918	0.73811	-3322.34445	-9.2	-3.0
Ga- <i>intra</i> -TS <sub>4',4</sub>	0.84316	0.73351	-3322.25585	42.6	49.7
Ga- <i>intra</i> -TS <sub>4',4'-W</sub>	0.87255	0.75828	-3398.72867	15.3	33.0
Ga- <i>inter</i> -TS <sub>4',4'-I</sub>	1.69615	1.49813	-6644.66313	-3.6	24.0
Ga- <i>inter</i> -IM <sub>4',4</sub>	1.70055	1.49863	-6644.68651	-15.6	9.6
Ga- <i>inter</i> -TS <sub>4',4'-II</sub>	1.69684	1.49843	-6644.68005	-13.8	13.5
Ga- <i>intra</i> -TS <sub>1,2'</sub>	0.84446	0.73380	-3322.28052	27.9	34.4
Ga- <i>intra</i> -IM <sub>1,2'</sub>	0.85086	0.74047	-3322.32200	5.9	12.6
Ga- <i>intra</i> -TS <sub>2',4</sub>	0.84356	0.73562	-3322.25780	41.6	49.8
Ga- <i>inter</i> -TS <sub>1,4'-I</sub>	1.67531	1.47803	-6643.47050	7.4	26.1
Ga- <i>inter</i> -IM <sub>1,4</sub>	1.68147	1.48134	-6643.50325	-9.3	7.7
Ga- <i>inter</i> -TS <sub>1,4'-II</sub>	1.69550	1.49929	-6644.68017	-14.7	14.0
Ga- <i>inter</i> -TS <sub>1,4'</sub>	1.67495	1.47882	-6643.45405	17.5	37.0
Ga- <i>inter</i> -IM <sub>1,4'</sub>	1.68016	1.48206	-6643.47171	9.7	27.9

a:  $H_c$  is the enthalpy correction calculated at the ONIOM[M06-2X/6-31++G\*\*//HF/3-21G\*] level in gas phase at 298 K;

b:  $G_c$  is the Gibbs free energy correction calculated at the ONIOM[M06-2X/6-31++G\*\*//HF/3-21G\*] level in gas phase at 298 K;

c:  $E_{sol}$  is the electron energy in the solvent after PCM correction calculated at the M06-2X/(SMD, benzene)//6-311++G(d, p) level;

d:  $\Delta H_{sol}$  is the relative enthalpy energy in the solvent at 298 K  $H_{sol} = H_c + E_{sol}$ .

e:  $\Delta G_{sol}$  is the relative Gibbs free energy in the solvent at 298 K.  $G_{sol} = G_c + E_{sol}$ .

**Table S3** Energies of the stationary points involved in H<sub>2</sub> activation with the [(BDI)Al'Bu] complex.

	<i>H</i> <sub>c</sub>	<i>G</i> <sub>c</sub>	<i>E</i> <sub>sol</sub>	$\Delta H_{\text{sol}}$	$\Delta G_{\text{sol}}$
(BDI)Al'Bu	0.83023	0.72015	-1638.78151	-	-
Al- <i>intra</i> - <b>TS<sub>1,4</sub></b>	0.84272	0.73426	-1639.89439	33.8	44.1
Al- <b>P<sub>1,4</sub></b>	0.84962	0.73982	-1640.00075	-28.6	-19.2
Al- <i>intra</i> - <b>TS<sub>1,4'</sub></b>	0.84369	0.73377	-1639.92464	15.4	24.8
Al- <i>intra</i> - <b>IM<sub>1,4'</sub></b>	0.84931	0.73949	-1639.96921	-9.0	0.4
Al- <i>intra</i> - <b>TS<sub>4',4</sub></b>	0.84324	0.73419	-1639.88056	42.8	52.7
Al- <i>intra</i> - <b>TS<sub>4',4-w</sub></b>	0.87262	0.75984	-1716.34982	17.7	38.7
Al- <i>inter</i> - <b>TS<sub>4',4-I</sub></b>	1.69522	1.49854	-3279.91516	-5.6	27.7
Al- <i>inter</i> - <b>IM<sub>4',4</sub></b>	1.69977	1.49893	-3279.93867	-17.5	13.2
Al- <i>inter</i> - <b>TS<sub>4',4-II</sub></b>	1.69695	1.49999	-3279.92896	-13.2	20.0
Al- <i>intra</i> - <b>TS<sub>1,2'</sub></b>	0.84488	0.73546	-1639.91282	23.6	33.3
Al- <i>intra</i> - <b>IM<sub>1,2'</sub></b>	0.85057	0.74110	-1639.94746	5.4	15.1
Al- <i>intra</i> - <b>TS<sub>2,4</sub></b>	0.84361	0.73663	-1639.88161	42.4	53.6
Al- <i>inter</i> - <b>TS<sub>1,4-I</sub></b>	1.67516	1.47810	-3278.72599	3.7	27.5
Al- <i>inter</i> - <b>IM<sub>1,4</sub></b>	1.68015	1.47813	-3278.75338	-10.3	10.3
Al- <i>inter</i> - <b>TS<sub>1,4-II</sub></b>	1.69652	1.50131	-3279.93686	-18.4	15.8
Al- <i>inter</i> - <b>TS<sub>1,4'</sub></b>	1.67477	1.48071	-3278.70990	13.6	39.3
Al- <i>inter</i> - <b>IM<sub>1,4'</sub></b>	1.67968	1.48199	-3278.72371	8.0	31.4

**Table S4** Energies of the stationary points involved in H<sub>2</sub> activation with the [(BDI)Si] complex.

	<i>H</i> <sub>c</sub>	<i>G</i> <sub>c</sub>	<i>E</i> <sub>sol</sub>	$\Delta H_{\text{sol}}$	$\Delta G_{\text{sol}}$
[(BDI)Si]	0.70083	0.60241		-	-
Si- <i>intra-TS</i> <sub>1,4</sub>	0.71364	0.61678	-1529.08512	45.9	56.1
Si- <b>P</b> <sub>1,4</sub>	0.72182	0.62250	-1529.184303	-11.2	-2.5
Si- <i>intra-TS</i> <sub>1,4'</sub>	0.71530	0.61785	-1529.119587	25.3	35.2
Si- <i>intra-IM</i> <sub>1,4'</sub>	0.72096	0.62123	-1529.156735	5.5	14.0
Si- <i>intra-TS</i> <sub>4,4</sub>	0.71513	0.61802	-1529.069388	56.7	66.8
Si- <i>inter-TS</i> <sub>4,4-I</sub>	1.43829	1.26276	-3058.278638	30.7	62.6
Si- <i>inter-IM</i> <sub>4,4</sub>	1.44291	1.26590	-3058.312993	12.0	43.0
Si- <i>inter-TS</i> <sub>4,4-II</sub>	1.43958	1.26588	-3058.306584	13.9	47.0
Si- <i>intra-TS</i> <sub>1,2</sub>	0.71530	0.61785	-1529.119587	25.3	35.2
Si- <i>intra-IM</i> <sub>1,2</sub>	0.72096	0.62123	-1529.156735	5.5	14.0
Si- <i>intra-TS</i> <sub>2,4</sub>	0.71513	0.61802	-1529.069388	56.7	66.8
Si- <i>intra-TS</i> <sub>1,1</sub>	0.71512	0.61738	-1529.085097	46.8	56.5
Si- <b>P</b> <sub>1,1</sub>	0.71834	0.61993	-1529.198947	-22.6	-13.3
Si- <i>inter-TS</i> <sub>1,4-I</sub>	1.41677	1.24306	-3057.125187	16.7	40.5
Si- <i>inter-IM</i> <sub>1,4</sub>	1.42243	1.24541	-3057.142906	9.1	30.8
Si- <i>inter-TS</i> <sub>1,4-II</sub>	1.43829	1.26369	-3058.301704	16.2	48.7
Si- <i>inter-TS</i> <sub>1,4'</sub>	1.41640	1.24327	-3057.097821	33.6	57.8
Si- <i>inter-IM</i> <sub>1,4'</sub>	1.42159	1.24495	-3057.110493	28.9	50.9

**Table S5** Energies of the stationary points involved in H<sub>2</sub> activation with the [(BDI)Ge] complex.

	<i>H</i> <sub>c</sub>	<i>G</i> <sub>c</sub>	<i>E</i> <sub>sol</sub>	$\Delta H_{\text{sol}}$	$\Delta G_{\text{sol}}$
[(BDI)Ge]	0.70097	0.60217		-	-
Ge- <i>intra-TS</i> <sub>1,4</sub>	0.71338	0.61503	-3316.584038	40.8	50.3
Ge- <b>P</b> <sub>1,4</sub>	0.72182	0.62222	-3316.683806	-16.5	-7.8
Ge- <i>intra-TS</i> <sub>1,4'</sub>	0.71499	0.61596	-3316.615778	21.9	31.0
Ge- <i>intra-IM</i> <sub>1,4'</sub>	0.72078	0.62002	-3316.656343	0.0	8.1
Ge- <i>intra-TS</i> <sub>4',4</sub>	0.71474	0.61620	-3316.568667	51.3	60.7
Ge- <i>inter-TS</i> <sub>4',4-I</sub>	1.43816	1.26062	-6633.277934	19.8	50.9
Ge- <i>inter-IM</i> <sub>4',4</sub>	1.44289	1.26514	-6633.311866	1.4	32.4
Ge- <i>inter-TS</i> <sub>4',4-II</sub>	1.43962	1.26397	-6633.305674	3.3	35.6
Ge- <i>intra-TS</i> <sub>1,2'</sub>	0.71549	0.61753	-3316.59662	34.2	44.0
Ge- <i>intra-IM</i> <sub>1,2'</sub>	0.72256	0.62432	-3316.634016	15.2	24.8
Ge- <i>intra-TS</i> <sub>2',4</sub>	0.71497	0.61731	-3316.558075	58.1	68.0
Ge- <i>intra-TS</i> <sub>1,1</sub>	0.71460	0.61512	-3316.557569	58.1	67.0
Ge- <b>P</b> <sub>1,1</sub>	0.71870	0.61877	-3316.664196	-6.2	2.4
Ge- <i>inter-TS</i> <sub>1,4-I</sub>	1.41740	1.24394	-6632.112095	14.0	38.4
Ge- <i>inter-IM</i> <sub>1,4</sub>	1.42310	1.24428	-6632.133278	4.3	25.3
Ge- <i>inter-TS</i> <sub>1,4-II</sub>	1.43869	1.26215	-6633.302041	5.0	
Ge- <i>inter-TS</i> <sub>1,4'</sub>	1.41753	1.24218	-6632.089575	28.2	51.4
Ge- <i>inter-IM</i> <sub>1,4'</sub>	1.42187	1.24322	-6632.103067	22.5	43.6

## S8: Cartesian coordinates of the optimized structures involved in this work

H <sub>2</sub>						
1	0.000000000	0.000000000	0.369040000	1	-3.132322000	-0.879796000
1	0.000000000	0.000000000	-0.369040000	1	-2.212454000	-0.002428000
				1	-5.164989000	-2.112992000
				1	-6.200333000	0.005787000
				1	-5.159445000	2.121076000
				6	0.808905000	1.232161000
				1	-1.955117000	0.877840000
				1	-1.956815000	-0.877539000
				6	-1.368560000	-0.000451000
				6	0.806629000	-1.237306000
				1	0.855678000	-1.232217000
				1	0.337359000	-2.179780000
				1	1.831676000	-1.228165000
				31	-0.036971000	-0.001326000
				6	2.764505000	-2.569078000
				1	1.699679000	-2.408920000
				6	2.759109000	2.569073000
				1	1.694387000	2.407123000
				6	3.267628000	-3.140698000
				1	4.340951000	-3.292647000
				1	3.039358000	-2.465812000
				6	2.794795000	-4.097886000
				6	3.016244000	-3.613685000
				1	2.406648000	-4.491520000
				1	2.768788000	-3.229017000
				1	4.051352000	-3.933260000
				6	3.258518000	3.141924000
				1	4.331641000	3.295822000
				1	2.783551000	4.098293000
				1	3.030018000	2.466785000
				6	3.011115000	3.613885000
				1	2.766905000	3.228341000
				1	2.399031000	4.490353000
				1	4.045485000	3.935898000
				6	-2.846056000	-2.544123000
						0.374006000

1	-2.075377000	-2.330651000	1.098147000	6	-4.692114000	1.198313000	-0.709033000
6	-2.179338000	-3.258090000	-0.819563000	6	-3.475801000	1.217674000	-0.040493000
1	-2.894575000	-3.428772000	-1.615914000	6	0.024409000	-0.001202000	-2.367755000
1	-1.369936000	-2.657035000	-1.211840000	1	-1.278116000	-0.000825000	-4.088454000
1	-1.769644000	-4.214294000	-0.511104000	1	0.335629000	2.176328000	-2.549219000
6	-3.880578000	-3.475828000	1.040825000	1	0.840708000	1.227342000	-3.948165000
1	-3.379690000	-4.351797000	1.439091000	1	1.828918000	1.221060000	-2.482394000
1	-4.388711000	-2.972396000	1.854902000	1	-0.051436000	-0.001051000	3.825938000
1	-4.625297000	-3.814086000	0.330460000	1	5.231042000	-2.113310000	-0.748485000
6	-2.839108000	2.544371000	0.377021000	1	6.366450000	0.001483000	-1.183419000
1	-2.070212000	2.328049000	1.102217000	1	5.228925000	2.115313000	-0.749224000
6	-2.168143000	3.256535000	-0.815246000	1	3.372298000	0.000299000	2.692943000
1	-1.755615000	4.211202000	-0.505808000	1	2.159604000	-0.000073000	4.094757000
1	-1.360188000	2.652894000	-1.206560000	1	-3.130514000	0.877522000	2.878477000
1	-2.881578000	3.429924000	-1.612626000	1	-3.130637000	-0.879605000	2.878544000
6	-3.871351000	3.479382000	1.042703000	1	-2.205742000	-0.001060000	4.107191000
1	-4.613649000	3.820852000	0.331342000	1	-5.184064000	-2.114216000	-0.955943000
1	-4.382644000	2.977274000	1.855621000	1	-6.224415000	0.004042000	-1.582581000
1	-3.367922000	4.353254000	1.442362000	1	-5.179470000	2.119942000	-0.955532000
				6	0.799794000	1.232094000	-2.848206000
[(BDI)Ga <sup>t</sup> Bu] in benzene solvent				1	-1.960738000	0.878320000	-2.716947000
7	-1.505375000	-0.001337000	0.790882000	1	-1.961191000	-0.879574000	-2.716944000
6	-1.287192000	-0.001151000	2.170651000	6	-1.373712000	-0.000778000	-2.991580000
6	-0.056800000	-0.001011000	2.741313000	6	0.798763000	-1.235474000	-2.847370000
6	1.295429000	-0.000588000	2.168224000	1	0.839297000	-1.231779000	-3.947343000
7	1.434429000	-0.000622000	0.766112000	1	0.334247000	-2.179198000	-2.547296000
6	2.778821000	-0.000067000	0.219246000	1	1.828027000	-1.224575000	-2.481924000
6	3.427668000	-1.218996000	-0.044513000	31	-0.040963000	-0.000813000	-0.383124000
6	4.720807000	-1.192770000	-0.550148000	6	2.769237000	-2.572071000	0.238700000
6	5.365527000	0.001050000	-0.797683000	1	1.705019000	-2.412524000	0.326889000
6	4.719630000	1.194327000	-0.550534000	6	2.766653000	2.571919000	0.237771000
6	3.426482000	1.219420000	-0.044907000	1	1.702568000	2.411366000	0.325728000
6	2.344875000	-0.000092000	3.027193000	6	3.284188000	-3.158068000	1.573669000
6	-2.505338000	-0.001077000	3.058127000	1	4.357002000	-3.313391000	1.523068000
6	-2.847708000	0.000210000	0.247172000	1	3.066868000	-2.493722000	2.396893000
6	-3.478419000	-1.215830000	-0.040741000	1	2.811513000	-4.116421000	1.769113000
6	-4.694700000	-1.193714000	-0.709260000	6	3.013236000	-3.606126000	-0.883422000
6	-5.288923000	0.002979000	-1.057936000	1	2.399355000	-4.483479000	-0.704382000

1	2.765140000	-3.212237000	-1.860151000	6	-1.226600000	-0.139679000	2.038251000
1	4.046623000	-3.931775000	-0.899940000	7	-1.475709000	0.018298000	0.699296000
6	3.280697000	3.158810000	1.572695000	6	-2.837596000	0.301817000	0.247316000
1	4.353351000	3.315297000	1.522254000	6	-3.138555000	1.671194000	0.113457000
1	2.806933000	4.116691000	1.767807000	6	-2.092889000	2.744627000	0.400789000
1	3.063960000	2.494426000	2.396045000	6	-2.397369000	3.442563000	1.744125000
6	3.009900000	3.605876000	-0.884597000	6	-1.998986000	3.781724000	-0.738465000
1	2.762196000	3.211525000	-1.861242000	6	-4.411502000	2.057554000	-0.265696000
1	2.395287000	4.482775000	-0.705831000	6	-5.387479000	1.119683000	-0.531403000
1	4.043026000	3.932357000	-0.901113000	6	-5.083532000	-0.217129000	-0.432312000
6	-2.853877000	-2.545369000	0.383877000	6	-3.818207000	-0.656231000	-0.051947000
1	-2.108737000	-2.335178000	1.135060000	6	-3.596738000	-2.169469000	-0.018515000
6	-2.140862000	-3.228222000	-0.800171000	6	-4.535053000	-2.872959000	0.993052000
1	-2.830884000	-3.408700000	-1.616835000	6	-3.859504000	-2.794299000	-1.411304000
1	-1.335214000	-2.604712000	-1.164860000	6	-1.924816000	-1.086986000	2.785060000
1	-1.715994000	-4.178469000	-0.491887000	6	2.354351000	1.148475000	2.776407000
6	-3.891298000	-3.505532000	1.002086000	6	2.779398000	0.258714000	0.119435000
1	-3.385172000	-4.375533000	1.408121000	6	3.081539000	1.376928000	-0.667887000
1	-4.439367000	-3.026894000	1.805822000	6	4.327434000	1.449137000	-1.275203000
1	-4.603374000	-3.854023000	0.263321000	6	5.255723000	0.441694000	-1.116916000
6	-2.848706000	2.545883000	0.384520000	6	4.955810000	-0.650862000	-0.329124000
1	-2.103085000	2.334035000	1.134742000	6	3.727420000	-0.757215000	0.305719000
6	-2.135999000	3.228738000	-0.799732000	6	3.439806000	-1.973402000	1.187717000
1	-1.709576000	4.178183000	-0.491133000	6	4.556864000	-2.204040000	2.229627000
1	-1.331534000	2.604485000	-1.165797000	6	3.249700000	-3.246283000	0.334180000
1	-2.826585000	3.410767000	-1.615571000	6	2.087417000	2.521112000	-0.859440000
6	-3.884127000	3.506935000	1.004702000	6	1.803347000	2.802450000	-2.351538000
1	-4.596824000	3.856628000	0.267108000	6	2.602940000	3.815227000	-0.188668000
1	-4.431638000	3.028418000	1.808892000	6	0.133681000	-1.443199000	-2.055835000
1	-3.376428000	4.376091000	1.410583000	1	1.451349000	-1.564113000	-3.760427000
				1	-0.339630000	-3.195010000	-3.247580000
<b>Ga-intra-TS<sub>1,4</sub></b>				1	-1.207520000	-3.155961000	-1.706074000
1	-0.967246000	-1.939967000	1.925206000	1	0.503466000	-3.574112000	-1.741042000
1	-0.368868000	-2.222828000	1.144195000	1	-0.022604000	0.545896000	3.678829000
31	0.042446000	-0.877363000	-0.146660000	1	-1.141868000	2.249229000	0.485265000
7	1.464030000	0.117867000	0.708078000	1	-1.635114000	4.182583000	1.967049000
6	1.227944000	0.525818000	1.993918000	1	-3.358999000	3.942519000	1.704342000
6	0.015365000	0.365068000	2.610746000	1	-2.419495000	2.721625000	2.552285000

1	-1.178590000	4.465410000	-0.543445000	6	1.507861000	-1.254393000	-2.705001000
1	-2.905429000	4.369561000	-0.821269000	6	-0.874959000	-0.557543000	-2.806525000
1	-1.819940000	3.292942000	-1.689399000	1	-0.887818000	-0.823590000	-3.874471000
1	-4.643849000	3.099540000	-0.352141000	1	-0.607376000	0.502905000	-2.735530000
1	-6.372530000	1.429561000	-0.820064000	1	-1.893918000	-0.654433000	-2.425830000
1	-5.841136000	-0.940860000	-0.653643000				
1	-2.572332000	-2.364504000	0.260401000				<b>Ga-P<sub>1,4</sub></b>
1	-4.467966000	-2.448517000	1.984286000	1	0.022586000	-2.463496000	-0.015494000
1	-4.284837000	-3.926907000	1.054745000	31	0.025544000	-0.914824000	-0.423021000
1	-5.565277000	-2.792583000	0.668069000	7	1.466770000	-0.142255000	0.741979000
1	-3.594894000	-3.846552000	-1.401786000	6	1.263458000	-0.182484000	2.057934000
1	-4.909089000	-2.717797000	-1.667021000	6	-0.004236000	-0.341365000	2.642503000
1	-3.289508000	-2.302592000	-2.184845000	6	-1.270082000	-0.217502000	2.038037000
1	-2.910030000	-1.397462000	2.476742000	7	-1.461171000	-0.161948000	0.721761000
1	-1.670158000	-1.217108000	3.832520000	6	-2.793395000	0.121005000	0.197644000
1	2.024860000	1.391825000	3.786966000	6	-3.132169000	1.448478000	-0.103278000
1	3.217333000	0.483789000	2.832728000	6	-2.149134000	2.588601000	0.151249000
1	2.691513000	2.064208000	2.289205000	6	-2.377765000	3.196866000	1.554184000
1	4.572519000	2.299395000	-1.879534000	6	-2.236935000	3.711866000	-0.903993000
1	6.210266000	0.509378000	-1.600655000	6	-4.390921000	1.715061000	-0.615967000
1	5.685429000	-1.425735000	-0.205727000	6	-5.296867000	0.697232000	-0.842117000
1	2.517981000	-1.797242000	1.719038000	6	-4.953656000	-0.602620000	-0.546163000
1	4.271340000	-3.006500000	2.901555000	6	-3.707019000	-0.915128000	-0.016739000
1	5.487527000	-2.485313000	1.751857000	6	-3.399809000	-2.371306000	0.329145000
1	4.734056000	-1.312249000	2.818753000	6	-4.410643000	-2.928005000	1.358106000
1	3.069214000	-4.104018000	0.973657000	6	-3.409743000	-3.255680000	-0.935544000
1	2.402405000	-3.138456000	-0.329491000	6	-2.430827000	-0.158666000	3.006641000
1	4.131212000	-3.442882000	-0.265048000	6	2.425363000	-0.062113000	3.017880000
1	1.161228000	2.233778000	-0.387748000	6	2.800167000	0.160748000	0.241655000
1	1.059338000	3.586702000	-2.442430000	6	3.097398000	1.482031000	-0.118076000
1	1.428627000	1.920254000	-2.851657000	6	4.369431000	1.774704000	-0.580956000
1	2.699576000	3.130502000	-2.864629000	6	5.321511000	0.782112000	-0.713313000
1	1.867145000	4.606510000	-0.289305000	6	5.008008000	-0.518584000	-0.386793000
1	2.795536000	3.663523000	0.865094000	6	3.749615000	-0.853550000	0.098851000
1	3.523045000	4.145993000	-0.656688000	6	3.441795000	-2.313271000	0.430903000
6	-0.255702000	-2.920881000	-2.184976000	6	4.508045000	-2.936485000	1.358936000
1	2.288951000	-1.852086000	-2.230616000	6	3.325638000	-3.144885000	-0.865567000
1	1.845337000	-0.218437000	-2.684124000	6	2.032708000	2.572736000	-0.014370000

6	2.158441000	3.646702000	-1.115659000	1	2.526929000	-2.766420000	-1.487928000
6	2.073057000	3.259566000	1.369650000	1	4.251422000	-3.108981000	-1.428370000
6	0.069218000	-0.482034000	-2.393657000	1	1.076862000	2.085037000	-0.124297000
1	1.442733000	0.156518000	-3.941531000	1	1.290016000	4.295683000	-1.085035000
1	-0.181694000	-1.609490000	-4.234427000	1	2.214645000	3.199566000	-2.099906000
1	-1.227169000	-2.170990000	-2.925947000	1	3.034919000	4.266325000	-0.965941000
1	0.488927000	-2.576608000	-2.908833000	1	1.332960000	4.052162000	1.416900000
1	-0.014896000	-0.405591000	3.723302000	1	1.861219000	2.557914000	2.164339000
1	-1.157295000	2.167213000	0.122134000	1	3.051734000	3.694510000	1.540896000
1	-1.685502000	4.014794000	1.726882000	6	-0.229278000	-1.784369000	-3.148263000
1	-3.389077000	3.580515000	1.632484000	1	2.254479000	-0.677751000	-2.610935000
1	-2.228443000	2.460584000	2.331150000	1	1.703048000	0.975525000	-2.397571000
1	-1.408952000	4.399324000	-0.766889000	6	1.444160000	0.017003000	-2.848050000
1	-3.153094000	4.281135000	-0.798357000	6	-0.967999000	0.565461000	-2.799918000
1	-2.190681000	3.315604000	-1.909673000	1	-0.912323000	0.749721000	-3.885241000
1	-4.667286000	2.722722000	-0.847467000	1	-0.786431000	1.520704000	-2.299077000
1	-6.264755000	0.919949000	-1.246091000	1	-1.990858000	0.255598000	-2.569993000
1	-5.661865000	-1.387164000	-0.720882000	1	-2.651730000	-1.178675000	3.336387000
1	-2.411142000	-2.421749000	0.756729000				
1	-4.453945000	-2.310006000	2.245993000				<i>Ga-intra-TS<sub>1,4'</sub> in gas phase</i>
1	-4.121461000	-3.931719000	1.651820000	31	0.006685000	-0.726261000	-0.352482000
1	-5.406175000	-2.977611000	0.932997000	7	1.480888000	-0.028058000	0.725782000
1	-3.153234000	-4.277555000	-0.676856000	6	1.286405000	-0.198316000	2.040798000
1	-4.388972000	-3.256505000	-1.400251000	6	0.061622000	-0.708474000	2.526927000
1	-2.688483000	-2.898567000	-1.655093000	6	-1.306551000	-0.312780000	2.078046000
1	-3.331306000	0.253838000	2.561003000	7	-1.480131000	-0.195097000	0.701049000
1	-2.159171000	0.421367000	3.889993000	6	-2.793644000	0.154653000	0.209988000
1	2.073399000	0.218125000	4.011032000	6	-3.122234000	1.503867000	0.023368000
1	2.928269000	-1.029595000	3.094067000	6	-2.133770000	2.617115000	0.352783000
1	3.165995000	0.658904000	2.678008000	6	-2.601137000	3.413896000	1.590942000
1	4.619093000	2.779103000	-0.853396000	6	-1.926244000	3.570856000	-0.843358000
1	6.299899000	1.023382000	-1.079685000	6	-4.385964000	1.833187000	-0.443973000
1	5.747000000	-1.284329000	-0.508846000	6	-5.317106000	0.855290000	-0.722602000
1	2.486784000	-2.357856000	0.930016000	6	-4.991993000	-0.471387000	-0.532805000
1	4.197409000	-3.933052000	1.654320000	6	-3.738989000	-0.844025000	-0.066549000
1	5.463441000	-3.022888000	0.855527000	6	-3.444664000	-2.325184000	0.159000000
1	4.650517000	-2.342738000	2.253960000	6	-4.207430000	-2.848795000	1.396846000
1	3.105408000	-4.180273000	-0.627832000	6	-3.802637000	-3.182136000	-1.075430000

6	-2.256178000	-0.097603000	3.017756000	1	-2.009537000	-0.200867000	4.066684000
6	2.387986000	0.014239000	3.048311000	1	2.523968000	-0.889183000	3.649465000
6	2.800514000	0.260918000	0.178121000	1	3.335405000	0.281508000	2.588121000
6	3.042087000	1.535405000	-0.348149000	1	2.086682000	0.814169000	3.730783000
6	4.286151000	1.802518000	-0.896292000	1	4.492987000	2.771251000	-1.299368000
6	5.266024000	0.830749000	-0.940439000	1	6.221470000	1.052182000	-1.373388000
6	5.012188000	-0.424342000	-0.433855000	1	5.774700000	-1.174785000	-0.481262000
6	3.783509000	-0.733273000	0.136150000	1	2.622436000	-2.166519000	1.211001000
6	3.553125000	-2.147207000	0.668607000	1	4.419662000	-3.557069000	2.065123000
6	4.674520000	-2.595978000	1.631372000	1	5.617244000	-2.708031000	1.110111000
6	3.428951000	-3.146475000	-0.501574000	1	4.812918000	-1.883201000	2.435108000
6	1.962141000	2.612847000	-0.302913000	1	3.258848000	-4.149232000	-0.123938000
6	2.073317000	3.636004000	-1.451496000	1	2.598319000	-2.879250000	-1.139855000
6	2.006390000	3.349266000	1.054436000	1	4.333455000	-3.151977000	-1.098359000
6	0.022206000	-0.898507000	-2.334733000	1	1.005823000	2.119546000	-0.388588000
1	1.290234000	-0.477331000	-4.035080000	1	1.200579000	4.277790000	-1.445280000
1	-0.177415000	-2.462754000	-3.823457000	1	2.126966000	3.143573000	-2.415286000
1	-1.033939000	-2.825653000	-2.318598000	1	2.945604000	4.268496000	-1.336152000
1	0.724412000	-2.978388000	-2.393801000	1	1.231755000	4.107537000	1.099240000
1	0.085006000	-0.928907000	3.590894000	1	1.852258000	2.660761000	1.874009000
1	-1.192074000	2.149824000	0.590413000	1	2.969436000	3.830858000	1.182659000
1	-1.877704000	4.186422000	1.834881000	6	-0.125241000	-2.374746000	-2.727954000
1	-3.555760000	3.891619000	1.399752000	1	2.212395000	-0.856860000	-2.572561000
1	-2.702973000	2.756274000	2.443281000	1	1.443034000	0.718355000	-2.742531000
1	-1.178684000	4.317850000	-0.596747000	6	1.317545000	-0.349372000	-2.941974000
1	-2.843058000	4.091182000	-1.093240000	6	-1.157343000	-0.107393000	-2.915527000
1	-1.594227000	3.029447000	-1.720870000	1	-1.140746000	-0.176717000	-4.013894000
1	-4.646290000	2.863057000	-0.585260000	1	-1.103751000	0.953359000	-2.652613000
1	-6.291305000	1.124835000	-1.080925000	1	-2.125389000	-0.479371000	-2.571268000
1	-5.723017000	-1.225742000	-0.743303000	1	0.166622000	-1.879469000	1.565331000
1	-2.388900000	-2.429439000	0.352428000	1	0.221603000	-2.235168000	0.683469000
1	-3.985248000	-3.899663000	1.556639000		<i>Ga-intra-TS<sub>1,4'</sub> in benzene</i>		
1	-5.277269000	-2.745142000	1.252515000				
1	-3.917455000	-2.296020000	2.279296000	31	0.000369000	-0.718932000	-0.366560000
1	-3.464523000	-4.202497000	-0.925676000	7	1.482518000	-0.041039000	0.723018000
1	-4.873930000	-3.209766000	-1.234581000	6	1.285009000	-0.215551000	2.036212000
1	-3.337584000	-2.793760000	-1.972892000	6	0.052535000	-0.713672000	2.517625000
1	-3.266905000	0.180114000	2.753751000	6	-1.306389000	-0.289445000	2.071569000

7	-1.484447000	-0.171562000	0.696208000	1	-2.875920000	4.053783000	-1.217918000
6	-2.804900000	0.166330000	0.211540000	1	-1.607201000	2.992390000	-1.805238000
6	-3.139188000	1.509892000	-0.009911000	1	-4.672426000	2.848921000	-0.642467000
6	-2.152320000	2.636595000	0.278644000	1	-6.322171000	1.095833000	-1.065760000
6	-2.615962000	3.471158000	1.492316000	1	-5.746503000	-1.244702000	-0.664858000
6	-1.953367000	3.554382000	-0.945771000	1	-2.401100000	-2.411278000	0.436024000
6	-4.409185000	1.823774000	-0.473652000	1	-3.988593000	-3.868891000	1.658099000
6	-5.343247000	0.837389000	-0.711199000	1	-5.297811000	-2.747843000	1.310587000
6	-5.014176000	-0.483233000	-0.485380000	1	-3.962940000	-2.250886000	2.346964000
6	-3.754790000	-0.840775000	-0.023743000	1	-3.456562000	-4.211371000	-0.824898000
6	-3.455678000	-2.316670000	0.233004000	1	-4.868288000	-3.229678000	-1.160496000
6	-4.227621000	-2.826002000	1.469981000	1	-3.326966000	-2.818892000	-1.890981000
6	-3.798366000	-3.194275000	-0.990852000	1	-3.260295000	0.233874000	2.759717000
6	-2.251543000	-0.058426000	3.015670000	1	-2.001661000	-0.164805000	4.064249000
6	2.385473000	-0.032541000	3.048437000	1	2.515561000	-0.952149000	3.626494000
6	2.805259000	0.255431000	0.182470000	1	3.336570000	0.242155000	2.600700000
6	3.059161000	1.544039000	-0.302566000	1	2.088063000	0.748534000	3.754133000
6	4.304871000	1.816715000	-0.846973000	1	4.521209000	2.797582000	-1.215926000
6	5.274018000	0.836824000	-0.928060000	1	6.229781000	1.062030000	-1.359133000
6	5.011264000	-0.430253000	-0.454568000	1	5.768268000	-1.184957000	-0.524241000
6	3.782840000	-0.744610000	0.113383000	1	2.613600000	-2.195097000	1.153881000
6	3.553947000	-2.165448000	0.629019000	1	4.403176000	-3.568326000	2.043923000
6	4.662894000	-2.608846000	1.608253000	1	5.612300000	-2.723366000	1.098980000
6	3.463863000	-3.160242000	-0.546886000	1	4.793528000	-1.894266000	2.412031000
6	2.001561000	2.640431000	-0.206796000	1	3.288840000	-4.165733000	-0.177300000
6	2.037726000	3.621423000	-1.395783000	1	2.649190000	-2.897758000	-1.207960000
6	2.167573000	3.416929000	1.117796000	1	4.383517000	-3.162892000	-1.120768000
6	0.014296000	-0.918954000	-2.349159000	1	1.034814000	2.162187000	-0.195463000
1	1.279252000	-0.505969000	-4.055096000	1	1.189235000	4.293293000	-1.336954000
1	-0.145389000	-2.515793000	-3.809385000	1	1.988566000	3.095993000	-2.342676000
1	-1.018174000	-2.860098000	-2.310678000	1	2.934710000	4.229052000	-1.385995000
1	0.741546000	-2.992881000	-2.358209000	1	1.403200000	4.182547000	1.206539000
1	0.073572000	-0.939116000	3.580704000	1	2.082413000	2.755521000	1.970829000
1	-1.207697000	2.180762000	0.525502000	1	3.139891000	3.896731000	1.151393000
1	-1.886813000	4.244878000	1.715749000	6	-0.109160000	-2.404044000	-2.714930000
1	-3.566880000	3.951929000	1.288409000	1	2.203609000	-0.858930000	-2.589310000
1	-2.724779000	2.842496000	2.366437000	1	1.419174000	0.708182000	-2.779253000
1	-1.218875000	4.320603000	-0.719708000	6	1.303411000	-0.363943000	-2.963187000

6	-1.171494000	-0.162068000	-2.958490000	6	-1.891299000	3.621253000	1.036425000
1	-1.148418000	-0.265316000	-4.054588000	6	-1.963725000	3.242130000	-1.456333000
1	-1.136876000	0.908121000	-2.732811000	6	0.024846000	-0.298018000	2.468827000
1	-2.137689000	-0.538705000	-2.612976000	1	-1.377561000	-0.104113000	4.112931000
1	0.142632000	-1.881849000	1.544997000	1	0.831148000	-1.149418000	4.301854000
1	0.196016000	-2.234633000	0.665396000	1	1.866798000	-1.401294000	2.890425000
				1	0.396741000	-2.370976000	3.092661000
Ga-intra-IM <sub>1,4'</sub> in gas phase				1	-0.077506000	-1.330862000	-3.449725000
31	0.041338000	-0.901366000	0.558243000	1	1.188878000	2.142529000	-0.376953000
7	-1.517315000	-0.263160000	-0.689961000	1	1.771679000	3.975664000	-1.983899000
6	-1.312503000	-0.470874000	-1.944801000	1	3.469523000	3.544208000	-1.827646000
6	-0.046127000	-1.163460000	-2.373069000	1	2.333660000	2.407199000	-2.547462000
6	1.265553000	-0.487098000	-2.011441000	1	1.444601000	4.411039000	0.481014000
7	1.431130000	-0.267216000	-0.654876000	1	3.180669000	4.247637000	0.586843000
6	2.770947000	0.080814000	-0.215720000	1	2.150560000	3.327340000	1.672623000
6	3.147306000	1.425679000	-0.070943000	1	4.737082000	2.747924000	0.443163000
6	2.179824000	2.564951000	-0.379263000	1	6.349071000	0.975752000	0.910975000
6	2.457107000	3.157361000	-1.780942000	1	5.700666000	-1.364174000	0.647390000
6	2.246839000	3.703304000	0.663512000	1	2.318125000	-2.504829000	-0.347332000
6	4.440153000	1.724804000	0.334438000	1	3.865552000	-4.005530000	-1.567450000
6	5.354106000	0.726437000	0.597771000	1	5.196830000	-2.899316000	-1.258467000
6	4.983846000	-0.592566000	0.450786000	1	3.859248000	-2.398889000	-2.288292000
6	3.703554000	-0.937787000	0.040870000	1	3.395776000	-4.297293000	0.905615000
6	3.376657000	-2.416395000	-0.167347000	1	4.789489000	-3.291897000	1.250509000
6	4.124274000	-2.963358000	-1.405120000	1	3.229606000	-2.899748000	1.956055000
6	3.721333000	-3.275016000	1.068954000	1	3.121754000	0.179094000	-2.812157000
6	2.139340000	-0.227900000	-3.007899000	1	1.879356000	-0.461855000	-4.032711000
6	-2.284246000	-0.154530000	-3.040616000	1	-2.561589000	-1.086617000	-3.544120000
6	-2.829986000	0.192771000	-0.220473000	1	-3.180453000	0.349000000	-2.689373000
6	-3.019484000	1.542623000	0.081032000	1	-1.769508000	0.462688000	-3.784040000
6	-4.271129000	1.947172000	0.517991000	1	-4.444583000	2.978035000	0.745621000
6	-5.297128000	1.036658000	0.673694000	1	-6.257967000	1.365894000	1.016367000
6	-5.082210000	-0.296327000	0.399853000	1	-5.879217000	-0.998020000	0.538779000
6	-3.848689000	-0.747840000	-0.050981000	1	-2.657448000	-2.408774000	-0.676305000
6	-3.662846000	-2.240627000	-0.325479000	1	-4.451650000	-3.782000000	-1.631585000
6	-4.650565000	-2.740307000	-1.403441000	1	-5.673566000	-2.663890000	-1.055077000
6	-3.830828000	-3.061527000	0.971606000	1	-4.562382000	-2.166050000	-2.317968000
6	-1.887421000	2.551980000	-0.076086000	1	-3.675234000	-4.114908000	0.764651000

1	-3.107021000	-2.750645000	1.711809000	6	3.682242000	-3.291638000	1.061512000
1	-4.824955000	-2.938264000	1.384472000	6	2.140536000	-0.224047000	-3.005047000
1	-0.957473000	2.008476000	-0.018106000	6	-2.282115000	-0.196038000	-3.051101000
1	-0.984226000	4.210128000	0.973375000	6	-2.833179000	0.187484000	-0.223812000
1	-1.936118000	3.167017000	2.017887000	6	-3.033815000	1.540312000	0.061035000
1	-2.730359000	4.298364000	0.928605000	6	-4.279343000	1.935879000	0.525359000
1	-1.151109000	3.951980000	-1.566468000	6	-5.290739000	1.015430000	0.717036000
1	-1.892401000	2.522768000	-2.261161000	6	-5.069085000	-0.317819000	0.448127000
1	-2.903048000	3.774884000	-1.554730000	6	-3.841025000	-0.761077000	-0.026651000
6	0.824370000	-1.369616000	3.2222809000	6	-3.654724000	-2.253008000	-0.309227000
1	-1.921031000	-1.231200000	2.866256000	6	-4.652240000	-2.744220000	-1.381317000
1	-2.014283000	0.506548000	2.577941000	6	-3.811756000	-3.085317000	0.980753000
6	-1.401210000	-0.280408000	3.025257000	6	-1.926454000	2.567340000	-0.152661000
6	0.681984000	1.056845000	2.718458000	6	-1.912913000	3.657144000	0.938567000
1	0.663029000	1.296534000	3.794175000	6	-2.071340000	3.231998000	-1.539627000
1	0.166205000	1.866958000	2.196015000	6	0.015533000	-0.261261000	2.477221000
1	1.726483000	1.062806000	2.396897000	1	-1.370490000	-0.126487000	4.141604000
1	-0.059215000	-2.142562000	-1.868454000	1	0.874265000	-1.080928000	4.302003000
1	-0.236664000	-2.469134000	0.348927000	1	1.904651000	-1.293135000	2.881122000
				1	0.475159000	-2.318395000	3.099532000
Ga-intra-IM <sub>1,4'</sub> in benzene solvent				1	-0.064498000	-1.343551000	-3.442257000
31	0.031723000	-0.866187000	0.564573000	1	1.227165000	2.169790000	-0.345943000
7	-1.519165000	-0.263236000	-0.696972000	1	1.837990000	4.004604000	-1.943447000
6	-1.313046000	-0.485532000	-1.949888000	1	3.527138000	3.538442000	-1.801275000
6	-0.038051000	-1.169884000	-2.366811000	1	2.364952000	2.432370000	-2.525278000
6	1.268209000	-0.4836668000	-2.005412000	1	1.526199000	4.423279000	0.529563000
7	1.437691000	-0.256331000	-0.650347000	1	3.260744000	4.237133000	0.613434000
6	2.782747000	0.074842000	-0.213594000	1	2.232009000	3.325949000	1.706538000
6	3.177712000	1.414154000	-0.058063000	1	4.787646000	2.711475000	0.460550000
6	2.226511000	2.572540000	-0.351754000	1	6.380257000	0.916026000	0.904537000
6	2.507454000	3.170776000	-1.749669000	1	5.700738000	-1.414627000	0.624359000
6	2.321053000	3.703312000	0.696778000	1	2.299827000	-2.503326000	-0.364340000
6	4.477008000	1.693068000	0.344849000	1	3.818839000	-4.029120000	-1.579642000
6	5.380502000	0.681400000	0.594193000	1	5.178390000	-2.964646000	-1.250860000
6	4.992719000	-0.632152000	0.437523000	1	3.870080000	-2.423144000	-2.296217000
6	3.705888000	-0.957571000	0.030768000	1	3.347334000	-4.311610000	0.899226000
6	3.358428000	-2.431856000	-0.179182000	1	4.748389000	-3.320199000	1.255303000
6	4.105607000	-2.995224000	-1.408739000	1	3.185268000	-2.910596000	1.943981000

1	3.121045000	0.192693000	-2.819601000	6	-1.310093000	-0.185631000	2.035374000
1	1.879307000	-0.467682000	-4.027964000	7	-1.474448000	-0.065935000	0.723728000
1	-2.530967000	-1.135384000	-3.556723000	6	-2.840215000	-0.001035000	0.200587000
1	-3.193744000	0.288732000	-2.713825000	6	-3.410319000	1.268913000	0.014725000
1	-1.775570000	0.430066000	-3.793433000	6	-2.687925000	2.532530000	0.479231000
1	-4.460158000	2.967763000	0.744342000	6	-3.123125000	2.876493000	1.924304000
1	-6.246699000	1.337975000	1.080070000	6	-2.943991000	3.758767000	-0.422626000
1	-5.856504000	-1.025917000	0.608363000	6	-4.673696000	1.355147000	-0.545596000
1	-2.653223000	-2.416500000	-0.672759000	6	-5.367057000	0.218383000	-0.913680000
1	-4.450193000	-3.781864000	-1.627002000	6	-4.810493000	-1.022158000	-0.702155000
1	-5.672238000	-2.679272000	-1.020388000	6	-3.548265000	-1.160039000	-0.133865000
1	-4.578691000	-2.158984000	-2.290567000	6	-3.021061000	-2.571198000	0.136458000
1	-3.649652000	-4.136489000	0.765052000	6	-3.965379000	-3.342427000	1.087929000
1	-3.087728000	-2.778344000	1.723303000	6	-2.844666000	-3.374360000	-1.169888000
1	-4.805021000	-2.974869000	1.400069000	6	-2.279754000	-0.603840000	2.972394000
1	-0.983564000	2.043040000	-0.122056000	6	2.490714000	-0.195534000	3.005528000
1	-1.013928000	4.254924000	0.841602000	6	2.858642000	0.074034000	0.227974000
1	-1.929526000	3.225608000	1.931416000	6	3.289082000	1.380348000	-0.044875000
1	-2.761084000	4.324398000	0.839004000	6	4.574452000	1.566118000	-0.526403000
1	-1.275794000	3.952994000	-1.697155000	6	5.407758000	0.489109000	-0.759723000
1	-2.024395000	2.500847000	-2.335779000	6	4.961512000	-0.790373000	-0.515729000
1	-3.021577000	3.750691000	-1.608109000	6	3.685844000	-1.023997000	-0.015773000
6	0.864211000	-1.300033000	3.222086000	6	3.237520000	-2.464128000	0.229419000
1	-1.887842000	-1.270393000	2.899835000	6	4.219180000	-3.222078000	1.151065000
1	-2.052384000	0.464407000	2.620569000	6	3.086911000	-3.217784000	-1.110483000
6	-1.401656000	-0.300762000	3.053028000	6	2.367002000	2.579844000	0.176940000
6	0.622891000	1.116808000	2.721286000	6	2.520613000	3.658574000	-0.917264000
1	0.597999000	1.361746000	3.796386000	6	2.614164000	3.225817000	1.559222000
1	0.080938000	1.909029000	2.197350000	6	-0.001847000	0.250643000	-2.344653000
1	1.667375000	1.155753000	2.402552000	1	1.355382000	0.564502000	-4.007384000
1	-0.048078000	-2.147623000	-1.860448000	1	-0.922597000	-0.277645000	-4.243077000
1	-0.219858000	-2.446166000	0.387477000	1	-1.922898000	-0.685069000	-2.839881000
				1	-0.508501000	-1.679896000	-3.243380000
<b>Ga-intra-TS<sub>4',4</sub></b>				1	0.032004000	0.003933000	3.710538000
31	0.019014000	-0.576441000	-0.517760000	1	-1.630960000	2.317186000	0.478194000
7	1.507739000	-0.112057000	0.745455000	1	-2.588742000	3.752137000	2.280126000
6	1.315249000	-0.179949000	2.055612000	1	-4.185968000	3.091657000	1.945739000
6	0.043568000	-0.276229000	2.661479000	1	-2.928576000	2.054484000	2.598823000

1	-2.290237000	4.569480000	-0.118217000	6	1.403886000	0.246539000	-2.952998000
1	-3.964427000	4.111064000	-0.327295000	6	-0.575287000	1.664899000	-2.388556000
1	-2.750432000	3.537950000	-1.463694000	1	-0.521235000	2.068698000	-3.412815000
1	-5.122922000	2.314600000	-0.696938000	1	-0.039897000	2.360446000	-1.735271000
1	-6.341209000	0.302958000	-1.353751000	1	-1.626465000	1.666226000	-2.092631000
1	-5.361945000	-1.899561000	-0.973276000	1	-0.882873000	-1.357081000	2.864606000
1	-2.055928000	-2.493327000	0.609248000	1	0.059761000	-2.171456000	-0.478105000
1	-3.540027000	-4.314652000	1.314783000				
1	-4.933961000	-3.499868000	0.628406000				<b>Ga-intra-TS<sub>4,4</sub>-w</b>
1	-4.109120000	-2.810282000	2.018458000	31	-0.021507000	-0.562585000	0.756650000
1	-2.469775000	-4.367002000	-0.942529000	7	-1.521911000	-0.319536000	-0.644695000
1	-3.789926000	-3.480702000	-1.689587000	6	-1.308780000	-0.777460000	-1.830828000
1	-2.138218000	-2.891023000	-1.827338000	6	0.012818000	-1.360551000	-2.213466000
1	-3.296602000	-0.792320000	2.662332000	6	1.313170000	-0.712033000	-1.802463000
1	-2.101775000	-0.413726000	4.025327000	7	1.425101000	-0.215306000	-0.606562000
1	2.902258000	-1.207693000	3.036832000	6	2.716067000	0.298067000	-0.128488000
1	3.291362000	0.466011000	2.682629000	6	2.937279000	1.681844000	-0.158666000
1	2.177321000	0.071106000	4.015535000	6	1.947228000	2.625021000	-0.840021000
1	4.926798000	2.555605000	-0.732120000	6	2.277716000	2.734620000	-2.347785000
1	6.397653000	0.649856000	-1.138899000	6	1.925093000	4.045398000	-0.237018000
1	5.608896000	-1.620347000	-0.714066000	6	4.107024000	2.172940000	0.395627000
1	2.267733000	-2.446175000	0.700824000	6	5.030293000	1.318267000	0.967840000
1	3.824866000	-4.207681000	1.374678000	6	4.812494000	-0.040099000	0.954247000
1	5.183106000	-3.350086000	0.673481000	6	3.664572000	-0.589019000	0.387089000
1	4.373610000	-2.695611000	2.085318000	6	3.538290000	-2.114326000	0.307054000
1	2.761531000	-4.236969000	-0.930032000	6	4.817707000	-2.728136000	-0.310853000
1	2.348049000	-2.734406000	-1.733818000	6	3.291827000	-2.729030000	1.700424000
1	4.030118000	-3.247698000	-1.643665000	6	2.393726000	-0.929630000	-2.757474000
1	1.353149000	2.212023000	0.148631000	6	-2.353592000	-0.874319000	-2.903462000
1	1.738842000	4.401560000	-0.801592000	6	-2.877355000	0.057411000	-0.224227000
1	2.439933000	3.230726000	-1.907723000	6	-3.227720000	1.409202000	-0.197488000
1	3.472642000	4.169808000	-0.836522000	6	-4.505001000	1.746065000	0.220414000
1	1.979381000	4.097150000	1.683000000	6	-5.400082000	0.772712000	0.619193000
1	2.396169000	2.537718000	2.364391000	6	-5.028545000	-0.553455000	0.605298000
1	3.648343000	3.540937000	1.644200000	6	-3.763227000	-0.942350000	0.183143000
6	-0.892025000	-0.653084000	-3.207887000	6	-3.406554000	-2.430158000	0.188331000
1	1.862522000	-0.748173000	-2.937865000	6	-4.380508000	-3.242777000	-0.694436000
1	2.085922000	0.922345000	-2.434884000	6	-3.403591000	-2.989715000	1.627608000

6	-2.240076000	2.487286000	-0.632311000	1	-3.140075000	-4.041487000	1.612643000
6	-2.378594000	3.790739000	0.181634000	1	-2.676810000	-2.469335000	2.235294000
6	-2.410429000	2.800608000	-2.135828000	1	-4.379687000	-2.887485000	2.086798000
6	-0.090085000	0.517620000	2.442697000	1	-1.246542000	2.097700000	-0.474074000
1	-1.510240000	0.934309000	4.023456000	1	-1.550488000	4.450292000	-0.051513000
1	0.794749000	0.248430000	4.407695000	1	-2.369493000	3.594086000	1.245894000
1	1.871082000	-0.224342000	3.084225000	1	-3.294115000	4.314195000	-0.066894000
1	0.521645000	-1.277237000	3.551956000	1	-1.697834000	3.557646000	-2.446013000
1	0.034748000	-1.520305000	-3.291887000	1	-2.253706000	1.919385000	-2.743167000
1	0.963093000	2.194516000	-0.736538000	1	-3.411145000	3.171718000	-2.325883000
1	1.568204000	3.391402000	-2.842318000	6	0.829012000	-0.233346000	3.418449000
1	3.272225000	3.147214000	-2.474358000	1	-1.910587000	-0.520584000	3.108331000
1	2.248496000	1.768965000	-2.830704000	1	-2.216647000	1.069711000	2.406093000
1	1.101743000	4.604927000	-0.668824000	6	-1.512981000	0.495156000	3.013203000
1	2.837418000	4.581808000	-0.469254000	6	0.390858000	1.962781000	2.355219000
1	1.798939000	4.024927000	0.836709000	1	0.312259000	2.443568000	3.343453000
1	4.300981000	3.224979000	0.386549000	1	-0.202748000	2.559374000	1.657928000
1	5.924319000	1.714582000	1.407835000	1	1.436519000	2.017084000	2.046901000
1	5.546986000	-0.695411000	1.374617000	1	0.119274000	-2.384534000	-1.785042000
1	2.746567000	-2.431471000	-0.364241000	1	-0.101022000	-2.142170000	0.874331000
1	4.626847000	-3.774002000	-0.519650000	8	1.917815000	-3.402351000	-1.902473000
1	5.672702000	-2.659782000	0.353225000	1	2.287217000	-4.288654000	-1.915945000
1	5.064571000	-2.243278000	-1.247741000	1	2.447685000	-2.105689000	-2.632302000
1	3.263999000	-3.810579000	1.618720000				
1	4.078455000	-2.458430000	2.398085000				Ga-inter-TS <sub>4',4</sub> I in gas phase
1	2.342729000	-2.405775000	2.105026000	31	3.944860000	0.810925000	0.711475000
1	3.333702000	-0.453779000	-2.495210000	7	3.421325000	0.526351000	-1.272192000
1	2.088786000	-0.717022000	-3.783867000	6	2.152846000	0.424373000	-1.478167000
1	-2.444799000	-1.924122000	-3.201713000	6	1.228978000	0.519696000	-0.297881000
1	-3.323042000	-0.496055000	-2.593339000	6	1.407044000	-0.497407000	0.809373000
1	-2.002804000	-0.328608000	-3.784338000	7	2.587732000	-0.460928000	1.429493000
1	-4.802015000	2.773493000	0.243272000	6	2.835058000	-1.284981000	2.612893000
1	-6.382524000	1.050841000	0.945331000	6	3.140387000	-2.646838000	2.501457000
1	-5.726322000	-1.299581000	0.926115000	6	3.187245000	-3.393811000	1.169754000
1	-2.408914000	-2.555754000	-0.200678000	6	2.077868000	-4.468904000	1.096377000
1	-4.057170000	-4.276884000	-0.739394000	6	4.553156000	-4.084357000	0.954753000
1	-5.383185000	-3.223099000	-0.284670000	6	3.397365000	-3.365063000	3.663024000
1	-4.420496000	-2.852857000	-1.704427000	6	3.361762000	-2.763487000	4.899976000

6	3.058384000	-1.421558000	4.999863000	1	0.318206000	0.426380000	3.414408000
6	2.788484000	-0.663552000	3.871686000	1	4.154338000	1.393062000	5.159594000
6	2.374119000	0.798855000	4.033771000	1	2.859154000	2.579105000	5.152688000
6	0.846299000	0.872123000	4.244753000	1	2.728087000	1.156128000	6.160246000
6	3.080668000	1.518547000	5.202051000	1	0.382949000	-2.064134000	1.842331000
6	0.276032000	-1.285035000	1.095648000	1	-0.278600000	-1.595660000	0.208928000
6	1.487714000	0.310983000	-2.810880000	1	0.815724000	1.166958000	-2.937564000
6	4.347324000	0.706890000	-2.397752000	1	2.188762000	0.259108000	-3.639348000
6	5.112483000	-0.374538000	-2.838354000	1	0.838748000	-0.571096000	-2.797003000
6	5.985401000	-0.169659000	-3.895343000	1	6.576585000	-0.982671000	-4.260005000
6	6.110373000	1.073525000	-4.482494000	1	6.793505000	1.214534000	-5.296267000
6	5.363230000	2.133247000	-4.018506000	1	5.475185000	3.095985000	-4.473413000
6	4.465987000	1.976195000	-2.970064000	1	2.992203000	2.890334000	-1.715289000
6	3.669466000	3.193685000	-2.497394000	1	2.219126000	4.608175000	-3.268581000
6	2.838732000	3.803461000	-3.648925000	1	3.483597000	4.213093000	-4.416757000
6	4.607705000	4.261450000	-1.893958000	1	2.194441000	3.063575000	-4.107762000
6	4.981068000	-1.752032000	-2.195841000	1	4.028179000	5.113774000	-1.556081000
6	6.317446000	-2.523282000	-2.171152000	1	5.145203000	3.859201000	-1.046732000
6	3.915155000	-2.589367000	-2.938442000	1	5.325448000	4.606502000	-2.628412000
6	5.866712000	0.636778000	1.243002000	1	4.656758000	-1.609069000	-1.175261000
1	7.791605000	1.368123000	0.563954000	1	6.207193000	-3.418143000	-1.571762000
1	7.025686000	1.471257000	2.882307000	1	7.111291000	-1.921699000	-1.746224000
1	5.409005000	0.941239000	3.359301000	1	6.611444000	-2.831577000	-3.167139000
1	5.613241000	2.452755000	2.456141000	1	3.816775000	-3.567338000	-2.480051000
1	0.193980000	0.510277000	-0.639904000	1	2.946679000	-2.107495000	-2.915838000
1	3.034438000	-2.679778000	0.374718000	1	4.205063000	-2.722944000	-3.974397000
1	2.099199000	-4.956541000	0.127362000	6	5.975142000	1.422550000	2.557191000
1	2.237771000	-5.225570000	1.855576000	1	6.440399000	2.352782000	-0.001487000
1	1.096220000	-4.043605000	1.238197000	1	6.763590000	0.790171000	-0.756423000
1	4.572195000	-4.560087000	-0.020180000	6	6.753584000	1.322670000	0.198298000
1	4.714855000	-4.854803000	1.698505000	6	6.378571000	-0.781175000	1.481944000
1	5.369107000	-3.379805000	1.012582000	1	7.425665000	-0.751219000	1.822649000
1	3.626057000	-4.408765000	3.594129000	1	6.354710000	-1.380519000	0.568388000
1	3.564554000	-3.336188000	5.783226000	1	5.798140000	-1.304307000	2.246374000
1	3.025309000	-0.963385000	5.965910000	1	1.435617000	1.502266000	0.154093000
1	2.611419000	1.328856000	3.125339000	1	3.335650000	2.285130000	0.859264000
1	0.530024000	1.905373000	4.344414000	31	-3.068240000	0.267486000	-0.933670000
1	0.573207000	0.339582000	5.149112000	7	-3.204036000	1.327972000	0.777069000

6	-2.732140000	0.750851000	1.876385000	1	-6.774343000	-3.902359000	1.633847000
6	-2.281568000	-0.600850000	1.930563000	1	-5.253060000	-3.232952000	2.221838000
6	-2.794967000	-1.748625000	1.122503000	1	-7.993620000	-1.111402000	0.814382000
7	-3.346011000	-1.477461000	-0.123268000	1	-8.153851000	-2.624019000	-0.048278000
6	-3.986151000	-2.573474000	-0.820435000	1	-7.496715000	-1.217721000	-0.870015000
6	-5.321997000	-2.899449000	-0.520839000	1	-6.946565000	-4.203190000	-0.960874000
6	-6.108531000	-2.142604000	0.546493000	1	-5.741504000	-5.482252000	-2.658670000
6	-6.230748000	-2.985473000	1.837128000	1	-3.423850000	-4.927502000	-3.182397000
6	-7.525275000	-1.749195000	0.070880000	1	-1.568223000	-2.085353000	-1.734466000
6	-5.931601000	-3.948665000	-1.190525000	1	0.110525000	-3.930089000	-1.600339000
6	-5.254461000	-4.673952000	-2.148889000	1	-1.189777000	-5.107266000	-1.740109000
6	-3.947528000	-4.355405000	-2.443531000	1	-1.093222000	-4.069262000	-0.322308000
6	-3.295087000	-3.316511000	-1.791383000	1	-0.481166000	-2.787514000	-3.787866000
6	-1.821759000	-3.064005000	-2.108968000	1	-1.605296000	-4.106076000	-4.017408000
6	-0.940247000	-4.111327000	-1.390359000	1	-2.159887000	-2.448269000	-4.182438000
6	-1.507741000	-3.102271000	-3.621570000	1	-2.998374000	-3.876056000	1.161774000
6	-2.668269000	-2.983687000	1.674432000	1	-2.267123000	-3.090837000	2.675272000
6	-2.567254000	1.567768000	3.137664000	1	-1.743967000	2.274371000	3.027351000
6	-3.577160000	2.736188000	0.810848000	1	-3.458829000	2.159080000	3.341793000
6	-4.927463000	3.076581000	0.969295000	1	-2.357335000	0.923891000	3.990912000
6	-5.275364000	4.417679000	1.019913000	1	-6.300852000	4.693459000	1.152340000
6	-4.321923000	5.406857000	0.889414000	1	-4.609581000	6.439085000	0.925885000
6	-3.002110000	5.062426000	0.699393000	1	-2.269071000	5.834651000	0.580844000
6	-2.606297000	3.732230000	0.659449000	1	-0.994727000	2.351278000	0.568491000
6	-1.131511000	3.410835000	0.427339000	1	0.817794000	3.817252000	1.293533000
6	-0.204346000	4.164312000	1.408081000	1	-0.215024000	5.230006000	1.214138000
6	-0.735601000	3.747027000	-1.027554000	1	-0.503343000	4.006828000	2.436912000
6	-6.008346000	2.003074000	1.077081000	1	0.321265000	3.552128000	-1.186338000
6	-7.308703000	2.401762000	0.345554000	1	-1.306311000	3.144120000	-1.718848000
6	-6.334566000	1.682865000	2.553087000	1	-0.921320000	4.792808000	-1.242086000
6	-4.201699000	0.816455000	-2.507030000	1	-5.619336000	1.110687000	0.614869000
1	-4.777707000	2.613692000	-3.580684000	1	-7.971099000	1.545218000	0.296846000
1	-4.024860000	0.545538000	-4.663084000	1	-7.106456000	2.734950000	-0.664241000
1	-3.481399000	-0.849296000	-3.719389000	1	-7.831660000	3.191325000	0.872718000
1	-2.460900000	0.591515000	-3.823581000	1	-7.130891000	0.947985000	2.608008000
1	-2.096705000	-0.917897000	2.954161000	1	-5.474725000	1.278694000	3.069462000
1	-5.552041000	-1.246701000	0.770026000	1	-6.659821000	2.580425000	3.068000000
1	-6.774338000	-2.429755000	2.596252000	6	-3.498914000	0.243354000	-3.742889000

1	-3.243579000	2.775359000	-2.720549000	6	3.101843000	3.932249000	-3.489948000
1	-4.755874000	2.830633000	-1.821806000	6	4.825227000	4.304240000	-1.678027000
6	-4.246315000	2.339730000	-2.654094000	6	5.039975000	-1.728840000	-2.243434000
6	-5.630034000	0.276247000	-2.480792000	6	6.339804000	-2.559177000	-2.231536000
1	-6.178238000	0.603583000	-3.379967000	6	3.965841000	-2.474350000	-3.066668000
1	-6.187313000	0.635748000	-1.612649000	6	5.900964000	0.525584000	1.361342000
1	-5.649909000	-0.816307000	-2.460776000	1	7.853032000	1.310463000	0.834937000
1	-0.868789000	-0.615451000	1.529615000	1	6.991887000	1.198299000	3.117826000
1	-1.499655000	0.429220000	-1.281431000	1	5.371102000	0.599249000	3.481549000
				1	5.580261000	2.201982000	2.751351000
Ga-inter-TS <sub>4,4-I</sub> in gas phase				1	0.276883000	0.560207000	-0.709950000
31	4.003462000	0.749496000	0.760249000	1	3.030065000	-2.704701000	0.293602000
7	3.525001000	0.554431000	-1.241568000	1	2.063818000	-4.954804000	-0.054797000
6	2.261158000	0.492030000	-1.489214000	1	2.130445000	-5.276640000	1.667839000
6	1.299562000	0.552826000	-0.334399000	1	1.037354000	-4.053101000	1.046295000
6	1.427588000	-0.497640000	0.749834000	1	4.541524000	-4.613722000	-0.099960000
7	2.590846000	-0.506661000	1.403425000	1	4.622402000	-4.949830000	1.613866000
6	2.785923000	-1.371439000	2.567718000	1	5.329623000	-3.474616000	0.984310000
6	3.063022000	-2.737202000	2.424191000	1	3.470281000	-4.544141000	3.476822000
6	3.141769000	-3.444908000	1.071605000	1	3.365968000	-3.536823000	5.695746000
6	2.015734000	-4.493719000	0.926665000	1	2.887848000	-1.156118000	5.935329000
6	4.499605000	-4.158509000	0.884066000	1	2.654832000	1.233820000	3.162022000
6	3.264891000	-3.497350000	3.570917000	1	0.540664000	1.853778000	4.303123000
6	3.205289000	-2.932707000	4.824466000	1	0.474963000	0.255807000	5.038904000
6	2.935405000	-1.585833000	4.956654000	1	0.320474000	0.425654000	3.298278000
6	2.719885000	-0.786921000	3.844542000	1	4.092636000	1.167671000	5.277142000
6	2.351659000	0.684388000	4.038487000	1	2.851813000	2.408399000	5.235462000
6	0.819970000	0.813020000	4.174415000	1	2.604326000	0.965914000	6.191955000
6	3.023705000	1.337284000	5.264149000	1	0.348427000	-2.079628000	1.699489000
6	0.272317000	-1.268034000	0.984423000	1	-0.271687000	-1.524229000	0.074238000
6	1.636625000	0.459379000	-2.844066000	1	0.984803000	1.333567000	-2.949520000
6	4.494316000	0.761139000	-2.327213000	1	2.358465000	0.434030000	-3.655426000
6	5.244442000	-0.320769000	-2.796300000	1	0.972457000	-0.409932000	-2.895599000
6	6.168833000	-0.087817000	-3.803419000	1	6.752819000	-0.897953000	-4.186222000
6	6.354879000	1.179707000	-4.318853000	1	7.076980000	1.340737000	-5.094755000
6	5.616363000	2.236171000	-3.833767000	1	5.771350000	3.216567000	-4.235527000
6	4.672438000	2.053564000	-2.830738000	1	3.184329000	2.952551000	-1.583419000
6	3.887186000	3.270406000	-2.336406000	1	2.494936000	4.745326000	-3.105204000

1	3.776941000	4.343523000	-4.231059000	6	-0.991314000	-4.007682000	-1.553589000
1	2.447677000	3.224453000	-3.984675000	6	-1.685144000	-3.077902000	-3.781569000
1	4.247079000	5.146958000	-1.312911000	6	-2.675108000	-2.982649000	1.583847000
1	5.351541000	3.8677787000	-0.840277000	6	-2.585523000	1.532831000	3.124418000
1	5.554405000	4.676747000	-2.388050000	6	-3.626892000	2.747213000	0.830692000
1	4.691049000	-1.634381000	-1.225119000	6	-4.978674000	3.077535000	1.004046000
1	6.174689000	-3.480917000	-1.686844000	6	-5.334030000	4.416349000	1.079197000
1	7.151494000	-2.023159000	-1.755032000	6	-4.387625000	5.413530000	0.956289000
1	6.645695000	-2.826732000	-3.236003000	6	-3.066913000	5.080010000	0.751552000
1	3.818327000	-3.476291000	-2.676987000	6	-2.662594000	3.752611000	0.688901000
1	3.015178000	-1.958717000	-3.038578000	6	-1.184512000	3.449797000	0.447044000
1	4.279342000	-2.553826000	-4.101774000	6	-0.264574000	4.207067000	1.430441000
6	5.952998000	1.170121000	2.752806000	6	-0.797156000	3.806618000	-1.004340000
1	6.527775000	2.366960000	0.343816000	6	-6.057635000	1.999663000	1.097788000
1	6.870709000	0.898362000	-0.576414000	6	-7.355517000	2.404157000	0.365536000
6	6.826948000	1.317030000	0.432932000	6	-6.390531000	1.667197000	2.568787000
6	6.408889000	-0.908373000	1.475499000	6	-4.229490000	0.889519000	-2.531533000
1	7.445231000	-0.914739000	1.850712000	1	-4.847839000	2.706493000	-3.549647000
1	6.414187000	-1.421528000	0.510138000	1	-4.017843000	0.698443000	-4.695151000
1	5.807796000	-1.499114000	2.171670000	1	-3.424869000	-0.702217000	-3.793524000
1	1.492696000	1.521047000	0.153229000	1	-2.467487000	0.780523000	-3.836261000
1	3.420899000	2.232440000	0.951777000	1	-2.076704000	-0.937287000	2.874144000
31	-3.105490000	0.308769000	-0.960237000	1	-5.571851000	-1.260479000	0.793108000
7	-3.242828000	1.341570000	0.766123000	1	-6.777974000	-2.445349000	2.617029000
6	-2.749182000	0.747075000	1.845653000	1	-6.840501000	-3.903737000	1.636866000
6	-2.280061000	-0.602408000	1.859794000	1	-5.290800000	-3.290434000	2.208060000
6	-2.813758000	-1.740155000	1.047810000	1	-8.024585000	-1.117539000	0.847647000
7	-3.391964000	-1.457342000	-0.183941000	1	-8.180848000	-2.603657000	-0.059820000
6	-4.047358000	-2.552793000	-0.870134000	1	-7.515761000	-1.177085000	-0.835405000
6	-5.368485000	-2.897995000	-0.525067000	1	-6.989330000	-4.227002000	-0.903679000
6	-6.137706000	-2.147957000	0.560290000	1	-5.826557000	-5.494954000	-2.639849000
6	-6.265629000	-3.005640000	1.839362000	1	-3.541600000	-4.899849000	-3.254851000
6	-7.550370000	-1.734793000	0.090798000	1	-1.686289000	-2.010116000	-1.921758000
6	-5.986737000	-3.958419000	-1.170362000	1	0.044187000	-3.797740000	-1.807797000
6	-5.334227000	-4.676733000	-2.150734000	1	-1.220261000	-5.019251000	-1.872819000
6	-4.044895000	-4.336028000	-2.495801000	1	-1.103169000	-3.951556000	-0.481064000
6	-3.384095000	-3.285216000	-1.870385000	1	-0.689469000	-2.706958000	-4.007577000
6	-1.932460000	-3.004304000	-2.258039000	1	-1.737777000	-4.098875000	-4.141583000

1	-2.400481000	-2.485173000	-4.335277000	6	-1.219057000	-0.604567000	-0.207270000
1	-3.005303000	-3.873359000	1.067959000	6	-1.537777000	0.163740000	1.052160000
1	-2.252438000	-3.100138000	2.575064000	7	-2.747350000	0.116637000	1.510038000
1	-1.822646000	2.303707000	3.011116000	6	-3.078880000	0.659588000	2.842176000
1	-3.509473000	2.049391000	3.384155000	6	-3.413967000	2.005811000	3.003780000
1	-2.302148000	0.880187000	3.949317000	6	-3.356045000	3.029532000	1.871371000
1	-6.359958000	4.684928000	1.224311000	6	-2.179719000	4.009611000	2.098292000
1	-4.681250000	6.443631000	1.010640000	6	-4.662056000	3.846618000	1.752026000
1	-2.339507000	5.858517000	0.639647000	6	-3.763089000	2.440246000	4.276283000
1	-1.030370000	2.391103000	0.578509000	6	-3.775362000	1.576212000	5.348262000
1	0.759584000	3.864574000	1.318149000	6	-3.424015000	0.254007000	5.172135000
1	-0.277554000	5.273373000	1.238482000	6	-3.067819000	-0.232394000	3.923821000
1	-0.562187000	4.047192000	2.459774000	6	-2.601390000	-1.684345000	3.791578000
1	0.264330000	3.641950000	-1.164084000	6	-1.120199000	-1.794959000	4.226208000
1	-1.348520000	3.194676000	-1.704343000	6	-3.448939000	-2.672507000	4.621510000
1	-1.009184000	4.848895000	-1.213482000	6	-0.379065000	0.841666000	1.666583000
1	-5.666327000	1.111629000	0.628091000	6	-1.225077000	-0.013255000	-2.667985000
1	-8.021398000	1.550250000	0.310425000	6	-4.132437000	-0.293443000	-2.586111000
1	-7.153434000	2.743338000	-0.642754000	6	-4.814314000	0.887624000	-2.885200000
1	-7.879870000	3.191466000	0.895006000	6	-5.601979000	0.913896000	-4.024903000
1	-7.181570000	0.925361000	2.615324000	6	-5.722351000	-0.201970000	-4.829659000
1	-5.531562000	1.266600000	3.089960000	6	-5.055989000	-1.362840000	-4.505844000
1	-6.727445000	2.557551000	3.089322000	6	-4.245407000	-1.436928000	-3.380125000
6	-3.491366000	0.388572000	-3.777127000	6	-3.532605000	-2.755303000	-3.072093000
1	-3.340359000	2.892349000	-2.648736000	6	-2.628975000	-3.193463000	-4.246617000
1	-4.872636000	2.853930000	-1.785827000	6	-4.552902000	-3.866761000	-2.742269000
6	-4.325224000	2.414200000	-2.622700000	6	-4.678441000	2.124501000	-2.002392000
6	-5.641506000	0.307066000	-2.542437000	6	-5.971139000	2.965218000	-1.950841000
1	-6.193899000	0.654768000	-3.432054000	6	-3.509236000	3.007281000	-2.494674000
1	-6.215838000	0.614899000	-1.664821000	6	-6.030616000	-0.795683000	0.812080000
1	-5.634912000	-0.785802000	-2.568604000	1	-7.910077000	-1.283448000	-0.147914000
1	-0.883451000	-0.606184000	1.441470000	1	-7.362788000	-1.829581000	2.182729000
1	-1.527732000	0.462809000	-1.283651000	1	-5.770126000	-1.493355000	2.870355000
				1	-5.967979000	-2.807721000	1.697497000
<b>Ga-inter-IM<sub>4',4</sub></b>				1	-0.153271000	-0.514692000	-0.437085000
31	-4.080841000	-0.971675000	0.424622000	1	-3.199569000	2.503130000	0.940865000
7	-3.308348000	-0.355811000	-1.369695000	1	-2.115603000	4.710620000	1.273747000
6	-2.023235000	-0.290186000	-1.439998000	1	-2.339296000	4.573927000	3.009406000

1	-1.232293000	3.497638000	2.179797000	1	-6.738864000	-0.546173000	-1.251990000
1	-4.595282000	4.509851000	0.896356000	6	-6.842199000	-1.237041000	-0.411334000
1	-4.813623000	4.462036000	2.629863000	6	-6.500134000	0.587031000	1.256393000
1	-5.524485000	3.208762000	1.628165000	1	-7.578227000	0.563362000	1.478389000
1	-4.018158000	3.468464000	4.427760000	1	-6.346599000	1.339193000	0.478761000
1	-4.046527000	1.933415000	6.321643000	1	-5.986556000	0.921611000	2.161224000
1	-3.418139000	-0.403921000	6.015463000	1	-1.435479000	-1.660929000	0.024496000
1	-2.676677000	-1.983138000	2.757982000	1	-3.440986000	-2.432779000	0.446026000
1	-0.772365000	-2.815612000	4.109847000	31	3.074407000	-0.116077000	-0.821878000
1	-1.019243000	-1.514554000	5.268269000	7	3.434575000	-1.380410000	0.643895000
1	-0.479580000	-1.149373000	3.641229000	6	3.077482000	-0.958558000	1.903904000
1	-4.504310000	-2.567890000	4.409398000	6	2.765769000	0.333028000	2.238578000
1	-3.150918000	-3.686553000	4.379727000	6	2.862575000	1.594962000	1.490434000
1	-3.293636000	-2.530959000	5.683877000	7	3.290076000	1.554075000	0.164834000
1	-0.589082000	1.290259000	2.633125000	6	3.782723000	2.782674000	-0.413205000
1	0.009490000	1.600771000	0.975243000	6	5.113331000	3.171647000	-0.160464000
1	-0.575664000	-0.875467000	-2.858894000	6	6.025628000	2.336765000	0.734757000
1	-1.840011000	0.197162000	-3.538487000	6	6.176021000	2.999589000	2.123593000
1	-0.539887000	0.814555000	-2.460931000	6	7.428820000	2.125164000	0.123437000
1	-6.128817000	1.807141000	-4.285637000	6	5.595614000	4.347607000	-0.710800000
1	-6.338497000	-0.164750000	-5.705750000	6	4.797910000	5.144265000	-1.507123000
1	-5.162725000	-2.224000000	-5.132812000	6	3.498340000	4.765663000	-1.757776000
1	-2.911157000	-2.626802000	-2.200056000	6	2.972719000	3.595692000	-1.221739000
1	-2.068747000	-4.078773000	-3.967238000	6	1.503549000	3.266598000	-1.483060000
1	-3.220848000	-3.434488000	-5.121066000	6	0.595712000	4.129704000	-0.576876000
1	-1.925594000	-2.416025000	-4.517463000	6	1.084171000	3.489492000	-2.954148000
1	-4.031827000	-4.791009000	-2.518249000	6	2.590807000	2.743297000	2.178350000
1	-5.148601000	-3.595913000	-1.881327000	6	3.000100000	-1.991806000	3.008883000
1	-5.216696000	-4.043986000	-3.579721000	6	3.849805000	-2.749636000	0.448737000
1	-4.457019000	1.788320000	-0.999557000	6	5.218259000	-3.067481000	0.471629000
1	-5.871702000	3.734024000	-1.194434000	6	5.611686000	-4.385667000	0.298783000
1	-6.831204000	2.353880000	-1.707689000	6	4.684530000	-5.384228000	0.079630000
1	-6.154560000	3.460415000	-2.896508000	6	3.344901000	-5.067535000	0.026038000
1	-3.401822000	3.880825000	-1.860498000	6	2.909429000	-3.762446000	0.210605000
1	-2.571749000	2.467622000	-2.486838000	6	1.413777000	-3.466681000	0.126245000
1	-3.699212000	3.340790000	-3.508219000	6	0.577951000	-4.385933000	1.045298000
6	-6.287567000	-1.790615000	1.953290000	6	0.922240000	-3.605308000	-1.331919000
1	-6.557231000	-2.233331000	-0.764431000	6	6.271225000	-1.980963000	0.672969000

6	7.499764000	-2.175004000	-0.242898000	1	1.422046000	-2.883565000	-1.961011000
6	6.739094000	-1.917605000	2.143976000	1	1.127451000	-4.599246000	-1.711757000
6	4.082726000	-0.327032000	-2.558932000	1	5.801948000	-1.043071000	0.426830000
1	4.682050000	-1.890785000	-3.943026000	1	8.130869000	-1.294267000	-0.192823000
1	3.740744000	0.273683000	-4.628177000	1	7.202738000	-2.324233000	-1.273104000
1	3.220858000	1.472488000	-3.433663000	1	8.095805000	-3.024613000	0.070796000
1	2.246446000	0.018878000	-3.702423000	1	7.510542000	-1.162443000	2.258556000
1	2.469363000	0.481230000	3.272059000	1	5.921724000	-1.661147000	2.803342000
1	5.550547000	1.377245000	0.860173000	1	7.148439000	-2.874744000	2.450043000
1	6.798192000	2.383115000	2.766321000	6	3.274765000	0.399860000	-3.636515000
1	6.648082000	3.972007000	2.024104000	1	3.205792000	-2.272975000	-3.051377000
1	5.209605000	3.122099000	2.589105000	1	4.764465000	-2.392157000	-2.243590000
1	7.988990000	1.426535000	0.737659000	6	4.189707000	-1.800228000	-2.959745000
1	7.987732000	3.053689000	0.093653000	6	5.484277000	0.279766000	-2.524252000
1	7.369518000	1.728080000	-0.880444000	1	5.997043000	0.120706000	-3.488226000
1	6.605818000	4.646430000	-0.515389000	1	6.105159000	-0.171192000	-1.746318000
1	5.186992000	6.051931000	-1.925992000	1	5.452895000	1.356910000	-2.340856000
1	2.881466000	5.391495000	-2.370803000	1	0.457261000	0.131244000	1.755503000
1	1.356561000	2.227325000	-1.233007000	1	1.473921000	-0.280384000	-1.096921000
1	-0.451984000	3.896482000	-0.755620000				
1	0.747788000	5.181450000	-0.793903000				<b>Ga-inter-TS<sub>4',4-II</sub></b>
1	0.822338000	3.955582000	0.464353000	31	-3.762713000	0.050475000	1.131465000
1	0.068853000	3.132886000	-3.105615000	7	-2.616834000	-1.501610000	0.466368000
1	1.094100000	4.542609000	-3.207905000	6	-1.609699000	-1.241693000	-0.316840000
1	1.735766000	2.966543000	-3.638796000	6	-1.285671000	0.146188000	-0.720022000
1	2.711085000	3.720864000	1.733931000	6	-2.367082000	1.037518000	-1.194888000
1	2.338402000	2.690131000	3.231241000	7	-3.552494000	1.040355000	-0.660248000
1	2.226577000	-2.733482000	2.802250000	6	-4.594454000	1.951730000	-1.165406000
1	3.936223000	-2.542352000	3.110278000	6	-5.501599000	1.475309000	-2.120918000
1	2.773756000	-1.510297000	3.961844000	6	-5.411294000	0.057792000	-2.684562000
1	6.652749000	-4.635297000	0.326944000	6	-4.519952000	0.031263000	-3.947444000
1	5.005915000	-6.398322000	-0.056834000	6	-6.793110000	-0.530529000	-3.043946000
1	2.629393000	-5.843791000	-0.160620000	6	-6.497250000	2.329991000	-2.564252000
1	1.270662000	-2.442709000	0.430905000	6	-6.613843000	3.610011000	-2.061528000
1	-0.465049000	-4.080058000	1.031164000	6	-5.721468000	4.058401000	-1.116055000
1	0.621764000	-5.415869000	0.712331000	6	-4.687729000	3.249593000	-0.657119000
1	0.931580000	-4.346824000	2.067817000	6	-3.711715000	3.834757000	0.363974000
1	-0.150942000	-3.437407000	-1.392170000	6	-3.138300000	5.183320000	-0.125916000

6	-4.404536000	4.037096000	1.727693000	1	-2.716613000	2.653309000	-2.601088000
6	-1.931389000	1.975988000	-2.278761000	1	-1.549388000	1.408616000	-3.130785000
6	-0.736607000	-2.313806000	-0.900407000	1	0.259439000	-1.920096000	-1.097590000
6	-2.861727000	-2.863621000	0.972105000	1	-0.670695000	-3.191658000	-0.259252000
6	-3.546068000	-3.806459000	0.198856000	1	-1.179808000	-2.617180000	-1.854783000
6	-3.830976000	-5.040118000	0.767497000	1	-4.354868000	-5.775258000	0.191757000
6	-3.453565000	-5.337400000	2.058403000	1	-3.690290000	-6.293374000	2.481157000
6	-2.759650000	-4.405738000	2.799578000	1	-2.453949000	-4.647924000	3.796421000
6	-2.443304000	-3.160210000	2.276713000	1	-1.375230000	-1.328756000	2.552745000
6	-1.639041000	-2.189627000	3.144560000	1	0.284356000	-2.094211000	4.133285000
6	-0.332672000	-2.842461000	3.649288000	1	-0.541113000	-3.625059000	4.368839000
6	-2.463813000	-1.699233000	4.353126000	1	0.232629000	-3.271407000	2.835273000
6	-3.979854000	-3.562578000	-1.245597000	1	-1.869218000	-1.017729000	4.951235000
6	-5.513746000	-3.654639000	-1.397900000	1	-3.351104000	-1.175116000	4.032965000
6	-3.316081000	-4.583884000	-2.200519000	1	-2.762598000	-2.532926000	4.977893000
6	-5.617429000	-0.309474000	1.850244000	1	-3.675550000	-2.568400000	-1.536738000
1	-6.875485000	-1.898065000	2.605633000	1	-5.789356000	-3.527142000	-2.438061000
1	-6.737629000	0.302888000	3.605198000	1	-6.011726000	-2.892071000	-0.816143000
1	-5.625845000	1.546966000	3.031648000	1	-5.874501000	-4.622440000	-1.073364000
1	-5.003293000	0.160912000	3.914993000	1	-3.537805000	-4.325915000	-3.230798000
1	-0.485213000	0.123012000	-1.462976000	1	-2.242058000	-4.612353000	-2.075147000
1	-4.961199000	-0.568305000	-1.927484000	1	-3.700566000	-5.579619000	-2.016817000
1	-4.458928000	-0.976742000	-4.344845000	6	-5.741261000	0.470218000	3.169623000
1	-4.943032000	0.674676000	-4.710205000	1	-5.156406000	-2.211517000	2.863577000
1	-3.517746000	0.373595000	-3.735783000	1	-5.847911000	-2.411928000	1.264686000
1	-6.682870000	-1.574486000	-3.307208000	6	-5.875163000	-1.788696000	2.158248000
1	-7.222578000	-0.025592000	-3.900206000	6	-6.722044000	0.179206000	0.908788000
1	-7.485282000	-0.456385000	-2.215393000	1	-7.706296000	-0.014764000	1.362954000
1	-7.197278000	1.993845000	-3.298818000	1	-6.698779000	-0.341993000	-0.051310000
1	-7.398770000	4.252489000	-2.407804000	1	-6.660738000	1.251277000	0.704757000
1	-5.818795000	5.052101000	-0.731206000	1	-0.695267000	0.730248000	0.179804000
1	-2.892250000	3.147025000	0.509134000	1	-2.724392000	0.865976000	2.018532000
1	-2.705768000	5.095052000	-1.113662000	1	-1.085708000	2.548646000	-1.886819000
1	-2.366788000	5.520608000	0.555382000	31	3.738388000	0.691287000	-1.063937000
1	-3.909074000	5.943340000	-0.157359000	7	3.670277000	-1.182796000	-0.390412000
1	-4.774666000	3.099944000	2.112534000	6	2.557563000	-1.547461000	0.293570000
1	-3.699841000	4.442251000	2.445351000	6	1.608204000	-0.673406000	0.790643000
1	-5.237077000	4.724909000	1.636102000	6	1.595903000	0.774528000	0.876240000

7	2.669599000	1.474539000	0.407993000	1	5.514252000	2.598551000	4.311993000
6	2.939132000	2.813331000	0.888781000	1	6.218871000	2.081223000	2.785853000
6	3.680195000	2.961384000	2.078075000	1	4.605924000	4.349892000	3.398627000
6	4.061896000	1.745562000	2.918551000	1	4.007975000	6.323004000	2.085528000
6	3.032574000	1.544638000	4.055724000	1	2.687849000	6.074028000	0.047606000
6	5.474736000	1.844507000	3.534049000	1	1.408557000	2.827951000	-1.225473000
6	4.042572000	4.229922000	2.495846000	1	-0.351212000	4.596963000	-1.580490000
6	3.702979000	5.348164000	1.758328000	1	0.510036000	5.653112000	-0.486321000
6	2.963631000	5.202738000	0.607844000	1	-0.190164000	4.162244000	0.121289000
6	2.555148000	3.947900000	0.166473000	1	1.511649000	4.435400000	-3.132682000
6	1.626820000	3.869791000	-1.044054000	1	2.523610000	5.504192000	-2.176652000
6	0.312797000	4.614785000	-0.722941000	1	3.108296000	3.913136000	-2.638665000
6	2.239445000	4.468919000	-2.326980000	1	0.397495000	2.425749000	1.583110000
6	0.443550000	1.355651000	1.425122000	1	-0.179833000	0.752001000	2.078840000
6	2.292453000	-3.024875000	0.494292000	1	2.066989000	-3.508667000	-0.458234000
6	4.575198000	-2.224678000	-0.837859000	1	3.160108000	-3.540091000	0.903021000
6	5.683820000	-2.563856000	-0.047044000	1	1.448642000	-3.173193000	1.164904000
6	6.531767000	-3.574827000	-0.472366000	1	7.374681000	-3.846907000	0.129794000
6	6.316057000	-4.229362000	-1.668064000	1	6.985688000	-5.004110000	-1.986722000
6	5.242683000	-3.873811000	-2.455214000	1	5.089046000	-4.374115000	-3.390491000
6	4.358262000	-2.880052000	-2.057594000	1	2.555166000	-1.824844000	-2.454722000
6	3.187774000	-2.526109000	-2.974653000	1	1.480310000	-3.465141000	-3.929221000
6	2.350843000	-3.769156000	-3.355464000	1	2.925650000	-4.453893000	-3.967286000
6	3.691645000	-1.832195000	-4.259044000	1	2.013497000	-4.306916000	-2.477540000
6	5.976074000	-1.828198000	1.258631000	1	2.855019000	-1.585168000	-4.905469000
6	7.474983000	-1.487183000	1.414667000	1	4.207880000	-0.916449000	-4.013069000
6	5.516396000	-2.645742000	2.486733000	1	4.368087000	-2.480125000	-4.804934000
6	5.594135000	1.424793000	-1.399155000	1	5.414688000	-0.909294000	1.229307000
1	7.420196000	0.812326000	-2.398061000	1	7.608921000	-0.822080000	2.261218000
1	6.504965000	3.012246000	-2.568709000	1	7.860961000	-0.996605000	0.531102000
1	5.006973000	3.492996000	-1.763487000	1	8.063659000	-2.378499000	1.599853000
1	4.946626000	2.469807000	-3.215338000	1	5.769943000	-2.118855000	3.401413000
1	0.761723000	-1.143217000	1.279567000	1	4.446624000	-2.803097000	2.479239000
1	4.027994000	0.888255000	2.265227000	1	6.009654000	-3.611905000	2.501446000
1	3.278152000	0.657397000	4.632454000	6	5.496458000	2.667421000	-2.286557000
1	3.048273000	2.401154000	4.722071000	1	5.971314000	0.080968000	-3.093912000
1	2.035183000	1.434374000	3.655784000	1	6.604799000	-0.520971000	-1.565814000
1	5.734813000	0.893741000	3.989201000	6	6.434129000	0.385238000	-2.148993000

6	6.325570000	1.821930000	-0.117610000	6	1.824384000	2.498949000	0.551795000
1	7.355639000	2.143858000	-0.347137000	6	1.400106000	3.458729000	-0.579395000
1	6.392983000	0.995268000	0.592664000	6	2.269942000	3.307968000	1.790533000
1	5.826218000	2.651791000	0.388060000	6	-0.004309000	-0.242355000	-2.451834000
1	2.731000000	0.700194000	-2.327807000	1	1.399610000	0.084813000	-4.058917000
				1	-0.463956000	-1.487660000	-4.162421000
<b>Ga-intra-TS<sub>1,2'</sub></b>				1	-1.558730000	-1.740573000	-2.797693000
1	1.186938000	-1.604214000	0.309231000	1	0.080367000	-2.420789000	-2.758517000
1	0.478251000	-2.200346000	-0.143432000	1	0.054057000	-0.387367000	3.759369000
31	-0.051847000	-0.467365000	-0.473696000	1	-1.545604000	2.252259000	-0.008267000
7	1.568961000	-0.402870000	0.739644000	1	-3.995061000	3.347599000	1.422809000
6	1.311144000	-0.375826000	2.138220000	1	-2.676365000	2.458066000	2.178008000
6	0.073869000	-0.325162000	2.675952000	1	-2.385346000	4.055503000	1.498724000
6	-1.280068000	-0.161163000	2.113119000	1	-2.182171000	4.351370000	-1.021199000
7	-1.447790000	-0.091020000	0.726252000	1	-3.878534000	3.930166000	-1.028485000
6	-2.803080000	-0.045587000	0.205262000	1	-2.765109000	3.090795000	-2.099336000
6	-3.362846000	1.183369000	-0.178971000	1	-5.088050000	2.128195000	-0.999106000
6	-2.596841000	2.492533000	0.000802000	1	-6.364088000	0.064184000	-1.251321000
6	-2.934162000	3.126916000	1.370496000	1	-5.395715000	-2.067694000	-0.556646000
6	-2.877608000	3.523561000	-1.113845000	1	-2.002587000	-2.441591000	0.918069000
6	-4.647642000	1.199299000	-0.701097000	1	-3.444193000	-4.069888000	2.072231000
6	-5.372806000	0.033250000	-0.843269000	1	-4.880181000	-3.319208000	1.393641000
6	-4.822794000	-1.168069000	-0.453395000	1	-3.879967000	-2.432797000	2.540900000
6	-3.542362000	-1.230634000	0.080776000	1	-2.556100000	-4.554377000	-0.225720000
6	-3.007011000	-2.582912000	0.554010000	1	-3.953801000	-3.810442000	-0.982959000
6	-3.862479000	-3.133114000	1.717514000	1	-2.335704000	-3.272593000	-1.403083000
6	-2.961928000	-3.616823000	-0.591689000	1	-3.322241000	0.067302000	2.688996000
6	-2.295577000	-0.059667000	3.001823000	1	-2.089791000	-0.108826000	4.063566000
6	2.511923000	-0.490009000	3.042924000	1	2.197583000	-0.494824000	4.087453000
6	2.824290000	0.157734000	0.251456000	1	3.060877000	-1.415032000	2.846121000
6	2.934820000	1.547240000	0.106627000	1	3.210124000	0.336040000	2.892469000
6	4.100708000	2.069716000	-0.430668000	1	4.202410000	3.130010000	-0.544124000
6	5.133109000	1.243555000	-0.825895000	1	6.023184000	1.661983000	-1.252508000
6	5.022040000	-0.119691000	-0.659143000	1	5.834069000	-0.751891000	-0.955445000
6	3.881418000	-0.686627000	-0.105143000	1	2.983468000	-2.443313000	0.712984000
6	3.841376000	-2.201331000	0.105330000	1	4.980806000	-3.754595000	1.096339000
6	5.093290000	-2.701530000	0.861352000	1	5.987024000	-2.589549000	0.260161000
6	3.698957000	-2.950688000	-1.236841000	1	5.233687000	-2.155406000	1.786361000

1	3.695802000	-4.022658000	-1.069712000	6	4.017484000	-2.828793000	-2.069763000
1	2.773100000	-2.682809000	-1.727694000	6	3.179076000	-3.554457000	0.209385000
1	4.522884000	-2.709275000	-1.898353000	6	2.167595000	0.358999000	-2.934859000
1	0.962253000	1.916753000	0.836129000	6	-2.488716000	-0.854271000	-2.980647000
1	0.576912000	4.080440000	-0.244272000	6	-2.823064000	0.218372000	-0.229969000
1	1.075839000	2.906069000	-1.450470000	6	-2.768012000	1.616772000	-0.260037000
1	2.214428000	4.110515000	-0.870915000	6	-3.902434000	2.327605000	0.100370000
1	1.464599000	3.954908000	2.121646000	6	-5.055040000	1.686078000	0.498542000
1	2.535100000	2.650839000	2.608662000	6	-5.089619000	0.311756000	0.536986000
1	3.129061000	3.924932000	1.553137000	6	-3.988505000	-0.452240000	0.171042000
6	-0.514708000	-1.553480000	-3.065559000	6	-4.168109000	-1.977864000	0.211085000
1	2.114114000	-0.775381000	-2.692219000	6	-5.217823000	-2.430687000	-0.830615000
1	1.835450000	0.954838000	-2.580396000	6	-4.592138000	-2.466360000	1.614950000
6	1.416059000	0.020831000	-2.960113000	6	-1.528097000	2.391282000	-0.702875000
6	-0.922176000	0.890706000	-2.917353000	6	-1.236364000	3.600415000	0.214615000
1	-0.903282000	0.947411000	-4.016355000	6	-1.707071000	2.899957000	-2.152458000
1	-0.602365000	1.864352000	-2.537650000	6	0.053713000	-0.514860000	2.439677000
1	-1.958242000	0.731164000	-2.609178000	1	-0.422097000	1.076022000	3.839318000
				1	-0.971282000	-1.370600000	4.157473000
<b>Ga-intra-IM<sub>1,z'</sub></b>				1	-0.636805000	-2.549754000	2.875364000
1	-1.862787000	-1.544340000	-0.477046000	1	-1.941426000	-1.367138000	2.680964000
1	-0.014965000	-2.505914000	0.136918000	1	-0.085769000	-0.320196000	-3.673717000
31	0.160038000	-0.948338000	0.493752000	1	1.393339000	2.142862000	0.358547000
7	-1.627374000	-0.568143000	-0.642512000	1	3.762854000	3.689721000	-0.764389000
6	-1.327413000	-0.534673000	-2.079420000	1	2.521870000	2.876649000	-1.712171000
6	-0.110108000	-0.291435000	-2.587902000	1	2.108409000	4.284956000	-0.740194000
6	1.221363000	0.017719000	-2.024795000	1	1.846259000	4.042335000	1.799153000
7	1.416478000	-0.053344000	-0.652551000	1	3.569139000	3.740557000	1.778941000
6	2.791501000	0.023225000	-0.179981000	1	2.495283000	2.619622000	2.603677000
6	3.282803000	1.219089000	0.362326000	1	4.973930000	2.176800000	1.235783000
6	2.416380000	2.470182000	0.424612000	1	6.414711000	0.207944000	1.124526000
6	2.720768000	3.388810000	-0.780959000	1	5.560113000	-1.876701000	0.179586000
6	2.597763000	3.261923000	1.737809000	1	2.140763000	-2.316259000	-1.188601000
6	4.590328000	1.266135000	0.823481000	1	3.637984000	-3.747255000	-2.506758000
6	5.407223000	0.156650000	0.760553000	1	5.049094000	-2.995024000	-1.781815000
6	4.922006000	-1.017109000	0.226812000	1	3.987402000	-2.052265000	-2.822947000
6	3.622789000	-1.105207000	-0.253537000	1	2.806208000	-4.479105000	-0.219133000
6	3.156293000	-2.431913000	-0.850873000	1	4.185928000	-3.728813000	0.570575000

1	2.551441000	-3.296656000	1.052770000	6	0.146940000	0.257097000	-2.316348000
1	3.180913000	0.596773000	-2.642968000	6	0.977780000	-0.629830000	-1.441017000
1	1.922837000	0.386777000	-3.989021000	7	1.618510000	-0.049978000	-0.418333000
1	-2.185370000	-0.793606000	-4.026845000	6	2.646222000	-0.791792000	0.317800000
1	-2.849640000	-1.872192000	-2.796220000	6	3.967564000	-0.554257000	-0.097957000
1	-3.327235000	-0.172879000	-2.818541000	6	4.271436000	0.387342000	-1.259753000
1	-3.881242000	3.396504000	0.072972000	6	4.538601000	-0.430962000	-2.543128000
1	-5.919740000	2.254604000	0.777455000	6	5.457894000	1.329429000	-0.968796000
1	-5.987968000	-0.180516000	0.846700000	6	5.005908000	-1.214122000	0.535480000
1	-3.240858000	-2.482667000	-0.022883000	6	4.760217000	-2.084256000	1.577601000
1	-5.295459000	-3.512585000	-0.830740000	6	3.466912000	-2.295942000	1.994910000
1	-6.190880000	-2.022566000	-0.587019000	6	2.388358000	-1.663531000	1.384063000
1	-4.955038000	-2.103897000	-1.827511000	6	0.996499000	-1.958396000	1.949136000
1	-4.636709000	-3.549908000	1.625132000	6	0.660842000	-3.467903000	1.907719000
1	-3.889191000	-2.145340000	2.369443000	6	0.891891000	-1.464833000	3.410729000
1	-5.572563000	-2.089051000	1.876256000	6	0.568318000	-1.967702000	-1.455080000
1	-0.676861000	1.731884000	-0.664312000	6	-2.088353000	1.424021000	-2.438075000
1	-0.285507000	4.037135000	-0.064708000	6	-2.673376000	-0.319149000	-0.084978000
1	-1.188271000	3.307515000	1.253977000	6	-3.323880000	0.425595000	0.912026000
1	-1.991699000	4.368973000	0.105822000	6	-4.556425000	-0.005057000	1.388606000
1	-0.803351000	3.400193000	-2.483172000	6	-5.179692000	-1.117906000	0.878734000
1	-1.913358000	2.087652000	-2.834240000	6	-4.581162000	-1.800654000	-0.155972000
1	-2.528507000	3.606532000	-2.197698000	6	-3.347309000	-1.418270000	-0.657216000
6	-0.926813000	-1.509736000	3.065863000	6	-2.803336000	-2.227206000	-1.834711000
1	-1.429699000	1.088225000	2.385062000	6	-3.805291000	-2.253531000	-3.012559000
1	0.245947000	1.653458000	2.308025000	6	-2.456835000	-3.667567000	-1.399650000
6	-0.414239000	0.904740000	2.750717000	6	-2.799889000	1.735839000	1.486351000
6	1.439462000	-0.740990000	3.057282000	6	-2.520874000	1.626514000	2.999160000
1	1.389467000	-0.607172000	4.150033000	6	-3.790074000	2.888786000	1.201354000
1	2.183429000	-0.042160000	2.668045000	6	0.619975000	3.057655000	-0.174796000
1	1.814155000	-1.754916000	2.874780000	1	-0.050586000	5.115444000	-0.023166000
				1	2.288205000	4.332788000	0.420018000
<b>Ga-intra-TS<sub>2,4</sub></b>				1	2.659856000	2.604768000	0.536068000
1	-0.503282000	-1.223522000	-0.784804000	1	1.628888000	3.368528000	1.752375000
1	0.259130000	0.951537000	1.967579000	1	0.505173000	0.629342000	-3.267686000
31	0.246400000	1.176297000	0.417345000	1	3.395758000	0.992697000	-1.415573000
7	-1.295646000	-0.010342000	-0.507316000	1	5.411048000	-1.061512000	-2.411883000
6	-1.070891000	0.530103000	-1.806433000	1	3.694334000	-1.069192000	-2.777801000

1	4.716787000	0.229727000	-3.385967000	1	-1.347716000	3.989142000	-0.432625000
1	5.555695000	2.049840000	-1.774341000	6	-0.440571000	4.103574000	0.170547000
1	6.392796000	0.786498000	-0.897221000	6	1.001558000	3.216925000	-1.645129000
1	5.302315000	1.870966000	-0.043251000	1	1.405537000	4.225279000	-1.828730000
1	6.013700000	-1.047430000	0.214592000	1	0.139253000	3.088359000	-2.308561000
1	5.572405000	-2.589074000	2.062586000	1	1.764255000	2.495301000	-1.954836000
1	3.284835000	-2.964589000	2.811279000				
1	0.255165000	-1.434338000	1.368681000				<i>Ga-inter-TS<sub>1,4</sub>-I in gas phase</i>
1	-0.359116000	-3.622864000	2.243856000	7	3.588335000	1.159833000	-0.746048000
1	1.316620000	-4.026878000	2.563944000	6	2.271593000	1.302518000	-1.142579000
1	0.756050000	-3.877558000	0.910936000	6	1.278816000	0.425511000	-0.804990000
1	-0.123796000	-1.592682000	3.771481000	6	1.320107000	-0.825494000	-0.079567000
1	1.552961000	-2.034864000	4.052940000	7	2.483541000	-1.240858000	0.531612000
1	1.153520000	-0.419689000	3.483961000	6	2.542575000	-2.570668000	1.136742000
1	1.028149000	-2.671377000	-0.775970000	6	2.914296000	-3.668699000	0.341238000
1	0.169358000	-2.368642000	-2.379695000	6	2.976467000	-4.922078000	0.930793000
1	-2.213728000	2.315634000	-1.813563000	6	2.691955000	-5.095045000	2.270082000
1	-1.764175000	1.734176000	-3.433783000	6	2.339204000	-4.011284000	3.042226000
1	-3.060937000	0.933725000	-2.509075000	6	2.254738000	-2.735926000	2.496973000
1	-5.036041000	0.552939000	2.166386000	6	0.116968000	-1.540587000	-0.006070000
1	-6.127091000	-1.437014000	1.265664000	6	1.928069000	2.472910000	-2.022401000
1	-5.078259000	-2.648110000	-0.581803000	6	4.634334000	2.007117000	-1.299689000
1	-1.909240000	-1.758524000	-2.199713000	6	5.273878000	1.605504000	-2.478195000
1	-3.356909000	-2.756773000	-3.863075000	6	6.364723000	2.335685000	-2.924595000
1	-4.711277000	-2.785239000	-2.750534000	6	6.800104000	3.449627000	-2.234981000
1	-4.076136000	-1.248730000	-3.314252000	6	6.129782000	3.865246000	-1.103656000
1	-2.021517000	-4.217889000	-2.227929000	6	5.033481000	3.162505000	-0.622230000
1	-1.750795000	-3.663990000	-0.579182000	6	5.861189000	-0.730784000	1.114508000
1	-3.348806000	-4.192020000	-1.077768000	1	7.916690000	-0.085331000	1.095417000
1	-1.883309000	1.990304000	0.990977000	1	5.407963000	0.408820000	2.952392000
1	-2.076601000	2.546611000	3.364069000	1	6.687661000	-0.799461000	3.113224000
1	-1.837214000	0.814527000	3.203005000	1	4.998920000	-1.313354000	3.028215000
1	-3.440516000	1.454583000	3.546099000	1	0.284223000	0.684378000	-1.152350000
1	-3.372128000	3.828353000	1.544650000	1	3.248360000	-5.772232000	0.340566000
1	-3.994413000	2.969477000	0.140122000	1	2.744143000	-6.072568000	2.707194000
1	-4.729573000	2.730097000	1.715779000	1	2.115281000	-4.156001000	4.079035000
6	1.868208000	3.350065000	0.682505000	1	0.123477000	-2.526742000	0.439956000
1	-0.730062000	4.068421000	1.226852000	1	-0.549224000	-1.412917000	-0.856121000

1	2.220029000	3.416422000	-1.558448000	1	6.752112000	-0.556834000	-3.364185000
1	2.458698000	2.405575000	-2.975841000	1	5.766141000	-1.092815000	-2.016603000
1	0.853664000	2.496444000	-2.207381000	1	5.410916000	-1.664430000	-3.637597000
1	6.876434000	2.036284000	-3.816610000	6	4.649958000	0.701866000	-4.776167000
1	7.649317000	4.000469000	-2.588052000	1	4.203839000	-0.146148000	-5.284374000
1	6.458699000	4.746696000	-0.591371000	1	4.016892000	1.566666000	-4.934216000
6	5.718488000	-0.592383000	2.636934000	1	5.612606000	0.894616000	-5.233507000
1	6.784762000	1.248477000	0.846218000	6	4.284776000	3.681356000	0.603427000
1	7.118661000	0.133996000	-0.467496000	1	3.404572000	3.073477000	0.738135000
6	6.970403000	0.199473000	0.612349000	6	5.141462000	3.570216000	1.882145000
6	6.248170000	-2.182508000	0.809845000	1	4.594229000	3.958843000	2.734330000
1	7.191116000	-2.415554000	1.326139000	1	5.396072000	2.538766000	2.085662000
1	6.418115000	-2.349672000	-0.256637000	1	6.061354000	4.134363000	1.781594000
1	5.495699000	-2.894477000	1.155702000	6	3.829854000	5.144269000	0.402187000
31	4.098612000	-0.294130000	0.317810000	1	4.680425000	5.812457000	0.341191000
6	3.223201000	-3.536759000	-1.152616000	1	3.247278000	5.251207000	-0.504289000
1	3.474106000	-2.505840000	-1.359643000	1	3.216068000	5.456390000	1.239700000
6	1.793095000	-1.585812000	3.391772000	7	-3.331391000	-1.052900000	-0.942306000
1	1.950993000	-0.658869000	2.860341000	6	-2.565553000	-0.567494000	-2.003645000
6	1.982895000	-3.902361000	-2.000593000	6	-2.091880000	0.704895000	-2.102039000
1	1.696777000	-4.929921000	-1.806375000	6	-2.337484000	1.918061000	-1.301731000
1	1.146966000	-3.261937000	-1.766384000	7	-3.027208000	1.792165000	-0.095504000
1	2.211909000	-3.804676000	-3.057100000	6	-3.266526000	2.991321000	0.680323000
6	4.409900000	-4.418204000	-1.603237000	6	-4.498911000	3.655895000	0.587253000
1	4.684082000	-4.157835000	-2.619784000	6	-4.714177000	4.788768000	1.357782000
1	5.275393000	-4.286471000	-0.968892000	6	-3.745149000	5.261457000	2.218787000
1	4.138921000	-5.466686000	-1.599923000	6	-2.536821000	4.605786000	2.309545000
6	0.284713000	-1.725655000	3.698359000	6	-2.276368000	3.478891000	1.542158000
1	0.095815000	-2.656188000	4.221743000	6	-1.890208000	3.100269000	-1.802343000
1	-0.043392000	-0.907784000	4.330266000	6	-2.201794000	-1.543952000	-3.099445000
1	-0.304261000	-1.711080000	2.795077000	6	-4.272488000	-2.120922000	-1.231342000
6	2.563742000	-1.524724000	4.730675000	6	-5.428162000	-1.834609000	-1.979748000
1	3.633928000	-1.501425000	4.582864000	6	-6.293772000	-2.864200000	-2.314633000
1	2.273782000	-0.630723000	5.272304000	6	-6.056748000	-4.158081000	-1.901146000
1	2.325788000	-2.377106000	5.355220000	6	-4.948761000	-4.429418000	-1.129387000
6	4.793023000	0.390224000	-3.271447000	6	-4.048490000	-3.430636000	-0.781800000
1	3.819697000	0.106900000	-2.901433000	6	-4.384782000	-0.332522000	2.270265000
6	5.742563000	-0.807682000	-3.061065000	1	-6.258192000	-1.307243000	2.772231000

1	-4.162579000	-1.480693000	4.103475000	1	-5.937217000	0.765505000	-4.235269000
1	-2.705653000	-0.587713000	3.644453000	1	-4.702439000	-0.476084000	-4.322073000
1	-3.132111000	-2.064628000	2.784057000	6	-7.181863000	-0.009100000	-1.932019000
1	-1.464038000	0.896066000	-2.967131000	1	-7.947530000	-0.624561000	-2.388960000
1	-5.649342000	5.305660000	1.289891000	1	-7.261277000	-0.108692000	-0.857175000
1	-3.932196000	6.134513000	2.813170000	1	-7.380621000	1.023398000	-2.197061000
1	-1.785849000	4.974641000	2.979731000	6	-5.590363000	3.167186000	-0.358976000
1	-2.036458000	4.038030000	-1.285902000	1	-5.386683000	2.130313000	-0.568833000
1	-1.411726000	3.122149000	-2.774209000	6	-7.006077000	3.274631000	0.248055000
1	-1.680033000	-2.408262000	-2.681369000	1	-7.309457000	4.308319000	0.364602000
1	-3.085734000	-1.929229000	-3.609308000	1	-7.721671000	2.796701000	-0.411542000
1	-1.550382000	-1.067179000	-3.834244000	1	-7.058259000	2.790669000	1.215687000
1	-7.166458000	-2.650832000	-2.898712000	6	-5.532706000	3.952967000	-1.688884000
1	-6.735127000	-4.944364000	-2.168768000	1	-4.563125000	3.841090000	-2.153227000
1	-4.775233000	-5.432790000	-0.795887000	1	-6.292635000	3.590501000	-2.375399000
6	-3.546836000	-1.164562000	3.247043000	1	-5.714129000	5.006919000	-1.504669000
1	-5.408460000	-2.085836000	1.425590000	6	-0.915532000	2.802124000	1.658080000
1	-6.258474000	-0.566935000	1.165060000	1	-0.864609000	2.027466000	0.913638000
6	-5.640641000	-1.120009000	1.879493000	6	0.233161000	3.794074000	1.388220000
6	-4.821305000	0.951665000	2.980775000	1	0.276393000	4.566448000	2.147762000
1	-5.382895000	0.695147000	3.893498000	1	1.179541000	3.264018000	1.391973000
1	-5.472218000	1.566738000	2.356618000	1	0.105405000	4.262508000	0.420721000
1	-3.977806000	1.581118000	3.275949000	6	-0.746993000	2.144674000	3.043375000
31	-3.291095000	0.051356000	0.638171000	1	-1.509850000	1.392996000	3.192793000
6	-2.846087000	-3.807006000	0.077870000	1	0.222881000	1.661168000	3.115504000
1	-2.347736000	-2.893630000	0.356476000	1	-0.824328000	2.880032000	3.836208000
6	-1.855528000	-4.696374000	-0.706617000	1	-0.889094000	-0.752434000	0.742185000
1	-0.992905000	-4.934569000	-0.092115000	1	-1.615099000	-0.333569000	1.165252000
1	-2.333835000	-5.625195000	-0.996439000				
1	-1.508740000	-4.201597000	-1.602711000				<i>Ga-inter-TS<sub>1,4</sub>-I in gas phase</i>
6	-3.272912000	-4.550796000	1.364591000	7	3.632432000	1.152910000	-0.758752000
1	-4.037152000	-4.005026000	1.900227000	6	2.317227000	1.314207000	-1.144117000
1	-3.659956000	-5.535816000	1.131858000	6	1.314866000	0.445205000	-0.808075000
1	-2.415965000	-4.677073000	2.018843000	6	1.343798000	-0.816828000	-0.099432000
6	-5.773248000	-0.413165000	-2.421094000	7	2.503568000	-1.252619000	0.504773000
1	-5.057441000	0.257230000	-1.976165000	6	2.543537000	-2.592807000	1.088478000
6	-5.695633000	-0.254709000	-3.955471000	6	2.862480000	-3.690370000	0.269486000
1	-6.400461000	-0.918136000	-4.444647000	6	2.881001000	-4.957055000	0.835931000

6	2.608463000	-5.143970000	2.175584000	1	3.413318000	-2.514095000	-1.425759000
6	2.320803000	-4.059414000	2.974920000	6	1.919137000	-1.613738000	3.384259000
6	2.283846000	-2.771613000	2.454324000	1	2.189306000	-0.690821000	2.892437000
6	0.133495000	-1.520751000	-0.044870000	6	1.942195000	-3.926046000	-2.078982000
6	1.979768000	2.495532000	-2.011173000	1	1.665926000	-4.958575000	-1.895346000
6	4.678799000	2.025343000	-1.272703000	1	1.097159000	-3.296146000	-1.846813000
6	5.337928000	1.668795000	-2.455873000	1	2.173787000	-3.818222000	-3.134373000
6	6.432026000	2.420079000	-2.859960000	6	4.370686000	-4.417161000	-1.667141000
6	6.850727000	3.512022000	-2.125343000	1	4.644647000	-4.162790000	-2.685795000
6	6.159592000	3.886498000	-0.991788000	1	5.234930000	-4.270054000	-1.033763000
6	5.059695000	3.161579000	-0.551964000	1	4.115136000	-5.469717000	-1.655169000
6	5.881499000	-0.783197000	1.105384000	6	0.397500000	-1.601660000	3.652135000
1	7.940653000	-0.148366000	1.135534000	1	0.094305000	-2.533958000	4.116659000
1	5.379453000	0.275796000	2.979948000	1	0.144130000	-0.790209000	4.326472000
1	6.683763000	-0.908730000	3.113622000	1	-0.162606000	-1.473667000	2.739402000
1	5.010058000	-1.456246000	2.983141000	6	2.654412000	-1.681458000	4.742273000
1	0.322424000	0.720197000	-1.149743000	1	3.721336000	-1.812824000	4.624167000
1	3.110459000	-5.806099000	0.225661000	1	2.483766000	-0.760169000	5.290150000
1	2.624333000	-6.131177000	2.593976000	1	2.277669000	-2.495384000	5.350145000
1	2.116002000	-4.213725000	4.014343000	6	4.870576000	0.483109000	-3.300716000
1	0.120219000	-2.509681000	0.392972000	1	3.882668000	0.202775000	-2.970354000
1	-0.527445000	-1.370817000	-0.895258000	6	5.796828000	-0.733274000	-3.098068000
1	2.293105000	3.433895000	-1.550647000	1	6.819487000	-0.489043000	-3.361702000
1	2.491812000	2.423630000	-2.974822000	1	5.782480000	-1.054080000	-2.063583000
1	0.903392000	2.536464000	-2.184729000	1	5.472676000	-1.565984000	-3.713740000
1	6.959771000	2.154664000	-3.753588000	6	4.780037000	0.839949000	-4.799014000
1	7.702838000	4.078993000	-2.445208000	1	4.325451000	0.018604000	-5.343331000
1	6.475563000	4.751874000	-0.444826000	1	4.174671000	1.725695000	-4.953872000
6	5.717540000	-0.704786000	2.628736000	1	5.760019000	1.016792000	-5.225711000
1	6.819936000	1.200087000	0.928381000	6	4.288428000	3.639007000	0.677282000
1	7.164009000	0.133647000	-0.426155000	1	3.407368000	3.025712000	0.778362000
6	7.000348000	0.159428000	0.653786000	6	5.123674000	3.490001000	1.965180000
6	6.266013000	-2.222549000	0.747225000	1	4.562710000	3.853712000	2.820238000
1	7.202655000	-2.483134000	1.262840000	1	5.374272000	2.452562000	2.144820000
1	6.445822000	-2.350848000	-0.323367000	1	6.046171000	4.055426000	1.898726000
1	5.507992000	-2.944111000	1.059965000	6	3.831752000	5.105325000	0.514460000
31	4.130065000	-0.311699000	0.306852000	1	4.680045000	5.778843000	0.479722000
6	3.172289000	-3.548005000	-1.224166000	1	3.254701000	5.238204000	-0.392806000

1	3.211350000	5.393768000	1.356294000	1	-5.381829000	-2.084952000	1.512782000
7	-3.384247000	-1.050683000	-0.924078000	1	-6.258387000	-0.577273000	1.264399000
6	-2.618333000	-0.580623000	-1.991296000	6	-5.611148000	-1.116762000	1.963809000
6	-2.135189000	0.688513000	-2.103474000	6	-4.792257000	0.969414000	3.027529000
6	-2.379219000	1.914064000	-1.322288000	1	-5.325896000	0.711312000	3.957062000
7	-3.061879000	1.807061000	-0.110373000	1	-5.471754000	1.571082000	2.419862000
6	-3.304384000	3.021064000	0.641830000	1	-3.952066000	1.613597000	3.299985000
6	-4.534335000	3.687918000	0.528274000	31	-3.311922000	0.069354000	0.646348000
6	-4.753293000	4.833796000	1.280620000	6	-2.832216000	-3.791763000	0.125899000
6	-3.789504000	5.318911000	2.140518000	1	-2.346950000	-2.867510000	0.391931000
6	-2.579813000	4.665790000	2.245485000	6	-1.828405000	-4.678471000	-0.643798000
6	-2.315495000	3.526436000	1.497557000	1	-0.962835000	-4.894493000	-0.025273000
6	-1.930011000	3.088939000	-1.841758000	1	-2.290591000	-5.620594000	-0.918063000
6	-2.262606000	-1.565912000	-3.080801000	1	-1.486619000	-4.195447000	-1.548391000
6	-4.302930000	-2.144441000	-1.192565000	6	-3.246993000	-4.525219000	1.422215000
6	-5.471501000	-1.892566000	-1.935325000	1	-4.020921000	-3.987989000	1.953770000
6	-6.311202000	-2.946624000	-2.262582000	1	-3.616718000	-5.520268000	1.202843000
6	-6.037209000	-4.232440000	-1.845625000	1	-2.387888000	-4.629614000	2.077940000
6	-4.918869000	-4.470850000	-1.077258000	6	-5.861145000	-0.482811000	-2.378303000
6	-4.043578000	-3.446686000	-0.736325000	1	-5.158428000	0.207891000	-1.943949000
6	-4.355061000	-0.311382000	2.312970000	6	-5.808298000	-0.327428000	-3.913321000
1	-6.201586000	-1.306126000	2.874867000	1	-6.504323000	-1.007191000	-4.393320000
1	-4.068187000	-1.451613000	4.144122000	1	-6.076680000	0.686472000	-4.193566000
1	-2.641284000	-0.531148000	3.651442000	1	-4.815567000	-0.526098000	-4.295428000
1	-3.056749000	-2.018337000	2.804135000	6	-7.274211000	-0.118147000	-1.872301000
1	-1.503980000	0.864473000	-2.969124000	1	-8.027671000	-0.759449000	-2.314712000
1	-5.686545000	5.352826000	1.196019000	1	-7.338769000	-0.212807000	-0.795238000
1	-3.979481000	6.201747000	2.719977000	1	-7.510921000	0.905399000	-2.141778000
1	-1.830837000	5.047538000	2.910837000	6	-5.620166000	3.202306000	-0.427047000
1	-2.066865000	4.036194000	-1.339976000	1	-5.381149000	2.186628000	-0.694760000
1	-1.446879000	3.093918000	-2.811941000	6	-7.026066000	3.225074000	0.209478000
1	-1.791052000	-2.455350000	-2.657747000	1	-7.353028000	4.237571000	0.415125000
1	-3.144183000	-1.907809000	-3.625357000	1	-7.745246000	2.782165000	-0.470975000
1	-1.569548000	-1.112463000	-3.792555000	1	-7.048292000	2.665041000	1.136905000
1	-7.192291000	-2.758807000	-2.843186000	6	-5.615121000	4.057552000	-1.713932000
1	-6.694843000	-5.038206000	-2.108356000	1	-4.650728000	4.005635000	-2.201315000
1	-4.717100000	-5.468062000	-0.740776000	1	-6.370751000	3.702078000	-2.409175000
6	-3.479379000	-1.124582000	3.272284000	1	-5.831871000	5.094637000	-1.478397000

6	-0.950448000	2.858109000	1.624335000	1	5.373964000	3.940629000	-3.454778000
1	-0.893246000	2.075658000	0.888331000	1	5.812740000	2.500844000	-5.368835000
6	0.195511000	3.852438000	1.350967000	1	4.944740000	0.221813000	-5.421052000
1	0.234084000	4.630249000	2.105642000	1	0.107308000	-1.682282000	1.907647000
1	1.143649000	3.326210000	1.362783000	1	1.135471000	-1.052702000	3.225086000
1	0.073980000	4.316673000	0.380176000	1	-0.074014000	-0.025751000	2.387258000
6	-0.780836000	2.216743000	3.016228000	1	4.642684000	-0.133750000	5.719889000
1	-1.535706000	1.458923000	3.175525000	1	5.264767000	-2.492142000	5.790135000
1	0.193626000	1.744374000	3.096044000	1	4.655781000	-3.982749000	3.955790000
1	-0.865629000	2.959223000	3.802311000	6	6.847945000	-0.798162000	-0.913168000
1	-0.903668000	-0.717405000	0.705770000	1	6.465904000	-1.595268000	1.736240000
1	-1.608576000	-0.295662000	1.126701000	1	6.428347000	0.011983000	2.445392000
				6	6.773394000	-0.559532000	1.582223000
<b>Ga-inter-IM<sub>1,4</sub></b>				6	6.782110000	1.455576000	0.088744000
7	2.993012000	-0.518655000	1.454316000	1	7.879622000	1.446016000	0.150725000
6	1.665041000	-0.398601000	1.231751000	1	6.424246000	2.135413000	0.865563000
6	1.133941000	0.098018000	0.032854000	1	6.511544000	1.863328000	-0.886612000
6	1.798849000	0.549225000	-1.107705000	31	4.286944000	0.004683000	0.180894000
7	3.150574000	0.614398000	-1.202784000	6	3.995795000	3.400810000	-1.172155000
6	3.816337000	1.150059000	-2.390990000	1	4.019740000	2.814576000	-0.262564000
6	4.288195000	2.472305000	-2.356607000	6	3.437245000	-1.080134000	-3.612772000
6	5.003211000	2.937951000	-3.449095000	1	2.762474000	-1.239507000	-2.786563000
6	5.249994000	2.124013000	-4.538087000	6	2.583151000	4.017260000	-1.301381000
6	4.762722000	0.836774000	-4.563805000	1	2.504355000	4.563736000	-2.233927000
6	4.024592000	0.328513000	-3.501303000	1	1.812454000	3.262506000	-1.278336000
6	0.679450000	-0.811717000	2.268700000	1	2.401552000	4.706096000	-0.483450000
6	3.508512000	-1.083894000	2.701078000	6	5.018832000	4.546173000	-1.017426000
6	3.771661000	-0.232594000	3.776758000	1	4.838232000	5.056951000	-0.078358000
6	4.416513000	-0.762739000	4.883901000	1	6.039002000	4.184960000	-1.018243000
6	4.760068000	-2.100161000	4.929619000	1	4.908438000	5.276401000	-1.809954000
6	4.424134000	-2.939715000	3.887576000	6	2.631399000	-1.239911000	-4.922525000
6	3.777650000	-2.451300000	2.760180000	1	3.284537000	-1.218566000	-5.786175000
6	6.273383000	0.016479000	0.252937000	1	2.114811000	-2.192546000	-4.918803000
1	7.872463000	-0.535547000	1.585935000	1	1.896597000	-0.452389000	-5.031669000
1	6.584280000	-1.857257000	-0.863996000	6	4.530239000	-2.166972000	-3.538229000
1	7.944936000	-0.740007000	-0.873451000	1	5.015061000	-2.160931000	-2.572051000
1	6.532269000	-0.397946000	-1.879930000	1	4.088737000	-3.146117000	-3.688059000
1	0.047776000	0.126258000	-0.011930000	1	5.283656000	-2.011654000	-4.301355000

6	3.335647000	1.232791000	3.753070000	6	-3.677459000	3.690549000	0.807632000
1	2.563535000	1.340137000	3.006485000	6	-4.111056000	0.625248000	-2.485822000
6	4.508718000	2.148933000	3.351745000	1	-5.425831000	2.063789000	-3.444412000
1	5.331919000	2.046160000	4.049048000	1	-3.472791000	0.967717000	-4.545733000
1	4.869053000	1.889428000	2.364566000	1	-2.332818000	-0.009756000	-3.599498000
1	4.195050000	3.186921000	3.335005000	1	-2.421564000	1.731404000	-3.339439000
6	2.739332000	1.687398000	5.101526000	1	-2.242047000	-0.727758000	3.163889000
1	2.322797000	2.682773000	4.995039000	1	-5.988813000	-5.040828000	-0.803786000
1	1.948888000	1.019281000	5.420589000	1	-4.461603000	-6.070347000	-2.413840000
1	3.494102000	1.726232000	5.877364000	1	-2.336246000	-4.986293000	-2.935393000
6	3.355492000	-3.400428000	1.638663000	1	-2.179473000	-3.770422000	1.242737000
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6	4.568042000	-3.801260000	0.773409000	1	-2.681366000	2.522867000	3.151069000
1	4.262244000	-4.469456000	-0.023835000	1	-4.272179000	1.909318000	3.537446000
1	5.022682000	-2.925444000	0.325347000	1	-2.838313000	1.064845000	4.146978000
1	5.320635000	-4.299580000	1.373279000	1	-7.507953000	3.867149000	1.119100000
6	2.642415000	-4.655649000	2.184562000	1	-6.203275000	5.926579000	0.993707000
1	3.319809000	-5.282488000	2.751610000	1	-3.774853000	5.820929000	0.752869000
1	1.809609000	-4.380193000	2.819450000	6	-3.023997000	0.838340000	-3.546863000
1	2.258035000	-5.241351000	1.357260000	1	-4.445692000	2.775600000	-2.152360000
7	-3.771726000	1.220317000	0.896725000	1	-5.823192000	1.766654000	-1.746748000
6	-3.219339000	0.732389000	2.055630000	6	-4.992711000	1.875323000	-2.446945000
6	-2.641927000	-0.505290000	2.179767000	6	-4.981883000	-0.560094000	-2.905685000
6	-2.628462000	-1.667678000	1.283014000	1	-5.505072000	-0.336431000	-3.850963000
7	-3.157164000	-1.528602000	0.003412000	1	-5.743116000	-0.783670000	-2.152438000
6	-3.502864000	-2.750316000	-0.680936000	1	-4.401588000	-1.474362000	-3.054670000
6	-4.731098000	-3.373261000	-0.395649000	31	-3.166679000	0.292372000	-0.731692000
6	-5.055510000	-4.562936000	-1.026356000	6	-2.162235000	3.665418000	0.613706000
6	-4.197230000	-5.147001000	-1.935871000	1	-1.817579000	2.659747000	0.792121000
6	-2.999972000	-4.531561000	-2.227108000	6	-1.421036000	4.624514000	1.570512000
6	-2.637945000	-3.337792000	-1.614898000	1	-0.347936000	4.497807000	1.458604000
6	-2.157629000	-2.846062000	1.801305000	1	-1.655660000	5.659244000	1.350406000
6	-3.252931000	1.604874000	3.293606000	1	-1.681971000	4.431063000	2.603849000
6	-4.421472000	2.507568000	0.911993000	6	-1.817739000	4.018232000	-0.849600000
6	-5.821563000	2.569949000	1.000684000	1	-2.265609000	3.296444000	-1.516497000
6	-6.441841000	3.808710000	1.040253000	1	-2.186963000	5.005352000	-1.104149000
6	-5.707379000	4.975792000	0.965439000	1	-0.742097000	4.002917000	-1.001108000
6	-4.337233000	4.912131000	0.835956000	6	-6.650550000	1.287420000	1.034465000

1	-6.076416000	0.533474000	0.519716000	6	-2.125704000	0.627323000	-2.187666000
6	-6.881375000	0.811367000	2.486010000	6	-2.837421000	-0.576774000	-2.086935000
1	-7.373357000	1.589167000	3.061061000	7	-3.638939000	-0.884858000	-1.054224000
1	-7.511081000	-0.072780000	2.495893000	6	-4.565080000	-2.027100000	-1.112000000
1	-5.945620000	0.558636000	2.963540000	6	-4.179268000	-3.285058000	-0.641168000
6	-8.014135000	1.433506000	0.325475000	6	-5.126113000	-4.303879000	-0.644568000
1	-8.689411000	2.066888000	0.889937000	6	-6.401124000	-4.092519000	-1.116072000
1	-7.899809000	1.849760000	-0.667843000	6	-6.760189000	-2.851328000	-1.605368000
1	-8.478094000	0.457558000	0.235088000	6	-5.858998000	-1.799370000	-1.611314000
6	-5.705488000	-2.772895000	0.612271000	6	-1.291576000	2.921001000	-1.744070000
1	-5.331396000	-1.795548000	0.869431000	6	-2.863557000	3.016051000	0.605751000
6	-7.124148000	-2.620866000	0.020921000	6	-1.880163000	3.315660000	1.549719000
1	-7.562720000	-3.586653000	-0.202991000	6	-2.017273000	4.487347000	2.284605000
1	-7.769795000	-2.122389000	0.737140000	6	-3.083216000	5.335459000	2.082959000
1	-7.105685000	-2.035521000	-0.889324000	6	-4.045203000	5.026114000	1.141459000
6	-5.763672000	-3.630755000	1.895750000	6	-3.960624000	3.863011000	0.392827000
1	-4.777977000	-3.718159000	2.330308000	6	-4.944643000	0.122417000	2.045503000
1	-6.426134000	-3.171225000	2.623829000	1	-5.530247000	1.233633000	3.795107000
1	-6.141032000	-4.623620000	1.672201000	1	-6.650221000	0.859275000	0.878634000
6	-1.292602000	-2.709078000	-1.964273000	1	-7.080245000	-0.006913000	2.357776000
1	-1.296818000	-1.699684000	-1.587031000	1	-6.528269000	-0.908662000	0.939185000
6	-0.135795000	-3.472721000	-1.280450000	1	-1.491779000	0.713036000	-3.061580000
1	-0.106112000	-4.500377000	-1.627497000	1	-4.850303000	-5.273735000	-0.284861000
1	0.818243000	-3.004052000	-1.515085000	1	-7.114368000	-4.892666000	-1.113266000
1	-0.271484000	-3.469467000	-0.208112000	1	-7.750422000	-2.704619000	-1.982346000
6	-1.054402000	-2.666118000	-3.489951000	1	-1.064845000	2.876559000	-2.809399000
1	-1.898692000	-2.226956000	-4.004568000	1	-1.775708000	3.865539000	-1.505748000
1	-0.172007000	-2.073669000	-3.711321000	1	-0.345964000	2.889736000	-1.192021000
1	-0.890296000	-3.659920000	-3.890215000	1	-1.275263000	4.735889000	3.014979000
1	-1.603121000	0.715561000	-0.817012000	1	-3.166601000	6.237640000	2.655787000
6	0.941460000	0.945889000	-2.275274000	1	-4.867187000	5.695314000	0.991770000
1	0.713272000	0.048599000	-2.858846000	6	-6.378253000	0.009433000	1.511676000
1	-0.020084000	1.323948000	-1.921527000	1	-5.108867000	2.280105000	2.431967000
1	1.429886000	1.660681000	-2.933089000	1	-3.839263000	1.495410000	3.359232000
				6	-4.840710000	1.356650000	2.947460000
<b>Ga-inter-TS<sub>1,4-II</sub></b>				6	-4.627523000	-1.129721000	2.867823000
7	-2.781281000	1.769398000	-0.165343000	1	-5.347448000	-1.215770000	3.693636000
6	-2.120477000	1.737673000	-1.331441000	1	-3.625556000	-1.097314000	3.309776000

1	-4.707954000	-2.038411000	2.265819000	6	-4.828351000	4.399034000	-1.923760000
31	-3.698030000	0.237417000	0.500922000	1	-4.856121000	5.455240000	-1.682855000
6	-2.753982000	-3.608979000	-0.200579000	1	-3.876296000	4.179986000	-2.388166000
1	-2.167528000	-2.708833000	-0.247605000	1	-5.612188000	4.191488000	-2.644660000
6	-6.275290000	-0.448248000	-2.197440000	6	-2.610280000	-1.568436000	-3.193942000
1	-5.670221000	0.319483000	-1.738049000	1	-2.491281000	-1.055378000	-4.148970000
6	-2.117287000	-4.647436000	-1.155161000	1	-1.667909000	-2.084886000	-2.976147000
1	-2.617924000	-5.604503000	-1.064894000	1	-3.400726000	-2.310451000	-3.263960000
1	-2.177229000	-4.330962000	-2.188214000	1	-2.253006000	-0.739009000	1.603123000
1	-1.073356000	-4.781580000	-0.898940000	1	-1.559858000	-0.673193000	1.268968000
6	-2.684891000	-4.151471000	1.243468000	7	3.850420000	0.997973000	-0.739480000
1	-1.651649000	-4.348518000	1.505818000	6	2.600016000	1.191273000	-1.250798000
1	-3.082626000	-3.441844000	1.954623000	6	1.486059000	0.472993000	-0.889586000
1	-3.238505000	-5.078215000	1.337884000	6	1.340662000	-0.730681000	-0.075090000
6	-6.005751000	-0.419676000	-3.720631000	7	2.454421000	-1.276226000	0.509502000
1	-6.567889000	-1.207814000	-4.207891000	6	2.360208000	-2.617261000	1.039634000
1	-6.315467000	0.532648000	-4.137843000	6	2.690823000	-3.702326000	0.204267000
1	-4.958129000	-0.560268000	-3.942198000	6	2.660624000	-4.988124000	0.717837000
6	-7.760112000	-0.102862000	-1.951367000	6	2.317939000	-5.221222000	2.036239000
1	-8.034760000	-0.222049000	-0.912279000	6	1.973877000	-4.162417000	2.845740000
1	-7.939257000	0.927626000	-2.238529000	6	1.969849000	-2.857385000	2.363617000
1	-8.411046000	-0.724409000	-2.553917000	6	0.072501000	-1.277069000	0.008743000
6	-0.671171000	2.418698000	1.803779000	6	2.395597000	2.294373000	-2.270839000
1	-0.651603000	1.626420000	1.072538000	6	4.955003000	1.759281000	-1.279734000
6	-0.759986000	1.770787000	3.202306000	6	5.737966000	1.201847000	-2.303692000
1	-0.779024000	2.527838000	3.977514000	6	6.791701000	1.934987000	-2.826179000
1	-1.651978000	1.164302000	3.293364000	6	7.096222000	3.189811000	-2.337169000
1	0.100969000	1.134844000	3.361829000	6	6.343042000	3.723323000	-1.314501000
6	0.658520000	3.194610000	1.682248000	6	5.266919000	3.029285000	-0.776807000
1	1.480623000	2.492559000	1.717754000	6	5.758590000	-0.949901000	1.314831000
1	0.715300000	3.737304000	0.746297000	1	7.866931000	-0.438575000	1.312820000
1	0.773480000	3.902786000	2.494710000	1	6.803888000	-1.699301000	3.067556000
6	-5.043127000	3.558334000	-0.643920000	1	5.071726000	-2.056908000	3.067397000
1	-4.967678000	2.516187000	-0.915996000	1	5.638958000	-0.414309000	3.437100000
6	-6.467805000	3.809816000	-0.102130000	1	0.563096000	0.768128000	-1.376202000
1	-7.197906000	3.438723000	-0.813433000	1	2.916475000	-5.816804000	0.089154000
1	-6.626228000	3.310698000	0.844824000	1	2.316669000	-6.221394000	2.424414000
1	-6.653342000	4.867611000	0.035159000	1	1.697737000	-4.348073000	3.864890000

1	-0.101353000	-2.221645000	0.502932000	1	3.375025000	-2.450663000	-1.346898000
1	-0.711866000	-0.849431000	-0.603063000	6	4.165985000	-4.407802000	-1.775908000
1	2.429578000	3.274951000	-1.789135000	1	3.816811000	-5.431237000	-1.858441000
1	3.174040000	2.294414000	-3.032624000	1	4.474594000	-4.088346000	-2.766617000
1	1.426811000	2.179941000	-2.762078000	1	5.030308000	-4.389355000	-1.126694000
1	7.388114000	1.520228000	-3.613302000	6	1.796882000	-3.659134000	-2.153166000
1	7.920237000	3.741862000	-2.745576000	1	1.011497000	-2.985208000	-1.843150000
1	6.592576000	4.691453000	-0.928021000	1	2.043328000	-3.459502000	-3.192532000
6	5.811935000	-1.294617000	2.805433000	1	1.438241000	-4.681420000	-2.077824000
1	6.816583000	0.958742000	1.566726000	6	1.476683000	-1.739295000	3.281822000
1	6.976671000	0.269521000	-0.045297000	1	1.449345000	-0.829198000	2.704676000
6	6.907257000	0.017552000	1.014714000	6	0.049370000	-2.049749000	3.790118000
6	5.987020000	-2.238371000	0.528150000	1	0.050133000	-2.917202000	4.439956000
1	6.992882000	-2.643140000	0.735290000	1	-0.334382000	-1.209107000	4.359872000
1	5.914190000	-2.082214000	-0.551036000	1	-0.619453000	-2.242350000	2.962671000
1	5.260741000	-3.007047000	0.802844000	6	2.406398000	-1.516834000	4.492885000
31	3.974366000	-0.076244000	0.928368000	1	3.379973000	-1.182507000	4.171855000
6	4.464546000	3.667987000	0.354600000	1	1.988535000	-0.756797000	5.146936000
1	3.607912000	3.043477000	0.544966000	1	2.521097000	-2.430290000	5.066224000
6	3.975496000	5.087657000	-0.012109000	1	3.451124000	0.907871000	2.095874000
1	3.323707000	5.465406000	0.769646000				
1	4.807961000	5.774610000	-0.110048000				<b>Ga-inter-TS<sub>1,4'</sub></b>
1	3.427138000	5.088508000	-0.946557000	1	-0.008001000	-0.197476000	-0.563860000
6	5.297025000	3.726986000	1.653765000	1	0.995700000	0.046586000	-0.389324000
1	5.563378000	2.730604000	1.973482000	7	3.277360000	-1.577592000	-0.162982000
1	6.204120000	4.302000000	1.503867000	6	3.157209000	-1.882168000	1.196332000
1	4.720823000	4.192914000	2.447379000	6	3.076966000	-0.962956000	2.198160000
6	5.445865000	-0.200548000	-2.830846000	6	3.249794000	0.502128000	2.209544000
1	4.869435000	-0.700781000	-2.070627000	7	3.280362000	1.174149000	0.987902000
6	4.603328000	-0.150946000	-4.125173000	6	3.401960000	2.616097000	0.993938000
1	5.121593000	0.419258000	-4.889185000	6	4.638306000	3.222501000	0.724745000
1	4.436086000	-1.155715000	-4.501749000	6	4.717499000	4.606548000	0.682108000
1	3.638662000	0.303502000	-3.945754000	6	3.602464000	5.392466000	0.887631000
6	6.732130000	-1.013579000	-3.093807000	6	2.390793000	4.795780000	1.159611000
1	7.270693000	-0.633081000	-3.954517000	6	2.276312000	3.414644000	1.231193000
1	7.392039000	-0.991522000	-2.236396000	6	3.406407000	1.111518000	3.414953000
1	6.472341000	-2.046966000	-3.298542000	6	3.060879000	-3.343867000	1.573606000
6	3.048332000	-3.474246000	-1.262734000	6	4.031074000	-2.512606000	-0.979728000

6	5.428877000	-2.583840000	-0.831460000	1	2.141322000	-2.313223000	-4.083666000
6	6.144466000	-3.530073000	-1.547903000	1	1.840712000	-4.034837000	-4.215913000
6	5.516771000	-4.383502000	-2.430435000	1	0.525247000	-2.953974000	-3.806499000
6	4.155943000	-4.283568000	-2.611477000	6	6.188818000	-1.636430000	0.093481000
6	3.398862000	-3.360724000	-1.901040000	1	5.502265000	-0.875213000	0.423198000
6	2.944914000	0.992495000	-2.429359000	6	6.730340000	-2.373383000	1.338157000
1	4.290988000	0.771377000	-4.121973000	1	7.416388000	-3.161040000	1.045358000
1	1.770350000	0.965116000	-4.266570000	1	7.261182000	-1.677878000	1.979945000
1	0.800094000	1.196113000	-2.801536000	1	5.925147000	-2.810643000	1.912626000
1	1.436750000	-0.399720000	-3.186444000	6	7.356841000	-0.949638000	-0.648696000
1	2.944019000	-1.373955000	3.193230000	1	8.115594000	-1.666683000	-0.938557000
1	5.657095000	5.077465000	0.479224000	1	7.006231000	-0.444799000	-1.539963000
1	3.679847000	6.461153000	0.838934000	1	7.823317000	-0.218163000	0.000907000
1	1.527290000	5.409671000	1.321761000	6	5.891496000	2.383319000	0.504085000
1	3.558645000	2.177900000	3.503593000	1	5.567788000	1.418346000	0.151658000
1	3.402530000	0.518316000	4.321083000	6	6.853577000	2.985612000	-0.542168000
1	2.169213000	-3.791342000	1.125341000	1	7.317621000	3.894680000	-0.177734000
1	3.916348000	-3.914264000	1.208976000	1	7.646620000	2.277093000	-0.753820000
1	2.999563000	-3.458060000	2.657627000	1	6.340076000	3.208711000	-1.469726000
1	7.205976000	-3.596353000	-1.419674000	6	6.635006000	2.192170000	1.846157000
1	6.084232000	-5.110388000	-2.977782000	1	5.993281000	1.711196000	2.570856000
1	3.671007000	-4.936469000	-3.309263000	1	7.522329000	1.582212000	1.705359000
6	1.669639000	0.669010000	-3.210049000	1	6.943001000	3.156769000	2.236641000
1	4.031241000	-0.739365000	-3.230479000	6	0.924873000	2.796170000	1.567994000
1	5.072868000	0.510108000	-2.553826000	1	1.076413000	1.744144000	1.739219000
6	4.149059000	0.341537000	-3.117396000	6	0.327243000	3.416693000	2.846712000
6	3.136862000	2.510087000	-2.428259000	1	0.133702000	4.474815000	2.719306000
1	3.176912000	2.880318000	-3.465757000	1	-0.615035000	2.936739000	3.086484000
1	4.061754000	2.809476000	-1.934063000	1	1.004577000	3.285915000	3.681163000
1	2.322225000	3.036396000	-1.922078000	6	-0.057215000	2.948028000	0.391330000
31	2.734169000	0.237661000	-0.588678000	1	0.361556000	2.517162000	-0.507443000
6	1.897858000	-3.317476000	-2.158158000	1	-0.984770000	2.425893000	0.613701000
1	1.507059000	-2.471951000	-1.615316000	1	-0.286041000	3.991260000	0.206048000
6	1.207584000	-4.606395000	-1.656320000	7	-2.462794000	-0.927350000	1.213769000
1	0.134531000	-4.552723000	-1.821419000	6	-1.442672000	-1.357503000	0.456107000
1	1.584434000	-5.467263000	-2.195842000	6	-1.157368000	-0.884280000	-0.852347000
1	1.391098000	-4.767240000	-0.602906000	6	-2.063129000	-0.183472000	-1.812096000
6	1.585512000	-3.139050000	-3.662473000	7	-3.203702000	0.465979000	-1.301290000

6	-4.104506000	1.104172000	-2.256060000	1	-5.816071000	2.440166000	-0.284544000
6	-5.141667000	0.360017000	-2.837776000	31	-3.703098000	0.339904000	0.475535000
6	-5.994265000	0.987193000	-3.734905000	6	-5.352764000	-1.125846000	-2.554523000
6	-5.835465000	2.317147000	-4.059372000	1	-4.683852000	-1.416988000	-1.759145000
6	-4.809059000	3.039921000	-3.491476000	6	-2.784709000	3.289694000	-2.034432000
6	-3.929450000	2.453180000	-2.592399000	1	-2.291079000	2.708267000	-1.275468000
6	-1.755207000	-0.221591000	-3.122517000	6	-4.999648000	-1.972300000	-3.798265000
6	-0.427400000	-2.318009000	0.993997000	1	-5.647072000	-1.715116000	-4.628559000
6	-2.825772000	-1.636716000	2.448400000	1	-3.972730000	-1.803331000	-4.090414000
6	-3.572802000	-2.815656000	2.335347000	1	-5.129027000	-3.028192000	-3.581303000
6	-3.958384000	-3.469012000	3.496506000	6	-6.802658000	-1.420481000	-2.110916000
6	-3.610762000	-2.977912000	4.736000000	1	-6.914614000	-2.473098000	-1.878694000
6	-2.872079000	-1.818125000	4.832272000	1	-7.068096000	-0.845638000	-1.232219000
6	-2.470477000	-1.123682000	3.699164000	1	-7.507142000	-1.179403000	-2.896526000
6	-5.088388000	1.333437000	1.472014000	6	-1.753498000	3.604552000	-3.141690000
1	-6.441227000	1.125080000	3.137978000	1	-2.210442000	4.190396000	-3.931395000
1	-3.592406000	2.283359000	2.778645000	1	-0.926247000	4.173301000	-2.730390000
1	-5.110189000	3.171960000	2.620486000	1	-1.360915000	2.691808000	-3.567967000
1	-3.934178000	3.196479000	1.301967000	6	-3.288627000	4.604631000	-1.399202000
1	-0.561654000	-1.623695000	-1.385886000	1	-4.055606000	4.417118000	-0.657642000
1	-6.786104000	0.428275000	-4.190433000	1	-2.464314000	5.119769000	-0.918226000
1	-6.502889000	2.784708000	-4.756077000	1	-3.700842000	5.268365000	-2.149572000
1	-4.681757000	4.069838000	-3.755947000	6	-3.990506000	-3.411929000	0.991974000
1	-2.357840000	0.277051000	-3.868040000	1	-3.555136000	-2.829062000	0.195457000
1	-0.867427000	-0.743900000	-3.454156000	6	-5.524927000	-3.351530000	0.835113000
1	-0.621727000	-2.622586000	2.017972000	1	-6.016006000	-3.903898000	1.626419000
1	-0.369035000	-3.200041000	0.354113000	1	-5.872382000	-2.325679000	0.872905000
1	0.552474000	-1.814977000	0.943020000	1	-5.823183000	-3.777842000	-0.115277000
1	-4.532212000	-4.370583000	3.429174000	6	-3.488489000	-4.863916000	0.834475000
1	-3.911765000	-3.497651000	5.623759000	1	-3.732782000	-5.232298000	-0.155934000
1	-2.600404000	-1.449012000	5.798819000	1	-2.415013000	-4.921293000	0.966487000
6	-4.379408000	2.560050000	2.072373000	1	-3.955497000	-5.518325000	1.560007000
1	-4.976780000	0.147601000	3.320142000	6	-1.624029000	0.133832000	3.860070000
1	-6.253635000	-0.368218000	2.215497000	1	-1.650983000	0.680038000	2.928183000
6	-5.713219000	0.502973000	2.597062000	6	-2.149987000	1.052027000	4.986355000
6	-6.194600000	1.812967000	0.525510000	1	-1.615890000	1.993755000	4.964803000
1	-6.922017000	2.406071000	1.098698000	1	-3.209063000	1.251971000	4.880408000
1	-6.736769000	0.980132000	0.071387000	1	-1.982967000	0.607558000	5.959540000

6	-0.157436000	-0.253417000	4.154211000	1	-2.228132000	3.683657000	1.381369000
1	-0.104481000	-0.815385000	5.080350000	1	-3.973554000	3.843742000	1.430681000
1	0.260576000	-0.857355000	3.362127000	1	-3.108712000	3.246847000	2.859896000
1	0.462545000	0.628534000	4.247555000	1	-7.199821000	3.826005000	-1.313440000
				1	-5.989677000	5.430046000	-2.708758000
<b>Ga-inter-IM<sub>1,4'</sub></b>				1	-3.571992000	5.213586000	-2.981248000
1	0.924143000	-0.511172000	-0.697040000	6	-1.597296000	-0.497185000	-3.220518000
1	-1.165528000	-0.095928000	-0.150639000	1	-3.868843000	1.066552000	-3.252381000
7	-3.370261000	1.604900000	-0.108263000	1	-5.014544000	-0.164084000	-2.737400000
6	-3.265499000	1.798702000	1.266738000	6	-4.049563000	-0.011134000	-3.233077000
6	-3.221203000	0.796732000	2.193767000	6	-3.225592000	-2.278270000	-2.659676000
6	-3.466448000	-0.657775000	2.092044000	1	-3.238219000	-2.566027000	-3.725083000
7	-3.531555000	-1.230457000	0.828856000	1	-4.195012000	-2.545967000	-2.235276000
6	-3.678915000	-2.662282000	0.726452000	1	-2.479899000	-2.903228000	-2.158548000
6	-4.923238000	-3.217234000	0.387732000	31	-2.723318000	-0.192088000	-0.610491000
6	-5.041300000	-4.590895000	0.242185000	6	-1.880343000	3.452503000	-1.909849000
6	-3.954091000	-5.423237000	0.412467000	1	-1.534989000	2.562796000	-1.407253000
6	-2.732264000	-4.880998000	0.744944000	6	-1.172997000	4.689594000	-1.309950000
6	-2.578487000	-3.511902000	0.915428000	1	-0.097677000	4.628915000	-1.461845000
6	-3.657635000	-1.339005000	3.259049000	1	-1.523620000	5.592879000	-1.794870000
6	-3.142324000	3.222756000	1.768592000	1	-1.371943000	4.781473000	-0.250810000
6	-4.068595000	2.620773000	-0.864008000	6	-1.525205000	3.355509000	-3.411481000
6	-5.468571000	2.720951000	-0.756154000	1	-2.069336000	2.554564000	-3.890900000
6	-6.136371000	3.741476000	-1.413951000	1	-1.762806000	4.280754000	-3.922760000
6	-5.459116000	4.645842000	-2.204971000	1	-0.460937000	3.175175000	-3.536000000
6	-4.096015000	4.521200000	-2.352522000	6	-6.275256000	1.714643000	0.059272000
6	-3.387547000	3.523216000	-1.695889000	1	-5.610261000	0.914516000	0.337638000
6	-2.934146000	-0.782586000	-2.524257000	6	-6.841207000	2.352065000	1.346964000
1	-4.154916000	-0.353648000	-4.276435000	1	-7.502838000	3.177455000	1.105076000
1	-1.651253000	-0.732573000	-4.296570000	1	-7.404367000	1.615181000	1.910421000
1	-0.785277000	-1.100726000	-2.793328000	1	-6.044881000	2.719478000	1.980123000
1	-1.300278000	0.553292000	-3.127394000	6	-7.430219000	1.120177000	-0.776526000
1	-3.090266000	1.123861000	3.220023000	1	-8.162136000	1.876949000	-1.033741000
1	-5.989864000	-5.017083000	-0.012676000	1	-7.056219000	0.680375000	-1.692732000
1	-4.060267000	-6.483391000	0.287559000	1	-7.936052000	0.349675000	-0.206354000
1	-1.888560000	-5.529810000	0.876556000	6	-6.142254000	-2.322917000	0.201121000
1	-3.876307000	-2.397506000	3.275044000	1	-5.773026000	-1.346388000	-0.062771000
1	-3.641021000	-0.805758000	4.201751000	6	-7.088269000	-2.809658000	-0.917016000

1	-7.586985000	-3.732407000	-0.643107000	1	3.250407000	-2.577787000	2.741332000
1	-7.855533000	-2.063858000	-1.093062000	1	4.694085000	-3.589147000	2.648375000
1	-6.550813000	-2.970368000	-1.844266000	1	3.618705000	-3.461166000	1.252600000
6	-6.917332000	-2.211732000	1.533984000	1	0.448525000	1.019322000	-1.356899000
1	-6.278870000	-1.812301000	2.309790000	1	7.495801000	-0.230437000	-3.729969000
1	-7.778799000	-1.559948000	1.420399000	1	6.984453000	-2.399314000	-4.724904000
1	-7.269471000	-3.192010000	1.839688000	1	4.907538000	-3.550302000	-4.151348000
6	-1.205974000	-2.972223000	1.309356000	1	3.213845000	0.929923000	-3.712956000
1	-1.303903000	-1.915762000	1.490325000	1	1.496752000	1.519645000	-3.318812000
6	-0.691890000	-3.647981000	2.597077000	1	0.579126000	2.523749000	1.911162000
1	-0.563480000	-4.714929000	2.458983000	1	0.378290000	2.904662000	0.169196000
1	0.271350000	-3.233051000	2.878547000	1	-0.551975000	1.589584000	0.857045000
1	-1.390193000	-3.483176000	3.407181000	1	4.408998000	4.060235000	3.744201000
6	-0.190076000	-3.163370000	0.162988000	1	3.587246000	3.133235000	5.847707000
1	-0.537088000	-2.654416000	-0.726063000	1	2.230697000	1.107009000	5.848727000
1	0.777137000	-2.746745000	0.445905000	6	4.059369000	-2.895098000	2.079741000
1	-0.048925000	-4.213475000	-0.066407000	1	4.792484000	-0.585310000	3.465840000
7	2.439503000	0.744644000	1.254784000	1	6.182151000	-0.155795000	2.459679000
6	1.444740000	1.126366000	0.507367000	6	5.540687000	-0.984312000	2.777616000
6	1.277458000	0.517902000	-0.860421000	6	6.031662000	-2.263925000	0.682280000
6	2.486725000	0.495455000	-1.771715000	1	6.646333000	-2.965037000	1.264496000
7	3.594158000	-0.220712000	-1.277951000	1	6.691865000	-1.476768000	0.312960000
6	4.530557000	-0.803194000	-2.232122000	1	5.646691000	-2.801720000	-0.187189000
6	5.714661000	-0.135675000	-2.562922000	31	3.755453000	-0.527674000	0.533769000
6	6.587324000	-0.731825000	-3.464176000	6	6.074712000	1.230973000	-1.988061000
6	6.300797000	-1.954832000	-4.029036000	1	5.306964000	1.505776000	-1.282087000
6	5.127752000	-2.603496000	-3.701882000	6	2.929133000	-2.790634000	-2.507463000
6	4.226595000	-2.046151000	-2.808380000	1	2.411220000	-2.260063000	-1.725480000
6	2.406175000	1.025971000	-2.999217000	6	6.110663000	2.307022000	-3.096219000
6	0.420023000	2.110566000	0.919218000	1	6.877895000	2.079841000	-3.826700000
6	2.735303000	1.403391000	2.543487000	1	5.158253000	2.368699000	-3.605483000
6	3.519938000	2.560136000	2.522567000	1	6.331558000	3.278765000	-2.666041000
6	3.816451000	3.168725000	3.733345000	6	7.432959000	1.188930000	-1.252938000
6	3.353989000	2.646619000	4.921799000	1	7.667040000	2.162252000	-0.837680000
6	2.588757000	1.499737000	4.920700000	1	7.416363000	0.467905000	-0.445020000
6	2.265986000	0.850312000	3.737008000	1	8.231512000	0.915103000	-1.930753000
6	4.917503000	-1.719164000	1.585499000	6	2.014673000	-2.814114000	-3.752540000
1	6.172435000	-1.686364000	3.340044000	1	2.487359000	-3.360091000	-4.560890000

1	1.074540000	-3.300416000	-3.516210000	6	-3.420035000	-1.218443000	-0.090595000
1	1.803575000	-1.808290000	-4.090370000	6	-2.370069000	0.000780000	2.964961000
6	3.192984000	-4.229087000	-2.011405000	6	2.491472000	0.001627000	3.002741000
1	3.844918000	-4.232078000	-1.145526000	6	2.813744000	0.000107000	0.206063000
1	2.255863000	-4.699701000	-1.736100000	6	3.448718000	1.215856000	-0.076289000
1	3.654865000	-4.831495000	-2.783852000	6	4.684553000	1.193703000	-0.706538000
6	4.055973000	3.186574000	1.236365000	6	5.293450000	-0.000617000	-1.032897000
1	3.768389000	2.573605000	0.395464000	6	4.684534000	-1.194550000	-0.705173000
6	5.597959000	3.249131000	1.264914000	6	3.448711000	-1.215965000	-0.074868000
1	5.946932000	3.877317000	2.074320000	6	-0.007874000	-0.001388000	-2.370626000
1	6.020859000	2.259982000	1.397094000	1	1.273803000	-0.002377000	-4.107449000
1	5.970055000	3.660107000	0.333914000	1	-0.302262000	-2.180435000	-2.577932000
6	3.464487000	4.596506000	1.016263000	1	-0.805679000	-1.221292000	-3.972336000
1	3.816121000	5.002398000	0.074182000	1	-1.807274000	-1.244500000	-2.515470000
1	2.382317000	4.568953000	0.994363000	1	0.034649000	0.001363000	3.797070000
1	3.770307000	5.267803000	1.809329000	1	-5.210851000	2.114920000	-0.818023000
6	1.381120000	-0.391560000	3.784472000	1	-6.333308000	0.001020000	-1.290997000
1	1.463223000	-0.908827000	2.838367000	1	-5.211523000	-2.113445000	-0.819072000
6	1.802887000	-1.362802000	4.909966000	1	-3.390032000	0.000562000	2.609406000
1	1.250378000	-2.288552000	4.810608000	1	-2.202808000	0.001329000	4.034936000
1	2.862467000	-1.585119000	4.876456000	1	3.114007000	-0.875470000	2.813949000
1	1.571308000	-0.950870000	5.884083000	1	3.113626000	0.878795000	2.813024000
6	-0.094242000	0.021606000	3.984052000	1	2.202836000	0.002121000	4.054598000
1	-0.201663000	0.556666000	4.921274000	1	5.175971000	2.116163000	-0.942669000
1	-0.445543000	0.655884000	3.184349000	1	6.244776000	-0.000910000	-1.527447000
1	-0.739315000	-0.846689000	4.004849000	1	5.175935000	-2.117282000	-0.940270000
				6	-0.774832000	-1.237523000	-2.871952000
[(BDI)Al <i>t</i> Bu]				1	1.978394000	-0.880042000	-2.744558000
7	1.461525000	0.000397000	0.736787000	1	1.978419000	0.876780000	-2.745530000
6	1.261473000	0.000938000	2.132069000	6	1.387797000	-0.001771000	-3.012377000
6	0.039328000	0.000888000	2.712861000	6	-0.774833000	1.234115000	-2.873529000
6	-1.307271000	0.000439000	2.128297000	1	-0.805860000	1.216369000	-3.973884000
7	-1.420959000	-0.000190000	0.713541000	1	-0.302055000	2.177353000	-2.580899000
6	-2.771236000	0.000106000	0.169467000	1	-1.807226000	1.241749000	-2.516892000
6	-3.419624000	1.218972000	-0.090059000	6	-2.783443000	2.570368000	0.242630000
6	-4.702765000	1.193587000	-0.619010000	1	-1.727557000	2.412071000	0.401256000
6	-5.340866000	0.000772000	-0.884771000	6	-2.784198000	-2.570160000	0.241432000
6	-4.703143000	-1.192387000	-0.619573000	1	-1.727876000	-2.412574000	0.397886000

6	-3.382276000	3.139279000	1.550785000		Al- <i>intra-TS</i> <sub>1,4</sub>			
1	-4.450337000	3.289209000	1.435995000	1	-0.958449000	-1.961953000	1.940222000	
1	-3.207579000	2.464382000	2.374819000	1	-0.347927000	-2.258476000	1.156491000	
1	-2.926317000	4.096984000	1.783062000	7	1.442862000	0.062090000	0.681490000	
6	-2.960398000	3.614950000	-0.882821000	6	1.220755000	0.502635000	1.963430000	
1	-2.382787000	4.502176000	-0.644405000	6	0.010349000	0.353349000	2.589606000	
1	-2.628145000	3.237850000	-1.840032000	6	-1.220349000	-0.169960000	2.020606000	
1	-3.996734000	3.916769000	-0.975351000	7	-1.454486000	-0.055771000	0.666813000	
6	-3.380874000	-3.137987000	1.551056000	6	-2.816774000	0.253083000	0.221005000	
1	-4.449324000	-3.286854000	1.438462000	6	-3.108147000	1.624889000	0.096622000	
1	-2.925417000	-4.096078000	1.782728000	6	-2.060728000	2.694505000	0.392543000	
1	-3.203844000	-2.462978000	2.374490000	6	-2.382716000	3.406107000	1.724825000	
6	-2.964174000	-3.615253000	-0.883064000	6	-1.945638000	3.721641000	-0.754193000	
1	-2.634251000	-3.238732000	-1.841315000	6	-4.378172000	2.022096000	-0.282805000	
1	-2.386135000	-4.502457000	-0.645617000	6	-5.360394000	1.093309000	-0.554869000	
1	-4.000788000	-3.916964000	-0.972815000	6	-5.067691000	-0.246227000	-0.457693000	
6	2.823364000	2.555688000	0.310604000	6	-3.806857000	-0.696401000	-0.076433000	
1	1.947555000	2.355044000	0.907873000	6	-3.604080000	-2.212092000	-0.030640000	
6	2.381509000	3.351802000	-0.936030000	6	-4.549820000	-2.891509000	0.990704000	
1	3.225768000	3.546390000	-1.587181000	6	-3.876316000	-2.850749000	-1.415223000	
1	1.639605000	2.802755000	-1.500701000	6	-1.920587000	-1.109289000	2.776876000	
1	1.949310000	4.302831000	-0.642567000	6	2.358073000	1.123234000	2.731378000	
6	3.793598000	3.407682000	1.159074000	6	2.766150000	0.196175000	0.096423000	
1	3.291993000	4.307655000	1.498815000	6	3.081007000	1.315830000	-0.683226000	
1	4.136044000	2.859076000	2.027901000	6	4.326440000	1.376627000	-1.292869000	
1	4.660416000	3.705713000	0.581686000	6	5.244725000	0.359746000	-1.139096000	
6	2.823315000	-2.555338000	0.313568000	6	4.935858000	-0.729725000	-0.351115000	
1	1.947447000	-2.353983000	0.910515000	6	3.706523000	-0.827056000	0.283600000	
6	2.381570000	-3.352981000	-0.932125000	6	3.420671000	-2.038124000	1.173524000	
1	1.949400000	-4.303673000	-0.637525000	6	4.519648000	-2.229746000	2.243163000	
1	1.639677000	-2.804661000	-1.497513000	6	3.279573000	-3.328349000	0.336959000	
1	3.225881000	-3.548329000	-1.582981000	6	2.105617000	2.477110000	-0.867062000	
6	3.793452000	-3.406324000	1.163173000	6	1.758011000	2.702737000	-2.354906000	
1	4.660289000	-3.705108000	0.586205000	6	2.680345000	3.782346000	-0.269996000	
1	4.135867000	-2.856660000	2.031341000	6	0.127651000	-1.541819000	-2.007398000	
1	3.291780000	-4.305850000	1.503996000	1	1.403832000	-1.745705000	-3.741304000	
13	0.025576000	-0.000312000	-0.383828000	1	-0.356400000	-3.341787000	-3.129622000	
				1	-1.214130000	-3.246210000	-1.586716000	

1	0.496329000	-3.666887000	-1.615505000	1	1.952195000	4.582356000	-0.355529000
1	-0.023516000	0.542540000	3.656282000	1	2.929510000	3.660514000	0.776389000
1	-1.111672000	2.198851000	0.495938000	1	3.577196000	4.084167000	-0.798232000
1	-1.618838000	4.142559000	1.953813000	6	-0.263997000	-3.028058000	-2.077854000
1	-3.339583000	3.912897000	1.664942000	1	2.276012000	-1.981054000	-2.223017000
1	-2.423893000	2.692725000	2.538929000	1	1.837506000	-0.359967000	-2.733531000
1	-1.126271000	4.404706000	-0.552778000	6	1.489725000	-1.393168000	-2.700775000
1	-2.849214000	4.310939000	-0.855126000	6	-0.890678000	-0.706760000	-2.808291000
1	-1.754271000	3.224318000	-1.698087000	1	-0.946356000	-1.078083000	-3.843955000
1	-4.602745000	3.066178000	-0.364121000	1	-0.597088000	0.347716000	-2.859869000
1	-6.342243000	1.411962000	-0.844800000	1	-1.899841000	-0.738249000	-2.391757000
1	-5.831261000	-0.963230000	-0.680081000	13	0.037292000	-0.911448000	-0.120163000
1	-2.582090000	-2.417649000	0.249459000				
1	-4.478176000	-2.454367000	1.976198000				
1	-4.311227000	-3.947191000	1.066416000	1	0.044284000	-2.381450000	-0.453619000
1	-5.579154000	-2.804006000	0.664833000	7	1.454137000	-0.233694000	0.695405000
1	-3.632247000	-3.907607000	-1.389287000	6	1.269941000	-0.388959000	2.007159000
1	-4.923825000	-2.757754000	-1.674121000	6	0.007660000	-0.597062000	2.590089000
1	-3.294375000	-2.382863000	-2.194382000	6	-1.257523000	-0.445805000	1.999840000
1	-2.898778000	-1.434710000	2.461342000	7	-1.437819000	-0.262708000	0.689348000
1	-1.679895000	-1.215225000	3.830431000	6	-2.771874000	0.026293000	0.167021000
1	2.028808000	1.406023000	3.731782000	6	-3.144309000	1.365965000	-0.028054000
1	3.202654000	0.438312000	2.812929000	6	-2.223940000	2.513770000	0.389931000
1	2.721399000	2.014252000	2.217444000	6	-2.491818000	2.907056000	1.861909000
1	4.578848000	2.226312000	-1.894968000	6	-2.371629000	3.773095000	-0.490848000
1	6.198877000	0.418713000	-1.624652000	6	-4.389075000	1.635018000	-0.573854000
1	5.659087000	-1.510464000	-0.227112000	6	-5.248033000	0.612142000	-0.926191000
1	2.484079000	-1.873499000	1.682338000	6	-4.877869000	-0.696954000	-0.717918000
1	4.239257000	-3.031822000	2.917700000	6	-3.644705000	-1.016623000	-0.160946000
1	5.466758000	-2.492596000	1.787815000	6	-3.323455000	-2.487072000	0.113897000
1	4.663017000	-1.328090000	2.826085000	6	-4.365133000	-3.102650000	1.078489000
1	3.096118000	-4.177721000	0.986613000	6	-3.277416000	-3.319801000	-1.185073000
1	2.452337000	-3.248842000	-0.354650000	6	-2.427700000	-0.535356000	2.952994000
1	4.182680000	-3.519272000	-0.231018000	6	2.433358000	-0.382791000	2.972875000
1	1.195886000	2.233694000	-0.341783000	6	2.793836000	0.038040000	0.179282000
1	1.042916000	3.512872000	-2.449695000	6	3.154917000	1.363224000	-0.097582000
1	1.323996000	1.813726000	-2.791066000	6	4.415426000	1.614064000	-0.615897000
1	2.641691000	2.965212000	-2.924555000	6	5.296328000	0.581808000	-0.871744000

6	4.927178000	-0.717269000	-0.603315000	1	5.614875000	-1.512662000	-0.807713000
6	3.679108000	-1.015267000	-0.070400000	1	2.366779000	-2.513994000	0.697975000
6	3.335808000	-2.475383000	0.226947000	1	4.052639000	-4.113201000	1.453773000
6	4.372466000	-3.113072000	1.180506000	1	5.341684000	-3.192496000	0.702738000
6	3.249478000	-3.301409000	-1.074791000	1	4.490027000	-2.530753000	2.086117000
6	2.197555000	2.518786000	0.185484000	1	3.007513000	-4.333307000	-0.842947000
6	2.296772000	3.651730000	-0.858014000	1	2.475909000	-2.911911000	-1.720199000
6	2.453992000	3.096952000	1.595886000	1	4.192816000	-3.282319000	-1.608282000
6	-0.001919000	-0.066257000	-2.397412000	1	1.194370000	2.124110000	0.159035000
1	1.330148000	0.070209000	-4.106693000	1	1.484152000	4.354080000	-0.705427000
1	-0.934051000	-0.677500000	-4.266486000	1	2.229046000	3.264736000	-1.866636000
1	-1.984278000	-0.894400000	-2.860674000	1	3.226042000	4.200393000	-0.758931000
1	-0.648765000	-2.026435000	-3.155327000	1	1.778123000	3.923022000	1.793214000
1	0.008076000	-0.754818000	3.662085000	1	2.302473000	2.347231000	2.360731000
1	-1.207108000	2.162591000	0.312237000	1	3.472623000	3.461718000	1.668589000
1	-1.853230000	3.736007000	2.150145000	6	-0.947436000	-0.972493000	-3.204452000
1	-3.525563000	3.211785000	1.982021000	1	1.792492000	-1.201610000	-2.974489000
1	-2.295651000	2.083564000	2.532652000	1	2.123164000	0.486928000	-2.579678000
1	-1.581814000	4.474800000	-0.244070000	6	1.391419000	-0.184644000	-3.035404000
1	-3.317166000	4.271248000	-0.310236000	6	-0.490597000	1.372723000	-2.576866000
1	-2.299021000	3.535670000	-1.543316000	1	-0.440322000	1.659657000	-3.640762000
1	-4.692096000	2.648954000	-0.731120000	1	0.111535000	2.096895000	-2.020510000
1	-6.203742000	0.839074000	-1.355980000	1	-1.530771000	1.481752000	-2.261671000
1	-5.554274000	-1.484177000	-0.982769000	1	-2.604973000	-1.591827000	3.176203000
1	-2.349663000	-2.547540000	0.573072000	13	0.016120000	-0.783034000	-0.517619000
1	-4.461609000	-2.520751000	1.986209000				
1	-4.067176000	-4.111173000	1.345852000				<i>Al-intra-TS<sub>1,4'</sub></i>
1	-5.339709000	-3.155980000	0.607789000	7	1.466927000	-0.075903000	0.689551000
1	-3.063152000	-4.356641000	-0.947669000	6	1.283324000	-0.195253000	2.014495000
1	-4.227959000	-3.280809000	-1.704587000	6	0.053936000	-0.679729000	2.518282000
1	-2.504404000	-2.959409000	-1.846447000	6	-1.306647000	-0.276325000	2.052831000
1	-3.341519000	-0.119981000	2.537667000	7	-1.465460000	-0.214113000	0.662288000
1	-2.190148000	-0.035888000	3.893684000	6	-2.789105000	0.125073000	0.175618000
1	2.148483000	0.116454000	3.900568000	6	-3.127449000	1.468704000	-0.031710000
1	2.685876000	-1.418740000	3.218299000	6	-2.141604000	2.597110000	0.250561000
1	3.319840000	0.090000000	2.559359000	6	-2.601144000	3.437730000	1.462286000
1	4.711586000	2.620124000	-0.828842000	6	-1.949231000	3.504434000	-0.983829000
1	6.264954000	0.792227000	-1.280462000	6	-4.401159000	1.783871000	-0.482289000

6	-5.333108000	0.798061000	-0.725333000	1	-5.228476000	-2.757720000	1.335871000
6	-4.997795000	-0.523298000	-0.518277000	1	-3.835841000	-2.291534000	2.309055000
6	-3.735027000	-0.882463000	-0.068421000	1	-3.482735000	-4.255647000	-0.875744000
6	-3.434328000	-2.359907000	0.174203000	1	-4.911797000	-3.280273000	-1.144095000
6	-4.154510000	-2.860045000	1.446879000	1	-3.410407000	-2.865507000	-1.952626000
6	-3.835158000	-3.240879000	-1.030150000	1	-3.275186000	0.227773000	2.694412000
6	-2.267260000	-0.042395000	2.975465000	1	-2.028722000	-0.117012000	4.028871000
6	2.402192000	0.002894000	3.005728000	1	2.529369000	-0.903426000	3.604436000
6	2.790149000	0.211428000	0.136731000	1	3.347313000	0.252965000	2.531857000
6	3.045236000	1.490822000	-0.368720000	1	2.122699000	0.807617000	3.691831000
6	4.287797000	1.749960000	-0.926381000	1	4.503136000	2.724269000	-1.312166000
6	5.253602000	0.767518000	-0.997022000	1	6.206853000	0.982333000	-1.437970000
6	4.990704000	-0.489803000	-0.499212000	1	5.745477000	-1.247211000	-0.558847000
6	3.765361000	-0.791764000	0.079935000	1	2.597223000	-2.230193000	1.141324000
6	3.541611000	-2.203114000	0.623142000	1	4.402327000	-3.576915000	2.060364000
6	4.647015000	-2.615521000	1.621381000	1	5.604592000	-2.711952000	1.124629000
6	3.470635000	-3.226551000	-0.530524000	1	4.750378000	-1.890857000	2.419380000
6	2.003007000	2.600926000	-0.275580000	1	3.300348000	-4.223166000	-0.137156000
6	1.997475000	3.526054000	-1.510137000	1	2.661951000	-2.985523000	-1.205771000
6	2.239758000	3.432987000	1.005146000	1	4.396346000	-3.233910000	-1.093748000
6	0.000570000	-1.040985000	-2.293714000	1	1.031247000	2.140223000	-0.197749000
1	1.240054000	-0.738615000	-4.045058000	1	1.158603000	4.208346000	-1.446376000
1	-0.218970000	-2.686030000	-3.697280000	1	1.904381000	2.955487000	-2.426302000
1	-1.065927000	-2.965356000	-2.170486000	1	2.900503000	4.121893000	-1.564443000
1	0.690726000	-3.131670000	-2.249224000	1	1.488935000	4.211064000	1.095164000
1	0.075919000	-0.880661000	3.586389000	1	2.188943000	2.808579000	1.888146000
1	-1.194550000	2.145568000	0.496367000	1	3.218127000	3.899175000	0.970747000
1	-1.877703000	4.220285000	1.671673000	6	-0.157424000	-2.539919000	-2.607588000
1	-3.558240000	3.906435000	1.262032000	1	2.188289000	-1.039181000	-2.582014000
1	-2.694822000	2.811723000	2.339146000	1	1.434153000	0.533176000	-2.833243000
1	-1.207852000	4.267808000	-0.771868000	6	1.291255000	-0.543742000	-2.962134000
1	-2.872696000	4.005071000	-1.248719000	6	-1.180459000	-0.292220000	-2.934547000
1	-1.617034000	2.930666000	-1.840569000	1	-1.173925000	-0.461931000	-4.022821000
1	-4.667780000	2.809861000	-0.638838000	1	-1.118847000	0.789160000	-2.775304000
1	-6.314876000	1.056921000	-1.070539000	1	-2.149361000	-0.623275000	-2.553189000
1	-5.728496000	-1.284482000	-0.702957000	1	0.148616000	-1.853097000	1.587942000
1	-2.372900000	-2.462972000	0.332700000	1	0.216395000	-2.255378000	0.711420000
1	-3.927789000	-3.908168000	1.617874000	13	-0.003197000	-0.775890000	-0.322468000

				1	-0.068727000	-1.341052000	-3.446547000
Al- <i>intra</i> -IM <sub>1,4'</sub>				1	1.157958000	2.091536000	-0.376444000
7	-1.487950000	-0.317021000	-0.653286000	1	1.749061000	3.885060000	-2.018381000
6	-1.305683000	-0.541891000	-1.911519000	1	3.447385000	3.463874000	-1.840488000
6	-0.039350000	-1.218942000	-2.363462000	1	2.322293000	2.307663000	-2.545696000
6	1.272320000	-0.559363000	-1.973221000	1	1.404481000	4.371319000	0.431725000
7	1.420555000	-0.345930000	-0.607536000	1	3.140300000	4.216736000	0.553924000
6	2.758300000	0.026685000	-0.170531000	1	2.104583000	3.317658000	1.652496000
6	3.120372000	1.378098000	-0.045515000	1	4.695582000	2.722244000	0.456498000
6	2.150901000	2.509478000	-0.381934000	1	6.321680000	0.974092000	0.959175000
6	2.436242000	3.073868000	-1.793870000	1	5.699010000	-1.375869000	0.724683000
6	2.207912000	3.670917000	0.636199000	1	2.336178000	-2.569049000	-0.272509000
6	4.408673000	1.695001000	0.361755000	1	3.908150000	-4.062060000	-1.469488000
6	5.331046000	0.709986000	0.644421000	1	5.224054000	-2.936029000	-1.166920000
6	4.975298000	-0.614571000	0.514108000	1	3.885481000	-2.464473000	-2.208933000
6	3.700474000	-0.978943000	0.103382000	1	3.435870000	-4.335314000	0.998740000
6	3.392653000	-2.464360000	-0.089269000	1	4.812440000	-3.306477000	1.341983000
6	4.153080000	-3.014994000	-1.317865000	1	3.243166000	-2.932923000	2.037906000
6	3.744842000	-3.306983000	1.156147000	1	3.157648000	0.069197000	-2.734157000
6	2.173231000	-0.322065000	-2.949974000	1	1.929182000	-0.550782000	-3.979966000
6	-2.311352000	-0.269975000	-2.989004000	1	-2.561428000	-1.216280000	-3.479768000
6	-2.808830000	0.117859000	-0.171159000	1	-3.218678000	0.202292000	-2.623835000
6	-3.030853000	1.468884000	0.104987000	1	-1.835140000	0.360279000	-3.746908000
6	-4.285816000	1.846349000	0.557906000	1	-4.484031000	2.876289000	0.768124000
6	-5.283433000	0.912265000	0.749582000	1	-6.246227000	1.222059000	1.104614000
6	-5.038629000	-0.418529000	0.492051000	1	-5.814976000	-1.138044000	0.653850000
6	-3.801688000	-0.845758000	0.027529000	1	-2.584234000	-2.494063000	-0.586747000
6	-3.592691000	-2.337357000	-0.240092000	1	-4.360250000	-3.891520000	-1.543963000
6	-4.573210000	-2.852038000	-1.318443000	1	-5.597056000	-2.788408000	-0.969932000
6	-3.755525000	-3.160409000	1.056194000	1	-4.493668000	-2.279284000	-2.234493000
6	-1.943892000	2.518885000	-0.104921000	1	-3.578978000	-4.210371000	0.849042000
6	-1.963901000	3.615586000	0.981164000	1	-3.043785000	-2.837787000	1.802208000
6	-2.086684000	3.171804000	-1.498436000	1	-4.755173000	-3.056697000	1.461068000
6	0.045980000	-0.318365000	2.479193000	1	-0.987294000	2.022817000	-0.059462000
1	-1.303322000	-0.264197000	4.181272000	1	-1.078220000	4.232268000	0.885604000
1	0.951792000	-1.102880000	4.296970000	1	-1.975182000	3.185191000	1.974049000
1	1.999647000	-1.232321000	2.879146000	1	-2.826897000	4.261704000	0.872751000
1	0.639044000	-2.353832000	3.081676000	1	-1.308109000	3.912255000	-1.647142000

1	-2.007387000	2.437218000	-2.288623000	6	4.927520000	-0.920197000	-0.559910000
1	-3.049917000	3.662495000	-1.582432000	6	3.638251000	-1.112913000	-0.078011000
6	0.960901000	-1.313949000	3.215289000	6	3.138238000	-2.542415000	0.129654000
1	-1.785369000	-1.434099000	2.950588000	6	4.073306000	-3.346641000	1.061199000
1	-2.059830000	0.291810000	2.680701000	6	3.002178000	-3.268691000	-1.226749000
6	-1.355702000	-0.436847000	3.093604000	6	2.485633000	2.548322000	0.201556000
6	0.585712000	1.086698000	2.750636000	6	2.677680000	3.628334000	-0.886051000
1	0.564188000	1.299068000	3.832641000	6	2.792742000	3.165483000	1.585301000
1	-0.003930000	1.864718000	2.257595000	6	-0.012956000	0.371529000	-2.348289000
1	1.621844000	1.188170000	2.418309000	1	1.304786000	0.608601000	-4.060493000
1	-0.060927000	-2.222824000	-1.908149000	1	-1.007082000	-0.048189000	-4.238680000
1	-0.241614000	-2.487012000	0.399589000	1	-2.010001000	-0.426348000	-2.830316000
13	0.046685000	-0.913526000	0.570786000	1	-0.673964000	-1.500932000	-3.284208000
				1	0.033926000	-0.049770000	3.677116000
<b>Al-intra-TS<sub>4',4</sub></b>				1	-1.694479000	2.316391000	0.490529000
7	1.488139000	-0.133946000	0.694467000	1	-2.700924000	3.674675000	2.322911000
6	1.307712000	-0.225902000	2.010314000	1	-4.272026000	2.957327000	1.982448000
6	0.041990000	-0.316399000	2.624738000	1	-2.971807000	1.959574000	2.611972000
6	-1.309384000	-0.224157000	1.995315000	1	-2.432739000	4.545461000	-0.062283000
7	-1.461886000	-0.102444000	0.677663000	1	-4.095412000	4.040898000	-0.256117000
6	-2.835272000	-0.051545000	0.159613000	1	-2.882622000	3.528161000	-1.421678000
6	-3.440493000	1.207541000	0.010668000	1	-5.188252000	2.222063000	-0.658886000
6	-2.759809000	2.485873000	0.499965000	1	-6.360773000	0.196158000	-1.349351000
6	-3.201660000	2.785011000	1.953302000	1	-5.320226000	-1.988064000	-1.030950000
6	-3.066523000	3.721801000	-0.373690000	1	-1.978858000	-2.539564000	0.482531000
6	-4.712110000	1.271917000	-0.534850000	1	-3.411941000	-4.410795000	1.171069000
6	-5.379888000	0.126793000	-0.921801000	1	-4.837111000	-3.601033000	0.545749000
6	-4.789057000	-1.103026000	-0.745126000	1	-3.986581000	-2.937312000	1.933262000
6	-3.517155000	-1.220925000	-0.194657000	1	-2.371225000	-4.373695000	-1.107986000
6	-2.953225000	-2.625681000	0.031113000	1	-3.745937000	-3.520225000	-1.792336000
6	-3.859309000	-3.439948000	0.983950000	1	-2.122117000	-2.865188000	-1.965475000
6	-2.789212000	-3.390853000	-1.299490000	1	-3.294830000	-0.857742000	2.597940000
6	-2.282131000	-0.662805000	2.917532000	1	-2.108976000	-0.495764000	3.975162000
6	2.489097000	-0.294809000	2.949909000	1	2.868324000	-1.319514000	2.958122000
6	2.853326000	0.012969000	0.184491000	1	3.308237000	0.347457000	2.635463000
6	3.342476000	1.306495000	-0.049513000	1	2.188673000	-0.039393000	3.966816000
6	4.639856000	1.448552000	-0.514919000	1	5.036025000	2.427178000	-0.690165000
6	5.429446000	0.344476000	-0.768543000	1	6.428958000	0.472813000	-1.134563000

1	5.541653000	-1.771599000	-0.771991000	6	3.636660000	-3.414932000	3.535356000
1	2.157084000	-2.504134000	0.574701000	6	3.599472000	-2.867445000	4.797692000
1	3.644826000	-4.324498000	1.253849000	6	3.223292000	-1.551254000	4.961408000
1	5.045302000	-3.493290000	0.605918000	6	2.887145000	-0.761569000	3.872385000
1	4.219026000	-2.844907000	2.010188000	6	2.378168000	0.659423000	4.114411000
1	2.628883000	-4.275645000	-1.072739000	6	0.863932000	0.603594000	4.414818000
1	2.305994000	-2.745816000	-1.866437000	6	3.092179000	1.388704000	5.272731000
1	3.961192000	-3.331298000	-1.728015000	6	0.363808000	-1.391439000	1.173698000
1	1.451800000	2.240949000	0.187782000	6	1.523209000	0.422042000	-2.800268000
1	1.935624000	4.408247000	-0.753298000	6	4.345645000	0.900674000	-2.309319000
1	2.562178000	3.212882000	-1.878177000	6	5.160075000	-0.117422000	-2.811787000
1	3.654961000	4.090750000	-0.814870000	6	6.043632000	0.197678000	-3.832380000
1	2.205866000	4.066540000	1.730618000	6	6.129424000	1.483120000	-4.327621000
1	2.556422000	2.480343000	2.388157000	6	5.325697000	2.474607000	-3.811944000
1	3.842992000	3.426803000	1.652692000	6	4.414786000	2.208599000	-2.797575000
6	-0.984087000	-0.451916000	-3.213164000	6	3.542060000	3.355684000	-2.284176000
1	1.749914000	-0.752863000	-3.026633000	6	2.708831000	3.975665000	-3.429400000
1	2.121398000	0.892740000	-2.515678000	6	4.401597000	4.445088000	-1.607110000
6	1.369648000	0.274856000	-3.011349000	6	5.068629000	-1.549232000	-2.290465000
6	-0.484343000	1.826603000	-2.386401000	6	6.427697000	-2.280475000	-2.318723000
1	-0.434050000	2.218748000	-3.416053000	6	4.037947000	-2.352285000	-3.116842000
1	0.119286000	2.489662000	-1.758868000	6	5.839444000	0.734107000	1.274102000
1	-1.523467000	1.908564000	-2.061064000	1	7.717529000	1.670854000	0.721519000
1	-0.881033000	-1.401679000	2.804935000	1	6.960095000	1.473713000	2.984859000
1	0.062375000	-2.092007000	-0.649296000	1	5.411767000	0.744533000	3.421742000
13	0.014773000	-0.502568000	-0.544990000	1	5.457807000	2.368776000	2.706067000
				1	0.176700000	0.249449000	-0.677207000
<b>AI-inter-TS<sub>4',4</sub>-I</b>				1	3.157285000	-2.625807000	0.284512000
7	3.414337000	0.604521000	-1.204672000	1	2.284157000	-4.917775000	-0.019587000
6	2.154499000	0.449785000	-1.446227000	1	2.467904000	-5.239185000	1.695739000
6	1.187681000	0.403594000	-0.296879000	1	1.282400000	-4.067643000	1.142534000
6	1.453796000	-0.569204000	0.831222000	1	4.736206000	-4.436532000	-0.221284000
7	2.644415000	-0.467644000	1.433860000	1	4.938910000	-4.792919000	1.479429000
6	2.946710000	-1.323638000	2.587448000	1	5.527867000	-3.272410000	0.833563000
6	3.315460000	-2.664264000	2.411526000	1	3.916236000	-4.441698000	3.417685000
6	3.352948000	-3.360240000	1.050830000	1	3.854252000	-3.464336000	5.650926000
6	2.271257000	-4.462958000	0.965510000	1	3.183000000	-1.137084000	5.946924000
6	4.732042000	-3.999581000	0.771899000	1	2.522038000	1.239033000	3.216429000

1	0.475918000	1.604435000	4.573457000	7	-3.195146000	1.287898000	0.760440000
1	0.687639000	0.020886000	5.312146000	6	-2.685268000	0.696313000	1.838280000
1	0.322505000	0.146088000	3.599377000	6	-2.235655000	-0.656850000	1.861602000
1	4.167569000	1.355536000	5.166193000	6	-2.756826000	-1.767311000	1.011403000
1	2.782697000	2.428187000	5.282070000	7	-3.325797000	-1.437484000	-0.218659000
1	2.825808000	0.961098000	6.231878000	6	-3.926790000	-2.530602000	-0.964042000
1	0.508148000	-2.110536000	1.973122000	6	-5.267626000	-2.887099000	-0.724163000
1	-0.175688000	-1.795660000	0.316070000	6	-6.099867000	-2.207001000	0.361861000
1	0.798312000	1.241749000	-2.858004000	6	-6.168667000	-3.098927000	1.624336000
1	2.240380000	0.494214000	-3.612696000	6	-7.540416000	-1.881593000	-0.093757000
1	0.931684000	-0.494531000	-2.887400000	6	-5.836713000	-3.913728000	-1.461624000
1	6.673638000	-0.563221000	-4.241241000	6	-5.113744000	-4.591800000	-2.421531000
1	6.823138000	1.708805000	-5.112839000	6	-3.797182000	-4.256238000	-2.642269000
1	5.401878000	3.469390000	-4.200004000	6	-3.183616000	-3.238927000	-1.921519000
1	2.863428000	2.977535000	-1.536728000	6	-1.694404000	-2.983406000	-2.151906000
1	2.037320000	4.727038000	-3.029214000	6	-0.859851000	-4.161247000	-1.597189000
1	3.350498000	4.455821000	-4.157918000	6	-1.345221000	-2.773018000	-3.641567000
1	2.117223000	3.226855000	-3.941355000	6	-2.598325000	-3.027920000	1.490115000
1	3.763813000	5.243668000	-1.244010000	6	-2.461109000	1.492345000	3.103448000
1	4.943648000	4.035792000	-0.766948000	6	-3.581688000	2.695662000	0.839228000
1	5.112409000	4.868091000	-2.306792000	6	-4.929691000	3.014237000	1.057369000
1	4.731598000	-1.511914000	-1.265081000	6	-5.292768000	4.349692000	1.137305000
1	6.340760000	-3.222303000	-1.791551000	6	-4.357685000	5.353500000	0.984287000
1	7.202269000	-1.692015000	-1.843491000	6	-3.040647000	5.030032000	0.748330000
1	6.733711000	-2.501819000	-3.333995000	6	-2.628529000	3.705697000	0.675931000
1	3.968831000	-3.369513000	-2.746734000	6	-1.153760000	3.412084000	0.411842000
1	3.053608000	-1.906716000	-3.064968000	6	-0.228380000	4.135160000	1.417974000
1	4.342260000	-2.384825000	-4.156689000	6	-0.771108000	3.815778000	-1.028640000
6	5.908329000	1.369178000	2.674508000	6	-5.990125000	1.925866000	1.216629000
1	6.309320000	2.625104000	0.255497000	6	-7.350740000	2.327469000	0.607134000
1	6.749849000	1.189865000	-0.679956000	6	-6.188459000	1.560840000	2.705374000
6	6.689275000	1.600926000	0.331658000	6	-4.314654000	0.886419000	-2.471702000
6	6.477542000	-0.653422000	1.365726000	1	-4.831446000	2.705223000	-3.542360000
1	7.521249000	-0.564175000	1.708356000	1	-4.215331000	0.681784000	-4.637656000
1	6.501739000	-1.161708000	0.398174000	1	-3.739287000	-0.782072000	-3.767879000
1	5.955006000	-1.297989000	2.077646000	1	-2.626325000	0.599599000	-3.854636000
1	1.213579000	1.412854000	0.146637000	1	-2.081021000	-1.002589000	2.881520000
1	3.249673000	2.276408000	0.945727000	1	-5.601195000	-1.286795000	0.619738000

1	-6.747396000	-2.604636000	2.399785000	6	-3.679790000	0.310303000	-3.748119000
1	-6.652838000	-4.040594000	1.387232000	1	-3.294112000	2.821093000	-2.682929000
1	-5.178047000	-3.298178000	2.003702000	1	-4.810880000	2.920324000	-1.785115000
1	-8.032685000	-1.284653000	0.668030000	6	-4.309296000	2.415253000	-2.614710000
1	-8.123708000	-2.785895000	-0.222556000	6	-5.767965000	0.408367000	-2.438807000
1	-7.552016000	-1.329641000	-1.022761000	1	-6.308479000	0.774379000	-3.328513000
1	-6.855950000	-4.189923000	-1.283150000	1	-6.309085000	0.773550000	-1.562228000
1	-5.572236000	-5.380951000	-2.984891000	1	-5.831917000	-0.682579000	-2.443997000
1	-3.233563000	-4.798353000	-3.374954000	1	-0.809631000	-0.705341000	1.526731000
1	-1.428477000	-2.089741000	-1.611510000	1	-1.596279000	0.549373000	-1.387566000
1	0.200668000	-3.970542000	-1.738015000	13	3.918476000	0.835464000	0.744129000
1	-1.109559000	-5.078815000	-2.118024000	13	-3.136570000	0.299450000	-0.946742000
1	-1.048327000	-4.297196000	-0.542043000				
1	-0.286302000	-2.549777000	-3.742145000	Al-inter-IM <sub>4',4</sub>			
1	-1.543872000	-3.666998000	-4.220439000	7	3.220336000	0.565084000	-1.284921000
1	-1.908643000	-1.955979000	-4.067572000	6	1.942046000	0.380364000	-1.332660000
1	-2.924922000	-3.897409000	0.938230000	6	1.145926000	0.370256000	-0.054026000
1	-2.171981000	-3.180556000	2.474848000	6	1.654791000	-0.430969000	1.118383000
1	-1.516841000	2.035029000	3.029346000	7	2.895061000	-0.316964000	1.480823000
1	-3.241673000	2.233256000	3.261860000	6	3.347340000	-0.936812000	2.746987000
1	-2.401841000	0.831094000	3.967827000	6	3.912714000	-2.216592000	2.734571000
1	-6.315549000	4.610488000	1.312136000	6	4.012073000	-3.062829000	1.465499000
1	-4.658092000	6.381025000	1.043142000	6	2.826851000	-4.054862000	1.392589000
1	-2.321249000	5.813331000	0.619832000	6	5.330107000	-3.864268000	1.375452000
1	-1.003395000	2.348939000	0.503655000	6	4.345849000	-2.745906000	3.941204000
1	0.797196000	3.805543000	1.284248000	6	4.227314000	-2.033997000	5.116744000
1	-0.253697000	5.207515000	1.266309000	6	3.660702000	-0.778796000	5.108600000
1	-0.520351000	3.934683000	2.441207000	6	3.204557000	-0.202950000	3.930047000
1	0.283737000	3.624770000	-1.203237000	6	2.519288000	1.165112000	4.000732000
1	-1.347900000	3.248453000	-1.744112000	6	1.165374000	1.046803000	4.740423000
1	-0.953005000	4.871552000	-1.191770000	6	3.396632000	2.223828000	4.704020000
1	-5.637979000	1.048376000	0.699555000	6	0.603858000	-1.203854000	1.815787000
1	-8.001422000	1.460807000	0.581372000	6	1.128316000	0.276437000	-2.576525000
1	-7.235955000	2.698173000	-0.403366000	6	3.990083000	0.765590000	-2.529427000
1	-7.841662000	3.088417000	1.202765000	6	4.729786000	-0.300946000	-3.047179000
1	-6.966681000	0.811265000	2.805074000	6	5.479969000	-0.077584000	-4.190673000
1	-5.282523000	1.158811000	3.137848000	6	5.506332000	1.165397000	-4.791325000
1	-6.483097000	2.439245000	3.269334000	6	4.772789000	2.203388000	-4.262362000

6	3.994025000	2.029034000	-3.125070000	1	2.592955000	2.902636000	-1.758688000
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6	2.216146000	3.744383000	-3.693046000	1	2.765580000	4.163125000	-4.527104000
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6	4.691165000	-1.687770000	-2.410899000	1	3.507375000	5.184735000	-1.760061000
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6	3.571167000	-2.537961000	-3.053742000	1	4.730604000	4.715972000	-2.931467000
6	6.005845000	0.945248000	0.746498000	1	4.468632000	-1.567678000	-1.361469000
1	7.787527000	1.771922000	-0.170071000	1	5.998007000	-3.335712000	-1.919090000
1	7.361364000	1.835385000	2.193994000	1	6.861167000	-1.828606000	-2.188808000
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1	3.963112000	-2.401684000	0.613533000	1	3.762601000	-2.660295000	-4.113408000
1	2.892196000	-4.649879000	0.487892000	6	6.275867000	1.735086000	2.040820000
1	2.855648000	-4.725131000	2.243741000	1	6.334310000	2.695022000	-0.547795000
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1	5.400605000	-4.325373000	0.396595000	6	6.715139000	1.679186000	-0.403148000
1	5.352743000	-4.660549000	2.108969000	6	6.640663000	-0.437604000	0.906926000
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1	4.775736000	-3.725023000	3.963288000	1	6.488106000	-1.073143000	0.030623000
1	4.569151000	-2.461864000	6.037965000	1	6.248522000	-0.960681000	1.782146000
1	3.560009000	-0.240719000	6.028255000	1	1.115722000	1.420693000	0.287352000
1	2.331145000	1.519178000	2.999607000	1	3.276865000	2.366226000	0.785830000
1	0.661044000	2.006904000	4.741990000	7	-3.427265000	1.262606000	0.737146000
1	1.322878000	0.744876000	5.769061000	6	-2.988162000	0.747303000	1.940182000
1	0.513972000	0.322117000	4.271071000	6	-2.631826000	-0.559821000	2.139258000
1	4.353078000	2.332355000	4.212906000	6	-2.774611000	-1.742610000	1.281542000
1	2.890863000	3.182688000	4.680240000	7	-3.256248000	-1.560907000	-0.018857000
1	3.568205000	1.964314000	5.741368000	6	-3.731951000	-2.751011000	-0.695788000
1	0.951277000	-1.719049000	2.706061000	6	-5.054635000	-3.184943000	-0.475628000
1	0.135448000	-1.913215000	1.121339000	6	-5.978827000	-2.465086000	0.504792000
1	0.394733000	1.091272000	-2.572599000	6	-6.063812000	-3.251224000	1.834397000
1	1.728194000	0.304384000	-3.481198000	6	-7.406460000	-2.261801000	-0.050281000
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1	6.050575000	-0.876334000	-4.614705000	6	-4.703650000	-5.030186000	-1.985484000
1	6.097254000	1.321020000	-5.671727000	6	-3.407656000	-4.615821000	-2.191527000
1	4.798810000	3.162265000	-4.737348000	6	-2.902498000	-3.486751000	-1.556819000

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6	-1.043381000	-3.100024000	-3.271682000	1	-2.606501000	-3.881811000	1.300559000
6	-2.465823000	-2.952802000	1.833084000	1	-2.163309000	-3.003397000	2.873144000
6	-2.868451000	1.679536000	3.128253000	1	-2.116555000	2.449645000	2.954694000
6	-3.856888000	2.646145000	0.701956000	1	-3.805957000	2.201382000	3.324365000
6	-5.223849000	2.949159000	0.817829000	1	-2.589815000	1.116914000	4.021186000
6	-5.627768000	4.275767000	0.799089000	1	-6.667189000	4.513571000	0.897620000
6	-4.714206000	5.298475000	0.647033000	1	-5.044474000	6.318715000	0.629911000
6	-3.376767000	4.999455000	0.508236000	1	-2.671851000	5.796296000	0.376809000
6	-2.929447000	3.685755000	0.536509000	1	-1.272261000	2.366935000	0.548126000
6	-1.435547000	3.416899000	0.367297000	1	0.472067000	3.945814000	1.266560000
6	-0.571069000	4.239728000	1.350552000	1	-0.631180000	5.298563000	1.129674000
6	-0.993658000	3.722834000	-1.080315000	1	-0.886083000	4.092192000	2.375554000
6	-6.269288000	1.845653000	0.964199000	1	0.073438000	3.547473000	-1.195066000
6	-7.541275000	2.124491000	0.133263000	1	-1.525016000	3.090005000	-1.775086000
6	-6.662791000	1.643644000	2.444748000	1	-1.192352000	4.758623000	-1.330250000
6	-4.204347000	0.523998000	-2.493863000	1	-5.822096000	0.932917000	0.607610000
1	-4.794006000	2.199774000	-3.747441000	1	-8.170147000	1.240644000	0.127966000
1	-3.925759000	0.146329000	-4.623130000	1	-7.294590000	2.374276000	-0.890652000
1	-3.421359000	-1.197351000	-3.589416000	1	-8.120328000	2.937116000	0.557122000
1	-2.400821000	0.250090000	-3.721207000	1	-7.428519000	0.878510000	2.527168000
1	-2.304189000	-0.802121000	3.145471000	1	-5.813240000	1.330053000	3.035509000
1	-5.544422000	-1.499469000	0.706315000	1	-7.054704000	2.566722000	2.858893000
1	-6.695789000	-2.721601000	2.541741000	6	-3.438405000	-0.106196000	-3.665775000
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1	-7.972851000	-1.636705000	0.633515000	6	-4.303312000	2.029999000	-2.773171000
1	-7.931792000	-3.206006000	-0.138468000	6	-5.619111000	-0.060878000	-2.511739000
1	-7.392693000	-1.783737000	-1.019682000	1	-6.124592000	0.188060000	-3.461305000
1	-6.520781000	-4.649037000	-0.961133000	1	-6.241719000	0.332299000	-1.703552000
1	-5.077617000	-5.904193000	-2.482354000	1	-5.605589000	-1.150625000	-2.425151000
1	-2.776005000	-5.181915000	-2.846530000	1	-0.223539000	-0.519380000	2.062410000
1	-1.273043000	-2.148133000	-1.356254000	1	-1.565516000	0.420024000	-1.178325000
1	0.529077000	-3.881134000	-1.194679000	13	4.031592000	0.992579000	0.494569000
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1	-0.727971000	-4.148578000	0.013994000				
1	-0.006449000	-2.793033000	-3.379752000				

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7	-2.649850000	-1.498564000	0.464150000	1	-4.664369000	-0.684261000	-4.400620000
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6	-2.451769000	1.048731000	-1.165598000	1	-6.823184000	-1.420878000	-3.297560000
7	-3.617450000	1.020973000	-0.588432000	1	-7.398577000	0.155524000	-3.779406000
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6	-3.663710000	3.784321000	0.545557000	1	-3.446099000	4.457000000	2.590151000
6	-3.086440000	5.105643000	-0.013984000	1	-5.054329000	4.725765000	1.934359000
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6	-3.549510000	-3.819933000	0.251939000	1	-1.227400000	-2.669841000	-1.820677000
6	-3.803939000	-5.048892000	0.844101000	1	-4.332616000	-5.798835000	0.292365000
6	-3.392043000	-5.320929000	2.130632000	1	-3.607257000	-6.273013000	2.573142000
6	-2.692950000	-4.370531000	2.842408000	1	-2.362299000	-4.594555000	3.835419000
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6	-4.030624000	-3.594223000	-1.181064000	1	-1.755113000	-0.944002000	4.922195000
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6	-3.392488000	-4.618892000	-2.149185000	1	-2.698061000	-2.428279000	4.972870000
6	-5.677144000	-0.447522000	1.807838000	1	-3.743066000	-2.600877000	-1.493212000
1	-6.802709000	-1.958435000	2.871780000	1	-5.887520000	-3.525983000	-2.300103000
1	-6.877871000	0.337365000	3.439676000	1	-6.047865000	-2.964257000	-0.643274000
1	-5.990842000	1.589132000	2.570081000	1	-5.907368000	-4.679554000	-0.979677000
1	-5.139630000	0.539676000	3.712310000	1	-3.660945000	-4.378209000	-3.172399000
1	-0.597784000	0.117636000	-1.559149000	1	-2.313600000	-4.630295000	-2.068995000
1	-5.063369000	-0.500513000	-1.938429000	1	-3.753764000	-5.617459000	-1.936627000

6	-5.921165000	0.564214000	2.944624000	6	3.811783000	-1.785756000	-4.332189000
1	-5.075261000	-2.044126000	3.210360000	6	5.979063000	-1.817889000	1.259701000
1	-5.695103000	-2.649205000	1.680976000	6	7.478339000	-1.491128000	1.445304000
6	-5.803487000	-1.853521000	2.419702000	6	5.496476000	-2.657387000	2.464643000
6	-6.828295000	-0.283620000	0.807771000	6	5.668022000	1.454043000	-1.394980000
1	-7.787789000	-0.459224000	1.320082000	1	7.492653000	0.880098000	-2.425730000
1	-6.767702000	-1.006810000	-0.008917000	1	6.601299000	3.055841000	-2.529954000
1	-6.869576000	0.716358000	0.371047000	1	5.099686000	3.541337000	-1.735623000
1	-0.715746000	0.725085000	0.084982000	1	5.047205000	2.537306000	-3.202532000
1	-2.872193000	0.790970000	2.072074000	1	0.786803000	-1.096216000	1.197646000
1	-1.215121000	2.622055000	-1.784399000	1	3.951993000	0.949921000	2.264843000
7	3.713079000	-1.119407000	-0.452843000	1	3.172256000	0.858414000	4.628123000
6	2.589368000	-1.498128000	0.218489000	1	2.991028000	2.609731000	4.632469000
6	1.633496000	-0.629357000	0.705691000	1	1.960777000	1.621610000	3.602101000
6	1.624232000	0.819510000	0.773737000	1	5.635927000	0.994233000	4.005759000
7	2.705148000	1.509614000	0.288058000	1	5.469263000	2.720570000	4.232607000
6	2.962459000	2.857866000	0.762524000	1	6.169350000	2.097252000	2.744692000
6	3.662095000	3.028534000	1.974090000	1	4.548602000	4.443123000	3.293663000
6	4.001699000	1.839861000	2.871803000	1	4.006239000	6.388927000	1.918762000
6	2.956972000	1.723442000	4.007223000	1	2.742445000	6.102227000	-0.149987000
6	5.411797000	1.926744000	3.496698000	1	1.474063000	2.840222000	-1.388765000
6	4.015974000	4.305537000	2.374887000	1	-0.271299000	4.604050000	-1.806520000
6	3.706081000	5.408724000	1.603381000	1	0.580003000	5.687498000	-0.730656000
6	2.999254000	5.241945000	0.435541000	1	-0.133410000	4.218614000	-0.088722000
6	2.599274000	3.979614000	0.008442000	1	1.627020000	4.410685000	-3.321209000
6	1.6966673000	3.883289000	-1.221302000	1	2.627621000	5.490473000	-2.364990000
6	0.381482000	4.643630000	-0.940095000	1	3.209833000	3.886866000	-2.785154000
6	2.339102000	4.454503000	-2.502141000	1	0.433531000	2.488126000	1.448814000
6	0.478099000	1.415068000	1.312488000	1	-0.154021000	0.823321000	1.968887000
6	2.321526000	-2.977165000	0.404427000	1	2.086825000	-3.448155000	-0.552214000
6	4.622392000	-2.171212000	-0.882647000	1	3.188917000	-3.502230000	0.800208000
6	5.705488000	-2.529594000	-0.064549000	1	1.481729000	-3.128589000	1.080069000
6	6.550620000	-3.549721000	-0.474694000	1	7.373979000	-3.836327000	0.147304000
6	6.357358000	-4.195684000	-1.678410000	1	7.025595000	-4.976790000	-1.984217000
6	5.307138000	-3.824844000	-2.488839000	1	5.169154000	-4.320369000	-3.428984000
6	4.424990000	-2.822249000	-2.108565000	1	2.640138000	-1.749972000	-2.551337000
6	3.276345000	-2.462173000	-3.051366000	1	1.578747000	-3.392301000	-4.031675000
6	2.434533000	-3.700565000	-3.438314000	1	3.014183000	-4.396095000	-4.033122000

1	2.074254000	-4.228040000	-2.563254000	6	4.794852000	-1.195664000	0.544926000
1	2.989418000	-1.534203000	-4.994874000	6	3.515871000	-1.271930000	0.008800000
1	4.334264000	-0.874317000	-4.084693000	6	2.985262000	-2.639004000	-0.428635000
1	4.489266000	-2.446849000	-4.860830000	6	3.841351000	-3.208547000	-1.583220000
1	5.426540000	-0.892942000	1.246253000	6	2.952054000	-3.652919000	0.735523000
1	7.602940000	-0.835904000	2.300992000	6	2.302544000	-0.169155000	-2.947542000
1	7.883477000	-0.995357000	0.573491000	6	-2.521560000	-0.531561000	-2.982611000
1	8.056048000	-2.389321000	1.631466000	6	-2.807581000	0.130073000	-0.194560000
1	5.741371000	-2.150798000	3.393049000	6	-2.943305000	1.516358000	-0.033626000
1	4.425753000	-2.807034000	2.439760000	6	-4.129478000	2.012410000	0.484345000
1	5.982724000	-3.627112000	2.466591000	6	-5.155459000	1.164960000	0.849196000
6	5.585781000	2.716426000	-2.263847000	6	-5.016769000	-0.193911000	0.673252000
1	6.044707000	0.155986000	-3.128813000	6	-3.856184000	-0.735986000	0.135959000
1	6.700235000	-0.483419000	-1.621690000	6	-3.794602000	-2.249317000	-0.083574000
6	6.512571000	0.436680000	-2.178878000	6	-5.017569000	-2.754611000	-0.883378000
6	6.433539000	1.836285000	-0.124970000	6	-3.694625000	-3.007700000	1.257573000
1	7.451778000	2.176920000	-0.382136000	6	-1.843583000	2.494587000	-0.445870000
1	6.541223000	0.998505000	0.567965000	6	-1.563897000	3.555917000	0.640109000
1	5.942035000	2.652907000	0.409960000	6	-2.218130000	3.195127000	-1.772056000
1	2.898048000	0.746769000	-2.424206000	6	0.034694000	-0.212439000	2.448924000
13	-3.828755000	-0.029157000	1.105626000	1	-1.327721000	0.022077000	4.112715000
13	3.807933000	0.716783000	-1.086827000	1	0.670708000	-1.322742000	4.201966000
				1	1.736455000	-1.547885000	2.810273000
<b>Al-intra-TS<sub>1,2'</sub></b>				1	0.165266000	-2.373387000	2.869701000
1	-1.182590000	-1.609393000	-0.250159000	1	-0.060131000	-0.452560000	-3.727673000
1	-0.481929000	-2.208608000	0.221939000	1	1.564205000	2.248225000	-0.138862000
7	-1.535692000	-0.403274000	-0.685863000	1	4.108990000	3.256008000	-1.466560000
6	-1.309367000	-0.394209000	-2.096256000	1	2.814956000	2.368749000	-2.266534000
6	-0.077658000	-0.370807000	-2.645612000	1	2.519758000	3.989701000	-1.649126000
6	1.272541000	-0.224099000	-2.072508000	1	2.189661000	4.367843000	0.839351000
7	1.419597000	-0.150324000	-0.675987000	1	3.873067000	3.912746000	0.955889000
6	2.782646000	-0.087989000	-0.163804000	1	2.683288000	3.132771000	1.988348000
6	3.354888000	1.153375000	0.159987000	1	5.087653000	2.119274000	0.937472000
6	2.619146000	2.467816000	-0.098206000	1	6.342047000	0.058049000	1.296567000
6	3.042850000	3.055740000	-1.465375000	1	5.361631000	-2.093854000	0.686621000
6	2.860329000	3.529487000	0.997877000	1	1.979395000	-2.512270000	-0.794148000
6	4.638753000	1.180998000	0.684591000	1	3.428429000	-4.155654000	-1.916150000
6	5.352432000	0.016961000	0.885440000	1	4.860821000	-3.380599000	-1.257323000

1	3.852697000	-2.526745000	-2.421884000	1	-0.004680000	-2.577980000	0.081737000
1	2.552699000	-4.599467000	0.385886000	7	1.579647000	-0.578337000	0.705443000
1	3.947356000	-3.833307000	1.124296000	6	1.290386000	-0.377915000	2.135472000
1	2.327893000	-3.301747000	1.545145000	6	0.068649000	-0.096284000	2.609485000
1	3.328417000	-0.065888000	-2.624522000	6	-1.250242000	0.133969000	1.986860000
1	2.106236000	-0.223426000	-4.011054000	7	-1.400385000	-0.075197000	0.616505000
1	-2.224064000	-0.482002000	-4.031104000	6	-2.769078000	-0.010976000	0.111231000
1	-3.019987000	-1.489913000	-2.813727000	6	-3.235614000	1.152502000	-0.517439000
1	-3.256801000	0.252420000	-2.792231000	6	-2.366270000	2.398538000	-0.637802000
1	-4.251994000	3.068818000	0.608073000	6	-2.737761000	3.413919000	0.467767000
1	-6.061126000	1.563955000	1.261298000	6	-2.480522000	3.074751000	-2.021731000
1	-5.822431000	-0.843145000	0.948955000	6	-4.531821000	1.179756000	-1.011700000
1	-2.915865000	-2.483178000	-0.664084000	6	-5.361205000	0.084111000	-0.897250000
1	-4.887484000	-3.804485000	-1.123418000	6	-4.902898000	-1.054286000	-0.271604000
1	-5.929875000	-2.656532000	-0.308383000	6	-3.617116000	-1.121702000	0.246958000
1	-5.136223000	-2.202035000	-1.807293000	6	-3.190681000	-2.404147000	0.961297000
1	-3.666788000	-4.077757000	1.081036000	6	-4.102738000	-2.695104000	2.173635000
1	-2.796534000	-2.729278000	1.791615000	6	-3.190274000	-3.606839000	-0.007149000
1	-4.550008000	-2.786379000	1.885142000	6	-2.232348000	0.527147000	2.834506000
1	-0.933752000	1.940838000	-0.616805000	6	2.447896000	-0.617079000	3.065631000
1	-0.698347000	4.145426000	0.357669000	6	2.779257000	0.168251000	0.213762000
1	-1.365380000	3.094227000	1.598186000	6	2.770777000	1.566256000	0.216747000
1	-2.401474000	4.233211000	0.753606000	6	3.932251000	2.229410000	-0.152927000
1	-1.430774000	3.880801000	-2.066726000	6	5.060386000	1.541022000	-0.538451000
1	-2.354454000	2.475185000	-2.567879000	6	5.037855000	0.165276000	-0.577856000
1	-3.137176000	3.757735000	-1.653024000	6	3.907203000	-0.551583000	-0.210962000
6	0.688957000	-1.439938000	3.107361000	6	3.996471000	-2.084461000	-0.284500000
1	-2.014297000	-0.934679000	2.798981000	6	4.841145000	-2.640458000	0.884483000
1	-1.903829000	0.815909000	2.639483000	6	4.610848000	-2.564271000	-1.621572000
6	-1.384415000	-0.068505000	3.016483000	6	1.556630000	2.404233000	0.617035000
6	0.849595000	1.019531000	2.862705000	6	1.264402000	3.509858000	-0.423045000
1	0.839249000	1.114599000	3.960054000	6	1.777648000	3.053859000	2.001744000
1	0.441166000	1.948364000	2.454591000	6	-0.015161000	-0.828337000	-2.363133000
1	1.892741000	0.941637000	2.548400000	1	0.532587000	0.545802000	-3.956839000
13	0.047801000	-0.511288000	0.481619000	1	0.999731000	-1.905646000	-3.962137000
				1	0.626396000	-2.921666000	-2.556773000
				1	1.961841000	-1.761133000	-2.489011000
1	1.835577000	-1.564120000	0.658477000	1	0.029301000	-0.012389000	3.691979000

1	-1.345242000	2.090843000	-0.490672000	1	2.613253000	3.743746000	1.962956000
1	-3.776516000	3.709768000	0.367880000	6	0.945132000	-1.917907000	-2.861520000
1	-2.592546000	2.981807000	1.448332000	1	1.515195000	0.736847000	-2.498858000
1	-2.122057000	4.305044000	0.386817000	1	-0.145017000	1.350157000	-2.537461000
1	-1.731853000	3.855399000	-2.109037000	6	0.500805000	0.527096000	-2.854759000
1	-3.451330000	3.536984000	-2.155915000	6	-1.388016000	-1.092335000	-3.003991000
1	-2.327046000	2.361987000	-2.822168000	1	-1.290303000	-1.101713000	-4.102292000
1	-4.896648000	2.065141000	-1.490733000	1	-2.125876000	-0.329649000	-2.743364000
1	-6.358513000	0.119788000	-1.289953000	1	-1.802269000	-2.064370000	-2.712460000
1	-5.552238000	-1.901687000	-0.180100000	13	-0.153130000	-1.045095000	-0.383334000
1	-2.187357000	-2.275212000	1.329258000				
1	-3.748904000	-3.577807000	2.697167000				<i>Al-intra-TS<sub>2',4</sub></i>
1	-5.124061000	-2.877628000	1.860314000	1	-0.483711000	-1.131319000	-0.789847000
1	-4.094657000	-1.861138000	2.863394000	1	0.253490000	0.999624000	1.974522000
1	-2.855182000	-4.500228000	0.509661000	7	-1.271191000	0.075948000	-0.475953000
1	-4.184027000	-3.792171000	-0.398033000	6	-1.050337000	0.648227000	-1.765754000
1	-2.520866000	-3.428669000	-0.838408000	6	0.169567000	0.389117000	-2.278601000
1	-3.241711000	0.711891000	2.495246000	6	0.997211000	-0.518799000	-1.422997000
1	-2.016265000	0.662591000	3.886731000	7	1.612607000	0.044077000	-0.372987000
1	2.168962000	-0.358631000	4.088259000	6	2.654260000	-0.703733000	0.341721000
1	2.734091000	-1.674271000	3.056075000	6	3.970781000	-0.456475000	-0.083247000
1	3.325934000	-0.032673000	2.783372000	6	4.268569000	0.504254000	-1.231537000
1	3.949471000	3.298904000	-0.140136000	6	4.541462000	-0.293769000	-2.526692000
1	5.948326000	2.072870000	-0.816552000	6	5.451148000	1.447175000	-0.925743000
1	5.912810000	-0.362518000	-0.894072000	6	5.015671000	-1.125702000	0.529786000
1	3.009883000	-2.525909000	-0.237352000	6	4.781123000	-2.014384000	1.558517000
1	4.895171000	-3.722053000	0.823622000	6	3.492081000	-2.237269000	1.982729000
1	5.848390000	-2.244559000	0.832515000	6	2.407071000	-1.596704000	1.392324000
1	4.424301000	-2.373261000	1.845078000	6	1.020449000	-1.910111000	1.959144000
1	4.501315000	-3.640163000	-1.698963000	6	0.692659000	-3.419977000	1.886854000
1	4.119285000	-2.107236000	-2.468550000	6	0.919447000	-1.443252000	3.429274000
1	5.667865000	-2.336293000	-1.670487000	6	0.602987000	-1.858601000	-1.475928000
1	0.690272000	1.766901000	0.667207000	6	-2.072727000	1.545866000	-2.386653000
1	0.344911000	4.017012000	-0.156774000	6	-2.652351000	-0.248601000	-0.067260000
1	1.153841000	3.095176000	-1.415498000	6	-3.304961000	0.461354000	0.952792000
1	2.053499000	4.251187000	-0.443967000	6	-4.543145000	0.018934000	1.403721000
1	0.891437000	3.605221000	2.296652000	6	-5.167557000	-1.070941000	0.848327000
1	1.981391000	2.309057000	2.758208000	6	-4.563434000	-1.719787000	-0.204722000

6	-3.323963000	-1.325691000	-0.682239000	1	-1.875603000	-1.623756000	-2.225295000
6	-2.770867000	-2.102882000	-1.877042000	1	-3.306800000	-2.582666000	-3.922063000
6	-3.764389000	-2.104108000	-3.062311000	1	-4.668902000	-2.647881000	-2.821134000
6	-2.423588000	-3.552622000	-1.474257000	1	-4.039269000	-1.093630000	-3.340223000
6	-2.778081000	1.743290000	1.585354000	1	-1.981857000	-4.082127000	-2.312630000
6	-2.503812000	1.567283000	3.092468000	1	-1.723166000	-3.567748000	-0.649040000
6	-3.763381000	2.911400000	1.347715000	1	-3.316639000	-4.086025000	-1.170822000
6	0.618334000	3.123285000	-0.080153000	1	-1.857492000	2.018173000	1.107042000
1	-0.044755000	5.173828000	0.215204000	1	-2.063435000	2.471828000	3.497987000
1	2.254659000	4.396822000	0.605634000	1	-1.816740000	0.750694000	3.262448000
1	2.698442000	2.686396000	0.525635000	1	-3.425080000	1.368785000	3.627677000
1	1.676968000	3.271812000	1.845804000	1	-3.340815000	3.833388000	1.730057000
1	0.535797000	0.798126000	-3.211669000	1	-3.966278000	3.037737000	0.290641000
1	3.392649000	1.111431000	-1.380885000	1	-4.703956000	2.735951000	1.854679000
1	5.417605000	-0.920800000	-2.404010000	6	1.880900000	3.374340000	0.773436000
1	3.701632000	-0.933888000	-2.772100000	1	-0.693553000	4.050533000	1.413675000
1	4.716519000	0.380493000	-3.359317000	1	-1.355927000	4.077200000	-0.230470000
1	5.546001000	2.179874000	-1.720434000	6	-0.432049000	4.151350000	0.354121000
1	6.388260000	0.907283000	-0.861679000	6	0.982721000	3.395163000	-1.542679000
1	5.292294000	1.974120000	0.007476000	1	1.367593000	4.421949000	-1.653612000
1	6.020233000	-0.951631000	0.202993000	1	0.118394000	3.299222000	-2.210222000
1	5.598764000	-2.525489000	2.027448000	1	1.760383000	2.714144000	-1.906145000
1	3.318254000	-2.921367000	2.787949000	13	0.252617000	1.210541000	0.421458000
1	0.273915000	-1.377358000	1.393322000				
1	-0.324878000	-3.587689000	2.224070000				<i>Al-inter-TS<sub>1,4</sub>-I</i>
1	1.354299000	-3.989682000	2.527780000	7	3.720443000	1.044884000	-0.686010000
1	0.785592000	-3.807314000	0.880712000	6	2.427709000	1.273254000	-1.145697000
1	-0.090211000	-1.597635000	3.796495000	6	1.373503000	0.445125000	-0.878061000
1	1.597591000	-2.010340000	4.056154000	6	1.336521000	-0.816553000	-0.172821000
1	1.158857000	-0.393766000	3.514779000	7	2.472353000	-1.282184000	0.469840000
1	1.059037000	-2.573814000	-0.806030000	6	2.454227000	-2.650529000	1.002043000
1	0.211118000	-2.240161000	-2.411564000	6	2.704545000	-3.723781000	0.131462000
1	-2.227698000	2.421250000	-1.746355000	6	2.702044000	-5.011132000	0.648271000
1	-1.737113000	1.883445000	-3.369371000	6	2.467042000	-5.241244000	1.987005000
1	-3.034234000	1.038895000	-2.485928000	6	2.227168000	-4.180893000	2.833458000
1	-5.025394000	0.549513000	2.198663000	6	2.213337000	-2.873753000	2.364520000
1	-6.119499000	-1.399182000	1.215905000	6	0.111011000	-1.498367000	-0.161333000
1	-5.060056000	-2.550234000	-0.663095000	6	2.189007000	2.483270000	-2.006539000

6	4.819978000	1.875137000	-1.175794000	1	1.925654000	-3.927292000	-3.246586000
6	5.496903000	1.483648000	-2.338019000	6	4.237220000	-4.258413000	-1.836987000
6	6.619059000	2.198843000	-2.728682000	1	4.416639000	-4.037198000	-2.883636000
6	7.054030000	3.287794000	-2.002255000	1	5.098155000	-3.940337000	-1.265932000
6	6.354548000	3.691511000	-0.884875000	1	4.144122000	-5.332714000	-1.739217000
6	5.227583000	3.003860000	-0.455756000	6	0.340115000	-1.670790000	3.535811000
6	5.789421000	-0.911649000	1.236882000	1	-0.026651000	-2.609599000	3.935723000
1	7.871807000	-0.364096000	1.361110000	1	0.092737000	-0.881416000	4.237125000
1	5.324325000	0.332014000	3.008005000	1	-0.168782000	-1.469317000	2.607434000
1	6.511520000	-0.946013000	3.280483000	6	2.533554000	-1.922000000	4.725357000
1	4.800713000	-1.354164000	3.140009000	1	3.591079000	-2.135694000	4.651401000
1	0.413353000	0.752159000	-1.281142000	1	2.406158000	-1.011330000	5.300369000
1	2.881861000	-5.841770000	-0.002974000	1	2.063495000	-2.724255000	5.280919000
1	2.467526000	-6.243310000	2.367931000	6	5.030171000	0.303509000	-3.190801000
1	2.039378000	-4.370780000	3.869585000	1	4.068070000	-0.022659000	-2.826781000
1	0.076040000	-2.497984000	0.251400000	6	6.013825000	-0.881784000	-3.081014000
1	-0.515617000	-1.321688000	-1.032140000	1	7.004064000	-0.588759000	-3.408677000
1	2.521260000	3.393732000	-1.507841000	1	6.089795000	-1.230806000	-2.058053000
1	2.748880000	2.406957000	-2.941890000	1	5.679958000	-1.709391000	-3.697128000
1	1.125237000	2.576616000	-2.228144000	6	4.852695000	0.707656000	-4.671193000
1	7.155631000	1.904970000	-3.607921000	1	4.430373000	-0.120732000	-5.229673000
1	7.926448000	3.827256000	-2.313696000	1	4.187097000	1.556968000	-4.764550000
1	6.685602000	4.552636000	-0.340631000	1	5.801621000	0.966630000	-5.124231000
6	5.580289000	-0.700395000	2.748290000	6	4.462876000	3.521930000	0.761087000
1	6.837222000	1.008856000	0.951053000	1	3.589034000	2.904501000	0.897523000
1	7.221929000	-0.192169000	-0.272867000	6	5.315074000	3.446704000	2.046443000
6	6.985239000	-0.058845000	0.785025000	1	4.743021000	3.810294000	2.893390000
6	6.150670000	-2.390799000	1.022888000	1	5.620915000	2.430793000	2.254339000
1	7.043398000	-2.628429000	1.620863000	1	6.206388000	4.055923000	1.953877000
1	6.400893000	-2.604863000	-0.020101000	6	3.993546000	4.978789000	0.541888000
1	5.355091000	-3.072877000	1.332314000	1	4.840462000	5.650080000	0.466828000
6	2.947802000	-3.546008000	-1.369523000	1	3.405541000	5.071900000	-0.361819000
1	3.048340000	-2.492109000	-1.583331000	1	3.382580000	5.298428000	1.378448000
6	1.870878000	-1.746965000	3.338946000	7	-3.456694000	-0.977877000	-0.828004000
1	2.204969000	-0.812954000	2.910861000	6	-2.705157000	-0.589909000	-1.945619000
6	1.748932000	-4.079557000	-2.186721000	6	-2.145258000	0.639455000	-2.110582000
1	1.619056000	-5.141534000	-2.013498000	6	-2.264181000	1.881566000	-1.328597000
1	0.837074000	-3.570727000	-1.913044000	7	-2.927120000	1.820176000	-0.095179000

6	-3.115183000	3.073713000	0.613725000	1	-3.827303000	1.830598000	3.293035000
6	-4.303452000	3.801782000	0.448198000	6	-2.935620000	-3.707526000	0.278494000
6	-4.480378000	4.977714000	1.162203000	1	-2.400302000	-2.795155000	0.482393000
6	-3.515521000	5.436286000	2.034486000	6	-2.006757000	-4.663675000	-0.503687000
6	-2.344720000	4.726367000	2.185899000	1	-1.116691000	-4.884940000	0.077249000
6	-2.121120000	3.554630000	1.475907000	1	-2.517018000	-5.597249000	-0.711597000
6	-1.720387000	3.012289000	-1.851267000	1	-1.700273000	-4.231060000	-1.445483000
6	-2.432440000	-1.636497000	-3.003003000	6	-3.312353000	-4.371483000	1.623510000
6	-4.413170000	-2.057606000	-1.031254000	1	-4.039420000	-3.782111000	2.164009000
6	-5.595820000	-1.800603000	-1.747851000	1	-3.728478000	-5.359049000	1.462868000
6	-6.480317000	-2.838473000	-1.997084000	1	-2.426751000	-4.480413000	2.241665000
6	-6.233846000	-4.113156000	-1.533716000	6	-5.951214000	-0.404759000	-2.257290000
6	-5.093824000	-4.356580000	-0.801260000	1	-5.211281000	0.286199000	-1.890463000
6	-4.173984000	-3.349484000	-0.538137000	6	-5.944970000	-0.342434000	-3.800911000
6	-4.301974000	-0.108777000	2.355447000	1	-6.678661000	-1.025155000	-4.215014000
1	-6.156675000	-1.022390000	3.021770000	1	-6.189438000	0.661567000	-4.132334000
1	-4.068257000	-1.141240000	4.255843000	1	-4.972401000	-0.599429000	-4.198981000
1	-2.586534000	-0.353716000	3.699238000	6	-7.331523000	0.042410000	-1.726921000
1	-3.109541000	-1.865047000	2.955801000	1	-8.121706000	-0.596461000	-2.102712000
1	-1.540898000	0.758164000	-3.004751000	1	-7.356809000	0.015905000	-0.645166000
1	-5.382567000	5.541184000	1.037412000	1	-7.539161000	1.056163000	-2.050829000
1	-3.673680000	6.342510000	2.586007000	6	-5.389283000	3.352368000	-0.523936000
1	-1.592026000	5.089032000	2.857470000	1	-5.183137000	2.328594000	-0.787888000
1	-1.772837000	3.965924000	-1.346236000	6	-6.802203000	3.426242000	0.094881000
1	-1.267045000	2.978164000	-2.835114000	1	-7.087890000	4.449797000	0.305597000
1	-1.878828000	-2.474486000	-2.571991000	1	-7.528839000	3.019235000	-0.598877000
1	-3.352821000	-2.050189000	-3.415533000	1	-6.855690000	2.859769000	1.016311000
1	-1.841899000	-1.210439000	-3.816174000	6	-5.333436000	4.202867000	-1.813485000
1	-7.374723000	-2.646346000	-2.554913000	1	-4.360770000	4.117629000	-2.278166000
1	-6.927658000	-4.905783000	-1.734614000	1	-6.087031000	3.866380000	-2.519824000
1	-4.909772000	-5.345287000	-0.431797000	1	-5.522970000	5.246191000	-1.583940000
6	-3.464482000	-0.913805000	3.362300000	6	-0.784924000	2.839572000	1.642233000
1	-5.426788000	-1.871983000	1.649510000	1	-0.758844000	2.015451000	0.951072000
1	-6.262352000	-0.342459000	1.393961000	6	0.392097000	3.776900000	1.303338000
6	-5.601600000	-0.883225000	2.079571000	1	0.457084000	4.598727000	2.007331000
6	-4.690855000	1.213036000	3.034423000	1	1.323039000	3.222010000	1.344985000
1	-5.235457000	0.996581000	3.968377000	1	0.277316000	4.180680000	0.305874000
1	-5.345870000	1.823584000	2.409392000	6	-0.623775000	2.280652000	3.071174000

1	-1.411132000	1.573430000	3.292011000	1	4.657176000	-0.469088000	5.726989000
1	0.329224000	1.768931000	3.169315000	1	4.912283000	-2.895381000	5.760192000
1	-0.660992000	3.076921000	3.805999000	1	4.203585000	-4.234711000	3.846461000
1	-0.871834000	-0.732164000	0.610109000	6	6.905003000	-0.834170000	-0.901295000
1	-1.572967000	-0.294276000	1.092326000	1	6.454357000	-1.931791000	1.613142000
13	4.088829000	-0.416604000	0.345150000	1	6.433630000	-0.420716000	2.512447000
13	-3.262854000	0.153078000	0.659349000	6	6.773139000	-0.887810000	1.587180000
Al-inter-IM <sub>1,4</sub>				6	6.833320000	1.294075000	0.373422000
7	3.026072000	-0.517540000	1.423765000	1	7.927021000	1.258170000	0.483862000
6	1.699122000	-0.330624000	1.202949000	1	6.443917000	1.873063000	1.217540000
6	1.205203000	0.226644000	0.015396000	1	6.616305000	1.835710000	-0.549126000
6	1.918273000	0.679129000	-1.092121000	6	4.136901000	3.455359000	-0.979394000
7	3.281223000	0.668783000	-1.150308000	1	4.048879000	2.827239000	-0.102871000
6	3.989477000	1.254525000	-2.296516000	6	3.615053000	-0.900658000	-3.653666000
6	4.470364000	2.569765000	-2.184978000	1	2.977186000	-1.132278000	-2.814077000
6	5.222325000	3.081018000	-3.231235000	6	2.775837000	4.160219000	-1.193112000
6	5.493973000	2.319867000	-4.351570000	1	2.810628000	4.759850000	-2.095141000
6	4.994087000	1.041574000	-4.456072000	1	1.966888000	3.451378000	-1.283086000
6	4.222343000	0.487569000	-3.441396000	1	2.558882000	4.812903000	-0.354467000
6	0.683185000	-0.751441000	2.206372000	6	5.206614000	4.529108000	-0.685464000
6	3.481258000	-1.173457000	2.655959000	1	4.982312000	5.001863000	0.264063000
6	3.855606000	-0.393699000	3.753965000	1	6.201879000	4.108237000	-0.630568000
6	4.368616000	-1.041257000	4.869121000	1	5.199311000	5.304000000	-1.442199000
6	4.507700000	-2.413649000	4.892426000	6	2.747795000	-0.920280000	-4.934869000
6	4.110233000	-3.168835000	3.808224000	1	3.364677000	-0.804492000	-5.817554000
6	3.578819000	-2.567692000	2.676594000	1	2.227923000	-1.868097000	-5.011103000
6	6.291297000	-0.147217000	0.329723000	1	2.012860000	-0.126191000	-4.928440000
1	7.872953000	-0.878952000	1.595070000	6	4.692961000	-2.001902000	-3.751634000
1	6.624306000	-1.889692000	-0.971852000	1	5.264400000	-2.079110000	-2.837550000
1	8.000890000	-0.799624000	-0.815144000	1	4.221455000	-2.960342000	-3.939160000
1	6.634320000	-0.337662000	-1.836373000	1	5.379050000	-1.798238000	-4.565023000
1	0.121502000	0.295566000	-0.058704000	6	3.670633000	1.123615000	3.785246000
1	5.600707000	4.079480000	-3.175888000	1	3.386215000	1.455047000	2.797138000
1	6.084203000	2.731320000	-5.145990000	6	4.964690000	1.864953000	4.186261000
1	5.192150000	0.469170000	-5.338954000	1	5.252592000	1.626081000	5.202336000
1	0.114497000	-1.609415000	1.809595000	1	5.787548000	1.607495000	3.531794000
1	1.109290000	-1.021572000	3.168059000	1	4.804831000	2.936283000	4.130619000
1	-0.066617000	0.038188000	2.320503000	6	2.530402000	1.503323000	4.758560000

1	2.376595000	2.576970000	4.751787000	1	-5.824203000	-5.033981000	-1.048474000
1	1.600993000	1.024382000	4.480937000	1	-4.272147000	-5.959396000	-2.697406000
1	2.781918000	1.201586000	5.768431000	1	-2.177800000	-4.798850000	-3.176138000
6	3.105598000	-3.435686000	1.509655000	1	-2.075337000	-3.740338000	1.043968000
1	2.560219000	-2.815208000	0.816101000	1	-1.824193000	-2.928512000	2.693043000
6	4.306842000	-4.049579000	0.757323000	1	-2.694977000	2.448621000	3.150239000
1	3.959466000	-4.665350000	-0.064757000	1	-4.310865000	1.873421000	3.491241000
1	4.951841000	-3.276667000	0.352577000	1	-2.914151000	0.980029000	4.117836000
1	4.900774000	-4.666688000	1.420974000	1	-7.589068000	3.748042000	1.160548000
6	2.140666000	-4.546288000	1.979422000	1	-6.344208000	5.845970000	1.053242000
1	2.641700000	-5.257723000	2.624356000	1	-3.913963000	5.810498000	0.811390000
1	1.297381000	-4.126370000	2.512943000	6	-2.906710000	0.989790000	-3.538959000
1	1.759755000	-5.083500000	1.118491000	1	-4.415699000	2.860661000	-2.163220000
7	-3.779840000	1.205124000	0.846264000	1	-5.807018000	1.828733000	-1.868311000
6	-3.250945000	0.694093000	2.013204000	6	-4.934157000	1.962461000	-2.510986000
6	-2.653619000	-0.534560000	2.116096000	6	-4.878669000	-0.445163000	-3.068788000
6	-2.594442000	-1.658061000	1.176250000	1	-5.308888000	-0.179537000	-4.050292000
7	-3.093168000	-1.467931000	-0.115200000	1	-5.715260000	-0.683232000	-2.404075000
6	-3.405573000	-2.678335000	-0.844035000	1	-4.299440000	-1.362962000	-3.199486000
6	-4.613485000	-3.348226000	-0.579230000	6	-2.238074000	3.717360000	0.658161000
6	-4.905070000	-4.522274000	-1.254094000	1	-1.863417000	2.716582000	0.797564000
6	-4.032850000	-5.047797000	-2.185031000	6	-1.552810000	4.653692000	1.678974000
6	-2.853470000	-4.389069000	-2.452187000	1	-0.473721000	4.566078000	1.590296000
6	-2.524307000	-3.208461000	-1.797212000	1	-1.815669000	5.689516000	1.499927000
6	-2.092113000	-2.843240000	1.645345000	1	-1.833345000	4.405321000	2.695046000
6	-3.295255000	1.545332000	3.265193000	6	-1.866909000	4.157935000	-0.774539000
6	-4.468335000	2.477207000	0.899207000	1	-2.274271000	3.464555000	-1.495256000
6	-5.868756000	2.501124000	1.003531000	1	-2.256389000	5.147779000	-0.984721000
6	-6.522413000	3.722156000	1.069070000	1	-0.786970000	4.181667000	-0.894592000
6	-5.822612000	4.909774000	1.007488000	6	-6.676366000	1.205520000	1.046330000
6	-4.451430000	4.885327000	0.875474000	1	-6.057340000	0.431046000	0.623933000
6	-3.757024000	3.684129000	0.824148000	6	-7.014867000	0.814248000	2.502538000
6	-4.035638000	0.718016000	-2.529724000	1	-7.582805000	1.605263000	2.981240000
1	-5.306618000	2.172338000	-3.529120000	1	-7.609836000	-0.093717000	2.519235000
1	-3.324008000	1.163189000	-4.545746000	1	-6.115934000	0.635143000	3.076124000
1	-2.205468000	0.151791000	-3.613591000	6	-7.981732000	1.290361000	0.225108000
1	-2.322558000	1.877990000	-3.269204000	1	-8.699475000	1.958157000	0.687755000
1	-2.263284000	-0.779274000	3.098819000	1	-7.788737000	1.636607000	-0.782118000

1	-8.436765000	0.307876000	0.167235000	6	-6.398245000	-4.025542000	-1.155896000
6	-5.607957000	-2.823700000	0.451673000	6	-6.742630000	-2.767232000	-1.610149000
1	-5.251200000	-1.863764000	0.786006000	6	-5.825307000	-1.728988000	-1.601070000
6	-7.014298000	-2.637963000	-0.158845000	6	-1.250854000	2.935546000	-1.666217000
1	-7.435523000	-3.586773000	-0.471003000	6	-2.866985000	2.996224000	0.671910000
1	-7.682459000	-2.204244000	0.578678000	6	-1.868413000	3.328243000	1.589402000
1	-6.978972000	-1.981127000	-1.018365000	6	-2.031461000	4.489858000	2.337457000
6	-5.684000000	-3.767596000	1.672158000	6	-3.136705000	5.292567000	2.180134000
1	-4.705353000	-3.879556000	2.117505000	6	-4.115549000	4.950685000	1.266600000
1	-6.361127000	-3.360739000	2.417733000	6	-4.004797000	3.801502000	0.501813000
1	-6.052108000	-4.744966000	1.377510000	6	-4.913662000	0.074374000	2.016000000
6	-1.193249000	-2.537643000	-2.123135000	1	-5.309397000	0.984708000	3.933998000
1	-1.222845000	-1.536497000	-1.725610000	1	-6.543915000	1.168734000	1.007362000
6	-0.024543000	-3.287916000	-1.444952000	1	-7.035757000	0.221060000	2.411772000
1	0.029418000	-4.308132000	-1.810585000	1	-6.666229000	-0.597903000	0.891291000
1	0.920613000	-2.794716000	-1.664836000	1	-1.423284000	0.750832000	-3.013926000
1	-0.167537000	-3.307398000	-0.373772000	1	-4.855871000	-5.252649000	-0.377223000
6	-0.941220000	-2.457607000	-3.645387000	1	-7.124401000	-4.813922000	-1.164114000
1	-1.795931000	-2.041675000	-4.161768000	1	-7.733846000	-2.597034000	-1.973759000
1	-0.080287000	-1.827312000	-3.845342000	1	-1.116108000	2.965388000	-2.747997000
1	-0.733643000	-3.436689000	-4.061556000	1	-1.667827000	3.875980000	-1.313991000
1	-1.602474000	0.829449000	-0.817509000	1	-0.262452000	2.816396000	-1.208096000
6	1.105331000	1.144949000	-2.265668000	1	-1.277587000	4.763048000	3.046237000
1	0.781962000	0.263321000	-2.828086000	1	-3.240373000	6.184552000	2.765417000
1	0.189299000	1.625963000	-1.915814000	1	-4.969355000	5.584821000	1.154237000
1	1.659797000	1.795208000	-2.937241000	6	-6.366541000	0.229625000	1.538592000
13	-3.153986000	0.334325000	-0.745426000	1	-4.785462000	2.159639000	2.718249000
13	4.315442000	-0.057845000	0.193671000	1	-3.610221000	1.082917000	3.476390000
				6	-4.629058000	1.142663000	3.084127000
<b>Al-inter-TS<sub>1,4-II</sub></b>				6	-4.791398000	-1.307135000	2.680369000
7	-2.771689000	1.754497000	-0.117904000	1	-5.538154000	-1.383699000	3.484081000
6	-2.086316000	1.750307000	-1.275233000	1	-3.811385000	-1.464415000	3.145925000
6	-2.066841000	0.650202000	-2.148278000	1	-4.980702000	-2.125684000	1.981454000
6	-2.778456000	-0.550054000	-2.062008000	6	-2.736623000	-3.623242000	-0.262452000
7	-3.588257000	-0.855346000	-1.023960000	1	-2.125020000	-2.740865000	-0.325880000
6	-4.531366000	-1.987613000	-1.115302000	6	-6.222241000	-0.365809000	-2.174208000
6	-4.159158000	-3.264929000	-0.686467000	1	-5.633960000	0.396414000	-1.685798000
6	-5.120872000	-4.269433000	-0.707535000	6	-2.137931000	-4.686225000	-1.214551000

1	-2.658996000	-5.630663000	-1.110322000	1	-3.338117000	-2.276596000	-3.251027000
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6	-2.666241000	-4.151415000	1.187196000	7	3.852883000	0.950659000	-0.701038000
1	-1.637001000	-4.379402000	1.440180000	6	2.610742000	1.132112000	-1.254239000
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1	-3.250268000	-5.057573000	1.297983000	6	1.332377000	-0.738249000	-0.031088000
6	-5.904294000	-0.314616000	-3.687836000	7	2.446069000	-1.239579000	0.607495000
1	-6.443224000	-1.101303000	-4.202786000	6	2.352269000	-2.571290000	1.172010000
1	-6.209331000	0.640436000	-4.102202000	6	2.716623000	-3.677956000	0.379668000
1	-4.848889000	-0.442302000	-3.877485000	6	2.683184000	-4.947621000	0.932670000
6	-7.713002000	-0.018052000	-1.971725000	6	2.303230000	-5.144797000	2.246238000
1	-8.022673000	-0.150554000	-0.944188000	6	1.924079000	-4.065979000	3.011923000
1	-7.876824000	1.017860000	-2.248149000	6	1.923398000	-2.776382000	2.490367000
1	-8.346668000	-0.625857000	-2.605910000	6	0.071904000	-1.295352000	0.052077000
6	-0.605529000	2.497080000	1.808203000	6	2.429199000	2.208212000	-2.306879000
1	-0.588541000	1.669029000	1.116753000	6	4.966645000	1.697790000	-1.255484000
6	-0.562962000	1.925346000	3.242598000	6	5.765939000	1.110728000	-2.250169000
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1	-1.436382000	1.323832000	3.456341000	6	7.116175000	3.103786000	-2.333015000
1	0.317322000	1.306268000	3.355690000	6	6.344041000	3.669092000	-1.342407000
6	0.673504000	3.331480000	1.568579000	6	5.263102000	2.989339000	-0.796673000
1	1.533355000	2.676599000	1.612360000	6	5.695306000	-0.881999000	1.465503000
1	0.659401000	3.816139000	0.600408000	1	7.795097000	-0.340877000	1.602017000
1	0.783490000	4.096346000	2.328442000	1	6.663471000	-1.585119000	3.283668000
6	-5.095263000	3.463793000	-0.516522000	1	4.942918000	-1.983514000	3.204132000
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6	-4.767971000	4.087639000	-1.892858000	1	-0.105763000	-2.211164000	0.596107000
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1	-3.852783000	3.685135000	-2.304055000	1	2.473710000	3.201537000	-1.854624000
1	-5.570039000	3.887942000	-2.595809000	1	3.211194000	2.175326000	-3.064533000
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1	6.581932000	4.652061000	-0.987731000	1	1.516382000	-4.744265000	-1.887720000
6	5.676538000	-1.206786000	2.966087000	6	1.390225000	-1.638117000	3.359907000
1	6.712322000	1.041661000	1.777802000	1	1.384227000	-0.742960000	2.759938000
1	6.995137000	0.349240000	0.180129000	6	-0.056724000	-1.941940000	3.814401000
6	6.852374000	0.101360000	1.234818000	1	-0.083834000	-2.803956000	4.470672000
6	6.027582000	-2.182801000	0.730341000	1	-0.460724000	-1.095516000	4.361134000
1	7.024881000	-2.548291000	1.033092000	1	-0.691671000	-2.140884000	2.961843000
1	6.047069000	-2.057913000	-0.355680000	6	2.267425000	-1.382926000	4.603397000
1	5.307397000	-2.970340000	0.965592000	1	3.252113000	-1.050769000	4.315684000
6	4.438018000	3.675519000	0.290513000	1	1.818275000	-0.611171000	5.222001000
1	3.581481000	3.056635000	0.497257000	1	2.362833000	-2.282253000	5.201944000
6	3.948697000	5.073981000	-0.152044000	1	3.400090000	0.989864000	2.090238000
1	3.281969000	5.484450000	0.600034000	13	3.921505000	-0.044415000	0.960989000
1	4.779674000	5.759890000	-0.267364000	13	-3.646382000	0.224839000	0.501013000
1	3.416883000	5.029570000	-1.094785000				
6	5.246438000	3.805535000	1.599438000				
1	5.517362000	2.829560000	1.972044000	1	-0.073994000	-0.141665000	-0.551768000
1	6.149984000	4.382965000	1.437741000	1	0.937427000	0.145930000	-0.292069000
1	4.650868000	4.303193000	2.358695000	7	3.194597000	-1.550084000	-0.236486000
6	5.492847000	-0.305453000	-2.751827000	6	3.100322000	-1.875112000	1.129121000
1	4.888854000	-0.795725000	-2.006787000	6	3.088611000	-0.964800000	2.139223000
6	4.702406000	-0.285201000	-4.079744000	6	3.315462000	0.492726000	2.143166000
1	5.255172000	0.260004000	-4.837627000	7	3.289030000	1.159702000	0.912042000
1	4.541633000	-1.298555000	-4.435502000	6	3.476121000	2.599578000	0.934132000
1	3.735398000	0.182136000	-3.951895000	6	4.732624000	3.156836000	0.651695000
6	6.790384000	-1.121025000	-2.946088000	6	4.871807000	4.537107000	0.626039000
1	7.356370000	-0.764974000	-3.799490000	6	3.798489000	5.368612000	0.865112000
1	7.420651000	-1.068504000	-2.068120000	6	2.569559000	4.820621000	1.160151000
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1	4.566952000	-4.165940000	-2.535786000	6	5.986658000	-3.608505000	-1.640283000
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1	2.139355000	-3.562735000	-3.035578000	6	2.808816000	1.002117000	-2.441096000

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1	0.640743000	1.198088000	-2.702242000	6	7.275037000	-1.051766000	-0.774651000
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1	2.961909000	-1.375379000	3.135514000	1	6.904587000	-0.518107000	-1.641021000
1	5.828915000	4.967753000	0.414233000	1	7.785943000	-0.347802000	-0.128020000
1	3.921673000	6.433467000	0.829251000	6	5.957643000	2.282014000	0.413208000
1	1.738720000	5.468809000	1.356170000	1	5.605385000	1.294239000	0.170689000
1	3.709219000	2.157892000	3.428436000	6	6.838319000	2.787063000	-0.750291000
1	3.551593000	0.496736000	4.243972000	1	7.309426000	3.732583000	-0.509311000
1	2.028918000	-3.738503000	1.042855000	1	7.627132000	2.070467000	-0.948964000
1	3.769712000	-3.938565000	1.112523000	1	6.256982000	2.914093000	-1.655312000
1	2.883540000	-3.458665000	2.572602000	6	6.796244000	2.193550000	1.709305000
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1	3.880255000	-0.710767000	-3.321550000	1	1.116953000	1.829243000	1.717370000
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6	2.980570000	2.526747000	-2.475154000	1	-0.409188000	3.057454000	3.218583000
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1	-1.027018000	-0.702514000	-3.488388000	1	-6.028265000	-4.135437000	1.781873000
1	-0.681359000	-2.612085000	1.983168000	1	-6.123971000	-2.490613000	1.180126000
1	-0.398647000	-3.153665000	0.312047000	1	-6.014485000	-3.836647000	0.054264000
1	0.491713000	-1.766354000	0.933486000	6	-3.512811000	-4.758111000	0.757158000
1	-4.539196000	-4.357266000	3.470910000	1	-3.837389000	-5.128771000	-0.209076000
1	-3.774290000	-3.536307000	5.639005000	1	-2.431108000	-4.712125000	0.760479000
1	-2.433673000	-1.503816000	5.772611000	1	-3.823815000	-5.468114000	1.513747000
6	-4.285619000	2.576826000	2.158601000	6	-1.557568000	0.107489000	3.824723000
1	-4.949505000	0.166221000	3.379743000	1	-1.587331000	0.658630000	2.895647000
1	-6.273579000	-0.276076000	2.298261000	6	-2.064847000	1.027312000	4.959560000
6	-5.684623000	0.565079000	2.677989000	1	-1.529337000	1.967959000	4.929549000
6	-6.172905000	1.946609000	0.659256000	1	-3.124709000	1.228786000	4.871167000
1	-6.833213000	2.571115000	1.279537000	1	-1.883079000	0.581277000	5.929354000
1	-6.789691000	1.158298000	0.220738000	6	-0.090932000	-0.289789000	4.106120000
1	-5.800221000	2.567344000	-0.158339000	1	-0.031320000	-0.844743000	5.035968000
6	-5.456383000	-1.020783000	-2.462723000	1	0.315128000	-0.901946000	3.314779000
1	-4.727425000	-1.351446000	-1.738839000	1	0.535475000	0.589192000	4.187163000
6	-2.801387000	3.347829000	-1.971292000	13	2.689621000	0.235840000	-0.595570000
1	-2.291047000	2.751483000	-1.234159000	13	-3.723958000	0.361863000	0.499931000
6	-5.230570000	-1.840450000	-3.753074000				
1	-5.944022000	-1.555251000	-4.517103000				

AI-inter-IM<sub>1,4'</sub>

1	-0.957450000	0.579166000	-0.676686000	6	1.587892000	0.607963000	-3.233775000
1	1.190097000	0.178578000	-0.216664000	1	3.844549000	-1.007490000	-3.348706000
7	3.314992000	-1.570791000	-0.203238000	1	5.019754000	0.225834000	-2.903495000
6	3.202026000	-1.798532000	1.172105000	6	4.023254000	0.071122000	-3.333286000
6	3.212681000	-0.817307000	2.118791000	6	3.265666000	2.338108000	-2.693930000
6	3.512011000	0.626316000	2.030013000	1	3.259364000	2.625690000	-3.760084000
7	3.563041000	1.205487000	0.762863000	1	4.249115000	2.591454000	-2.292687000
6	3.793429000	2.633187000	0.697022000	1	2.539948000	2.975990000	-2.180329000
6	5.073493000	3.128276000	0.404069000	6	1.732789000	-3.335951000	-2.028141000
6	5.268809000	4.497805000	0.302176000	1	1.421213000	-2.441374000	-1.512016000
6	4.225687000	5.383080000	0.474221000	6	0.969956000	-4.552359000	-1.453276000
6	2.969886000	4.899278000	0.769358000	1	-0.101862000	-4.435920000	-1.597768000
6	2.737784000	3.536881000	0.896279000	1	1.273706000	-5.459520000	-1.961794000
6	3.716307000	1.293320000	3.201803000	1	1.169587000	-4.680730000	-0.397992000
6	2.990634000	-3.223877000	1.638335000	6	1.387792000	-3.198672000	-3.529284000
6	3.961426000	-2.618271000	-0.971010000	1	1.969212000	-2.415845000	-3.994150000
6	5.352928000	-2.798753000	-0.856524000	1	1.584965000	-4.125793000	-4.054164000
6	5.967508000	-3.845041000	-1.526034000	1	0.333382000	-2.968084000	-3.653884000
6	5.246653000	-4.701048000	-2.331299000	6	6.216082000	-1.859969000	-0.018308000
6	3.892596000	-4.503118000	-2.478785000	1	5.599048000	-1.035604000	0.295602000
6	3.235385000	-3.476901000	-1.812112000	6	6.761330000	-2.567281000	1.241631000
6	2.948547000	0.843062000	-2.555300000	1	7.382086000	-3.413663000	0.966967000
1	4.064097000	0.417540000	-4.380657000	1	7.362369000	-1.877092000	1.824777000
1	1.634829000	0.868345000	-4.305247000	1	5.952882000	-2.919318000	1.868607000
1	0.799731000	1.225493000	-2.782762000	6	7.389092000	-1.295298000	-0.849477000
1	1.260218000	-0.435007000	-3.166358000	1	8.076538000	-2.078809000	-1.146087000
1	3.065449000	-1.154597000	3.139671000	1	7.024829000	-0.802780000	-1.742548000
1	6.245978000	4.877595000	0.083333000	1	7.942279000	-0.573443000	-0.259417000
1	4.391712000	6.438960000	0.383022000	6	6.258165000	2.186410000	0.228608000
1	2.160868000	5.589367000	0.907922000	1	5.856110000	1.207154000	0.033642000
1	3.962135000	2.345320000	3.228756000	6	7.171769000	2.587095000	-0.949650000
1	3.694774000	0.747865000	4.137424000	1	7.683179000	3.522835000	-0.755772000
1	2.051657000	-3.617608000	1.237154000	1	7.928809000	1.825706000	-1.100882000
1	3.783370000	-3.887339000	1.289006000	1	6.603477000	2.689600000	-1.866291000
1	2.949841000	-3.270126000	2.728712000	6	7.077777000	2.124235000	1.537849000
1	7.024242000	-3.988269000	-1.421796000	1	6.454388000	1.788331000	2.355420000
1	5.736484000	-5.505444000	-2.844337000	1	7.912475000	1.437130000	1.431169000
1	3.334334000	-5.159881000	-3.115965000	1	7.473110000	3.105992000	1.778386000

6	1.332543000	3.067714000	1.265374000	1	-3.327636000	-0.686401000	-3.704631000
1	1.366081000	2.001327000	1.406739000	1	-1.610345000	-1.304800000	-3.355221000
6	0.856508000	3.721535000	2.580072000	1	-0.585016000	-2.390627000	1.917764000
1	0.781499000	4.798015000	2.481309000	1	-0.384260000	-2.782069000	0.177918000
1	-0.126402000	3.345002000	2.850017000	1	0.490102000	-1.417004000	0.830775000
1	1.546824000	3.492356000	3.381208000	1	-4.393973000	-4.060812000	3.810046000
6	0.331966000	3.368815000	0.128800000	1	-3.484561000	-3.143254000	5.881013000
1	0.632937000	2.861888000	-0.777972000	1	-2.127940000	-1.117779000	5.834062000
1	-0.664428000	3.024782000	0.404025000	6	-4.131705000	2.811230000	2.086160000
1	0.275039000	4.433121000	-0.070031000	1	-4.807193000	0.545662000	3.572111000
7	-2.549981000	-0.722451000	1.250949000	1	-6.267576000	0.118173000	2.672648000
6	-1.529300000	-1.055678000	0.501605000	6	-5.590356000	0.941916000	2.922305000
6	-1.362992000	-0.430496000	-0.855731000	6	-6.205855000	2.195335000	0.847135000
6	-2.577845000	-0.349920000	-1.752862000	1	-6.750606000	2.923532000	1.465664000
7	-3.682017000	0.345992000	-1.204659000	1	-6.918450000	1.421889000	0.552393000
6	-4.636172000	0.934187000	-2.142759000	1	-5.880478000	2.709648000	-0.060401000
6	-5.793942000	0.239117000	-2.509106000	6	-6.104883000	-1.170246000	-2.010758000
6	-6.689104000	0.847388000	-3.379902000	1	-5.303874000	-1.481379000	-1.357644000
6	-6.446905000	2.105620000	-3.884499000	6	-3.099210000	2.981606000	-2.329927000
6	-5.295815000	2.778177000	-3.528233000	1	-2.584446000	2.456218000	-1.541700000
6	-4.375289000	2.212361000	-2.660126000	6	-6.169556000	-2.175272000	-3.182758000
6	-2.513460000	-0.820489000	-3.005010000	1	-6.977165000	-1.925779000	-3.860116000
6	-0.457164000	-1.982326000	0.919962000	1	-5.242221000	-2.179184000	-3.739791000
6	-2.781572000	-1.391148000	2.553172000	1	-6.345059000	-3.177090000	-2.804117000
6	-3.563579000	-2.550491000	2.559929000	6	-7.431961000	-1.201393000	-1.220013000
6	-3.805548000	-3.167193000	3.778434000	1	-7.637644000	-2.205178000	-0.866484000
6	-3.292279000	-2.651126000	4.948669000	1	-7.393049000	-0.538294000	-0.364585000
6	-2.527474000	-1.504775000	4.920478000	1	-8.259206000	-0.890982000	-1.845789000
6	-2.257005000	-0.846155000	3.728369000	6	-2.164269000	3.028156000	-3.559852000
6	-5.034576000	1.630721000	1.667157000	1	-2.638031000	3.563759000	-4.374637000
1	-6.169339000	1.672294000	3.506264000	1	-1.240393000	3.537224000	-3.307531000
1	-3.271366000	2.500870000	2.683827000	1	-1.922838000	2.028774000	-3.896037000
1	-4.716909000	3.510166000	2.701482000	6	-3.395513000	4.414232000	-1.834673000
1	-3.761089000	3.375922000	1.223997000	1	-4.083748000	4.407749000	-0.997490000
1	-0.556216000	-0.951210000	-1.370243000	1	-2.473310000	4.888669000	-1.517967000
1	-7.579928000	0.327864000	-3.669647000	1	-3.826782000	5.019909000	-2.622162000
1	-7.147278000	2.558934000	-4.557643000	6	-4.139445000	-3.181850000	1.292832000
1	-5.109052000	3.751324000	-3.934058000	1	-3.921001000	-2.547234000	0.446555000

6	-5.673616000	-3.325319000	1.390663000	6	5.129621000	-0.000235000	-1.358233000
1	-5.950878000	-4.000158000	2.190072000	6	4.514149000	-1.194315000	-1.046174000
1	-6.144461000	-2.367234000	1.579095000	6	3.276665000	-1.216457000	-0.419584000
1	-6.066755000	-3.724949000	0.463216000	1	0.031452000	0.000074000	3.616305000
6	-3.488530000	-4.557122000	1.022297000	1	-4.995906000	2.117681000	-1.310187000
1	-3.871825000	-4.974171000	0.097619000	1	-6.077233000	0.000195000	-1.872314000
1	-2.412301000	-4.471930000	0.939393000	1	-4.995719000	-2.117416000	-1.311031000
1	-3.712672000	-5.248258000	1.825545000	1	-3.408986000	-0.000815000	2.276310000
6	-1.370297000	0.397019000	3.759159000	1	-2.304684000	-0.000776000	3.769585000
1	-1.434608000	0.895368000	2.801787000	1	3.105739000	-0.877116000	2.478247000
6	-1.812158000	1.393042000	4.856202000	1	3.105365000	0.878329000	2.478135000
1	-1.256259000	2.316036000	4.746864000	1	2.265021000	0.000512000	3.770086000
1	-2.869912000	1.615890000	4.799409000	1	4.997300000	2.116294000	-1.297949000
1	-1.599413000	1.000052000	5.842385000	1	6.084481000	-0.000340000	-1.845957000
6	0.102851000	-0.005773000	3.998504000	1	4.997263000	-2.116740000	-1.297108000
1	0.200100000	-0.488714000	4.964562000	6	-2.634480000	2.556821000	-0.086677000
1	0.464219000	-0.682117000	3.239178000	1	-1.710187000	2.361891000	0.433140000
1	0.746109000	0.864246000	3.980814000	6	-2.634273000	-2.556843000	-0.087677000
13	2.763377000	0.214646000	-0.644852000	1	-1.710005000	-2.362047000	0.432240000
13	-3.898701000	0.460825000	0.572150000	6	-3.535201000	3.381993000	0.857086000
				1	-4.477333000	3.628366000	0.381640000
[(BDI)Si]				1	-3.737318000	2.827160000	1.764543000
7	1.330056000	0.000128000	0.500761000	1	-3.039852000	4.309831000	1.124658000
6	1.220094000	0.000193000	1.907840000	6	-2.312192000	3.353820000	-1.369986000
6	0.024353000	0.000015000	2.532094000	1	-1.812359000	4.283734000	-1.118089000
6	-1.303778000	-0.000260000	1.923284000	1	-1.666060000	2.782110000	-2.026251000
7	-1.339081000	-0.000049000	0.503013000	1	-3.219102000	3.593977000	-1.912498000
6	-2.661030000	-0.000003000	-0.124713000	6	-3.534948000	-3.382455000	0.855746000
6	-3.277566000	1.216529000	-0.429714000	1	-4.477055000	-3.628704000	0.380187000
6	-4.511641000	1.194493000	-1.063081000	1	-3.039536000	-4.310365000	1.122952000
6	-5.124293000	0.000139000	-1.380634000	1	-3.737119000	-2.828005000	1.763424000
6	-4.511536000	-1.194284000	-1.063560000	6	-2.311900000	-3.353320000	-1.371288000
6	-3.277455000	-1.216465000	-0.430198000	1	-1.665811000	-2.781302000	-2.027326000
6	-2.411956000	-0.000647000	2.691693000	1	-1.811989000	-4.283287000	-1.119741000
6	2.496127000	0.000491000	2.703757000	1	-3.218782000	-3.593349000	-1.913900000
6	2.660006000	0.000035000	-0.109843000	6	2.614531000	2.558022000	-0.116719000
6	3.276686000	1.216394000	-0.420060000	1	1.739183000	2.374519000	0.486746000
6	4.514169000	1.193974000	-1.046655000	6	2.164493000	3.238753000	-1.429445000

1	3.020558000	3.450603000	-2.059539000	6	-2.659266000	-2.829723000	-2.362038000
1	1.487245000	2.599261000	-1.982865000	6	-1.873664000	-1.569279000	2.407464000
1	1.657920000	4.174093000	-1.214612000	6	2.411200000	0.759295000	2.567184000
6	3.547408000	3.497177000	0.678282000	6	2.659962000	0.153465000	-0.190398000
1	3.016314000	4.406026000	0.940486000	6	2.810550000	1.378587000	-0.846781000
1	3.888001000	3.025786000	1.592505000	6	4.003717000	1.638269000	-1.505776000
1	4.416011000	3.775408000	0.093986000	6	5.019979000	0.706390000	-1.525909000
6	2.614415000	-2.557925000	-0.115742000	6	4.853838000	-0.507548000	-0.891834000
1	1.739124000	-2.374135000	0.487721000	6	3.678196000	-0.805429000	-0.218951000
6	2.164217000	-3.239026000	-1.428223000	6	3.508927000	-2.176085000	0.431124000
1	1.657572000	-4.174253000	-1.213068000	6	4.675577000	-2.516856000	1.383522000
1	1.486990000	-2.599643000	-1.981796000	6	3.374468000	-3.264175000	-0.658570000
1	3.020219000	-3.451142000	-2.058313000	6	1.690031000	2.413266000	-0.890322000
6	3.547234000	-3.496923000	0.679513000	6	1.161342000	2.563132000	-2.334768000
1	4.415738000	-3.775513000	0.095242000	6	2.148017000	3.781239000	-0.340292000
1	3.887983000	-3.025240000	1.593528000	1	0.037564000	0.024797000	3.546001000
1	3.016027000	-4.405591000	0.942108000	1	-1.373998000	2.007986000	0.835780000
14	-0.014202000	0.000087000	-0.648155000	1	-2.390335000	3.401841000	2.621322000
				1	-3.997153000	2.957618000	2.056910000
<b>Si-<i>intra-TS</i><sub>1,4</sub></b>				1	-2.941210000	1.735757000	2.748442000
1	-0.830490000	-2.250461000	1.556394000	1	-1.734973000	4.358170000	0.326479000
1	-0.128501000	-2.337496000	0.740544000	1	-3.378982000	4.058222000	-0.197649000
7	1.409818000	-0.151583000	0.494238000	1	-2.034035000	3.417414000	-1.130924000
6	1.248039000	0.172447000	1.817496000	1	-4.862656000	2.446685000	-0.328083000
6	0.066627000	-0.061431000	2.466675000	1	-6.170154000	0.686298000	-1.411635000
6	-1.136768000	-0.535885000	1.817425000	1	-5.236241000	-1.553832000	-1.643101000
7	-1.298694000	-0.282199000	0.479348000	1	-1.961923000	-2.654776000	-0.348331000
6	-2.652038000	-0.090941000	-0.054508000	1	-4.093486000	-3.364592000	0.768586000
6	-3.178033000	1.206739000	0.060256000	1	-3.456299000	-4.562588000	-0.348672000
6	-2.393876000	2.335031000	0.724938000	1	-4.823062000	-3.568871000	-0.814843000
6	-2.967631000	2.625107000	2.130044000	1	-2.268683000	-3.834687000	-2.484595000
6	-2.389911000	3.621674000	-0.128187000	1	-3.586549000	-2.754310000	-2.918235000
6	-4.449186000	1.463580000	-0.423783000	1	-1.945335000	-2.132651000	-2.779953000
6	-5.189486000	0.472538000	-1.034531000	1	-2.834856000	-1.852142000	1.996714000
6	-4.660456000	-0.790693000	-1.160821000	1	-1.678920000	-1.818956000	3.445467000
6	-3.395737000	-1.102319000	-0.672921000	1	2.140932000	0.927372000	3.610433000
6	-2.898853000	-2.534259000	-0.864382000	1	3.282091000	0.103531000	2.520986000
6	-3.884480000	-3.568675000	-0.274516000	1	2.706031000	1.711912000	2.121352000

1	4.134938000	2.572189000	-2.014053000	6	-2.453814000	-0.311691000	2.667139000
1	5.934850000	0.921130000	-2.042330000	6	2.453902000	-0.312687000	2.667056000
1	5.642165000	-1.231948000	-0.926618000	6	2.711861000	0.027074000	-0.105346000
1	2.596339000	-2.168792000	1.006248000	6	3.097401000	1.349377000	-0.336323000
1	4.479734000	-3.461084000	1.880482000	6	4.364186000	1.593155000	-0.848063000
1	5.609386000	-2.612526000	0.842769000	6	5.223529000	0.556998000	-1.142968000
1	4.798883000	-1.752195000	2.141773000	6	4.821889000	-0.745930000	-0.936650000
1	3.217490000	-4.235666000	-0.201358000	6	3.568342000	-1.035384000	-0.418329000
1	2.535614000	-3.051516000	-1.309827000	6	3.154388000	-2.496002000	-0.247957000
1	4.273418000	-3.310421000	-1.262658000	6	4.200395000	-3.312998000	0.542148000
1	0.878479000	2.057608000	-0.275542000	6	2.917317000	-3.137388000	-1.634193000
1	0.335516000	3.266237000	-2.360483000	6	2.166685000	2.527707000	-0.070943000
1	0.814209000	1.609644000	-2.713854000	6	1.907498000	3.309704000	-1.377277000
1	1.941298000	2.929801000	-2.992071000	6	2.740444000	3.468251000	1.011596000
1	1.312522000	4.473282000	-0.329400000	1	-0.000045000	-0.755072000	3.446573000
1	2.526773000	3.688830000	0.671048000	1	-1.222779000	2.138877000	0.276319000
1	2.929129000	4.208770000	-0.957540000	1	-2.044077000	4.277561000	1.208390000
14	0.095436000	-0.974563000	-0.501579000	1	-3.677958000	3.903679000	0.685220000
				1	-2.916424000	2.938331000	1.938294000
				1	-1.219102000	4.126364000	-1.194395000
Si-P <sub>1,4</sub>				1	-2.827602000	3.727264000	-1.768580000
1	-0.000173000	-2.152869000	-0.304473000	1	-1.477694000	2.657879000	-2.129477000
7	1.387021000	-0.257251000	0.450028000	1	-4.676287000	2.602601000	-1.024817000
6	1.248813000	-0.412733000	1.766002000	1	-6.197541000	0.762659000	-1.541379000
6	-0.000030000	-0.621062000	2.373415000	1	-5.487490000	-1.547215000	-1.185120000
6	-1.248833000	-0.412358000	1.766016000	1	-2.222388000	-2.530957000	0.293319000
7	-1.387047000	-0.257076000	0.450030000	1	-4.406764000	-2.862443000	1.507669000
6	-2.711879000	0.027206000	-0.105374000	1	-3.828031000	-4.317517000	0.710143000
6	-3.097293000	1.349474000	-0.336840000	1	-2.133974000	-3.390510000	-0.000919000
6	-2.166414000	2.527796000	-0.072026000	1	-2.584664000	-4.163949000	-1.517986000
6	-2.739972000	3.468905000	1.010124000	1	-3.832988000	-3.135821000	-2.214111000
6	-1.907225000	3.309136000	-1.378761000	1	-2.161157000	-2.592102000	-2.182411000
6	-4.364079000	1.593184000	-0.848580000	1	-2.895324000	0.683999000	2.596278000
6	-5.223549000	0.556998000	-1.143054000	1	-2.171078000	-0.498901000	3.703269000
6	-4.822022000	-0.745887000	-0.936303000	1	2.171162000	-0.499986000	3.703171000
6	-3.568470000	-1.035276000	-0.417933000	1	3.224634000	-1.023578000	2.369673000
6	-3.154642000	-2.495873000	-0.247087000	1	2.895840000	0.682813000	2.596346000
6	-4.200697000	-3.312501000	0.543331000	1	4.676474000	2.602607000	-1.023946000
6	-2.917678000	-3.137738000	-1.633119000	1			

1	6.197520000	0.762696000	-1.541280000	6	2.428501000	-0.253752000	2.674065000
1	5.487282000	-1.547223000	-1.185776000	6	2.686326000	0.090573000	-0.142354000
1	2.222153000	-2.531182000	0.292478000	6	2.994453000	1.420570000	-0.429756000
1	3.827650000	-4.318041000	0.708618000	6	4.240841000	1.710282000	-0.968687000
1	5.133648000	-3.390895000	-0.002158000	6	5.150043000	0.710442000	-1.233329000
1	4.406536000	-2.863300000	1.506638000	6	4.824811000	-0.602801000	-0.963621000
1	2.584200000	-4.163603000	-1.519388000	6	3.597077000	-0.938649000	-0.414312000
1	2.160844000	-2.591496000	-2.183295000	6	3.276899000	-2.411349000	-0.164961000
1	3.832616000	-3.135377000	-2.215202000	6	4.401374000	-3.134452000	0.608606000
1	1.223024000	2.138744000	0.277284000	6	3.011111000	-3.126174000	-1.509339000
1	1.219416000	4.126870000	-1.192462000	6	2.009270000	2.559809000	-0.192852000
1	1.477910000	2.658866000	-2.128325000	6	1.691857000	3.279291000	-1.522379000
1	2.827870000	3.728010000	-1.766917000	6	2.553048000	3.562941000	0.847899000
1	2.044685000	4.276926000	1.210272000	1	0.073538000	-1.315613000	3.272860000
1	2.916890000	2.937255000	1.939522000	1	-1.223751000	2.104700000	0.376370000
1	3.678471000	3.903024000	0.686808000	1	-2.117229000	3.946091000	1.792076000
1	-3.224890000	-1.022290000	2.369944000	1	-3.753094000	3.527551000	1.300415000
14	-0.000038000	-0.702796000	-0.797317000	1	-2.803101000	2.392569000	2.254926000
				1	-1.380469000	4.349067000	-0.611333000
<b>Si-<i>intra-TS</i><sub>1,4'</sub></b>				1	-3.024323000	4.052111000	-1.132516000
7	1.376435000	-0.236872000	0.433132000	1	-1.703482000	3.144500000	-1.854416000
6	1.255146000	-0.439577000	1.752211000	1	-4.669463000	2.623193000	-0.903228000
6	0.048677000	-0.999093000	2.234462000	1	-6.138709000	0.809924000	-1.621083000
6	-1.300712000	-0.564259000	1.785256000	1	-5.413579000	-1.512817000	-1.397521000
7	-1.363629000	-0.289382000	0.412261000	1	-2.168292000	-2.549834000	0.082030000
6	-2.675064000	0.010576000	-0.151536000	1	-3.803434000	-4.298799000	0.594934000
6	-3.085019000	1.341993000	-0.279716000	1	-5.117090000	-3.290697000	0.013120000
6	-2.203769000	2.501981000	0.168291000	1	-4.211287000	-2.813933000	1.446228000
6	-2.757260000	3.131504000	1.466234000	1	-2.668531000	-4.196003000	-1.688097000
6	-2.071886000	3.576821000	-0.931776000	1	-3.938797000	-3.159027000	-2.320240000
6	-4.340460000	1.608494000	-0.807141000	1	-2.261533000	-2.640226000	-2.403614000
6	-5.173453000	0.586719000	-1.210585000	1	-3.327469000	-0.240445000	2.342355000
6	-4.762194000	-0.722663000	-1.082575000	1	-2.158386000	-0.733533000	3.701935000
6	-3.520413000	-1.033100000	-0.547577000	1	2.175816000	-0.592239000	3.679125000
6	-3.125212000	-2.500536000	-0.408873000	1	3.318060000	-0.776756000	2.323952000
6	-4.134043000	-3.272717000	0.468611000	1	2.680666000	0.809057000	2.722032000
6	-2.989688000	-3.164932000	-1.796724000	1	4.495812000	2.726738000	-1.188973000
6	-2.329257000	-0.510453000	2.656390000	1	6.105924000	0.950657000	-1.655083000

1	5.531778000	-1.375272000	-1.186327000	6	2.280983000	-0.166989000	2.708909000
1	2.377263000	-2.475973000	0.424974000	6	2.725882000	0.073432000	-0.141343000
1	4.087458000	-4.145596000	0.843881000	6	3.010956000	1.414840000	-0.387636000
1	5.308042000	-3.198154000	0.020004000	6	4.269985000	1.735412000	-0.875416000
1	4.633522000	-2.625456000	1.536959000	6	5.205018000	0.755679000	-1.132579000
1	2.753703000	-4.165821000	-1.336219000	6	4.891805000	-0.568928000	-0.912491000
1	2.194273000	-2.653975000	-2.039865000	6	3.650755000	-0.937949000	-0.414677000
1	3.894446000	-3.090351000	-2.136526000	6	3.339470000	-2.421243000	-0.222619000
1	1.091093000	2.142867000	0.188447000	6	4.365839000	-3.103415000	0.707786000
1	0.966749000	4.066700000	-1.356143000	6	3.287828000	-3.133210000	-1.592566000
1	1.283916000	2.582623000	-2.244847000	6	1.995691000	2.527417000	-0.152812000
1	2.584272000	3.726493000	-1.943323000	6	1.744341000	3.308659000	-1.460709000
1	1.819510000	4.340178000	1.033799000	6	2.464515000	3.480794000	0.968266000
1	2.771358000	3.070156000	1.788113000	1	0.050598000	-1.322849000	3.224532000
1	3.462109000	4.034001000	0.493035000	1	-1.212671000	2.070161000	0.322757000
1	0.117209000	-2.017076000	1.200714000	1	-2.018945000	4.036642000	1.616583000
1	0.147611000	-2.212404000	0.233107000	1	-3.674744000	3.657944000	1.165999000
14	-0.020554000	-0.724309000	-0.713384000	1	-2.767772000	2.551483000	2.191359000
				1	-1.329364000	4.265344000	-0.813725000
<i>Si-intra-IM<sub>1,4'</sub></i>				1	-2.969677000	3.936649000	-1.330595000
7	1.414922000	-0.323138000	0.399156000	1	-1.645417000	2.963473000	-1.957301000
6	1.260188000	-0.509778000	1.667854000	1	-4.698493000	2.631998000	-0.830573000
6	0.022411000	-1.214001000	2.139794000	1	-6.228387000	0.832112000	-1.449976000
6	-1.293717000	-0.594785000	1.724362000	1	-5.518432000	-1.499014000	-1.248055000
7	-1.378337000	-0.335442000	0.360051000	1	-2.194113000	-2.545960000	0.047648000
6	-2.702269000	0.001317000	-0.148944000	1	-3.805647000	-4.295054000	0.670874000
6	-3.102157000	1.335182000	-0.272013000	1	-5.147337000	-3.285042000	0.160817000
6	-2.179717000	2.489190000	0.097961000	1	-4.160613000	-2.803777000	1.536945000
6	-2.695937000	3.229816000	1.351286000	1	-2.804063000	-4.199525000	-1.680738000
6	-2.022490000	3.474400000	-1.079951000	1	-4.104674000	-3.158048000	-2.241817000
6	-4.379624000	1.613282000	-0.738601000	1	-2.432614000	-2.644981000	-2.416874000
6	-5.246044000	0.599751000	-1.087737000	1	-3.227490000	-0.012344000	2.389473000
6	-4.843506000	-0.714052000	-0.971150000	1	-2.054591000	-0.634222000	3.689144000
6	-3.579533000	-1.033461000	-0.498951000	1	2.574338000	-1.083489000	3.232089000
6	-3.181941000	-2.501426000	-0.378719000	1	3.163656000	0.314306000	2.297030000
6	-4.139365000	-3.268045000	0.558664000	1	1.808538000	0.485362000	3.451227000
6	-3.128315000	-3.167587000	-1.770955000	1	4.516003000	2.760676000	-1.061335000
6	-2.250200000	-0.392876000	2.651742000	1	6.171057000	1.022579000	-1.512811000

1	5.616301000	-1.326040000	-1.132580000	6	-2.478402000	-0.423554000	2.666782000
1	2.362433000	-2.518390000	0.222004000	6	-2.691791000	-0.004541000	-0.126585000
1	4.079748000	-4.136004000	0.876864000	6	-3.495517000	-1.086154000	-0.508893000
1	5.355519000	-3.099723000	0.267551000	6	-4.730153000	-0.817453000	-1.083714000
1	4.420452000	-2.601408000	1.667313000	6	-5.162350000	0.477038000	-1.275186000
1	3.029557000	-4.178289000	-1.458800000	6	-4.355537000	1.532000000	-0.905335000
1	2.541516000	-2.674852000	-2.228947000	6	-3.109025000	1.313640000	-0.337729000
1	4.248604000	-3.079352000	-2.090956000	6	-2.240723000	2.513384000	0.030590000
1	1.060265000	2.082313000	0.147442000	6	-2.890047000	3.344527000	1.159862000
1	1.002366000	4.079613000	-1.294284000	6	-1.986604000	3.406644000	-1.203040000
1	1.381455000	2.642340000	-2.232873000	6	-3.072615000	-2.545098000	-0.333445000
1	2.652301000	3.785962000	-1.809025000	6	-2.886345000	-3.222544000	-1.709483000
1	1.712389000	4.241623000	1.147183000	6	-4.098581000	-3.339818000	0.506659000
1	2.633592000	2.945319000	1.895477000	1	0.007912000	-1.147859000	3.338401000
1	3.387178000	3.976500000	0.689820000	1	2.187337000	-2.529330000	0.218782000
1	0.075413000	-2.218004000	1.684400000	1	3.832398000	-4.107115000	1.169036000
1	0.140458000	-2.140439000	-0.588304000	1	5.157784000	-3.112608000	0.585579000
14	-0.062136000	-0.648866000	-0.896424000	1	4.085762000	-2.498176000	1.836833000
				1	2.928205000	-4.380607000	-1.203287000
<b>Si-intra-TS<sub>4',4</sub></b>				1	4.240169000	-3.407780000	-1.847096000
7	-1.376123000	-0.245645000	0.469076000	1	2.567540000	-2.963949000	-2.179480000
6	-1.258334000	-0.417644000	1.783696000	1	5.471596000	-1.579952000	-1.248783000
6	-0.008791000	-0.578548000	2.413253000	1	6.143302000	0.719590000	-1.726872000
6	1.320458000	-0.406204000	1.744849000	1	4.632098000	2.569401000	-1.218321000
7	1.408163000	-0.266511000	0.435973000	1	1.220109000	2.129000000	0.201027000
6	2.715793000	0.015010000	-0.158825000	1	2.095975000	4.235963000	1.185171000
6	3.568574000	-1.054209000	-0.451088000	1	3.720078000	3.816913000	0.663942000
6	3.198677000	-2.505125000	-0.152501000	1	2.908953000	2.843721000	1.884919000
6	4.130616000	-3.091041000	0.931219000	1	1.217304000	4.157742000	-1.191033000
6	3.239727000	-3.366758000	-1.432486000	1	2.829023000	3.796536000	-1.777810000
6	4.803077000	-0.775119000	-1.019690000	1	1.485639000	2.737656000	-2.193107000
6	5.183750000	0.521957000	-1.290985000	1	3.224888000	0.404077000	2.423204000
6	4.328718000	1.564980000	-1.003431000	1	2.185538000	-0.434381000	3.705127000
6	3.081665000	1.333437000	-0.440788000	1	-2.960850000	0.555555000	2.650747000
6	2.167064000	2.516837000	-0.139216000	1	-3.214513000	-1.147559000	2.320131000
6	2.764884000	3.407832000	0.972627000	1	-2.197700000	-0.653453000	3.695539000
6	1.910644000	3.353553000	-1.411207000	1	-5.357496000	-1.631269000	-1.385326000
6	2.262079000	0.005570000	2.715200000	1	-6.121316000	0.663170000	-1.717144000

1	-4.694008000	2.535484000	-1.065092000	6	-3.964930000	-4.043994000	0.308166000
1	-1.287391000	2.145164000	0.374023000	6	-4.093220000	-5.333372000	0.805384000
1	-2.243599000	4.172017000	1.433146000	6	-3.313647000	-5.775851000	1.851847000
1	-3.841884000	3.751032000	0.838412000	6	-2.398387000	-4.921352000	2.428657000
1	-3.061420000	2.742727000	2.044094000	6	-2.230422000	-3.628319000	1.955773000
1	-1.325792000	4.224352000	-0.936720000	6	-1.246082000	-2.704229000	2.663598000
1	-1.523360000	2.834998000	-1.996425000	6	0.150432000	-3.345663000	2.814452000
1	-2.911575000	3.831741000	-1.574079000	6	-1.801687000	-2.299169000	4.046876000
1	-2.120938000	-2.571043000	0.173530000	6	-4.911900000	-3.582602000	-0.794328000
1	-2.563355000	-4.249723000	-1.574896000	6	-6.364533000	-3.597730000	-0.268279000
1	-2.134094000	-2.702194000	-2.285981000	6	-4.791971000	-4.455582000	-2.062534000
1	-3.817533000	-3.228111000	-2.264384000	1	-1.150994000	-0.352891000	-2.095087000
1	-3.734449000	-4.348579000	0.669806000	1	-5.511279000	-0.403793000	-1.481025000
1	-4.266344000	-2.879489000	1.472882000	1	-6.345459000	-0.359353000	-3.829368000
1	-5.051315000	-3.407633000	-0.004289000	1	-6.878665000	1.301827000	-3.605533000
1	0.808721000	0.516047000	2.888444000	1	-5.161070000	0.913301000	-3.544643000
1	0.002156000	0.701590000	-1.394416000	1	-7.814187000	-1.178029000	-1.919740000
14	-0.000949000	-0.682441000	-0.783589000	1	-8.434979000	0.444209000	-1.706283000
				1	-7.728556000	-0.407685000	-0.338598000
<b>Si-inter-TS<sub>4',4</sub>-I</b>				1	-7.789286000	2.523561000	-1.565434000
7	-2.831820000	-1.844884000	0.347159000	1	-7.369156000	4.602565000	-0.354358000
6	-1.980603000	-1.626741000	-0.650283000	1	-5.290235000	4.882988000	0.902911000
6	-1.746473000	-0.332944000	-1.182971000	1	-2.573796000	2.351697000	0.993635000
7	-3.768373000	0.702661000	-0.257841000	1	-2.313994000	4.448255000	-0.328440000
6	-4.758638000	1.767622000	-0.287389000	1	-1.545920000	4.559594000	1.248926000
6	-5.953069000	1.602972000	-0.998294000	1	-3.085096000	5.355660000	0.967697000
6	-6.255529000	0.322031000	-1.765026000	1	-3.995728000	2.311045000	3.022521000
6	-6.151421000	0.562276000	-3.287548000	1	-2.596342000	3.352023000	3.260647000
6	-7.648339000	-0.237420000	-1.405305000	1	-4.176104000	4.058297000	2.941094000
6	-6.876587000	2.638303000	-1.016109000	1	-0.451946000	-2.417427000	-1.943760000
6	-6.641740000	3.814318000	-0.335509000	1	-0.641901000	-3.315624000	-0.409239000
6	-5.468195000	3.970067000	0.370348000	1	-1.827663000	-3.499852000	-1.681826000
6	-4.513369000	2.963893000	0.398889000	1	-4.821400000	-5.991669000	0.376716000
6	-3.226019000	3.186422000	1.185725000	1	-3.430585000	-6.773516000	2.226972000
6	-2.499622000	4.472567000	0.737906000	1	-1.815884000	-5.259174000	3.261901000
6	-3.519315000	3.229225000	2.701500000	1	-1.151613000	-1.804877000	2.079715000
6	-1.167525000	-2.775373000	-1.200899000	1	0.846033000	-2.620524000	3.227404000
6	-3.005915000	-3.197927000	0.872688000	1	0.123673000	-4.194583000	3.486289000

1	0.528557000	-3.689511000	1.856878000	6	4.693860000	-3.606149000	-3.402069000
1	-1.120956000	-1.612638000	4.540444000	6	5.413279000	-1.332041000	-4.274302000
1	-2.760500000	-1.810440000	3.936539000	6	6.207861000	-0.267833000	1.568715000
1	-1.927462000	-3.172863000	4.676376000	6	7.226310000	0.880918000	1.737491000
1	-4.664581000	-2.565548000	-1.052313000	6	6.207071000	-1.182789000	2.813392000
1	-7.043890000	-3.252761000	-1.038297000	1	3.003412000	1.188378000	2.137315000
1	-6.458208000	-2.946541000	0.591424000	1	2.148687000	1.182118000	4.449442000
1	-6.659149000	-4.600241000	0.019662000	1	1.634967000	2.851721000	4.293113000
1	-5.443134000	-4.069252000	-2.839357000	1	0.845267000	1.603276000	3.344943000
1	-3.777499000	-4.460741000	-2.444247000	1	4.568564000	1.845441000	3.903012000
1	-5.082613000	-5.479696000	-1.859275000	1	4.049801000	3.516810000	3.793782000
1	-0.681649000	0.193502000	-0.283959000	1	4.907872000	2.784562000	2.448968000
1	-2.416911000	0.095517000	1.774940000	1	2.251434000	4.712383000	3.013349000
7	4.220655000	-0.689837000	-0.590783000	1	1.555853000	6.417316000	1.409822000
6	3.236104000	-1.421610000	-0.196942000	1	1.266634000	5.836376000	-0.943396000
6	1.509570000	0.489184000	0.071413000	1	1.636655000	2.413636000	-2.323835000
7	2.400295000	1.436867000	-0.227421000	1	0.072085000	3.652498000	-3.719580000
6	2.158432000	2.814543000	0.235209000	1	0.109491000	5.027406000	-2.635435000
6	2.352129000	3.140378000	1.582647000	1	-0.598319000	3.504627000	-2.104436000
6	2.836298000	2.136388000	2.624960000	1	2.586918000	3.899355000	-4.056503000
6	1.794779000	1.930046000	3.746754000	1	2.648361000	5.228750000	-2.908704000
6	4.179792000	2.602124000	3.228756000	1	3.681538000	3.827811000	-2.679883000
6	2.118759000	4.446221000	1.984609000	1	-0.078894000	1.647545000	0.935473000
6	1.727770000	5.411753000	1.080825000	1	-0.068530000	-0.131556000	1.332133000
6	1.563881000	5.081273000	-0.245773000	1	2.796762000	-3.493511000	-0.294518000
6	1.768487000	3.782940000	-0.693229000	1	4.403154000	-3.142448000	0.396816000
6	1.579942000	3.481546000	-2.178092000	1	2.909841000	-2.845948000	1.334335000
6	0.198754000	3.948811000	-2.683292000	1	8.498251000	-1.518540000	0.922674000
6	2.700906000	4.150625000	-3.007193000	1	9.067653000	-2.776046000	-1.090247000
6	0.227349000	0.651199000	0.636523000	1	7.428580000	-3.032438000	-2.882043000
6	3.370158000	-2.810684000	0.342262000	1	3.958377000	-1.698821000	-2.763483000
6	5.578904000	-1.258887000	-0.710392000	1	3.944882000	-3.690394000	-4.181885000
6	6.5111192000	-1.068778000	0.307157000	1	5.607768000	-4.056289000	-3.769131000
6	7.767062000	-1.638004000	0.150229000	1	4.358927000	-4.174626000	-2.541868000
6	8.090881000	-2.347410000	-0.986379000	1	4.698565000	-1.415201000	-5.085763000
6	7.162469000	-2.495578000	-1.994946000	1	5.536397000	-0.283930000	-4.032323000
6	5.889627000	-1.956289000	-1.881307000	1	6.364892000	-1.720864000	-4.616249000
6	4.910821000	-2.119638000	-3.043630000	1	5.228561000	0.175141000	1.470619000

1	6.987852000	1.459523000	2.621355000	6	5.417014000	-4.579223000	-2.159321000
1	7.200782000	1.537576000	0.876973000	6	4.113849000	-4.360539000	-2.553110000
1	8.231960000	0.495824000	1.851777000	6	3.371732000	-3.317704000	-2.019183000
1	5.953173000	-0.608016000	3.697195000	6	1.957432000	-3.075975000	-2.535737000
1	5.487144000	-1.987004000	2.711402000	6	1.101654000	-4.361895000	-2.525878000
1	7.185630000	-1.622259000	2.966027000	6	2.015970000	-2.487522000	-3.963604000
1	3.287169000	0.609246000	-2.420619000	6	6.006866000	-1.729165000	0.267018000
6	-2.765615000	0.749925000	-1.220463000	6	7.123675000	-0.977376000	-0.492400000
6	-2.665045000	1.683167000	-2.200131000	6	6.586726000	-2.474603000	1.488398000
1	-3.361233000	2.504756000	-2.286838000	1	1.156313000	-0.826011000	2.116852000
1	-1.891285000	1.584971000	-2.951101000	1	4.146084000	0.744120000	2.045239000
6	1.837981000	-0.910889000	-0.391333000	1	4.174493000	1.155545000	4.487613000
1	1.123444000	-1.610089000	0.044468000	1	4.459714000	2.867857000	4.210028000
1	1.677997000	-0.912570000	-1.486900000	1	2.935525000	2.137481000	3.711976000
14	4.011433000	1.175544000	-1.199535000	1	6.293291000	0.525189000	3.193654000
14	-3.774189000	-0.389135000	1.236479000	1	6.620432000	2.238376000	3.015962000
				1	6.575707000	1.208117000	1.595201000
<b>Si-inter-IM<sub>4',4</sub></b>				1	5.587793000	4.122360000	2.454138000
7	3.195937000	-1.377574000	-0.494919000	1	5.267832000	5.964119000	0.876488000
6	2.448852000	-1.564118000	0.638895000	1	3.818740000	5.653581000	-1.065475000
6	1.756820000	-0.551124000	1.252410000	1	1.881446000	2.592510000	-1.779419000
7	2.840878000	1.296447000	0.095859000	1	0.736311000	4.624687000	-0.840995000
6	3.480734000	2.579518000	0.302371000	1	0.594907000	4.518802000	-2.596254000
6	4.330296000	2.761266000	1.411791000	1	1.732476000	5.636189000	-1.869654000
6	4.606197000	1.645166000	2.414869000	1	3.910967000	2.851364000	-3.165731000
6	4.000766000	1.975868000	3.796954000	1	2.512925000	3.548217000	-3.974752000
6	6.122660000	1.390284000	2.560366000	1	3.684058000	4.600062000	-3.190794000
6	4.948336000	3.984708000	1.605266000	1	1.733083000	-2.962651000	2.109256000
6	4.770801000	5.026840000	0.718396000	1	2.060939000	-3.697549000	0.517505000
6	3.953352000	4.847295000	-0.372355000	1	3.391755000	-3.261472000	1.567420000
6	3.291059000	3.644444000	-0.590002000	1	7.019112000	-3.893118000	-0.951832000
6	2.373868000	3.550832000	-1.805000000	1	5.978818000	-5.390533000	-2.579427000
6	1.289808000	4.652493000	-1.771854000	1	3.674582000	-5.001507000	-3.290860000
6	3.177267000	3.643958000	-3.120516000	1	1.494941000	-2.340694000	-1.896826000
6	2.396706000	-2.949548000	1.240947000	1	0.088120000	-4.139129000	-2.847944000
6	3.957490000	-2.477482000	-1.061660000	1	1.500158000	-5.104009000	-3.206130000
6	5.290940000	-2.676780000	-0.686908000	1	1.061410000	-4.800509000	-1.534666000
6	5.998595000	-3.735934000	-1.238090000	1	1.014737000	-2.281511000	-4.332033000

1	2.580760000	-1.564599000	-3.965373000	6	-4.355228000	-3.775688000	-2.159755000
1	2.492942000	-3.186616000	-4.641304000	1	-4.390887000	0.518547000	-2.044884000
1	5.290533000	-1.001997000	0.613050000	1	-4.381467000	0.697778000	-4.511733000
1	7.628216000	-0.282078000	0.169114000	1	-4.729629000	2.415715000	-4.405398000
1	6.701485000	-0.421656000	-1.320272000	1	-3.190629000	1.798679000	-3.831642000
1	7.860558000	-1.672359000	-0.879186000	1	-6.508326000	0.138028000	-3.217492000
1	7.046340000	-1.768072000	2.170717000	1	-6.910929000	1.839827000	-3.124454000
1	5.809344000	-3.008100000	2.023945000	1	-6.815700000	0.881683000	-1.651856000
1	7.343325000	-3.189974000	1.187140000	1	-5.936506000	3.824116000	-2.785709000
1	1.593731000	0.083116000	-1.677565000	1	-5.634519000	5.812551000	-1.402459000
7	-3.082140000	-1.369059000	0.719230000	1	-4.185311000	5.736247000	0.560017000
6	-1.896702000	-1.387822000	0.206046000	1	-2.204707000	2.763239000	1.600021000
6	-1.923790000	1.080378000	-0.563023000	1	-1.046221000	4.752311000	2.373765000
7	-3.119904000	1.320522000	-0.138536000	1	-2.178319000	5.805953000	1.547250000
6	-3.811928000	2.575800000	-0.506092000	1	-1.092755000	4.779979000	0.621370000
6	-4.651637000	2.591075000	-1.619631000	1	-2.996639000	3.764004000	3.704072000
6	-4.873566000	1.368001000	-2.504231000	1	-4.157148000	4.750871000	2.826168000
6	-4.250356000	1.584988000	-3.901434000	1	-4.342637000	3.004199000	2.865424000
6	-6.376623000	1.038965000	-2.628922000	1	-0.130153000	-2.519064000	0.381989000
6	-5.295694000	3.779237000	-1.929422000	1	-1.612385000	-3.531759000	0.255763000
6	-5.125781000	4.903890000	-1.149100000	1	-0.936703000	-2.674488000	-1.159414000
6	-4.305450000	4.859977000	-0.042540000	1	-5.858589000	-4.998317000	0.127354000
6	-3.628726000	3.698385000	0.303561000	1	-5.409940000	-5.832533000	2.377002000
6	-2.744087000	3.695909000	1.549831000	1	-3.905415000	-4.612620000	3.863284000
6	-1.701522000	4.833966000	1.514207000	1	-2.104933000	-1.490577000	2.927452000
6	-3.620071000	3.809695000	2.818004000	1	-0.711561000	-2.686501000	4.541776000
6	-1.117879000	-2.625817000	-0.081561000	1	-1.761243000	-4.089672000	4.479510000
6	-3.728349000	-2.621937000	1.165601000	1	-0.818211000	-3.638878000	3.068378000
6	-4.600367000	-3.291062000	0.308014000	1	-2.687240000	-1.248602000	5.298118000
6	-5.192873000	-4.457632000	0.767933000	1	-4.137440000	-1.149682000	4.308858000
6	-4.940453000	-4.930443000	2.038777000	1	-3.778812000	-2.622292000	5.199152000
6	-4.088881000	-4.241826000	2.875976000	1	-4.442181000	-1.837682000	-1.243743000
6	-3.464361000	-3.074395000	2.460093000	1	-6.634361000	-2.213029000	-2.281494000
6	-2.538382000	-2.340879000	3.429754000	1	-6.823577000	-1.910126000	-0.558491000
6	-1.385122000	-3.251065000	3.906551000	1	-6.960488000	-3.546099000	-1.192643000
6	-3.340981000	-1.806332000	4.636787000	1	-4.549179000	-3.396222000	-3.157206000
6	-4.913755000	-2.798343000	-1.101250000	1	-3.285999000	-3.910717000	-2.047211000
6	-6.433629000	-2.605170000	-1.291237000	1	-4.829130000	-4.745760000	-2.069756000

1	-3.163780000	0.579415000	2.210171000	6	-3.383878000	-5.317046000	2.527917000
6	1.857730000	0.890646000	1.002728000	6	-2.644809000	-4.373188000	3.208490000
6	1.059012000	1.757763000	1.693971000	6	-2.385393000	-3.128779000	2.653062000
1	1.164937000	2.829457000	1.584453000	6	-1.604572000	-2.100565000	3.470100000
1	0.426268000	1.390480000	2.497989000	6	-0.294509000	-2.683464000	4.042538000
6	-1.172718000	-0.111904000	-0.067405000	6	-2.491526000	-1.565350000	4.617771000
1	-0.296734000	-0.292755000	-0.700945000	6	-4.318222000	-3.496202000	-0.661825000
1	-0.718207000	0.226883000	0.887692000	6	-5.856641000	-3.527465000	-0.520008000
6	-1.129379000	1.975303000	-1.444291000	6	-3.862531000	-4.497067000	-1.746765000
1	-0.216000000	2.226050000	-0.888250000	1	-0.442342000	-0.107506000	-1.249462000
1	-0.794530000	1.413161000	-2.322607000	1	-4.750980000	-0.329202000	-1.881693000
1	-1.660672000	2.876572000	-1.734139000	1	-5.139487000	-0.438425000	-4.323202000
14	3.132400000	0.256657000	-1.423793000	1	-5.844679000	1.169607000	-4.301227000
14	-4.142845000	0.222461000	1.106239000	1	-4.139658000	0.958557000	-3.948066000
				1	-6.885129000	-1.260892000	-2.658891000
<b>Si-inter-TS<sub>4',4-II</sub></b>				1	-7.627677000	0.324485000	-2.634246000
7	-2.621976000	-1.535965000	0.781088000	1	-7.116304000	-0.424832000	-1.127334000
6	-1.557382000	-1.358985000	0.045518000	1	-7.074453000	2.474175000	-2.632909000
6	-1.218569000	-0.030715000	-0.483182000	1	-7.052673000	4.620708000	-1.471757000
6	-2.286637000	0.890774000	-0.901893000	1	-5.379565000	5.066800000	0.249392000
7	-3.422694000	0.942313000	-0.274074000	1	-2.644229000	2.732243000	1.182084000
6	-4.433084000	1.962651000	-0.620972000	1	-2.225843000	4.871437000	-0.075218000
6	-5.398944000	1.679493000	-1.587432000	1	-1.906171000	4.994083000	1.646512000
6	-5.468964000	0.345083000	-2.323387000	1	-3.373792000	5.681509000	0.979407000
6	-5.122317000	0.521940000	-3.818832000	1	-4.586833000	2.579593000	2.738104000
6	-6.867149000	-0.292458000	-2.172420000	1	-3.374204000	3.711841000	3.319777000
6	-6.331380000	2.662229000	-1.885629000	1	-4.848323000	4.308463000	2.567269000
6	-6.321089000	3.875349000	-1.230806000	1	-2.632342000	2.595922000	-2.192220000
6	-5.373975000	4.126551000	-0.261814000	1	-1.759383000	1.221451000	-2.928558000
6	-4.410813000	3.181487000	0.062653000	1	0.220389000	-2.152993000	-0.847121000
6	-3.396983000	3.504061000	1.159317000	1	-0.316204000	-3.024448000	0.603467000
6	-2.684090000	4.849607000	0.905164000	1	-1.202124000	-3.232386000	-0.898581000
6	-4.099803000	3.525247000	2.535756000	1	-4.482947000	-5.755364000	0.768596000
6	-1.903561000	1.810052000	-2.016958000	1	-3.570295000	-6.274634000	2.971866000
6	-0.649794000	-2.506200000	-0.297475000	1	-2.268655000	-4.602379000	4.183866000
6	-2.893231000	-2.858694000	1.378214000	1	-1.347804000	-1.268414000	2.833840000
6	-3.670955000	-3.789188000	0.688375000	1	0.276554000	-1.894668000	4.519141000
6	-3.894959000	-5.022960000	1.282533000	1	-0.493481000	-3.445629000	4.785692000

1	0.316129000	-3.120194000	3.262406000	6	4.075811000	-2.819745000	-2.166364000
1	-1.958310000	-0.804209000	5.176764000	6	2.670209000	-2.818685000	-2.758938000
1	-3.404743000	-1.130057000	4.232180000	6	2.043304000	-4.229624000	-2.793431000
1	-2.756246000	-2.368482000	5.295661000	6	2.700050000	-2.211335000	-4.179305000
1	-4.033890000	-2.502537000	-0.974245000	6	6.236196000	-0.885528000	0.344612000
1	-6.323922000	-3.301887000	-1.471208000	6	7.248546000	0.091149000	-0.295020000
1	-6.185586000	-2.799418000	0.210422000	6	6.853095000	-1.577272000	1.579415000
1	-6.190794000	-4.508518000	-0.205434000	1	1.085700000	-1.001879000	1.761231000
1	-4.300951000	-4.231219000	-2.702647000	1	3.753576000	1.111613000	2.062607000
1	-2.785007000	-4.501161000	-1.856456000	1	3.504447000	1.387664000	4.509460000
1	-4.180105000	-5.503070000	-1.501773000	1	3.464964000	3.135225000	4.323209000
1	-0.601270000	0.626810000	0.344715000	1	2.159621000	2.152651000	3.668493000
1	-2.819497000	0.543982000	2.081136000	1	5.802876000	1.252540000	3.380039000
1	-0.930748000	2.245051000	-1.771199000	1	5.800851000	3.003615000	3.292915000
7	3.462463000	-1.010553000	-0.598365000	1	6.065994000	2.058708000	1.836634000
6	2.672669000	-1.396753000	0.435827000	1	4.462673000	4.681158000	2.717855000
6	1.725912000	-0.566474000	1.000703000	1	3.913750000	6.504801000	1.183922000
6	1.583287000	0.860312000	0.817736000	1	2.711526000	6.024665000	-0.886258000
7	2.515333000	1.507443000	0.031640000	1	1.440906000	2.692052000	-1.858256000
6	2.866337000	2.881137000	0.342214000	1	-0.065169000	4.407939000	-2.768957000
6	3.577687000	3.159640000	1.524008000	1	0.798223000	5.672810000	-1.921831000
6	3.993042000	2.064923000	2.502894000	1	-0.105379000	4.482379000	-1.005599000
6	3.226866000	2.194859000	3.837925000	1	2.102610000	3.809350000	-3.971526000
6	5.514585000	2.100594000	2.766724000	1	2.993763000	5.022592000	-3.062035000
6	3.929240000	4.467604000	1.813457000	1	3.523248000	3.341168000	-3.045993000
6	3.621667000	5.499364000	0.951413000	1	0.399072000	2.577267000	1.348545000
6	2.942411000	5.224120000	-0.212650000	1	-0.014511000	1.007293000	2.236292000
6	2.544346000	3.930761000	-0.528729000	1	2.612520000	-3.546241000	0.210043000
6	1.767888000	3.720440000	-1.824935000	1	3.843105000	-2.972403000	1.319279000
6	0.517873000	4.627728000	-1.879333000	1	2.144319000	-2.951783000	1.819497000
6	2.659699000	3.990899000	-3.056905000	1	7.702794000	-2.768689000	-0.888179000
6	0.500137000	1.500201000	1.415034000	1	7.046569000	-4.359264000	-2.623739000
6	2.820473000	-2.797476000	0.977967000	1	4.751448000	-4.369439000	-3.463346000
6	4.447348000	-1.930036000	-1.149637000	1	2.053345000	-2.182128000	-2.146717000
6	5.768764000	-1.897924000	-0.693712000	1	1.019933000	-4.170915000	-3.152096000
6	6.688644000	-2.786025000	-1.233498000	1	2.588312000	-4.885865000	-3.460928000
6	6.322864000	-3.681352000	-2.215262000	1	2.036244000	-4.681123000	-1.807715000
6	5.025408000	-3.688570000	-2.682599000	1	1.697844000	-2.174052000	-4.596108000

1	3.098337000	-1.205484000	-4.149478000	6	5.087097000	0.909090000	-1.320909000
1	3.321837000	-2.810125000	-4.835263000	6	4.902234000	-0.409828000	-0.966034000
1	5.378608000	-0.314952000	0.662091000	6	3.723926000	-0.832802000	-0.367602000
1	7.565074000	0.833191000	0.429932000	6	3.565983000	-2.311573000	-0.016593000
1	6.794494000	0.601262000	-1.135225000	6	4.796551000	-2.876177000	0.726851000
1	8.127913000	-0.439085000	-0.642957000	6	3.296814000	-3.129567000	-1.300157000
1	7.129921000	-0.835567000	2.320786000	6	1.803014000	2.500738000	-0.295243000
1	6.148356000	-2.265291000	2.033017000	6	1.380135000	3.120506000	-1.645845000
1	7.744627000	-2.132391000	1.311459000	6	2.276892000	3.604946000	0.675620000
1	1.745065000	0.168996000	-1.909032000	1	0.052355000	-0.313600000	3.530267000
14	-3.891884000	-0.156849000	1.267663000	1	-1.500289000	2.128986000	0.427142000
14	3.174075000	0.627714000	-1.489283000	1	-4.195998000	3.300829000	1.222957000
				1	-3.185451000	2.269982000	2.231739000
<b>Si-intra-TS<sub>1,z'</sub></b>				1	-2.630050000	3.877415000	1.778572000
1	1.036344000	-1.532970000	0.208505000	1	-1.838259000	4.323519000	-0.614739000
1	0.319203000	-2.131541000	-0.208575000	1	-3.429383000	3.861651000	-1.181401000
7	1.448544000	-0.311781000	0.462372000	1	-2.004933000	3.075108000	-1.845394000
6	1.273448000	-0.181228000	1.863031000	1	-4.944509000	2.261301000	-0.962074000
6	0.065136000	-0.321304000	2.445718000	1	-6.193374000	0.290909000	-1.684364000
6	-1.265295000	-0.421309000	1.835172000	1	-5.234634000	-1.938017000	-1.402751000
7	-1.358351000	-0.255901000	0.434468000	1	-1.950021000	-2.599104000	0.210615000
6	-2.699615000	-0.112960000	-0.134292000	1	-3.395713000	-4.519846000	0.638891000
6	-3.247030000	1.166388000	-0.286082000	1	-4.778339000	-3.690229000	-0.052190000
6	-2.506989000	2.417682000	0.172146000	1	-4.048782000	-3.095125000	1.435116000
6	-3.175316000	3.003235000	1.436233000	1	-2.156417000	-4.300727000	-1.577201000
6	-2.442596000	3.483787000	-0.942488000	1	-3.490143000	-3.406552000	-2.293831000
6	-4.510797000	1.289211000	-0.843370000	1	-1.876540000	-2.713921000	-2.283431000
6	-5.219929000	0.177506000	-1.249046000	1	-3.346355000	-0.637736000	2.246756000
6	-4.676831000	-1.078861000	-1.089349000	1	-2.195051000	-0.690855000	3.703122000
6	-3.420336000	-1.247446000	-0.523744000	1	2.242420000	0.047874000	3.751932000
6	-2.872416000	-2.660978000	-0.343250000	1	3.234040000	-0.782430000	2.536849000
6	-3.841479000	-3.544626000	0.472154000	1	3.012962000	0.957198000	2.440744000
6	-2.579271000	-3.310726000	-1.714082000	1	4.235950000	2.851302000	-1.368803000
6	-2.338301000	-0.597590000	2.633401000	1	6.005756000	1.218223000	-1.778978000
6	2.510922000	0.021397000	2.694677000	1	5.681858000	-1.118213000	-1.156258000
6	2.713351000	0.109046000	-0.142593000	1	2.719756000	-2.428719000	0.643548000
6	2.887130000	1.447969000	-0.506051000	1	4.592289000	-3.892496000	1.045803000
6	4.086630000	1.828368000	-1.088973000	1	5.669670000	-2.899941000	0.087077000

1	5.029837000	-2.282400000	1.602805000	6	5.040073000	1.396174000	-0.775422000
1	3.144470000	-4.175737000	-1.056501000	6	4.965309000	0.029056000	-0.941366000
1	2.416215000	-2.765070000	-1.814451000	6	3.826348000	-0.675424000	-0.584598000
1	4.140940000	-3.052624000	-1.975649000	6	3.786217000	-2.188148000	-0.832873000
1	0.939868000	2.025912000	0.144895000	6	5.153492000	-2.876219000	-0.630596000
1	0.584064000	3.839374000	-1.492114000	6	3.261771000	-2.460400000	-2.262093000
1	1.026593000	2.354210000	-2.324643000	6	1.613554000	2.255216000	0.597497000
1	2.212545000	3.634512000	-2.111244000	6	1.290486000	3.416000000	-0.368407000
1	1.477241000	4.318594000	0.843214000	6	1.912360000	2.806443000	2.008747000
1	2.564439000	3.186271000	1.632189000	1	0.035057000	-0.626846000	3.407442000
1	3.126490000	4.139209000	0.267059000	1	-1.286055000	2.122402000	-0.323550000
14	-0.081485000	-0.519866000	-0.771349000	1	-3.815630000	3.790187000	0.001859000
				1	-2.908877000	3.038026000	1.309199000
<b>Si-intra-IM<sub>1,z'</sub></b>							
1	1.693605000	-1.673132000	0.108067000	1	-1.428157000	3.890330000	-2.041997000
1	-0.122540000	-2.228093000	-0.544307000	1	-3.048710000	3.377618000	-2.470689000
7	1.517398000	-0.700121000	0.345185000	1	-1.684222000	2.306568000	-2.766158000
6	1.291111000	-0.738879000	1.793483000	1	-4.765193000	2.211565000	-1.608869000
6	0.079918000	-0.539970000	2.325506000	1	-6.233176000	0.259467000	-1.684453000
6	-1.221393000	-0.206467000	1.720394000	1	-5.448456000	-1.891430000	-0.829965000
7	-1.335498000	-0.177694000	0.331302000	1	-2.098591000	-2.450501000	0.665337000
6	-2.686825000	-0.050189000	-0.215397000	1	-3.665401000	-3.982842000	1.780212000
6	-3.133199000	1.180102000	-0.708429000	1	-5.034908000	-3.173328000	1.038605000
6	-2.257504000	2.423719000	-0.672972000	1	-4.037084000	-2.318147000	2.210115000
6	-2.830864000	3.462769000	0.315769000	1	-2.692244000	-4.528695000	-0.513264000
6	-2.096836000	3.036867000	-2.080582000	1	-4.040289000	-3.724873000	-1.304036000
6	-4.415264000	1.271577000	-1.232376000	1	-2.390474000	-3.242694000	-1.673720000
6	-5.245656000	0.173016000	-1.275169000	1	-3.213169000	0.355798000	2.243121000
6	-4.800517000	-1.038990000	-0.790983000	1	-2.036976000	0.065810000	3.649464000
6	-3.527745000	-1.173326000	-0.256933000	1	2.211562000	-1.153330000	3.679325000
6	-3.093291000	-2.541333000	0.264323000	1	2.883767000	-2.084037000	2.332946000
6	-4.021755000	-3.031872000	1.396467000	1	3.299442000	-0.380054000	2.509195000
6	-3.052703000	-3.574147000	-0.883463000	1	4.023858000	3.145747000	-0.149959000
6	-2.222171000	0.089585000	2.582865000	1	5.934589000	1.920709000	-1.046572000
6	2.489779000	-1.103733000	2.625227000	1	5.804998000	-0.493266000	-1.347282000
6	2.740826000	0.045771000	-0.067237000	1	3.117978000	-2.663674000	-0.125038000
6	2.787533000	1.429149000	0.079446000	1	5.018858000	-3.951249000	-0.670713000
6	3.961660000	2.084214000	-0.269145000	1	5.852779000	-2.606116000	-1.411424000

1	5.584828000	-2.618488000	0.329359000	6	-4.963725000	-0.279304000	1.203707000
1	3.199106000	-3.527505000	-2.446168000	6	-4.392145000	-1.289619000	0.463516000
1	2.281728000	-2.025931000	-2.414693000	6	-3.185387000	-1.110469000	-0.192666000
1	3.939081000	-2.022343000	-2.985615000	6	-2.666419000	-2.292678000	-1.012025000
1	0.740802000	1.627473000	0.654018000	6	-3.717217000	-2.781520000	-2.036069000
1	0.413496000	3.946508000	-0.017379000	6	-2.245091000	-3.455653000	-0.087880000
1	1.091317000	3.041510000	-1.364412000	6	-2.606445000	2.607717000	0.666021000
1	2.107128000	4.125381000	-0.420323000	6	-2.274982000	3.038841000	2.109911000
1	1.058658000	3.365710000	2.375837000	6	-3.615277000	3.589654000	0.026750000
1	2.117131000	2.004450000	2.706010000	1	0.514557000	-0.054569000	-3.553967000
1	2.769873000	3.469418000	1.983935000	1	3.283478000	1.319879000	-1.835408000
14	-0.134718000	-0.735086000	-0.935183000	1	5.520344000	-0.697931000	-2.291631000
				1	3.819309000	-0.986533000	-2.614914000
<b>Si-intra-TS<sub>2',4</sub></b>				1	4.701399000	0.210773000	-3.557759000
1	-0.352108000	-0.993622000	-0.582997000	1	5.310418000	2.473888000	-2.490410000
1	0.343472000	1.519213000	1.172109000	1	6.281809000	1.573058000	-1.345860000
7	-1.163811000	0.255742000	-0.676551000	1	5.076189000	2.715881000	-0.764688000
6	-1.032396000	0.300538000	-2.093584000	1	6.092208000	0.115586000	0.249693000
6	0.192773000	-0.067878000	-2.520961000	1	5.802550000	-0.909921000	2.450899000
6	1.063245000	-0.585436000	-1.416646000	1	3.562758000	-1.352005000	3.302605000
7	1.631555000	0.310354000	-0.595068000	1	0.410994000	-0.674553000	1.506271000
6	2.719700000	-0.054687000	0.312278000	1	0.037070000	-2.578737000	2.991348000
6	4.008368000	0.235202000	-0.166549000	1	1.733028000	-2.641942000	3.427764000
6	4.216797000	0.870157000	-1.539277000	1	1.236453000	-3.068451000	1.803759000
6	4.586304000	-0.221775000	-2.568842000	1	-0.026857000	-0.177492000	3.859960000
6	5.292473000	1.976304000	-1.526434000	1	1.686672000	-0.276076000	4.237901000
6	5.105897000	-0.088016000	0.612432000	1	1.085786000	1.022589000	3.216388000
6	4.945232000	-0.665735000	1.854968000	1	1.220599000	-2.311164000	-0.147068000
6	3.679210000	-0.917908000	2.330667000	1	0.357356000	-2.569935000	-1.760822000
6	2.545744000	-0.621595000	1.580875000	1	-2.251385000	1.922369000	-2.706771000
6	1.185017000	-0.911827000	2.216115000	1	-1.851945000	0.776353000	-4.007248000
6	1.043530000	-2.395764000	2.629635000	1	-3.069576000	0.360049000	-2.773442000
6	0.971645000	-0.023257000	3.463612000	1	-4.797737000	1.743006000	1.797529000
6	0.739973000	-1.882771000	-1.014526000	1	-5.891233000	-0.438585000	1.717045000
6	-2.117646000	0.862663000	-2.951935000	1	-4.889405000	-2.235410000	0.395107000
6	-2.510315000	0.123798000	-0.086047000	1	-1.808538000	-1.980315000	-1.577563000
6	-3.131742000	1.176784000	0.605527000	1	-3.284240000	-3.554697000	-2.662455000
6	-4.339482000	0.942927000	1.253394000	1	-4.586157000	-3.200060000	-1.544391000

1	-4.045347000	-1.969320000	-2.673625000	1	-5.342652000	-1.592686000	-1.508928000
1	-1.829052000	-4.270972000	-0.671470000	1	-4.702648000	2.554412000	-0.953614000
1	-1.502051000	-3.130733000	0.629035000	1	-6.098744000	0.717595000	-1.754383000
1	-3.101015000	-3.833352000	0.458995000	6	-2.289953000	2.471791000	0.240568000
1	-1.710259000	2.683011000	0.078663000	6	-2.937390000	3.077533000	1.505983000
1	-1.834378000	4.030326000	2.107314000	6	-2.108356000	3.558737000	-0.840531000
1	-1.572291000	2.352965000	2.563714000	1	-1.316732000	2.094104000	0.510922000
1	-3.171034000	3.070036000	2.719123000	1	-3.028262000	2.325921000	2.278601000
1	-3.187811000	4.586329000	-0.000030000	1	-2.328726000	3.892492000	1.885332000
1	-3.853104000	3.291082000	-0.987540000	1	-3.923730000	3.466332000	1.278323000
1	-4.537168000	3.632623000	0.593920000	1	-1.689048000	3.139736000	-1.747517000
14	0.344015000	1.719466000	-0.323111000	1	-3.052771000	4.029041000	-1.086457000
				1	-1.439484000	4.331642000	-0.476132000
<b>Si-intra-TS<sub>1,1</sub></b>				6	-3.073515000	-2.539848000	-0.419210000
6	1.234865000	-0.204485000	1.851938000	6	-2.841235000	-3.192202000	-1.800723000
6	0.036396000	-0.391044000	2.456710000	6	-4.116043000	-3.347711000	0.383982000
6	-1.307011000	-0.453091000	1.868222000	1	-2.149549000	-2.566875000	0.135505000
6	-2.393202000	-0.578737000	2.656207000	1	-2.113630000	-2.633542000	-2.378063000
7	1.392082000	-0.200723000	0.454030000	1	-2.481006000	-4.208842000	-1.680376000
7	-1.391336000	-0.294681000	0.459597000	1	-3.764547000	-3.225214000	-2.367564000
14	0.004131000	-0.646962000	-0.513499000	1	-4.273701000	-2.902555000	1.358072000
1	0.046380000	-0.430034000	3.539910000	1	-5.065527000	-3.391353000	-0.136218000
1	-3.396659000	-0.594506000	2.255717000	1	-3.763393000	-4.364065000	0.526082000
6	2.692160000	0.064897000	-0.152741000	6	2.064718000	2.538630000	-0.353195000
6	3.586172000	-0.991262000	-0.366391000	6	1.651651000	3.102393000	-1.731447000
6	3.026254000	1.368868000	-0.531679000	6	2.680360000	3.652877000	0.520701000
6	4.813143000	-0.718479000	-0.952746000	1	1.179549000	2.176290000	0.145059000
6	4.265206000	1.598246000	-1.113156000	1	1.187519000	2.332609000	-2.337363000
6	5.154328000	0.565824000	-1.321334000	1	0.946175000	3.916089000	-1.609123000
1	5.505396000	-1.517162000	-1.126056000	1	2.515542000	3.479789000	-2.265609000
1	4.533924000	2.592183000	-1.408680000	1	2.975633000	3.267689000	1.489301000
1	6.107007000	0.759939000	-1.773377000	1	3.552915000	4.084438000	0.044968000
6	-2.691578000	-0.024666000	-0.141761000	1	1.955233000	4.444863000	0.675667000
6	-3.496038000	-1.082259000	-0.575815000	6	3.239205000	-2.432837000	-0.004516000
6	-3.122462000	1.300936000	-0.269508000	6	4.323196000	-3.090882000	0.877233000
6	-4.720101000	-0.792398000	-1.163081000	6	3.033689000	-3.266543000	-1.290264000
6	-4.356752000	1.545897000	-0.851879000	1	2.313634000	-2.431823000	0.549244000
6	-5.149033000	0.509772000	-1.301901000	1	4.502468000	-2.512145000	1.774973000

1	4.002024000	-4.084397000	1.171408000	1	-4.858574000	2.258363000	-1.380711000
1	5.260041000	-3.187971000	0.342190000	1	-6.068212000	0.214392000	-1.952048000
1	2.280729000	-2.819319000	-1.928103000	6	-2.499688000	2.547899000	-0.109608000
1	3.956933000	-3.326578000	-1.854902000	6	-3.300505000	3.326411000	0.957400000
1	2.719725000	-4.274242000	-1.039161000	6	-2.257191000	3.430669000	-1.353218000
1	0.096859000	-1.964183000	-1.212760000	1	-1.542885000	2.292152000	0.316177000
6	2.472123000	0.022473000	2.676692000	1	-3.429950000	2.722146000	1.845640000
1	2.219539000	-0.013904000	3.737134000	1	-2.771592000	4.233637000	1.232076000
1	3.238712000	-0.725876000	2.471132000	1	-4.277086000	3.604765000	0.577788000
1	2.911187000	0.998970000	2.457911000	1	-1.706392000	2.887941000	-2.111948000
1	-2.265391000	-0.648643000	3.729404000	1	-3.193852000	3.765039000	-1.783466000
1	0.101231000	-2.297501000	-0.057027000	1	-1.684267000	4.309713000	-1.076116000
				6	-2.840621000	-2.558975000	-0.092779000
<b>Si-P<sub>1,1</sub></b>				6	-2.680272000	-3.454786000	-1.340652000
6	1.226042000	-0.133630000	1.899091000	6	-3.760336000	-3.240850000	0.943973000
6	0.020273000	-0.143844000	2.510504000	1	-1.870673000	-2.430670000	0.359845000
6	-1.316339000	-0.095799000	1.914788000	1	-2.040742000	-2.982862000	-2.076691000
6	-2.411930000	-0.055454000	2.701749000	1	-2.237077000	-4.404687000	-1.059812000
7	1.373271000	-0.110000000	0.501657000	1	-3.640448000	-3.656611000	-1.800722000
7	-1.386510000	-0.082719000	0.503845000	1	-3.838972000	-2.633271000	1.835798000
1	0.030018000	-0.173597000	3.594869000	1	-4.753022000	-3.395310000	0.536805000
1	-3.413670000	-0.015527000	2.298099000	1	-3.353651000	-4.208048000	1.221898000
6	2.670836000	-0.001121000	-0.150760000	6	2.465315000	2.548738000	-0.044522000
6	3.361935000	-1.161054000	-0.521487000	6	2.170588000	3.437952000	-1.272561000
6	3.188386000	1.266426000	-0.446061000	6	3.289050000	3.336894000	0.998341000
6	4.573397000	-1.029978000	-1.185448000	1	1.524576000	2.277212000	0.407237000
6	4.403350000	1.351154000	-1.109564000	1	1.599443000	2.894336000	-2.014621000
6	5.091577000	0.213876000	-1.478130000	1	1.598169000	4.308400000	-0.969363000
1	5.115242000	-1.907823000	-1.474091000	1	3.089019000	3.783972000	-1.731859000
1	4.813969000	2.313381000	-1.339837000	1	3.491741000	2.730281000	1.872405000
1	6.029110000	0.297121000	-1.991714000	1	4.235800000	3.655731000	0.577949000
6	-2.686094000	-0.003743000	-0.147240000	1	2.743371000	4.220078000	1.313597000
6	-3.376333000	-1.179233000	-0.464389000	6	2.834300000	-2.556982000	-0.202149000
6	-3.215121000	1.250638000	-0.474131000	6	3.786605000	-3.298533000	0.762620000
6	-4.596357000	-1.077218000	-1.117808000	6	2.631680000	-3.386932000	-1.489116000
6	-4.438089000	1.306563000	-1.125913000	1	1.877831000	-2.451330000	0.284445000
6	-5.123715000	0.153467000	-1.447869000	1	3.932016000	-2.735392000	1.676193000
1	-5.138514000	-1.967058000	-1.366673000	1	3.372796000	-4.267793000	1.020534000

1	4.754734000	-3.456459000	0.301899000	1	0.493828000	1.319438000	-1.173908000
1	1.967470000	-2.878070000	-2.176330000	1	-3.034509000	-3.184299000	-1.278948000
1	3.576292000	-3.561234000	-1.990710000	1	-3.310284000	-2.303073000	-2.773133000
1	2.198044000	-4.350726000	-1.243723000	1	-1.644992000	-2.596409000	-2.213120000
1	0.004092000	0.916522000	-1.527459000	1	-7.590840000	-1.437712000	-3.164695000
6	2.477427000	-0.151892000	2.748406000	1	-8.423686000	-3.152327000	-1.639358000
1	2.503223000	0.726069000	3.399112000	1	-7.159635000	-3.729839000	0.366641000
1	2.484638000	-1.039883000	3.385952000	6	-2.876043000	3.879408000	-1.082232000
1	3.383828000	-0.155232000	2.147697000	1	-2.874083000	2.866167000	-1.453480000
1	-2.290293000	-0.059269000	3.777536000	6	-1.740457000	1.411095000	3.272626000
1	-0.013980000	-1.459038000	-1.320530000	1	-1.687786000	0.580460000	2.585368000
14	-0.016994000	-0.194021000	-0.558174000	6	-1.831954000	4.674497000	-1.896425000
				1	-1.820871000	5.716369000	-1.600305000
<b>Si-inter-TS<sub>1,4-I</sub></b>				1	-0.840167000	4.265238000	-1.753210000
7	-3.872906000	-0.641334000	-0.576378000	1	-2.074206000	4.627697000	-2.952904000
6	-2.670380000	-1.074107000	-1.129128000	6	-4.288864000	4.468193000	-1.294764000
6	-1.520267000	-0.354445000	-0.996563000	1	-4.554547000	4.432494000	-2.345972000
6	-1.362720000	0.886318000	-0.291618000	1	-5.030050000	3.912266000	-0.732323000
7	-2.445234000	1.382133000	0.418277000	1	-4.325793000	5.501587000	-0.972173000
6	-2.298621000	2.674667000	1.113029000	6	-0.404576000	1.463836000	4.044148000
6	-2.522524000	3.858851000	0.403242000	1	-0.405532000	2.261100000	4.777215000
6	-2.422321000	5.062035000	1.085153000	1	-0.248037000	0.529479000	4.569346000
6	-2.116267000	5.092377000	2.429905000	1	0.427106000	1.612898000	3.368042000
6	-1.900064000	3.916009000	3.114886000	6	-2.915558000	1.166613000	4.247081000
6	-1.980402000	2.688119000	2.472220000	1	-3.858884000	1.106903000	3.715980000
6	-0.103597000	1.504693000	-0.285585000	1	-2.765203000	0.239158000	4.789564000
6	-2.662678000	-2.364265000	-1.896245000	1	-2.985158000	1.974060000	4.966557000
6	-5.112792000	-1.371708000	-0.886665000	6	-5.364888000	0.063183000	-2.998251000
6	-5.830846000	-1.028612000	-2.037153000	1	-4.373523000	0.377656000	-2.710101000
6	-7.023932000	-1.687773000	-2.291396000	6	-6.305930000	1.285918000	-2.905762000
6	-7.497100000	-2.655601000	-1.430119000	1	-7.309890000	1.015647000	-3.210538000
6	-6.781083000	-2.980953000	-0.298278000	1	-6.352478000	1.664034000	-1.891258000
6	-5.579718000	-2.350667000	-0.005474000	1	-5.954729000	2.081128000	-3.554709000
1	-0.617898000	-0.757388000	-1.447596000	6	-5.290325000	-0.443378000	-4.455256000
1	-2.588580000	5.981370000	0.561800000	1	-4.888467000	0.335467000	-5.094156000
1	-2.047448000	6.031321000	2.942500000	1	-4.649364000	-1.313040000	-4.534729000
1	-1.665474000	3.950677000	4.158599000	1	-6.271633000	-0.708112000	-4.828907000
1	-0.023133000	2.496166000	0.139991000	6	-4.832713000	-2.732206000	1.269686000

1	-3.870945000	-2.243665000	1.261711000	1	7.147156000	4.658162000	-0.320516000
6	-5.613025000	-2.249072000	2.513484000	1	4.996753000	4.938092000	0.806166000
1	-5.061198000	-2.485832000	3.416939000	6	2.913138000	3.277223000	0.948323000
1	-5.775905000	-1.178357000	2.479443000	1	2.270833000	2.440155000	0.744416000
1	-6.579656000	-2.735903000	2.567202000	6	2.210174000	4.557646000	0.444940000
6	-4.582502000	-4.253760000	1.354651000	1	1.242848000	4.665701000	0.925790000
1	-5.513815000	-4.800069000	1.438520000	1	2.796095000	5.440161000	0.672719000
1	-4.052890000	-4.612098000	0.480297000	1	2.058674000	4.520731000	-0.627958000
1	-3.982701000	-4.477343000	2.229565000	6	3.133307000	3.351906000	2.475271000
7	3.505917000	0.788767000	-0.549640000	1	3.586247000	2.437370000	2.836747000
6	2.824782000	0.612416000	-1.754803000	1	3.781654000	4.182866000	2.729292000
6	2.161013000	-0.529765000	-2.062727000	1	2.184837000	3.493826000	2.983586000
6	2.114430000	-1.788119000	-1.312880000	6	6.141883000	0.381057000	-1.790197000
7	2.732175000	-1.796897000	-0.050020000	1	5.317200000	-0.308216000	-1.714794000
6	2.835381000	-3.081973000	0.633986000	6	6.451838000	0.607460000	-3.286503000
6	3.980830000	-3.871001000	0.463217000	1	7.299833000	1.271318000	-3.409875000
6	4.056908000	-5.098125000	1.105921000	1	6.692085000	-0.338332000	-3.761122000
6	3.037458000	-5.542547000	1.920214000	1	5.603770000	1.037752000	-3.803685000
6	1.918698000	-4.758971000	2.095571000	6	7.365902000	-0.253466000	-1.094076000
6	1.796525000	-3.533809000	1.455118000	1	8.228985000	0.398284000	-1.160612000
6	1.501706000	-2.864083000	-1.867891000	1	7.157416000	-0.439998000	-0.048020000
6	2.762731000	1.784944000	-2.701823000	1	7.617522000	-1.194695000	-1.569893000
6	4.505531000	1.849087000	-0.464800000	6	5.139693000	-3.432926000	-0.423360000
6	5.752983000	1.676914000	-1.084472000	1	4.987397000	-2.395842000	-0.671946000
6	6.683540000	2.703643000	-1.030780000	6	6.492535000	-3.568312000	0.308640000
6	6.414043000	3.876384000	-0.358426000	1	6.712385000	-4.603219000	0.541017000
6	5.200256000	4.031389000	0.272813000	1	7.292807000	-3.195291000	-0.318959000
6	4.233126000	3.036548000	0.226898000	1	6.487280000	-3.002528000	1.232972000
1	1.620840000	-0.543080000	-3.004240000	6	5.151036000	-4.248946000	-1.735211000
1	4.923923000	-5.711852000	0.970649000	1	4.213769000	-4.126473000	-2.261907000
1	3.116430000	-6.490958000	2.414906000	1	5.958265000	-3.914241000	-2.380152000
1	1.129686000	-5.102679000	2.734063000	1	5.298464000	-5.302905000	-1.524809000
1	1.448122000	-3.821629000	-1.370651000	6	0.529438000	-2.719025000	1.674254000
1	1.096494000	-2.781304000	-2.870320000	1	0.564181000	-1.862558000	1.023098000
1	2.303071000	2.647226000	-2.207421000	6	-0.731381000	-3.534110000	1.320846000
1	3.754021000	2.102482000	-3.025208000	1	-0.856197000	-4.378744000	1.988219000
1	2.171270000	1.527215000	-3.582894000	1	-1.610396000	-2.904737000	1.408920000
1	7.633678000	2.579112000	-1.510005000	1	-0.671134000	-3.900801000	0.303974000

6	0.455653000	-2.222062000	3.133460000	6	4.675577000	-2.516856000	1.383522000
1	1.312913000	-1.603189000	3.367170000	6	3.374468000	-3.264175000	-0.658570000
1	-0.445229000	-1.635834000	3.285297000	6	1.690031000	2.413266000	-0.890322000
1	0.436511000	-3.058595000	3.8222886000	6	1.161342000	2.563132000	-2.334768000
1	0.768970000	0.721955000	0.493228000	6	2.148017000	3.781239000	-0.340292000
1	1.527852000	0.258032000	0.962368000	1	0.037564000	0.024797000	3.546001000
14	3.193116000	-0.309711000	0.881965000	1	-1.373998000	2.007986000	0.835780000
14	-4.115255000	0.774953000	0.461445000	1	-2.390335000	3.401841000	2.621322000
				1	-3.997153000	2.957618000	2.056910000
<i>Si-inter-IM<sub>1,4</sub></i>				1	-2.941210000	1.735757000	2.748442000
1	-0.830490000	-2.250461000	1.556394000	1	-1.734973000	4.358170000	0.326479000
1	-0.128501000	-2.337496000	0.740544000	1	-3.378982000	4.058222000	-0.197649000
7	1.409818000	-0.151583000	0.494238000	1	-2.034035000	3.417414000	-1.130924000
6	1.248039000	0.172447000	1.817496000	1	-4.862656000	2.446685000	-0.328083000
6	0.0666627000	-0.061431000	2.466675000	1	-6.170154000	0.686298000	-1.411635000
6	-1.136768000	-0.535885000	1.817425000	1	-5.236241000	-1.553832000	-1.643101000
7	-1.298694000	-0.282199000	0.479348000	1	-1.961923000	-2.654776000	-0.348331000
6	-2.652038000	-0.090941000	-0.054508000	1	-4.093486000	-3.364592000	0.768586000
6	-3.178033000	1.206739000	0.060256000	1	-3.456299000	-4.562588000	-0.348672000
6	-2.393876000	2.335031000	0.724938000	1	-4.823062000	-3.568871000	-0.814843000
6	-2.967631000	2.625107000	2.130044000	1	-2.268683000	-3.834687000	-2.484595000
6	-2.389911000	3.621674000	-0.128187000	1	-3.586549000	-2.754310000	-2.918235000
6	-4.449186000	1.463580000	-0.423783000	1	-1.945335000	-2.132651000	-2.779953000
6	-5.189486000	0.472538000	-1.034531000	1	-2.834856000	-1.852142000	1.996714000
6	-4.660456000	-0.790693000	-1.160821000	1	-1.678920000	-1.818956000	3.445467000
6	-3.395737000	-1.102319000	-0.672921000	1	2.140932000	0.927372000	3.610433000
6	-2.898853000	-2.534259000	-0.864382000	1	3.282091000	0.103531000	2.520986000
6	-3.884480000	-3.568675000	-0.274516000	1	2.706031000	1.711912000	2.121352000
6	-2.659266000	-2.829723000	-2.362038000	1	4.134938000	2.572189000	-2.014053000
6	-1.873664000	-1.569279000	2.407464000	1	5.934850000	0.921130000	-2.042330000
6	2.411200000	0.759295000	2.567184000	1	5.642165000	-1.231948000	-0.926618000
6	2.659962000	0.153465000	-0.190398000	1	2.596339000	-2.168792000	1.006248000
6	2.810550000	1.378587000	-0.846781000	1	4.479734000	-3.461084000	1.880482000
6	4.003717000	1.638269000	-1.505776000	1	5.609386000	-2.612526000	0.842769000
6	5.019979000	0.706390000	-1.525909000	1	4.798883000	-1.752195000	2.141773000
6	4.853838000	-0.507548000	-0.891834000	1	3.217490000	-4.235666000	-0.201358000
6	3.678196000	-0.805429000	-0.218951000	1	2.535614000	-3.051516000	-1.309827000
6	3.508927000	-2.176085000	0.431124000	1	4.273418000	-3.310421000	-1.262658000

1	0.878479000	2.057608000	-0.275542000	6	-2.829304000	-3.726309000	-0.034332000
1	0.335516000	3.266237000	-2.360483000	1	-2.143234000	-2.902866000	-0.120857000
1	0.814209000	1.609644000	-2.713854000	6	-6.156669000	-0.213619000	-1.782517000
1	1.941298000	2.929801000	-2.992071000	1	-5.322528000	0.441562000	-1.585310000
1	1.312522000	4.473282000	-0.329400000	6	-2.207063000	-4.927650000	-0.779695000
1	2.526773000	3.688830000	0.671048000	1	-2.789318000	-5.829200000	-0.634044000
1	2.929129000	4.208770000	-0.957540000	1	-2.133937000	-4.736580000	-1.844181000
14	0.095436000	-0.974563000	-0.501579000	1	-1.208424000	-5.108050000	-0.400716000
				6	-2.993450000	-4.057330000	1.466637000
<b>Si-inter-TS<sub>1,4-II</sub></b>				1	-2.032045000	-4.310825000	1.897562000
7	-2.589315000	1.372552000	0.368865000	1	-3.398431000	-3.211930000	2.010347000
6	-1.703439000	1.407030000	-0.646884000	1	-3.663284000	-4.899149000	1.598900000
6	-1.711385000	0.428307000	-1.647514000	6	-6.538429000	-0.058431000	-3.271248000
6	-2.616086000	-0.625674000	-1.759044000	1	-7.404418000	-0.661755000	-3.513634000
7	-3.476093000	-0.927721000	-0.764139000	1	-6.779042000	0.977213000	-3.485955000
6	-4.485578000	-1.994103000	-0.961781000	1	-5.723825000	-0.359529000	-3.918947000
6	-4.173956000	-3.315693000	-0.624698000	6	-7.333021000	0.220098000	-0.878231000
6	-5.147610000	-4.286143000	-0.811663000	1	-7.061563000	0.149346000	0.168804000
6	-6.387812000	-3.964622000	-1.318836000	1	-7.614687000	1.243321000	-1.094381000
6	-6.682506000	-2.656659000	-1.635888000	1	-8.197556000	-0.409631000	-1.045991000
6	-5.747214000	-1.647598000	-1.456067000	6	-1.310934000	1.672918000	3.058505000
6	-0.644950000	2.459848000	-0.704818000	1	-1.092944000	0.914363000	2.323114000
6	-2.826819000	2.583903000	1.186528000	6	-2.005387000	1.007344000	4.269138000
6	-2.234280000	2.720126000	2.443005000	1	-2.209486000	1.741941000	5.039271000
6	-2.510631000	3.869549000	3.173688000	1	-2.942411000	0.545686000	3.981543000
6	-3.330360000	4.854978000	2.673337000	1	-1.362729000	0.244427000	4.689639000
6	-3.907099000	4.704853000	1.429141000	6	0.036907000	2.291064000	3.490857000
6	-3.679981000	3.568916000	0.669175000	1	0.702976000	1.508452000	3.830353000
1	-0.987093000	0.547353000	-2.440350000	1	0.519560000	2.793401000	2.664101000
1	-4.930485000	-5.302119000	-0.555374000	1	-0.098449000	2.997251000	4.301301000
1	-7.124924000	-4.729897000	-1.459766000	6	-4.354255000	3.456047000	-0.697228000
1	-7.652155000	-2.414059000	-2.019363000	1	-4.215801000	2.453345000	-1.070315000
1	-0.342537000	2.653993000	-1.734818000	6	-5.873589000	3.716791000	-0.598601000
1	-0.933948000	3.381794000	-0.207686000	1	-6.341824000	3.519321000	-1.557021000
1	0.228192000	2.035578000	-0.185341000	1	-6.330419000	3.080293000	0.148638000
1	-2.069274000	3.992335000	4.140520000	1	-6.077151000	4.747850000	-0.339151000
1	-3.521502000	5.738251000	3.249656000	6	-3.719538000	4.439939000	-1.706400000
1	-4.542909000	5.477046000	1.048230000	1	-3.847428000	5.460907000	-1.366982000

1	-2.660378000	4.254015000	-1.827817000	1	5.028370000	5.319250000	-0.840194000
1	-4.196744000	4.341144000	-2.675711000	6	2.945810000	3.801455000	-0.087715000
6	-2.618016000	-1.448506000	-3.014514000	1	2.279101000	2.956837000	-0.052120000
1	-1.831481000	-1.109166000	-3.688642000	6	2.261583000	4.944102000	-0.869460000
1	-2.460241000	-2.503009000	-2.782286000	1	1.311171000	5.193222000	-0.406707000
1	-3.582247000	-1.372893000	-3.520791000	1	2.870991000	5.839737000	-0.870141000
1	-1.503680000	-0.933330000	0.994747000	1	2.078743000	4.659958000	-1.899828000
1	-0.869355000	-1.197106000	0.588447000	6	3.224985000	4.241554000	1.366945000
7	3.474988000	0.988239000	-0.722025000	1	3.659959000	3.424640000	1.928320000
6	2.553622000	0.668121000	-1.676842000	1	3.912957000	5.079410000	1.385548000
6	1.597723000	-0.304294000	-1.496404000	1	2.303334000	4.544864000	1.854856000
6	1.535166000	-1.314791000	-0.453666000	6	6.102277000	0.134919000	-1.720940000
7	2.561686000	-1.334532000	0.472267000	1	5.246002000	-0.460134000	-1.449568000
6	2.864732000	-2.585590000	1.138964000	6	6.469783000	-0.166388000	-3.189985000
6	3.573495000	-3.583583000	0.447346000	1	7.350566000	0.387992000	-3.493460000
6	3.873651000	-4.773702000	1.089476000	1	6.680052000	-1.223687000	-3.311552000
6	3.506151000	-4.990475000	2.401774000	1	5.656277000	0.097013000	-3.856420000
6	2.815085000	-4.012266000	3.079157000	6	7.268438000	-0.243764000	-0.780229000
6	2.473169000	-2.814367000	2.463104000	1	8.147400000	0.352867000	-0.996392000
6	0.498672000	-2.227907000	-0.464603000	1	6.982769000	-0.079155000	0.251347000
6	2.580679000	1.414017000	-2.990331000	1	7.529953000	-1.288211000	-0.904979000
6	4.493358000	1.987236000	-1.006830000	6	4.021296000	-3.396794000	-0.997919000
6	5.736456000	1.599835000	-1.519583000	1	3.843320000	-2.368120000	-1.264827000
6	6.682471000	2.572969000	-1.810565000	6	5.528360000	-3.689873000	-1.162147000
6	6.425864000	3.907540000	-1.583968000	1	5.742719000	-4.741162000	-1.008303000
6	5.215070000	4.283505000	-1.042293000	1	5.848845000	-3.430015000	-2.166162000
6	4.241730000	3.341474000	-0.745040000	1	6.109686000	-3.115308000	-0.453207000
1	0.900989000	-0.452172000	-2.312247000	6	3.205880000	-4.301109000	-1.948780000
1	4.409416000	-5.537171000	0.561810000	1	2.150291000	-4.082951000	-1.862906000
1	3.757966000	-5.912438000	2.888961000	1	3.512644000	-4.137479000	-2.977964000
1	2.530048000	-4.180233000	4.098585000	1	3.368352000	-5.346697000	-1.708710000
1	0.495810000	-3.075064000	0.208337000	6	1.662433000	-1.798156000	3.259104000
1	-0.155467000	-2.263821000	-1.330554000	1	1.416883000	-0.977017000	2.604255000
1	2.483919000	2.491678000	-2.842011000	6	0.341010000	-2.422585000	3.759350000
1	3.528835000	1.252874000	-3.508253000	1	0.529528000	-3.230065000	4.456865000
1	1.771321000	1.068110000	-3.637934000	1	-0.256090000	-1.675386000	4.270158000
1	7.633430000	2.280312000	-2.208464000	1	-0.234782000	-2.813047000	2.929428000
1	7.168554000	4.647005000	-1.812038000	6	2.478862000	-1.249099000	4.449642000

1	3.390589000	-0.785866000	4.096860000	1	-6.712250000	4.333893000	-0.351463000
1	1.901596000	-0.505859000	4.992647000	1	-5.252145000	6.285055000	-0.529159000
1	2.734576000	-2.046247000	5.139015000	1	-2.827510000	6.006473000	-0.383499000
1	1.915651000	0.948588000	1.169011000	6	-1.390700000	3.770825000	-0.030023000
14	3.316654000	0.289930000	1.027107000	1	-1.167445000	2.753416000	0.243649000
14	-3.495092000	-0.130219000	0.874943000	6	-0.732087000	4.717597000	0.996993000
				1	0.340477000	4.545992000	1.029681000
<b>Si-inter-TS<sub>1,4</sub>'</b>				1	-0.890019000	5.755036000	0.728938000
1	-0.047482000	0.484491000	-0.181716000	1	-1.134863000	4.560205000	1.990395000
1	-1.078643000	0.386294000	-0.592709000	6	-0.818350000	4.034197000	-1.441394000
7	-3.179145000	1.469303000	0.350077000	1	-1.268537000	3.362003000	-2.161286000
6	-3.043351000	1.065748000	1.676191000	1	-1.027789000	5.052104000	-1.749100000
6	-2.689591000	-0.198156000	2.025870000	1	0.257474000	3.889160000	-1.456076000
6	-2.559442000	-1.374826000	1.164241000	6	-6.085575000	1.755914000	-0.004331000
7	-2.954174000	-1.215230000	-0.175801000	1	-5.505904000	0.864232000	0.167393000
6	-3.327101000	-2.416506000	-0.906643000	6	-7.114520000	1.894407000	1.138532000
6	-4.600882000	-2.973992000	-0.703398000	1	-7.747911000	2.761501000	0.990242000
6	-4.957476000	-4.119010000	-1.396418000	1	-7.749845000	1.015709000	1.173531000
6	-4.090134000	-4.712406000	-2.291139000	1	-6.619745000	1.993304000	2.097544000
6	-2.843698000	-4.164637000	-2.489386000	6	-6.804204000	1.611574000	-1.365002000
6	-2.440229000	-3.027967000	-1.798871000	1	-7.385361000	2.498382000	-1.589889000
6	-2.141774000	-2.551402000	1.692853000	1	-6.081453000	1.463212000	-2.158164000
6	-3.284788000	2.086743000	2.759480000	1	-7.477015000	0.762601000	-1.346781000
6	-3.742947000	2.786397000	0.076421000	6	-5.601046000	-2.362230000	0.270532000
6	-5.129171000	2.941742000	-0.050041000	1	-5.203523000	-1.414766000	0.594777000
6	-5.651897000	4.210157000	-0.260971000	6	-6.966587000	-2.116027000	-0.407136000
6	-4.831644000	5.312098000	-0.366068000	1	-7.455503000	-3.051335000	-0.653740000
6	-3.465605000	5.152036000	-0.277248000	1	-7.619846000	-1.568264000	0.264944000
6	-2.906312000	3.901902000	-0.060026000	1	-6.847204000	-1.543137000	-1.317763000
1	-2.545331000	-0.390652000	3.084321000	6	-5.783774000	-3.265961000	1.509980000
1	-5.925805000	-4.550096000	-1.239784000	1	-4.835680000	-3.417836000	2.006672000
1	-4.385784000	-5.593590000	-2.826525000	1	-6.473943000	-2.805615000	2.210991000
1	-2.170173000	-4.625464000	-3.184177000	1	-6.187385000	-4.230388000	1.220333000
1	-2.085840000	-3.456293000	1.104576000	6	-1.034773000	-2.493387000	-2.041768000
1	-1.937219000	-2.614132000	2.755393000	1	-0.868828000	-1.666561000	-1.372711000
1	-2.636676000	2.957841000	2.643662000	6	0.032917000	-3.565275000	-1.732508000
1	-4.312643000	2.454972000	2.731840000	1	-0.043198000	-4.405447000	-2.412834000
1	-3.103753000	1.638835000	3.738623000	1	1.025549000	-3.137610000	-1.836990000

1	-0.081301000	-3.932324000	-0.719554000	6	3.827003000	-1.769501000	-3.063649000
6	-0.883579000	-1.985094000	-3.491620000	1	3.047884000	-1.745601000	-2.317207000
1	-1.628653000	-1.229521000	-3.704581000	6	3.919175000	4.182418000	-1.934503000
1	0.098776000	-1.548798000	-3.633685000	1	4.611230000	4.613168000	-2.648202000
1	-1.003712000	-2.799222000	-4.198050000	1	3.016230000	3.895365000	-2.458540000
7	2.638287000	-0.447635000	1.448265000	1	3.667460000	4.945973000	-1.205565000
6	1.545771000	0.328778000	1.310557000	6	5.816225000	3.365543000	-0.452333000
6	1.164430000	0.904176000	0.065879000	1	5.576919000	4.120699000	0.289503000
6	1.955795000	0.738839000	-1.191793000	1	6.250652000	2.510215000	0.053131000
7	3.308898000	0.324675000	-1.040864000	1	6.562408000	3.776934000	-1.121182000
6	4.228793000	0.593664000	-2.156764000	6	3.162219000	-2.108013000	-4.415760000
6	4.844441000	1.848240000	-2.228377000	1	3.901867000	-2.222043000	-5.198795000
6	5.751629000	2.082069000	-3.249077000	1	2.615914000	-3.040841000	-4.331713000
6	6.044990000	1.101650000	-4.175226000	1	2.466042000	-1.332513000	-4.708705000
6	5.423734000	-0.125772000	-4.099576000	6	4.846966000	-2.866868000	-2.683671000
6	4.500864000	-0.401006000	-3.098628000	1	5.315555000	-2.653466000	-1.729922000
6	1.404763000	1.019231000	-2.380352000	1	4.353784000	-3.831026000	-2.618114000
6	0.604899000	0.525645000	2.450282000	1	5.626978000	-2.934319000	-3.433055000
6	2.978334000	-1.044513000	2.757586000	6	4.113974000	1.167009000	3.447298000
6	3.697285000	-0.285071000	3.686886000	1	3.703899000	1.503755000	2.506177000
6	4.063622000	-0.890351000	4.880523000	6	5.653814000	1.281633000	3.364944000
6	3.737271000	-2.203577000	5.139420000	1	6.106498000	0.999454000	4.307542000
6	3.034759000	-2.938992000	4.207843000	1	6.051245000	0.636434000	2.591342000
6	2.641486000	-2.378329000	3.001472000	1	5.939425000	2.304352000	3.143578000
1	0.807345000	1.924675000	0.209143000	6	3.572907000	2.104929000	4.550077000
1	6.234664000	3.035501000	-3.319771000	1	3.832461000	3.131976000	4.317918000
1	6.753678000	1.296585000	-4.955637000	1	2.495502000	2.036443000	4.634321000
1	5.654147000	-0.878083000	-4.825760000	1	4.005285000	1.859949000	5.511990000
1	1.969726000	0.964138000	-3.300795000	6	1.907179000	-3.230208000	1.968183000
1	0.363982000	1.316055000	-2.430479000	1	1.322353000	-2.581663000	1.332477000
1	1.098143000	0.540214000	3.418507000	6	2.939754000	-3.989268000	1.102435000
1	0.004652000	1.425180000	2.303727000	1	2.435341000	-4.580324000	0.346847000
1	-0.100271000	-0.320543000	2.434751000	1	3.621591000	-3.310295000	0.604427000
1	4.613441000	-0.330571000	5.608919000	1	3.529176000	-4.651554000	1.725955000
1	4.032142000	-2.655725000	6.065444000	6	0.937268000	-4.244156000	2.609747000
1	2.790642000	-3.957774000	4.421044000	1	1.472283000	-5.035254000	3.121345000
6	4.543507000	2.959919000	-1.227744000	1	0.269921000	-3.759884000	3.309747000
1	3.822052000	2.588603000	-0.517719000	1	0.335318000	-4.699687000	1.833567000

14	4.068818000	-0.475901000	0.296524000	1	1.205710000	-1.845133000	-1.732071000
14	-2.720118000	0.367227000	-1.047661000	6	0.416990000	-3.755585000	-2.333153000
				1	-0.609955000	-3.401322000	-2.389323000
<b>Si-inter-IM<sub>1,4'</sub></b>				1	0.551947000	-4.488030000	-3.119479000
1	-1.025900000	0.755487000	-0.750522000	1	0.560914000	-4.257772000	-1.382381000
1	1.382172000	0.293351000	-0.691395000	6	1.214566000	-1.900202000	-3.870331000
7	3.203265000	-1.375597000	-0.504007000	1	1.875233000	-1.047928000	-3.957485000
6	2.998563000	-1.673446000	0.837437000	1	1.428773000	-2.595515000	-4.673891000
6	2.952322000	-0.717167000	1.803787000	1	0.189786000	-1.556142000	-3.988329000
6	3.276916000	0.711865000	1.695574000	6	6.033076000	-2.158323000	-0.362699000
7	3.450421000	1.229047000	0.405950000	1	5.517552000	-1.376296000	0.169811000
6	3.794124000	2.634375000	0.294402000	6	6.641615000	-3.135642000	0.666604000
6	5.127623000	3.021939000	0.118331000	1	7.198939000	-3.923276000	0.171837000
6	5.436558000	4.371922000	0.027071000	1	7.321642000	-2.603198000	1.323566000
6	4.453108000	5.335470000	0.090892000	1	5.873445000	-3.592963000	1.277466000
6	3.138341000	4.953024000	0.250516000	6	7.158940000	-1.508785000	-1.196958000
6	2.794164000	3.614068000	0.360252000	1	7.728631000	-2.261495000	-1.730074000
6	3.429990000	1.429993000	2.839644000	1	6.744371000	-0.815941000	-1.917842000
6	2.762889000	-3.117164000	1.213995000	1	7.838398000	-0.967367000	-0.547349000
6	3.696735000	-2.422694000	-1.377328000	6	6.247754000	1.994221000	0.041193000
6	5.033211000	-2.843486000	-1.289156000	1	5.785650000	1.027611000	-0.067189000
6	5.476741000	-3.877280000	-2.100090000	6	7.160406000	2.240638000	-1.179027000
6	4.637430000	-4.480751000	-3.012524000	1	7.679102000	3.189004000	-1.099865000
6	3.335852000	-4.043844000	-3.124910000	1	7.909431000	1.459984000	-1.246589000
6	2.849762000	-3.025793000	-2.316932000	1	6.578834000	2.240019000	-2.093411000
1	2.745222000	-1.055449000	2.814002000	6	7.069897000	1.999267000	1.348910000
1	6.457346000	4.672356000	-0.096934000	1	6.427707000	1.788207000	2.194407000
1	4.708560000	6.374548000	0.013584000	1	7.850129000	1.244390000	1.308396000
1	2.373453000	5.703289000	0.289950000	1	7.539660000	2.965846000	1.499539000
1	3.691014000	2.478201000	2.833884000	6	1.326206000	3.239915000	0.526485000
1	3.340341000	0.928586000	3.795777000	1	1.279898000	2.183979000	0.733407000
1	1.924385000	-3.533099000	0.645358000	6	0.669873000	3.993936000	1.702177000
1	3.627464000	-3.742841000	0.989737000	1	0.642667000	5.062303000	1.523403000
1	2.542644000	-3.197982000	2.280967000	1	-0.355150000	3.656108000	1.838002000
1	6.495090000	-4.203301000	-2.027554000	1	1.218715000	3.809554000	2.616993000
1	4.998260000	-5.274021000	-3.637694000	6	0.561339000	3.513794000	-0.786394000
1	2.689138000	-4.499644000	-3.848352000	1	0.999953000	2.952517000	-1.601591000
6	1.405366000	-2.578277000	-2.495737000	1	-0.482851000	3.225374000	-0.685849000

1	0.595254000	4.568743000	-1.035754000	1	-5.868994000	-1.691209000	-3.502106000
7	-2.623955000	-0.635340000	1.219032000	1	-6.743625000	-2.841125000	-2.501343000
6	-1.585416000	-0.849324000	0.440895000	6	-7.491265000	-1.112896000	-0.473165000
6	-1.534278000	-0.215971000	-0.909898000	1	-7.611257000	-2.156986000	-0.206307000
6	-2.836877000	-0.017077000	-1.636460000	1	-7.280665000	-0.547610000	0.427768000
7	-3.880104000	0.545477000	-0.858230000	1	-8.430871000	-0.758669000	-0.878880000
6	-4.979407000	1.218239000	-1.571896000	6	-2.929530000	3.899979000	-2.943089000
6	-6.155704000	0.520503000	-1.860230000	1	-3.587988000	4.627012000	-3.402891000
6	-7.184557000	1.202876000	-2.495913000	1	-1.986916000	4.388195000	-2.724688000
6	-7.050715000	2.530692000	-2.838807000	1	-2.744869000	3.102832000	-3.652612000
6	-5.878462000	3.202224000	-2.558182000	6	-3.804307000	4.471035000	-0.624560000
6	-4.823792000	2.562411000	-1.926806000	1	-4.223304000	4.078242000	0.295648000
6	-2.943922000	-0.278980000	-2.943464000	1	-2.876635000	4.981286000	-0.390106000
6	-0.368043000	-1.556204000	0.860141000	1	-4.499262000	5.197737000	-1.028078000
6	-2.7113666000	-1.241794000	2.567641000	6	-3.849482000	-3.285145000	1.499782000
6	-3.326376000	-2.489333000	2.694232000	1	-3.784826000	-2.671571000	0.612908000
6	-3.443641000	-3.023848000	3.968278000	6	-5.331252000	-3.676773000	1.690446000
6	-2.982027000	-2.336119000	5.071591000	1	-5.448162000	-4.368262000	2.515161000
6	-2.389326000	-1.100622000	4.921684000	1	-5.943071000	-2.804876000	1.887903000
6	-2.238722000	-0.525909000	3.667436000	1	-5.700354000	-4.162474000	0.793737000
1	-0.841061000	-0.780272000	-1.533250000	6	-2.986813000	-4.546575000	1.269031000
1	-8.096643000	0.690082000	-2.723228000	1	-3.341891000	-5.087533000	0.398825000
1	-7.856973000	3.041639000	-3.326496000	1	-1.947050000	-4.288475000	1.110647000
1	-5.782375000	4.232876000	-2.831889000	1	-3.044657000	-5.206016000	2.126476000
1	-3.848228000	-0.062697000	-3.496169000	6	-1.559688000	0.836423000	3.549409000
1	-2.098045000	-0.689311000	-3.480976000	1	-1.479486000	1.101949000	2.504865000
1	-0.392490000	-1.920143000	1.883618000	6	-2.395981000	1.927880000	4.254275000
1	-0.154386000	-2.371016000	0.162048000	1	-1.920943000	2.893588000	4.124516000
1	0.480580000	-0.848327000	0.717236000	1	-3.399736000	1.977919000	3.848099000
1	-3.899594000	-3.983453000	4.098321000	1	-2.468281000	1.727298000	5.316311000
1	-3.083666000	-2.764598000	6.048588000	6	-0.127450000	0.789605000	4.125871000
1	-2.033044000	-0.577432000	5.784528000	1	-0.149294000	0.603425000	5.193055000
6	-6.356612000	-0.951934000	-1.510006000	1	0.462670000	0.018380000	3.650065000
1	-5.441282000	-1.332400000	-1.081764000	1	0.375196000	1.731477000	3.952978000
6	-3.542805000	3.338562000	-1.642150000	14	2.890267000	0.356782000	-1.119129000
1	-2.823997000	2.661942000	-1.210433000	14	-4.088836000	0.484205000	0.862989000
6	-6.659621000	-1.793349000	-2.769534000				
1	-7.593053000	-1.488486000	-3.226007000				[(BDI)Ge]

7	1.367869000	0.000030000	0.544935000	1	-3.022728000	4.310187000	1.177117000
6	1.226751000	-0.000005000	1.942111000	6	-2.363469000	3.347862000	-1.333946000
6	0.024413000	-0.000061000	2.556840000	1	-1.852979000	4.275608000	-1.095883000
6	-1.310023000	-0.000089000	1.959562000	1	-1.735532000	2.771730000	-2.004424000
7	-1.375865000	-0.000023000	0.548054000	1	-3.281308000	3.591489000	-1.856003000
6	-2.697461000	-0.000001000	-0.064979000	6	-3.527622000	-3.383203000	0.924804000
6	-3.315525000	1.216344000	-0.368203000	1	-4.482352000	-3.630684000	0.475455000
6	-4.557438000	1.194788000	-0.985789000	1	-3.022669000	-4.310301000	1.176682000
6	-5.175338000	0.000053000	-1.292950000	1	-3.704941000	-2.830021000	1.838316000
6	-4.557419000	-1.194708000	-0.985933000	6	-2.363494000	-3.347762000	-1.334318000
6	-3.315504000	-1.216319000	-0.368349000	1	-1.735593000	-2.771573000	-2.004779000
6	-2.406390000	-0.000166000	2.746512000	1	-1.852986000	-4.275522000	-1.096351000
6	2.491613000	0.000029000	2.756326000	1	-3.281354000	-3.591358000	-1.856352000
6	2.698468000	0.000009000	-0.048981000	6	2.639435000	2.554275000	-0.072551000
6	3.316809000	1.216195000	-0.356932000	1	1.748699000	2.363093000	0.505314000
6	4.562568000	1.194451000	-0.966644000	6	2.217278000	3.228495000	-1.397947000
6	5.183531000	-0.000049000	-1.267502000	1	3.085565000	3.442041000	-2.010354000
6	4.562570000	-1.194525000	-0.966520000	1	1.555681000	2.583030000	-1.963866000
6	3.316814000	-1.216210000	-0.356811000	1	1.700601000	4.161759000	-1.198868000
1	0.031299000	-0.000081000	3.641785000	6	3.544911000	3.500863000	0.743822000
1	-5.043820000	2.118052000	-1.228981000	1	3.003572000	4.408931000	0.987149000
1	-6.135141000	0.000074000	-1.771112000	1	3.861388000	3.034726000	1.669238000
1	-5.043787000	-2.117951000	-1.229234000	1	4.428699000	3.779214000	0.182574000
1	-3.408703000	-0.000182000	2.344066000	6	2.639409000	-2.554252000	-0.072325000
1	-2.287098000	-0.000213000	3.823018000	1	1.748713000	-2.363012000	0.505582000
1	3.104016000	-0.877484000	2.537111000	6	2.217149000	-3.228500000	-1.397676000
1	3.103967000	0.877573000	2.537097000	1	1.700452000	-4.161741000	-1.198543000
1	2.251021000	0.000031000	3.820036000	1	1.555543000	-2.583029000	-1.963577000
1	5.047882000	2.116961000	-1.213687000	1	3.085397000	-3.442087000	-2.010125000
1	6.145549000	-0.000073000	-1.740953000	6	3.544883000	-3.500855000	0.744031000
1	5.047890000	-2.117057000	-1.213470000	1	4.428606000	-3.779309000	0.182733000
6	-2.657462000	2.553531000	-0.042164000	1	3.861465000	-3.034688000	1.669396000
1	-1.719668000	2.350651000	0.449786000	1	3.003495000	-4.408869000	0.987452000
6	-2.657432000	-2.553537000	-0.042458000	32	-0.014120000	0.000050000	-0.678908000
1	-1.719618000	-2.350705000	0.449473000				
6	-3.527684000	3.383119000	0.925133000				
1	-4.482391000	3.630657000	0.475767000	1	-0.814184000	-2.198290000	1.580198000
1	-3.705050000	2.829858000	1.838589000	1	-0.112856000	-2.310649000	0.791401000

7	1.446067000	-0.082062000	0.539437000	1	-2.079492000	3.456566000	-1.141549000
6	1.246024000	0.292296000	1.840228000	1	-4.916703000	2.503112000	-0.277533000
6	0.063790000	0.036741000	2.484140000	1	-6.232928000	0.723808000	-1.320202000
6	-1.139058000	-0.459115000	1.845897000	1	-5.289649000	-1.513551000	-1.545123000
7	-1.335311000	-0.199577000	0.515006000	1	-1.979217000	-2.570442000	-0.300007000
6	-2.692515000	-0.023048000	-0.001770000	1	-4.076322000	-3.309621000	0.860958000
6	-3.222458000	1.274027000	0.102659000	1	-3.447774000	-4.502902000	-0.266085000
6	-2.427504000	2.411287000	0.737568000	1	-4.835891000	-3.526677000	-0.706462000
6	-2.981707000	2.728892000	2.144185000	1	-2.304335000	-3.766184000	-2.424336000
6	-2.428144000	3.680990000	-0.140310000	1	-3.653641000	-2.716634000	-2.835974000
6	-4.500898000	1.520252000	-0.366876000	1	-2.025314000	-2.059494000	-2.739331000
6	-5.245780000	0.518826000	-0.955338000	1	-2.809139000	-1.805835000	2.040980000
6	-4.711630000	-0.742879000	-1.077378000	1	-1.639904000	-1.761335000	3.475255000
6	-3.438461000	-1.042417000	-0.604509000	1	2.106770000	1.085786000	3.634863000
6	-2.927737000	-2.468538000	-0.798226000	1	3.273009000	0.271840000	2.565297000
6	-3.886448000	-3.514056000	-0.185459000	1	2.672008000	1.866275000	2.145259000
6	-2.713607000	-2.769006000	-2.299102000	1	4.150058000	2.603901000	-2.030472000
6	-1.844779000	-1.513771000	2.438369000	1	5.966755000	0.971403000	-1.997913000
6	2.389552000	0.912254000	2.595996000	1	5.685872000	-1.156250000	-0.830172000
6	2.690309000	0.226240000	-0.142089000	1	2.628964000	-2.043841000	1.121355000
6	2.829493000	1.430660000	-0.837547000	1	4.502989000	-3.346618000	2.006292000
6	4.024772000	1.683939000	-1.495532000	1	5.633511000	-2.545819000	0.932414000
6	5.050457000	0.761839000	-1.481868000	1	4.856526000	-1.637695000	2.219942000
6	4.891472000	-0.437630000	-0.817393000	1	3.225302000	-4.150833000	-0.046751000
6	3.714997000	-0.726020000	-0.142846000	1	2.501363000	-2.986147000	-1.147145000
6	3.536265000	-2.079693000	0.539331000	1	4.240398000	-3.242999000	-1.163032000
6	4.709085000	-2.418925000	1.483053000	1	0.866420000	2.068901000	-0.336868000
6	3.365536000	-3.187179000	-0.525506000	1	0.365034000	3.269593000	-2.431577000
6	1.691382000	2.443720000	-0.922153000	1	0.893555000	1.626745000	-2.775915000
6	1.206508000	2.586417000	-2.382609000	1	1.996513000	2.974243000	-3.015094000
6	2.105191000	3.819669000	-0.358101000	1	1.260646000	4.500252000	-0.383441000
1	0.026273000	0.142918000	3.561530000	1	2.444034000	3.735895000	0.667712000
1	-1.408630000	2.079038000	0.840976000	1	2.905486000	4.254555000	-0.945253000
1	-2.394863000	3.511632000	2.614184000	32	0.095844000	-0.926719000	-0.524376000
1	-4.010864000	3.064378000	2.079073000				
1	-2.950132000	1.850168000	2.777402000		Ge-P <sub>1,4</sub>		
1	-1.769216000	4.425637000	0.294922000	1	0.000064000	-2.107163000	-0.381513000
1	-3.417379000	4.117019000	-0.211748000	7	1.422487000	-0.213333000	0.520486000

6	1.255038000	-0.303611000	1.834881000	1	-4.727294000	2.596992000	-1.008005000
6	-0.000020000	-0.497060000	2.438468000	1	-6.233246000	0.734534000	-1.488370000
6	-1.255033000	-0.303563000	1.834828000	1	-5.502957000	-1.563454000	-1.092113000
7	-1.422437000	-0.213317000	0.520425000	1	-2.207482000	-2.473167000	0.384953000
6	-2.746395000	0.055903000	-0.030905000	1	-4.359840000	-2.820966000	1.646520000
6	-3.140385000	1.370626000	-0.290392000	1	-3.783697000	-4.283039000	0.860076000
6	-2.211904000	2.556835000	-0.053305000	1	-5.113467000	-3.379455000	0.161596000
6	-2.794305000	3.535553000	0.989554000	1	-2.574507000	-4.151843000	-1.387497000
6	-1.935832000	3.292742000	-1.382885000	1	-3.841275000	-3.149967000	-2.089079000
6	-4.407557000	1.593898000	-0.809768000	1	-2.175017000	-2.586086000	-2.078577000
6	-5.258128000	0.544392000	-1.085093000	1	-2.847086000	0.848013000	2.694321000
6	-4.845596000	-0.751562000	-0.855527000	1	-2.165093000	-0.375010000	3.780452000
6	-3.589860000	-1.019383000	-0.331095000	1	2.164857000	-0.374948000	3.780602000
6	-3.149973000	-2.468854000	-0.138448000	1	3.250655000	-0.841032000	2.451380000
6	-4.169792000	-3.284440000	0.685193000	1	2.847116000	0.847893000	2.694460000
6	-2.921450000	-3.131828000	-1.515665000	1	4.727391000	2.596869000	-1.008062000
6	-2.447684000	-0.166689000	2.748482000	1	6.233135000	0.734341000	-1.488761000
6	2.447605000	-0.166766000	2.748643000	1	5.502746000	-1.563626000	-1.092508000
6	2.746431000	0.055855000	-0.030870000	1	2.207377000	-2.473176000	0.384908000
6	3.140477000	1.370578000	-0.290351000	1	3.783587000	-4.283068000	0.860065000
6	4.407594000	1.593791000	-0.809846000	1	5.113350000	-3.379482000	0.161573000
6	5.258060000	0.544231000	-1.085363000	1	4.359705000	-2.820960000	1.646475000
6	4.845475000	-0.751693000	-0.855816000	1	2.574265000	-4.151954000	-1.387424000
6	3.589774000	-1.019457000	-0.331226000	1	2.174814000	-2.586221000	-2.078593000
6	3.149854000	-2.468907000	-0.138513000	1	3.841050000	-3.150187000	-2.089126000
6	4.169669000	-3.284467000	0.685162000	1	1.273078000	2.176824000	0.317660000
6	2.921248000	-3.131964000	-1.515680000	1	1.247022000	4.114213000	-1.218301000
6	2.212104000	2.556815000	-0.052992000	1	1.498678000	2.614507000	-2.104497000
6	1.935503000	3.292672000	-1.382500000	1	2.850710000	3.698412000	-1.797070000
6	2.794903000	3.535580000	0.989601000	1	2.097409000	4.346956000	1.170197000
1	-0.000045000	-0.586461000	3.516363000	1	2.987115000	3.037211000	1.932236000
1	-1.272742000	2.176806000	0.316967000	1	3.725921000	3.964193000	0.637631000
1	-2.096772000	4.346956000	1.169857000	1	-3.250772000	-0.840821000	2.451055000
1	-3.725496000	3.964125000	0.637993000	32	0.000041000	-0.569691000	-0.805526000
1	-2.986071000	3.037165000	1.932269000				
1	-1.247342000	4.114318000	-1.218905000				Ge-intra- <b>TS<sub>1,4'</sub></b>
1	-2.851210000	3.698438000	-1.797124000	7	1.409862000	-0.172807000	0.489234000
1	-1.499218000	2.614624000	-2.105056000	6	1.267137000	-0.374168000	1.803901000

6	0.054984000	-0.932997000	2.277935000	1	-6.163331000	0.861877000	-1.554535000
6	-1.303439000	-0.510242000	1.840325000	1	-5.438855000	-1.462194000	-1.337658000
7	-1.394707000	-0.242079000	0.473760000	1	-2.177939000	-2.486147000	0.130723000
6	-2.702442000	0.058401000	-0.082770000	1	-3.795873000	-4.258441000	0.640999000
6	-3.108349000	1.390391000	-0.215894000	1	-5.120041000	-3.259231000	0.066898000
6	-2.212257000	2.540984000	0.224642000	1	-4.215076000	-2.781360000	1.500342000
6	-2.740236000	3.169614000	1.533147000	1	-2.678076000	-4.137064000	-1.642424000
6	-2.084073000	3.619401000	-0.871889000	1	-3.938759000	-3.090548000	-2.278880000
6	-4.363064000	1.659108000	-0.742973000	1	-2.258669000	-2.578321000	-2.342696000
6	-5.197983000	0.637471000	-1.144872000	1	-3.324757000	-0.207964000	2.424443000
6	-4.787523000	-0.672899000	-1.019868000	1	-2.133733000	-0.682203000	3.772035000
6	-3.545876000	-0.984025000	-0.485250000	1	2.185226000	-0.585978000	3.728392000
6	-3.137772000	-2.448314000	-0.355114000	1	3.342647000	-0.649431000	2.375659000
6	-4.136077000	-3.234809000	0.520399000	1	2.628429000	0.883554000	2.848468000
6	-2.994942000	-3.104147000	-1.746264000	1	4.490864000	2.776984000	-1.211747000
6	-2.319925000	-0.466135000	2.727803000	1	6.120153000	1.005447000	-1.629019000
6	2.427420000	-0.186726000	2.743287000	1	5.572029000	-1.312957000	-1.097206000
6	2.715084000	0.151783000	-0.083558000	1	2.441972000	-2.388580000	0.583766000
6	3.005721000	1.475280000	-0.412777000	1	4.152114000	-4.059563000	0.973897000
6	4.247771000	1.764394000	-0.961715000	1	5.346059000	-3.149157000	0.073703000
6	5.167509000	0.766948000	-1.199018000	1	4.744666000	-2.528746000	1.603263000
6	4.857111000	-0.542687000	-0.893038000	1	2.762437000	-4.120340000	-1.162142000
6	3.634528000	-0.875641000	-0.331311000	1	2.137337000	-2.627652000	-1.847596000
6	3.317937000	-2.341713000	-0.042327000	1	3.837473000	-3.034436000	-2.037801000
6	4.466859000	-3.058643000	0.699392000	1	1.082661000	2.164820000	0.159049000
6	2.992173000	-3.078766000	-1.360977000	1	0.947158000	4.077827000	-1.397442000
6	1.998732000	2.600319000	-0.205821000	1	1.315073000	2.597019000	-2.271729000
6	1.693045000	3.306269000	-1.544928000	1	2.582916000	3.771744000	-1.951210000
6	2.505499000	3.617259000	0.839433000	1	1.758733000	4.386660000	1.004309000
1	0.081742000	-1.251182000	3.315724000	1	2.709487000	3.132888000	1.787180000
1	-1.235538000	2.126990000	0.415087000	1	3.416676000	4.096286000	0.500384000
1	-2.087657000	3.976331000	1.853743000	1	0.132391000	-1.980872000	1.247450000
1	-3.734439000	3.576157000	1.382795000	1	0.154850000	-2.202148000	0.289059000
1	-2.782195000	2.427233000	2.318698000	32	-0.013513000	-0.692129000	-0.711756000
1	-1.378804000	4.381915000	-0.558169000				
1	-3.033779000	4.106897000	-1.056196000				
1	-1.734654000	3.187538000	-1.802303000	7	1.446730000	-0.279352000	0.484072000
1	-4.689903000	2.674412000	-0.841452000	6	1.276319000	-0.421741000	1.754159000

6	0.016719000	-1.078240000	2.243247000	1	-6.238036000	0.851092000	-1.418505000
6	-1.298445000	-0.462487000	1.812085000	1	-5.544186000	-1.474658000	-1.116095000
7	-1.403394000	-0.271656000	0.444496000	1	-2.222126000	-2.471300000	0.235509000
6	-2.720828000	0.053756000	-0.074058000	1	-3.832888000	-4.211835000	0.891515000
6	-3.108337000	1.383297000	-0.263357000	1	-5.172602000	-3.231036000	0.323027000
6	-2.167537000	2.539813000	0.045379000	1	-4.214829000	-2.694819000	1.699416000
6	-2.661423000	3.345790000	1.266562000	1	-2.805064000	-4.189059000	-1.448374000
6	-2.005530000	3.465670000	-1.178998000	1	-4.080243000	-3.152586000	-2.076039000
6	-4.383187000	1.649975000	-0.743214000	1	-2.398569000	-2.658789000	-2.214898000
6	-5.257611000	0.627839000	-1.045468000	1	-3.220274000	0.161330000	2.471570000
6	-4.864622000	-0.682909000	-0.871289000	1	-2.040659000	-0.408507000	3.787383000
6	-3.603691000	-0.989107000	-0.383269000	1	2.547084000	-0.981895000	3.357332000
6	-3.203578000	-2.450075000	-0.206387000	1	3.203746000	0.350698000	2.371298000
6	-4.172126000	-3.192019000	0.738052000	1	1.845141000	0.624728000	3.502522000
6	-3.118334000	-3.157724000	-1.576349000	1	4.548877000	2.785079000	-0.998591000
6	-2.242665000	-0.212946000	2.741832000	1	6.196107000	1.038915000	-1.449254000
6	2.298358000	-0.076362000	2.793547000	1	5.630252000	-1.307751000	-1.070962000
6	2.754177000	0.106900000	-0.061349000	1	2.372877000	-2.470314000	0.314241000
6	3.041196000	1.445991000	-0.316058000	1	4.071096000	-4.134547000	0.891266000
6	4.299737000	1.761311000	-0.808192000	1	5.351539000	-3.121783000	0.253878000
6	5.230045000	0.776700000	-1.065818000	1	4.474268000	-2.619541000	1.690014000
6	4.911088000	-0.547017000	-0.845713000	1	2.959513000	-4.118029000	-1.417023000
6	3.670419000	-0.909122000	-0.342377000	1	2.455881000	-2.593574000	-2.133438000
6	3.337409000	-2.388108000	-0.159573000	1	4.163552000	-3.016628000	-2.076185000
6	4.376883000	-3.106990000	0.726302000	1	1.082330000	2.099495000	0.188451000
6	3.223741000	-3.073087000	-1.539571000	1	1.036799000	4.111535000	-1.231342000
6	2.020208000	2.554574000	-0.088808000	1	1.447531000	2.690071000	-2.180396000
6	1.788719000	3.349170000	-1.392143000	1	2.698811000	3.838977000	-1.716588000
6	2.465836000	3.499157000	1.048557000	1	1.709964000	4.258049000	1.219721000
1	0.042993000	-1.150891000	3.331125000	1	2.618733000	2.957012000	1.974427000
1	-1.206494000	2.112737000	0.281041000	1	3.393312000	3.997062000	0.790165000
1	-1.970390000	4.153811000	1.488647000	1	0.052394000	-2.098066000	1.822202000
1	-3.635442000	3.779494000	1.068837000	1	0.095313000	-2.198515000	-0.467152000
1	-2.735943000	2.708280000	2.137716000	32	-0.056803000	-0.655952000	-0.859488000
1	-1.302048000	4.260267000	-0.955268000				
1	-2.948791000	3.926210000	-1.447031000				
1	-1.639333000	2.908868000	-2.032977000	7	-1.414112000	-0.187551000	0.531316000
1	-4.693502000	2.665851000	-0.883923000	6	-1.270057000	-0.289075000	1.845791000

6	-0.013537000	-0.429512000	2.468577000	1	6.193973000	0.665070000	-1.661929000
6	1.323128000	-0.297331000	1.807089000	1	4.718062000	2.549268000	-1.174873000
7	1.441366000	-0.210860000	0.498815000	1	1.298522000	2.182432000	0.253074000
6	2.752651000	0.043104000	-0.088976000	1	2.205715000	4.297716000	1.193907000
6	3.582160000	-1.045390000	-0.376136000	1	3.821706000	3.847913000	0.673745000
6	3.172171000	-2.483106000	-0.067510000	1	3.003555000	2.908872000	1.916835000
6	4.053713000	-3.066628000	1.058559000	1	1.304411000	4.182460000	-1.173312000
6	3.238482000	-3.370420000	-1.328573000	1	2.915341000	3.805508000	-1.755300000
6	4.823030000	-0.796874000	-0.944451000	1	1.567047000	2.746627000	-2.154274000
6	5.230156000	0.490449000	-1.225612000	1	3.235862000	0.498345000	2.473311000
6	4.395411000	1.553087000	-0.949276000	1	2.168341000	-0.260659000	3.779818000
6	3.144165000	1.351626000	-0.384550000	1	-2.836060000	0.798474000	2.814787000
6	2.248514000	2.553430000	-0.097479000	1	-3.294049000	-0.835122000	2.365314000
6	2.862917000	3.456990000	0.994623000	1	-2.213330000	-0.564290000	3.753814000
6	1.994940000	3.372186000	-1.381931000	1	-5.372324000	-1.672337000	-1.270535000
6	2.262949000	0.131024000	2.771643000	1	-6.168517000	0.601966000	-1.667615000
6	-2.474458000	-0.229966000	2.748664000	1	-4.763815000	2.512152000	-1.080046000
6	-2.729578000	0.029552000	-0.062505000	1	-1.353509000	2.205854000	0.378081000
6	-3.516128000	-1.073763000	-0.416517000	1	-2.327603000	4.269936000	1.344728000
6	-4.755993000	-0.841025000	-0.994389000	1	-3.918177000	3.821128000	0.750499000
6	-5.206223000	0.441970000	-1.222691000	1	-3.150427000	2.865519000	2.005417000
6	-4.412492000	1.518663000	-0.888067000	1	-1.384868000	4.225499000	-1.018951000
6	-3.162965000	1.335072000	-0.314284000	1	-1.576417000	2.793404000	-2.021030000
6	-2.305992000	2.554973000	0.012586000	1	-2.967909000	3.805657000	-1.648737000
6	-2.969411000	3.430249000	1.099166000	1	-2.088565000	-2.501010000	0.269371000
6	-2.044554000	3.397344000	-1.255190000	1	-2.551773000	-4.257167000	-1.392444000
6	-3.058817000	-2.516445000	-0.201419000	1	-2.194266000	-2.729370000	-2.182804000
6	-2.908214000	-3.245281000	-1.555243000	1	-3.858854000	-3.299127000	-2.073173000
6	-4.037118000	-3.292463000	0.708964000	1	-3.657295000	-4.292661000	0.888563000
1	0.001120000	-0.941040000	3.426642000	1	-4.164373000	-2.801542000	1.666304000
1	2.147992000	-2.476036000	0.268149000	1	-5.011218000	-3.382770000	0.243284000
1	3.730776000	-4.073737000	1.302393000	1	0.811107000	0.675556000	2.897024000
1	5.091942000	-3.109329000	0.749322000	1	0.005745000	0.890824000	-1.368623000
1	3.986811000	-2.457571000	1.951941000	32	-0.002615000	-0.575069000	-0.794573000
1	2.889449000	-4.370439000	-1.092807000				
1	4.252278000	-3.448599000	-1.703345000				<i>Ge-inter-TS<sub>4',4-I</sub></i>
1	2.608081000	-2.964052000	-2.109626000	7	3.726732000	0.500634000	-0.944616000
1	5.475328000	-1.616880000	-1.166659000	6	2.539267000	0.353325000	-1.423776000

6	1.382086000	0.438565000	-0.475073000	1	2.667277000	-2.947787000	6.145305000
6	1.393433000	-0.481062000	0.721679000	1	2.147588000	-0.561751000	6.066094000
7	2.474219000	-0.404113000	1.499848000	1	1.806471000	1.383952000	2.914229000
6	2.517194000	-1.132422000	2.767940000	1	0.377189000	2.418356000	4.592702000
6	2.838397000	-2.491549000	2.803336000	1	0.755204000	1.171269000	5.765547000
6	3.173457000	-3.289484000	1.548774000	1	-0.174451000	0.767358000	4.330683000
6	2.192683000	-4.463281000	1.335667000	1	4.026398000	1.712893000	3.966004000
6	4.622735000	-3.816693000	1.629014000	1	2.891158000	2.942167000	4.506279000
6	2.877488000	-3.128385000	4.034971000	1	3.298117000	1.592639000	5.559214000
6	2.627092000	-2.439080000	5.202536000	1	0.262471000	-1.958037000	1.765843000
6	2.331194000	-1.093796000	5.155043000	1	-0.255536000	-1.601002000	0.059163000
6	2.265623000	-0.420217000	3.944203000	1	1.553323000	1.050940000	-3.159168000
6	1.942602000	1.071318000	3.936980000	1	3.079622000	0.192121000	-3.513298000
6	0.640458000	1.372010000	4.707262000	1	1.607859000	-0.694498000	-3.005042000
6	3.117191000	1.881240000	4.530428000	1	7.373818000	-0.926421000	-3.373388000
6	0.232138000	-1.232377000	0.959446000	1	7.815101000	1.324181000	-4.207283000
6	2.201954000	0.215663000	-2.873264000	1	6.421345000	3.195834000	-3.486509000
6	4.877625000	0.708592000	-1.837209000	1	3.455356000	2.862447000	-1.263382000
6	5.692192000	-0.363036000	-2.195282000	1	3.150636000	4.845956000	-2.642252000
6	6.743922000	-0.117318000	-3.066753000	1	4.613607000	4.513749000	-3.546799000
6	6.995975000	1.153730000	-3.537403000	1	3.228673000	3.444877000	-3.702110000
6	6.203806000	2.208431000	-3.134772000	1	4.570237000	4.923421000	-0.504123000
6	5.130865000	2.010149000	-2.278827000	1	5.470118000	3.498305000	-0.002441000
6	4.309981000	3.213467000	-1.818870000	1	6.035738000	4.460988000	-1.361672000
6	3.795239000	4.053735000	-3.006904000	1	4.729184000	-1.724068000	-0.876346000
6	5.154395000	4.081123000	-0.858771000	1	6.580897000	-3.320818000	-0.631725000
6	5.467553000	-1.773535000	-1.662181000	1	7.132459000	-1.692421000	-0.264525000
6	6.767463000	-2.340744000	-1.051491000	1	7.540306000	-2.443188000	-1.802935000
6	4.942247000	-2.705640000	-2.775960000	1	4.759699000	-3.698158000	-2.378363000
1	0.435472000	0.339950000	-1.008311000	1	4.016234000	-2.333513000	-3.198249000
1	3.103152000	-2.627361000	0.699786000	1	5.669604000	-2.788404000	-3.575217000
1	2.433196000	-4.983304000	0.413999000	1	1.436570000	1.461005000	-0.061005000
1	2.264248000	-5.175333000	2.149342000	1	3.308234000	2.012505000	1.042812000
1	1.170339000	-4.115645000	1.272490000	7	-3.162673000	1.404208000	0.297060000
1	4.874872000	-4.352549000	0.720299000	6	-2.784357000	0.902795000	1.466980000
1	4.736159000	-4.500178000	2.461618000	6	-2.334287000	-0.438980000	1.623915000
1	5.321722000	-2.999749000	1.758749000	6	-2.816314000	-1.604573000	0.827809000
1	3.113123000	-4.172101000	4.080747000	7	-3.344127000	-1.338153000	-0.431554000

6	-3.936810000	-2.439667000	-1.161304000	1	0.249247000	-3.801945000	-2.113787000
6	-5.284573000	-2.770211000	-0.964595000	1	-1.009916000	-4.897669000	-2.657144000
6	-6.153942000	-1.994849000	0.016006000	1	-0.952844000	-4.392922000	-0.971598000
6	-6.449015000	-2.839974000	1.274633000	1	-0.418782000	-2.112261000	-3.906583000
6	-7.474503000	-1.534433000	-0.637023000	1	-1.735139000	-3.126920000	-4.473488000
6	-5.831445000	-3.830228000	-1.671231000	1	-2.062227000	-1.479334000	-3.953098000
6	-5.076433000	-4.552504000	-2.572544000	1	-2.979678000	-3.733960000	0.840628000
6	-3.754383000	-4.219901000	-2.772545000	1	-2.295902000	-2.947100000	2.378172000
6	-3.168447000	-3.174888000	-2.072191000	1	-2.218850000	2.711225000	2.519368000
6	-1.697574000	-2.855050000	-2.310194000	1	-3.807034000	2.087497000	2.920307000
6	-0.797545000	-4.068176000	-1.992808000	1	-2.368700000	1.266646000	3.546329000
6	-1.466019000	-2.361621000	-3.754670000	1	-6.232275000	4.820652000	0.180747000
6	-2.680387000	-2.840444000	1.370328000	1	-4.498025000	6.519026000	-0.100069000
6	-2.780988000	1.792095000	2.686507000	1	-2.153707000	5.851491000	-0.275172000
6	-3.532908000	2.807527000	0.178255000	1	-0.967864000	2.346259000	0.071352000
6	-4.878484000	3.177726000	0.226040000	1	0.888172000	3.853933000	0.613015000
6	-5.204044000	4.523987000	0.133613000	1	-0.129886000	5.263352000	0.404119000
6	-4.228808000	5.483584000	-0.029143000	1	-0.424176000	4.161662000	1.739419000
6	-2.905541000	5.104188000	-0.120376000	1	0.366279000	3.266339000	-1.829167000
6	-2.537634000	3.771332000	-0.023125000	1	-1.290434000	2.881444000	-2.296180000
6	-1.072139000	3.385283000	-0.195517000	1	-0.817070000	4.552363000	-2.015548000
6	-0.130213000	4.220838000	0.697972000	1	-5.544208000	1.167931000	0.337376000
6	-0.677940000	3.530413000	-1.683145000	1	-7.702795000	1.488621000	-0.831974000
6	-5.995104000	2.146663000	0.335780000	1	-6.361473000	2.079022000	-1.803976000
6	-6.925653000	2.240609000	-0.893816000	1	-7.400658000	3.213252000	-0.947667000
6	-6.802060000	2.320622000	1.640274000	1	-7.561996000	1.549772000	1.713271000
1	-2.218299000	-0.709944000	2.671484000	1	-6.160133000	2.246698000	2.510336000
1	-5.594253000	-1.122217000	0.309721000	1	-7.295947000	3.285388000	1.663725000
1	-7.047971000	-2.269991000	1.979277000	1	-0.891838000	-0.502438000	1.283921000
1	-7.000103000	-3.735738000	1.008135000	1	-1.468390000	0.260465000	-1.130080000
1	-5.525695000	-3.127744000	1.758177000	32	4.076080000	0.619557000	1.065714000
1	-8.027080000	-0.903469000	0.052228000	32	-3.052025000	0.313986000	-1.381309000
1	-8.104897000	-2.380064000	-0.885971000				
1	-7.280924000	-0.972184000	-1.542333000				<i>Ge-inter-IM<sub>4',4</sub></i>
1	-6.859085000	-4.092717000	-1.518821000	7	3.158026000	-1.415665000	-0.412643000
1	-5.516802000	-5.366447000	-3.114805000	6	2.428403000	-1.526668000	0.739886000
1	-3.169898000	-4.779808000	-3.475725000	6	1.723761000	-0.486393000	1.294867000
1	-1.432580000	-2.057555000	-1.638568000	7	2.804164000	1.367488000	0.118932000

6	3.414583000	2.662695000	0.309577000	1	0.566941000	4.448662000	-2.715937000
6	4.234603000	2.895577000	1.432152000	1	1.676620000	5.611069000	-2.017858000
6	4.509348000	1.815323000	2.473512000	1	3.932697000	2.831233000	-3.154870000
6	3.859046000	2.168260000	3.829275000	1	2.533685000	3.456980000	-4.017868000
6	6.026964000	1.602247000	2.666097000	1	3.659948000	4.568501000	-3.250792000
6	4.825624000	4.135821000	1.600708000	1	1.619886000	-2.867815000	2.215809000
6	4.653269000	5.146067000	0.676378000	1	2.034383000	-3.659752000	0.674452000
6	3.867748000	4.916545000	-0.428452000	1	3.305435000	-3.198052000	1.786700000
6	3.231800000	3.695747000	-0.621564000	1	7.041169000	-3.883438000	-0.484560000
6	2.345417000	3.541288000	-1.852716000	1	6.139048000	-5.458467000	-2.121032000
6	1.244864000	4.626492000	-1.885861000	1	3.896824000	-5.116377000	-3.031132000
6	3.175748000	3.603099000	-3.153825000	1	1.607634000	-2.417157000	-1.902369000
6	2.335223000	-2.889637000	1.390849000	1	0.273606000	-4.249163000	-2.902118000
6	3.980169000	-2.516413000	-0.873517000	1	1.710184000	-5.220339000	-3.122630000
6	5.287059000	-2.678084000	-0.399420000	1	1.144934000	-4.867291000	-1.499407000
6	6.042951000	-3.750864000	-0.851091000	1	1.312048000	-2.449305000	-4.373348000
6	5.540114000	-4.637190000	-1.778820000	1	2.824036000	-1.686896000	-3.894272000
6	4.271203000	-4.445707000	-2.283896000	1	2.830428000	-3.327371000	-4.531047000
6	3.481435000	-3.393037000	-1.847206000	1	5.189654000	-0.917819000	0.779329000
6	2.113053000	-3.172588000	-2.481034000	1	7.557365000	-0.230875000	0.486276000
6	1.259807000	-4.459051000	-2.497823000	1	6.759955000	-0.473412000	-1.062966000
6	2.281950000	-2.623262000	-3.915653000	1	7.871903000	-1.688654000	-0.441148000
6	5.926957000	-1.669210000	0.546535000	1	6.817125000	-1.583304000	2.523607000
6	7.107779000	-0.970599000	-0.166067000	1	5.580021000	-2.821038000	2.367312000
6	6.401679000	-2.331238000	1.857595000	1	7.169651000	-3.071264000	1.663154000
1	1.114257000	-0.732911000	2.161190000	1	1.599226000	0.084208000	-1.720833000
1	4.081324000	0.893675000	2.116203000	7	-2.945629000	-1.453765000	0.631495000
1	4.035312000	1.372638000	4.547627000	6	-1.784274000	-1.399371000	0.072396000
1	4.283994000	3.083443000	4.227873000	6	-1.898056000	1.096577000	-0.629072000
1	2.792735000	2.298993000	3.711882000	7	-3.086468000	1.314612000	-0.178567000
1	6.201351000	0.758725000	3.326603000	6	-3.818969000	2.547264000	-0.517760000
1	6.491349000	2.473946000	3.112215000	6	-4.707356000	2.539940000	-1.592320000
1	6.510642000	1.406714000	1.718453000	6	-4.938714000	1.299624000	-2.448877000
1	5.441317000	4.312140000	2.459974000	6	-4.272036000	1.464042000	-3.832863000
1	5.130072000	6.096592000	0.816558000	6	-6.443761000	0.999063000	-2.611151000
1	3.737314000	5.697242000	-1.151184000	6	-5.384468000	3.714524000	-1.883056000
1	1.870331000	2.575170000	-1.799098000	6	-5.204064000	4.846174000	-1.114982000
1	0.675329000	4.631362000	-0.964326000	6	-4.343618000	4.821610000	-0.038205000

6	-3.631522000	3.674753000	0.283957000	1	-5.145861000	-6.044915000	2.086733000
6	-2.712682000	3.678636000	1.504485000	1	-3.698122000	-4.833928000	3.636007000
6	-1.734581000	4.872120000	1.490704000	1	-1.947696000	-1.651828000	2.808869000
6	-3.563326000	3.692635000	2.794952000	1	-0.648856000	-2.809319000	4.512223000
6	-0.985112000	-2.590980000	-0.329715000	1	-1.704147000	-4.206711000	4.449521000
6	-3.553459000	-2.739146000	1.015079000	1	-0.692878000	-3.810491000	3.068256000
6	-4.401618000	-3.398470000	0.127644000	1	-2.673125000	-1.378295000	5.150040000
6	-4.960684000	-4.600756000	0.535499000	1	-4.043907000	-1.256883000	4.056610000
6	-4.702473000	-5.115992000	1.788229000	1	-3.785001000	-2.731032000	4.977900000
6	-3.881609000	-4.432734000	2.660731000	1	-4.273967000	-1.875723000	-1.353669000
6	-3.290907000	-3.232012000	2.295256000	1	-6.488380000	-2.227656000	-2.374076000
6	-2.414380000	-2.489478000	3.302270000	1	-6.642311000	-1.989812000	-0.637094000
6	-1.295615000	-3.391501000	3.865204000	1	-6.781344000	-3.601630000	-1.327110000
6	-3.288310000	-1.928100000	4.446427000	1	-4.403920000	-3.335553000	-3.341485000
6	-4.738193000	-2.845204000	-1.252595000	1	-3.126854000	-3.909743000	-2.277300000
6	-6.262983000	-2.653983000	-1.403685000	1	-4.671949000	-4.739179000	-2.322355000
6	-4.196796000	-3.766609000	-2.367891000	1	-2.839149000	0.524039000	2.187918000
1	-4.488721000	0.456348000	-1.946922000	6	1.822957000	0.953028000	1.017657000
1	-4.414472000	0.568513000	-4.428493000	6	0.981652000	1.816831000	1.663806000
1	-4.712376000	2.299255000	-4.364709000	1	1.070771000	2.887793000	1.531795000
1	-3.208550000	1.647073000	-3.739521000	1	0.337161000	1.456714000	2.461669000
1	-6.575860000	0.078499000	-3.167423000	6	-1.115375000	-0.082127000	-0.145970000
1	-6.944514000	1.788444000	-3.157250000	1	-0.214973000	-0.207796000	-0.756492000
1	-6.920142000	0.890308000	-1.644703000	1	-0.715146000	0.247822000	0.836754000
1	-6.060125000	3.743758000	-2.712623000	32	-4.005412000	0.160346000	1.186967000
1	-5.738490000	5.744361000	-1.352435000	32	3.193064000	0.250506000	-1.424491000
1	-4.220732000	5.701247000	0.558824000	6	-1.129023000	2.016516000	-1.506532000
1	-2.122835000	2.776012000	1.505465000	1	-0.240189000	2.307292000	-0.930396000
1	-1.047496000	4.786053000	2.324476000	1	-0.754379000	1.467125000	-2.376082000
1	-2.259404000	5.814879000	1.585719000	1	-1.693506000	2.894511000	-1.806341000
1	-1.154125000	4.891413000	0.577369000				
1	-2.918303000	3.665496000	3.666174000		<b>Ge-inter-TS<sub>4',4-II</sub></b>		
1	-4.168460000	4.590343000	2.842305000	7	-2.547146000	-1.574075000	0.715038000
1	-4.222992000	2.834123000	2.831358000	6	-1.493960000	-1.373479000	-0.024861000
1	0.057634000	-2.422474000	-0.041140000	6	-1.165788000	-0.028662000	-0.528616000
1	-1.367261000	-3.519524000	0.085305000	6	-2.228092000	0.888016000	-0.982718000
1	-0.990675000	-2.647759000	-1.423647000	7	-3.367217000	0.960818000	-0.368469000
1	-5.606810000	-5.134296000	-0.130874000	6	-4.379262000	1.962401000	-0.740950000

6	-5.328412000	1.661964000	-1.718097000	1	-1.969610000	5.027027000	1.622739000
6	-5.378020000	0.315515000	-2.432646000	1	-3.461428000	5.690427000	0.987286000
6	-5.011171000	0.466224000	-3.925776000	1	-4.559085000	2.470013000	2.595402000
6	-6.774792000	-0.327651000	-2.291635000	1	-3.428602000	3.655743000	3.229697000
6	-6.265932000	2.633053000	-2.038698000	1	-4.924029000	4.183635000	2.465107000
6	-6.279337000	3.850004000	-1.391340000	1	-2.531290000	2.590585000	-2.283900000
6	-5.353942000	4.115540000	-0.404560000	1	-1.738114000	1.171228000	-3.023571000
6	-4.386836000	3.182751000	-0.058993000	1	0.322192000	-2.120130000	-0.875750000
6	-3.402735000	3.507588000	1.063366000	1	-0.307467000	-3.102467000	0.464325000
6	-2.741364000	4.889151000	0.873833000	1	-1.106082000	-3.162125000	-1.102668000
6	-4.128216000	3.448907000	2.427359000	1	-4.384721000	-5.799758000	0.628731000
6	-1.830391000	1.777514000	-2.116537000	1	-3.518699000	-6.327671000	2.848950000
6	-0.581261000	-2.503194000	-0.405801000	1	-2.263456000	-4.651837000	4.104944000
6	-2.823189000	-2.899158000	1.290604000	1	-1.318057000	-1.313708000	2.779703000
6	-3.582066000	-3.828317000	0.579478000	1	0.215559000	-1.906178000	4.555618000
6	-3.812394000	-5.067426000	1.160350000	1	-0.575178000	-3.446054000	4.824393000
6	-3.328667000	-5.365966000	2.415542000	1	0.312148000	-3.164644000	3.335283000
6	-2.614920000	-4.420094000	3.121021000	1	-2.045016000	-0.817359000	5.091958000
6	-2.350587000	-3.171393000	2.578749000	1	-3.433634000	-1.122027000	4.060046000
6	-1.609519000	-2.132283000	3.418010000	1	-2.879337000	-2.366273000	5.169154000
6	-0.334533000	-2.705336000	4.071761000	1	-3.922386000	-2.521277000	-1.067940000
6	-2.555997000	-1.572981000	4.505384000	1	-6.206484000	-3.319853000	-1.607599000
6	-4.209839000	-3.520307000	-0.775903000	1	-6.089718000	-2.836266000	0.081113000
6	-5.749970000	-3.555164000	-0.653726000	1	-6.086296000	-4.539901000	-0.353450000
6	-3.740910000	-4.506599000	-1.867910000	1	-4.165398000	-4.227242000	-2.826263000
1	-0.360754000	-0.085813000	-1.265921000	1	-2.662126000	-4.512224000	-1.961991000
1	-4.662840000	-0.343802000	-1.964288000	1	-4.064259000	-5.515004000	-1.640637000
1	-5.012878000	-0.503672000	-4.411915000	1	-0.602816000	0.611532000	0.337208000
1	-5.732559000	1.098010000	-4.430346000	1	-2.668668000	0.578260000	2.024793000
1	-4.031096000	0.909480000	-4.049925000	1	-0.833557000	2.170298000	-1.902418000
1	-6.781094000	-1.303486000	-2.762969000	7	3.462181000	-1.072466000	-0.524973000
1	-7.531808000	0.278010000	-2.773636000	6	2.664985000	-1.422250000	0.513922000
1	-7.039056000	-0.444978000	-1.248300000	6	1.710138000	-0.579941000	1.050459000
1	-6.995137000	2.432032000	-2.796294000	6	1.569445000	0.853563000	0.888994000
1	-7.014072000	4.586432000	-1.649586000	7	2.491755000	1.526763000	0.118539000
1	-5.381117000	5.057022000	0.103570000	6	2.821640000	2.895886000	0.449472000
1	-2.621182000	2.764608000	1.070274000	6	3.518079000	3.176131000	1.639834000
1	-2.284499000	4.974357000	-0.103649000	6	3.942228000	2.076977000	2.608999000

6	3.164062000	2.177494000	3.939264000	1	2.117667000	3.819335000	-3.870219000
6	5.461249000	2.132368000	2.883183000	1	2.958279000	5.059457000	-2.949158000
6	3.848798000	4.486518000	1.941637000	1	3.537592000	3.397166000	-2.922339000
6	3.537715000	5.520351000	1.082663000	1	0.356980000	2.547289000	1.423635000
6	2.878046000	5.243681000	-0.092517000	1	-0.067492000	0.956841000	2.269828000
6	2.501360000	3.947054000	-0.420176000	1	2.582915000	-3.569481000	0.282769000
6	1.749858000	3.724999000	-1.728566000	1	3.778906000	-3.017846000	1.441381000
6	0.483123000	4.606413000	-1.798910000	1	2.063213000	-2.972739000	1.874951000
6	2.653612000	4.018740000	-2.946758000	1	7.707501000	-2.836868000	-0.627447000
6	0.468447000	1.470176000	1.475828000	1	7.122466000	-4.420273000	-2.394710000
6	2.773430000	-2.825889000	1.061144000	1	4.869677000	-4.411310000	-3.344225000
6	4.468639000	-1.988195000	-1.027585000	1	2.131743000	-2.209223000	-2.124949000
6	5.770276000	-1.957847000	-0.517392000	1	1.120858000	-4.171890000	-3.209299000
6	6.709377000	-2.849115000	-1.017260000	1	2.694787000	-4.896907000	-3.462610000
6	6.384061000	-3.739982000	-2.017685000	1	2.074109000	-4.713131000	-1.830967000
6	5.109971000	-3.737231000	-2.546520000	1	1.881896000	-2.169501000	-4.594135000
6	4.142169000	-2.867088000	-2.068502000	1	3.245203000	-1.197668000	-4.053354000
6	2.764895000	-2.843217000	-2.722266000	1	3.523597000	-2.783924000	-4.762685000
6	2.127322000	-4.246272000	-2.808218000	1	5.331327000	-0.343153000	0.783216000
6	2.861576000	-2.207078000	-4.126886000	1	7.551195000	0.750684000	0.686225000
6	6.194025000	-0.940142000	0.534852000	1	6.889895000	0.507748000	-0.926118000
6	7.271076000	0.002723000	-0.047370000	1	8.161477000	-0.550641000	-0.323373000
6	6.711397000	-1.627228000	1.816729000	1	6.966377000	-0.881846000	2.562178000
1	1.061661000	-1.012933000	1.805323000	1	5.959414000	-2.285125000	2.237197000
1	3.720526000	1.126638000	2.153201000	1	7.599105000	-2.214416000	1.610971000
1	3.450144000	1.367156000	4.603436000	1	1.756877000	0.186509000	-1.900004000
1	3.382118000	3.116040000	4.437496000	32	3.247971000	0.637991000	-1.446660000
1	2.099199000	2.118730000	3.760014000	32	-3.834655000	-0.143588000	1.245846000
1	5.758579000	1.282347000	3.489307000				
1	5.730698000	3.033998000	3.420602000		Ge-intra-TS <sub>1,2'</sub>		
1	6.018934000	2.108681000	1.955915000	1	1.064214000	-1.596073000	0.193183000
1	4.369854000	4.701039000	2.853127000	1	0.310792000	-2.150763000	-0.250599000
1	3.813589000	6.527924000	1.325522000	7	1.492069000	-0.388162000	0.513678000
1	2.646566000	6.045213000	-0.765015000	6	1.299361000	-0.328809000	1.918401000
1	1.447695000	2.689006000	-1.765635000	6	0.075899000	-0.305765000	2.483026000
1	-0.073308000	4.393343000	-2.706891000	6	-1.258218000	-0.165798000	1.882033000
1	0.743207000	5.657515000	-1.813526000	7	-1.373436000	-0.132789000	0.484865000
1	-0.157806000	4.429795000	-0.944154000	6	-2.713070000	-0.080584000	-0.089343000

6	-3.273592000	1.147233000	-0.453586000	1	-4.692691000	-3.614364000	0.651371000
6	-2.532814000	2.462222000	-0.245442000	1	-3.895109000	-2.778997000	1.980865000
6	-3.221431000	3.310365000	0.846001000	1	-2.121732000	-4.429878000	-0.890268000
6	-2.425719000	3.258838000	-1.563831000	1	-3.499483000	-3.682976000	-1.688904000
6	-4.545343000	1.161102000	-1.009239000	1	-1.900859000	-2.969130000	-1.843369000
6	-5.246181000	-0.009476000	-1.209014000	1	-3.328018000	0.060514000	2.340355000
6	-4.683081000	-1.217399000	-0.852786000	1	-2.168028000	-0.081289000	3.781371000
6	-3.418407000	-1.273803000	-0.287192000	1	2.267179000	-0.408891000	3.826074000
6	-2.826091000	-2.626374000	0.096525000	1	3.104709000	-1.317555000	2.552757000
6	-3.731990000	-3.378045000	1.093811000	1	3.207521000	0.437221000	2.584668000
6	-2.572596000	-3.481727000	-1.164439000	1	4.219794000	3.045804000	-0.836439000
6	-2.318706000	-0.052276000	2.709247000	1	6.011514000	1.519909000	-1.494984000
6	2.539091000	-0.406207000	2.769484000	1	5.715205000	-0.888846000	-1.259039000
6	2.744042000	0.123567000	-0.041102000	1	2.813296000	-2.498443000	0.373659000
6	2.894048000	1.504743000	-0.201759000	1	4.653660000	-4.041887000	0.317938000
6	4.085577000	1.989743000	-0.718645000	1	5.671454000	-2.925732000	-0.564526000
6	5.097660000	1.130879000	-1.091390000	1	5.216452000	-2.567759000	1.096398000
6	4.928959000	-0.230506000	-0.953064000	1	3.005289000	-3.892664000	-1.668028000
6	3.759627000	-0.758381000	-0.423903000	1	2.260892000	-2.346034000	-2.054000000
6	3.596244000	-2.273584000	-0.334891000	1	3.949491000	-2.625526000	-2.447765000
6	4.869892000	-2.990781000	0.160595000	1	0.907799000	1.919277000	0.441522000
6	3.173259000	-2.821983000	-1.717152000	1	0.584459000	4.022520000	-0.781998000
6	1.783281000	2.484960000	0.164276000	1	1.127572000	2.771029000	-1.892665000
6	1.415085000	3.376507000	-1.041499000	1	2.248578000	4.004053000	-1.332397000
6	2.185496000	3.357484000	1.372750000	1	1.374625000	4.029294000	1.633321000
1	0.054488000	-0.349086000	3.567098000	1	2.409033000	2.745355000	2.237225000
1	-1.537371000	2.224220000	0.091879000	1	3.059828000	3.953651000	1.137871000
1	-4.232922000	3.566014000	0.551003000	32	-0.064522000	-0.422891000	-0.783596000
1	-3.258763000	2.765399000	1.780387000				
1	-2.671500000	4.232433000	1.007088000				<i>Ge-intra-IM<sub>1,2'</sub></i>
1	-1.848139000	4.163338000	-1.406913000	1	1.064214000	-1.596073000	0.193183000
1	-3.404902000	3.548832000	-1.925302000	1	0.310792000	-2.150763000	-0.250599000
1	-1.939096000	2.668893000	-2.331869000	7	1.492069000	-0.388162000	0.513678000
1	-4.990123000	2.094853000	-1.288286000	6	1.299361000	-0.328809000	1.918401000
1	-6.226723000	0.019172000	-1.642242000	6	0.075899000	-0.305765000	2.483026000
1	-5.231041000	-2.123697000	-1.015039000	6	-1.258218000	-0.165798000	1.882033000
1	-1.878231000	-2.450489000	0.576061000	7	-1.373436000	-0.132789000	0.484865000
1	-3.260542000	-4.309422000	1.390582000	6	-2.713070000	-0.080584000	-0.089343000

6	-3.273592000	1.147233000	-0.453586000	1	-4.692691000	-3.614364000	0.651371000
6	-2.532814000	2.462222000	-0.245442000	1	-3.895109000	-2.778997000	1.980865000
6	-3.221431000	3.310365000	0.846001000	1	-2.121732000	-4.429878000	-0.890268000
6	-2.425719000	3.258838000	-1.563831000	1	-3.499483000	-3.682976000	-1.688904000
6	-4.545343000	1.161102000	-1.009239000	1	-1.900859000	-2.969130000	-1.843369000
6	-5.246181000	-0.009476000	-1.209014000	1	-3.328018000	0.060514000	2.340355000
6	-4.683081000	-1.217399000	-0.852786000	1	-2.168028000	-0.081289000	3.781371000
6	-3.418407000	-1.273803000	-0.287192000	1	2.267179000	-0.408891000	3.826074000
6	-2.826091000	-2.626374000	0.096525000	1	3.104709000	-1.317555000	2.552757000
6	-3.731990000	-3.378045000	1.093811000	1	3.207521000	0.437221000	2.584668000
6	-2.572596000	-3.481727000	-1.164439000	1	4.219794000	3.045804000	-0.836439000
6	-2.318706000	-0.052276000	2.709247000	1	6.011514000	1.519909000	-1.494984000
6	2.539091000	-0.406207000	2.769484000	1	5.715205000	-0.888846000	-1.259039000
6	2.744042000	0.123567000	-0.041102000	1	2.813296000	-2.498443000	0.373659000
6	2.894048000	1.504743000	-0.201759000	1	4.653660000	-4.041887000	0.317938000
6	4.085577000	1.989743000	-0.718645000	1	5.671454000	-2.925732000	-0.564526000
6	5.097660000	1.130879000	-1.091390000	1	5.216452000	-2.567759000	1.096398000
6	4.928959000	-0.230506000	-0.953064000	1	3.005289000	-3.892664000	-1.668028000
6	3.759627000	-0.758381000	-0.423903000	1	2.260892000	-2.346034000	-2.054000000
6	3.596244000	-2.273584000	-0.334891000	1	3.949491000	-2.625526000	-2.447765000
6	4.869892000	-2.990781000	0.160595000	1	0.907799000	1.919277000	0.441522000
6	3.173259000	-2.821983000	-1.717152000	1	0.584459000	4.022520000	-0.781998000
6	1.783281000	2.484960000	0.164276000	1	1.127572000	2.771029000	-1.892665000
6	1.415085000	3.376507000	-1.041499000	1	2.248578000	4.004053000	-1.332397000
6	2.185496000	3.357484000	1.372750000	1	1.374625000	4.029294000	1.633321000
1	0.054488000	-0.349086000	3.567098000	1	2.409033000	2.745355000	2.237225000
1	-1.537371000	2.224220000	0.091879000	1	3.059828000	3.953651000	1.137871000
1	-4.232922000	3.566014000	0.551003000	32	-0.064522000	-0.422891000	-0.783596000
1	-3.258763000	2.765399000	1.780387000				
1	-2.671500000	4.232433000	1.007088000				<i>Ge-intra-TS<sub>2',4</sub></i>
1	-1.848139000	4.163338000	-1.406913000	1	-0.352108000	-0.993622000	-0.582997000
1	-3.404902000	3.548832000	-1.925302000	1	0.343472000	1.519213000	1.172109000
1	-1.939096000	2.668893000	-2.331869000	7	-1.163811000	0.255742000	-0.676551000
1	-4.990123000	2.094853000	-1.288286000	6	-1.032396000	0.300538000	-2.093584000
1	-6.226723000	0.019172000	-1.642242000	6	0.192773000	-0.067878000	-2.520961000
1	-5.231041000	-2.123697000	-1.015039000	6	1.063245000	-0.585436000	-1.416646000
1	-1.878231000	-2.450489000	0.576061000	7	1.631555000	0.310354000	-0.595068000
1	-3.260542000	-4.309422000	1.390582000	6	2.719700000	-0.054687000	0.312278000

6	4.008368000	0.235202000	-0.166549000	1	1.733028000	-2.641942000	3.427764000
6	4.216797000	0.870157000	-1.539277000	1	1.236453000	-3.068451000	1.803759000
6	4.586304000	-0.221775000	-2.568842000	1	-0.026857000	-0.177492000	3.859960000
6	5.292473000	1.976304000	-1.526434000	1	1.686672000	-0.276076000	4.237901000
6	5.105897000	-0.088016000	0.612432000	1	1.085786000	1.022589000	3.216388000
6	4.945232000	-0.665735000	1.854968000	1	1.220599000	-2.311164000	-0.147068000
6	3.679210000	-0.917908000	2.330667000	1	0.357356000	-2.569935000	-1.760822000
6	2.545744000	-0.621595000	1.580875000	1	-2.251385000	1.922369000	-2.706771000
6	1.185017000	-0.911827000	2.216115000	1	-1.851945000	0.776353000	-4.007248000
6	1.043530000	-2.395764000	2.629635000	1	-3.069576000	0.360049000	-2.773442000
6	0.971645000	-0.023257000	3.463612000	1	-4.797737000	1.743006000	1.797529000
6	0.739973000	-1.882771000	-1.014526000	1	-5.891233000	-0.438585000	1.717045000
6	-2.117646000	0.862663000	-2.951935000	1	-4.889405000	-2.235410000	0.395107000
6	-2.510315000	0.123798000	-0.086047000	1	-1.808538000	-1.980315000	-1.577563000
6	-3.131742000	1.176784000	0.605527000	1	-3.284240000	-3.554697000	-2.662455000
6	-4.339482000	0.942927000	1.253394000	1	-4.586157000	-3.200060000	-1.544391000
6	-4.963725000	-0.279304000	1.203707000	1	-4.045347000	-1.969320000	-2.673625000
6	-4.392145000	-1.289619000	0.463516000	1	-1.829052000	-4.270972000	-0.671470000
6	-3.185387000	-1.110469000	-0.192666000	1	-1.502051000	-3.130733000	0.629035000
6	-2.666419000	-2.292678000	-1.012025000	1	-3.101015000	-3.833352000	0.458995000
6	-3.717217000	-2.781520000	-2.036069000	1	-1.710259000	2.683011000	0.078663000
6	-2.245091000	-3.455653000	-0.087880000	1	-1.834378000	4.030326000	2.107314000
6	-2.606445000	2.607717000	0.666021000	1	-1.572291000	2.352965000	2.563714000
6	-2.274982000	3.038841000	2.109911000	1	-3.171034000	3.070036000	2.719123000
6	-3.615277000	3.589654000	0.026750000	1	-3.187811000	4.586329000	-0.000030000
1	0.514557000	-0.054569000	-3.553967000	1	-3.853104000	3.291082000	-0.987540000
1	3.283478000	1.319879000	-1.835408000	1	-4.537168000	3.632623000	0.593920000
1	5.520344000	-0.697931000	-2.291631000	14	0.344015000	1.719466000	-0.323111000
1	3.819309000	-0.986533000	-2.614914000				
1	4.701399000	0.210773000	-3.557759000				<i>Ge-intra-TS<sub>1,1</sub></i>
1	5.310418000	2.473888000	-2.490410000	6	1.244652000	-0.334685000	1.878511000
1	6.281809000	1.573058000	-1.345860000	6	0.020544000	-0.399004000	2.455919000
1	5.076189000	2.715881000	-0.764688000	6	-1.315974000	-0.177843000	1.886343000
1	6.092208000	0.115586000	0.249693000	6	-2.364900000	0.020105000	2.712658000
1	5.802550000	-0.909921000	2.450899000	7	1.446860000	-0.275355000	0.493484000
1	3.562758000	-1.352005000	3.302605000	7	-1.443286000	-0.160484000	0.483539000
1	0.410994000	-0.674553000	1.506271000	1	0.015708000	-0.486220000	3.536074000
1	0.037070000	-2.578737000	2.991348000	1	-3.365188000	0.194444000	2.343070000

6	2.754719000	0.027895000	-0.064729000	6	2.254907000	2.521634000	0.186246000
6	3.584897000	-1.019803000	-0.475096000	6	1.822928000	3.306171000	-1.072644000
6	3.159578000	1.359095000	-0.208350000	6	2.938689000	3.466362000	1.197507000
6	4.823156000	-0.714837000	-1.021578000	1	1.370209000	2.118069000	0.653361000
6	4.406317000	1.621477000	-0.756151000	1	1.314352000	2.655340000	-1.774448000
6	5.234388000	0.594219000	-1.158895000	1	1.150244000	4.112405000	-0.801334000
1	5.468759000	-1.506738000	-1.343476000	1	2.684638000	3.734770000	-1.570594000
1	4.729920000	2.635911000	-0.874059000	1	3.254317000	2.926614000	2.082052000
1	6.194575000	0.813829000	-1.582521000	1	3.807934000	3.942884000	0.760261000
6	-2.749183000	0.044942000	-0.115911000	1	2.246660000	4.244148000	1.502282000
6	-3.584715000	-1.057150000	-0.325350000	6	3.151027000	-2.477369000	-0.359485000
6	-3.158335000	1.331995000	-0.478550000	6	4.179334000	-3.327446000	0.417352000
6	-4.828008000	-0.851404000	-0.904789000	6	2.922509000	-3.077845000	-1.765180000
6	-4.411050000	1.495290000	-1.052048000	1	2.214935000	-2.504983000	0.175275000
6	-5.240815000	0.414276000	-1.265233000	1	4.362077000	-2.914381000	1.401950000
1	-5.477656000	-1.686706000	-1.072736000	1	3.805244000	-4.338753000	0.536565000
1	-4.741471000	2.475321000	-1.331165000	1	5.124167000	-3.380119000	-0.110253000
1	-6.206077000	0.558342000	-1.709587000	1	2.202871000	-2.490708000	-2.323603000
6	-2.276525000	2.553334000	-0.245966000	1	3.848437000	-3.096369000	-2.328331000
6	-2.878621000	3.457060000	0.851987000	1	2.550229000	-4.093661000	-1.684714000
6	-2.064707000	3.351112000	-1.550815000	1	-0.044562000	-1.610009000	-1.582402000
1	-1.316130000	2.206409000	0.101324000	6	2.484518000	-0.366436000	2.730822000
1	-2.983450000	2.905397000	1.777028000	1	2.210818000	-0.518527000	3.775360000
1	-2.232801000	4.311166000	1.030470000	1	3.158705000	-1.168302000	2.423783000
1	-3.853324000	3.824880000	0.551911000	1	3.041214000	0.570119000	2.650999000
1	-1.646354000	2.719736000	-2.326433000	1	-2.207267000	0.006172000	3.783488000
1	-2.999420000	3.761453000	-1.913250000	1	-0.044410000	-2.221744000	-0.432894000
1	-1.384387000	4.177134000	-1.375352000	32	-0.009000000	-0.437169000	-0.595772000
6	-3.163623000	-2.468345000	0.071301000				
6	-3.076095000	-3.381457000	-1.171317000				
6	-4.129561000	-3.067657000	1.115404000	6	-1.233843000	-0.000860000	1.915706000
1	-2.184667000	-2.410430000	0.517848000	6	-0.019806000	-0.000835000	2.514143000
1	-2.397875000	-2.966016000	-1.908033000	6	1.325467000	-0.000344000	1.935029000
1	-2.713743000	-4.364181000	-0.888157000	6	2.407948000	0.000314000	2.743121000
1	-4.048210000	-3.499218000	-1.635953000	7	-1.418993000	-0.000822000	0.529338000
1	-4.166649000	-2.440878000	1.996967000	7	1.431985000	-0.000539000	0.532808000
1	-5.131152000	-3.163702000	0.712138000	1	-0.030596000	-0.001017000	3.599098000
1	-3.788528000	-4.054736000	1.410848000	1	3.416313000	0.000688000	2.354347000

6	-2.724631000	0.000102000	-0.102519000	6	-2.688507000	-2.556403000	-0.091058000
6	-3.334562000	1.217723000	-0.428435000	6	-2.495125000	-3.422718000	-1.355124000
6	-3.335903000	-1.216672000	-0.429084000	6	-3.526257000	-3.323433000	0.955636000
6	-4.566807000	1.196016000	-1.065050000	1	-1.716544000	-2.357757000	0.331842000
6	-4.568108000	-1.193275000	-1.065725000	1	-1.916951000	-2.892203000	-2.101609000
6	-5.181523000	0.001791000	-1.379828000	1	-1.969491000	-4.336942000	-1.100049000
1	-5.048995000	2.119184000	-1.316007000	1	-3.449133000	-3.694792000	-1.790931000
1	-5.051289000	-2.115782000	-1.317203000	1	-3.657059000	-2.735841000	1.855753000
1	-6.134700000	0.002450000	-1.870874000	1	-4.506426000	-3.563300000	0.559829000
6	2.737413000	0.000042000	-0.096728000	1	-3.031465000	-4.251637000	1.221829000
6	3.352209000	1.217592000	-0.411225000	6	-2.685658000	2.556547000	-0.089725000
6	3.353392000	-1.217017000	-0.410885000	6	-3.522163000	3.323620000	0.957931000
6	4.590203000	1.195748000	-1.036669000	6	-2.491970000	3.423613000	-1.353224000
6	4.591339000	-1.194152000	-1.036370000	1	-1.713706000	2.356608000	0.332592000
6	5.206723000	0.001057000	-1.346651000	1	-3.653085000	2.735501000	1.857686000
1	5.076623000	2.118806000	-1.280106000	1	-3.026364000	4.251161000	1.224559000
1	5.078642000	-2.116801000	-1.279580000	1	-4.502296000	3.564688000	0.562762000
1	6.164802000	0.001452000	-1.828419000	1	-1.914570000	2.893115000	-2.100321000
6	2.707191000	-2.554914000	-0.064094000	1	-3.445885000	3.696902000	-1.788468000
6	3.520332000	-3.287415000	1.025199000	1	-1.965400000	4.337163000	-1.097673000
6	2.552506000	-3.448928000	-1.313801000	1	0.007419000	-1.260110000	-1.483734000
1	1.724854000	-2.353089000	0.331881000	6	-2.468980000	-0.001246000	2.789565000
1	3.586528000	-2.679456000	1.917601000	1	-2.473594000	-0.884810000	3.432939000
1	3.038839000	-4.225639000	1.282548000	1	-2.473132000	0.881248000	3.434397000
1	4.522691000	-3.505523000	0.674160000	1	-3.384724000	-0.000550000	2.203250000
1	1.994264000	-2.937490000	-2.089012000	1	2.270392000	0.000440000	3.816712000
1	3.518911000	-3.727967000	-1.716786000	1	0.007073000	1.256066000	-1.485634000
1	2.023169000	-4.359875000	-1.053695000	32	0.016395000	-0.001351000	-0.609360000
6	2.704718000	2.554963000	-0.064858000				
6	2.549565000	3.448605000	-1.314766000				<b>Ge-inter-TS<sub>1,4</sub>-I</b>
6	3.516927000	3.288372000	1.024518000	7	-4.010512000	-0.644643000	-0.467954000
1	1.722459000	2.352319000	0.330896000	6	-2.862158000	-1.258020000	-0.947438000
1	1.991585000	2.936693000	-2.089852000	6	-1.642693000	-0.653016000	-0.906813000
1	2.019763000	4.359340000	-1.054875000	6	-1.329124000	0.668714000	-0.438392000
1	3.515821000	3.728047000	-1.717827000	7	-2.310238000	1.420991000	0.164673000
1	3.583698000	2.680482000	1.916926000	6	-1.995380000	2.754566000	0.682823000
1	4.519082000	3.507580000	0.673576000	6	-2.057882000	3.855130000	-0.177141000
1	3.034370000	4.226063000	1.281816000	6	-1.802136000	5.113784000	0.345451000

6	-1.501907000	5.278065000	1.682856000	1	0.471901000	1.502754000	3.118593000
6	-1.460278000	4.184164000	2.521467000	6	-2.884153000	1.835930000	3.990867000
6	-1.704465000	2.904556000	2.040572000	1	-3.826527000	1.887383000	3.457082000
6	-0.012705000	1.125062000	-0.589930000	1	-2.907712000	0.974732000	4.650262000
6	-2.987816000	-2.638415000	-1.525461000	1	-2.794254000	2.727433000	4.600109000
6	-5.307219000	-1.309564000	-0.603264000	6	-5.588031000	-0.180515000	-2.883570000
6	-6.070303000	-1.087625000	-1.753793000	1	-4.564879000	0.098345000	-2.683898000
6	-7.317114000	-1.687885000	-1.845642000	6	-6.437707000	1.110200000	-2.925065000
6	-7.798252000	-2.481909000	-0.825344000	1	-7.474330000	0.877221000	-3.137316000
6	-7.039502000	-2.684721000	0.308245000	1	-6.397838000	1.629762000	-1.974429000
6	-5.785960000	-2.105234000	0.441457000	1	-6.071939000	1.777679000	-3.698144000
1	-0.796607000	-1.208859000	-1.300610000	6	-5.626490000	-0.891554000	-4.253131000
1	-1.845566000	5.971570000	-0.294345000	1	-5.212375000	-0.241836000	-5.016474000
1	-1.309147000	6.258260000	2.071635000	1	-5.046723000	-1.806438000	-4.233998000
1	-1.240229000	4.324864000	3.559817000	1	-6.641974000	-1.137284000	-4.538496000
1	0.170732000	2.182646000	-0.443062000	6	-4.989860000	-2.325418000	1.725366000
1	0.544820000	0.664363000	-1.400142000	1	-4.006555000	-1.901859000	1.592180000
1	-3.413394000	-3.329777000	-0.795586000	6	-5.671935000	-1.597471000	2.906304000
1	-3.651971000	-2.638713000	-2.392474000	1	-5.086981000	-1.720125000	3.811679000
1	-2.005770000	-3.002190000	-1.829882000	1	-5.772542000	-0.537632000	2.702399000
1	-7.918609000	-1.528606000	-2.717299000	1	-6.661784000	-2.001691000	3.082133000
1	-8.765110000	-2.936853000	-0.911197000	6	-4.818629000	-3.825072000	2.048749000
1	-7.426411000	-3.295194000	1.098428000	1	-5.772880000	-4.291325000	2.261306000
6	-2.430312000	3.714687000	-1.651169000	1	-4.356852000	-4.352120000	1.222766000
1	-2.508529000	2.664388000	-1.884556000	1	-4.186211000	-3.942149000	2.921678000
6	-1.692645000	1.725042000	3.011052000	7	3.732873000	0.729770000	-0.550734000
1	-1.805108000	0.814234000	2.442351000	6	3.289194000	0.562833000	-1.858742000
6	-1.354779000	4.322207000	-2.576122000	6	2.498931000	-0.466468000	-2.263395000
1	-1.265321000	5.390759000	-2.422220000	6	2.059589000	-1.652919000	-1.524004000
1	-0.390270000	3.865189000	-2.395910000	7	2.532455000	-1.812049000	-0.211291000
1	-1.624594000	4.154581000	-3.613416000	6	2.564144000	-3.160356000	0.332312000
6	-3.804881000	4.370464000	-1.915747000	6	3.553410000	-4.059926000	-0.099525000
1	-4.094766000	4.230959000	-2.951949000	6	3.587780000	-5.335680000	0.438307000
1	-4.569815000	3.935244000	-1.282302000	6	2.684148000	-5.729103000	1.404676000
1	-3.766471000	5.434170000	-1.713674000	6	1.723434000	-4.842660000	1.834170000
6	-0.365206000	1.630909000	3.791161000	6	1.639719000	-3.561864000	1.301397000
1	-0.198991000	2.518625000	4.389177000	6	1.231609000	-2.541799000	-2.130826000
1	-0.395021000	0.779029000	4.460948000	6	3.675899000	1.621321000	-2.861726000

6	4.754122000	1.733590000	-0.279782000	6	4.596249000	-3.673931000	-1.142025000
6	6.110820000	1.419171000	-0.431531000	1	4.484175000	-2.622026000	-1.346582000
6	7.061642000	2.404620000	-0.205262000	6	6.025700000	-3.916712000	-0.611208000
6	6.694485000	3.672602000	0.189848000	1	6.216170000	-4.974369000	-0.471973000
6	5.361152000	3.966378000	0.378963000	1	6.753879000	-3.538697000	-1.321833000
6	4.380533000	3.012769000	0.150819000	1	6.174110000	-3.415448000	0.336927000
1	2.162981000	-0.437609000	-3.294636000	6	4.381009000	-4.452885000	-2.457733000
1	4.335473000	-6.027671000	0.106414000	1	3.391117000	-4.263322000	-2.848650000
1	2.732896000	-6.717265000	1.818849000	1	5.111859000	-4.143747000	-3.199017000
1	1.025463000	-5.147231000	2.588096000	1	4.496148000	-5.518716000	-2.292382000
1	0.907482000	-3.449535000	-1.639249000	6	0.538292000	-2.633086000	1.794247000
1	0.952393000	-2.391519000	-3.167722000	1	0.545813000	-1.755448000	1.169801000
1	3.364768000	2.613200000	-2.525805000	6	-0.850133000	-3.296411000	1.677864000
1	4.758333000	1.659878000	-2.998519000	1	-0.944003000	-4.133797000	2.359286000
1	3.209852000	1.412732000	-3.826138000	1	-1.623997000	-2.576420000	1.922933000
1	8.100321000	2.173322000	-0.330254000	1	-1.019736000	-3.653217000	0.669847000
1	7.442371000	4.421679000	0.362285000	6	0.798150000	-2.204882000	3.255083000
1	5.079094000	4.945525000	0.710096000	1	1.740378000	-1.678772000	3.336839000
6	2.925522000	3.365619000	0.421785000	1	0.006866000	-1.548419000	3.602585000
1	2.323533000	2.552649000	0.057306000	1	0.831307000	-3.072091000	3.905178000
6	2.485290000	4.661496000	-0.291615000	1	0.847923000	0.616720000	0.409927000
1	1.425616000	4.828766000	-0.129465000	1	1.599783000	0.345855000	0.985714000
1	3.019951000	5.522754000	0.091479000	32	3.237643000	-0.429694000	0.871952000
1	2.664586000	4.598828000	-1.358982000	32	-4.103785000	1.012317000	0.346825000
6	2.695006000	3.485456000	1.944343000				
1	2.949539000	2.553681000	2.435014000				<i>Ge-inter-IM<sub>1,4</sub></i>
1	3.313100000	4.272413000	2.362034000	7	3.080228000	-0.597839000	1.341579000
1	1.655795000	3.715795000	2.151305000	6	1.744261000	-0.442773000	1.221235000
6	6.585996000	0.016767000	-0.795547000	6	1.174623000	0.189998000	0.106911000
1	5.718640000	-0.613292000	-0.905936000	6	1.850967000	0.745817000	-0.964786000
6	7.368092000	0.003017000	-2.126590000	7	3.211181000	0.742463000	-1.039575000
1	8.269156000	0.601014000	-2.052733000	6	3.891718000	1.395868000	-2.167970000
1	7.656820000	-1.012504000	-2.377291000	6	4.248771000	2.741552000	-2.050438000
1	6.764861000	0.393536000	-2.937084000	6	4.938785000	3.327632000	-3.100975000
6	7.457926000	-0.554562000	0.345818000	6	5.267142000	2.600551000	-4.226387000
1	8.336712000	0.059283000	0.503545000	6	4.913802000	1.270587000	-4.320586000
1	6.894066000	-0.589409000	1.270365000	6	4.221101000	0.641622000	-3.296316000
1	7.786411000	-1.557808000	0.102740000	6	0.807791000	-0.962862000	2.244548000

6	3.657599000	-1.312698000	2.491086000	6	5.269793000	1.632472000	3.804118000
6	4.068819000	-0.582488000	3.607740000	1	5.791016000	1.337077000	4.706349000
6	4.657303000	-1.274314000	4.656041000	1	5.894934000	1.378848000	2.955185000
6	4.833076000	-2.641249000	4.593213000	1	5.138388000	2.708892000	3.826367000
6	4.425780000	-3.342992000	3.477542000	6	3.006725000	1.313123000	4.912274000
6	3.831833000	-2.695175000	2.404323000	1	2.853690000	2.386515000	4.933490000
1	0.086992000	0.238944000	0.085576000	1	2.038870000	0.831409000	4.848247000
1	5.224583000	4.357469000	-3.037013000	1	3.473411000	1.020888000	5.845001000
1	5.801591000	3.069429000	-5.028380000	6	3.410047000	-3.501342000	1.177314000
1	5.180327000	0.715902000	-5.196474000	1	2.915756000	-2.841745000	0.480386000
1	0.242808000	-1.809016000	1.811328000	6	4.651868000	-4.092696000	0.472272000
1	1.297265000	-1.280192000	3.160749000	1	4.352351000	-4.627240000	-0.422487000
1	0.036701000	-0.210514000	2.444300000	1	5.348758000	-3.310775000	0.189759000
1	4.979444000	-0.740568000	5.526629000	1	5.170151000	-4.785487000	1.124028000
1	5.288611000	-3.159458000	5.413340000	6	2.411350000	-4.618886000	1.548351000
1	4.569862000	-4.403181000	3.439588000	1	2.866956000	-5.342953000	2.212858000
6	3.934035000	3.566800000	-0.803662000	1	1.532084000	-4.211731000	2.031464000
1	3.310709000	2.977765000	-0.147832000	1	2.093216000	-5.137731000	0.651309000
6	3.874755000	-0.840934000	-3.420963000	7	-3.638010000	1.220927000	0.649031000
1	3.217813000	-1.112788000	-2.608094000	6	-3.187858000	0.729600000	1.846630000
6	3.162829000	4.859295000	-1.147607000	6	-2.535986000	-0.471441000	1.975254000
1	3.765225000	5.524298000	-1.753835000	6	-2.484372000	-1.603074000	1.045952000
1	2.249840000	4.638915000	-1.686885000	7	-3.015647000	-1.415218000	-0.223248000
1	2.899838000	5.383421000	-0.235503000	6	-3.305641000	-2.583565000	-1.018168000
6	5.239061000	3.904084000	-0.046481000	6	-4.522911000	-3.260399000	-0.850632000
1	5.015245000	4.456627000	0.859665000	6	-4.782236000	-4.389633000	-1.610962000
1	5.776429000	3.001756000	0.223967000	6	-3.869992000	-4.851171000	-2.538700000
1	5.891510000	4.510467000	-0.662838000	6	-2.680987000	-4.177535000	-2.713820000
6	3.140027000	-1.153734000	-4.742236000	6	-2.382971000	-3.049540000	-1.961499000
1	3.784811000	-0.990253000	-5.596780000	6	-1.986150000	-2.797116000	1.497837000
1	2.829470000	-2.192241000	-4.750281000	6	-3.417152000	1.555688000	3.091968000
1	2.257765000	-0.536562000	-4.856254000	6	-4.322698000	2.493546000	0.598271000
6	5.158185000	-1.696080000	-3.309726000	6	-5.720927000	2.543526000	0.617153000
1	5.675446000	-1.507283000	-2.375557000	6	-6.355792000	3.777526000	0.593465000
1	4.911404000	-2.750960000	-3.359534000	6	-5.632972000	4.949458000	0.531156000
1	5.838369000	-1.465414000	-4.120808000	6	-4.255611000	4.897007000	0.471823000
6	3.895989000	0.931516000	3.708923000	6	-3.586798000	3.682923000	0.499494000
1	3.404659000	1.283124000	2.813907000	1	-2.212084000	-0.720647000	2.981046000

1	-5.708222000	-4.913256000	-1.479901000	1	-4.675704000	-3.828472000	1.837409000	
1	-4.087937000	-5.724985000	-3.121725000	1	-6.357483000	-3.369984000	2.089742000	
1	-1.975976000	-4.531720000	-3.440464000	1	-5.966450000	-4.724853000	1.037424000	
1	-1.982914000	-3.685356000	0.882093000	6	-1.056070000	-2.335308000	-2.183854000	
1	-1.709005000	-2.899273000	2.541784000	1	-1.013166000	-1.515834000	-1.486941000	
1	-3.000617000	2.559961000	3.000917000	6	0.141406000	-3.267405000	-1.901298000	
1	-4.488043000	1.673795000	3.277041000	1	0.159305000	-4.104177000	-2.590506000	
1	-2.972898000	1.062547000	3.958768000	1	1.075387000	-2.720360000	-2.011303000	
1	-7.426538000	3.819872000	0.616815000	1	0.082321000	-3.651051000	-0.890045000	
1	-6.138321000	5.895458000	0.513725000	6	-0.980936000	-1.762477000	-3.615657000	
1	-3.697565000	5.809105000	0.395692000	1	-1.794061000	-1.066795000	-3.781103000	
6	-2.068150000	3.661096000	0.360205000	1	-0.041699000	-1.238474000	-3.767478000	
1	-1.734243000	2.652397000	0.541468000	1	-1.047176000	-2.553602000	-4.353984000	
6	-1.365219000	4.605472000	1.358469000	1	-1.570183000	0.584173000	-0.596359000	
1	-0.287519000	4.500327000	1.270625000	6	1.061601000	1.368883000	-2.073797000	
1	-1.613766000	5.641958000	1.163108000	1	1.287903000	0.878419000	-3.022309000	
1	-1.647569000	4.375029000	2.378848000	1	-0.006537000	1.282710000	-1.867794000	
6	-1.682989000	4.035255000	-1.088990000	1	1.323735000	2.423051000	-2.182334000	
1	-2.118706000	3.327783000	-1.783366000	32	-3.102429000	0.355465000	-1.019534000	
1	-2.044372000	5.027070000	-1.335791000	32	4.404178000	-0.001997000	0.170535000	
1	-0.603399000	4.025452000	-1.210682000					
6	-6.559835000	1.272513000	0.623002000	<b>Ge-inter-TS<sub>1,4-II</sub></b>				
1	-5.879631000	0.437308000	0.607441000	7	-2.764602000	1.789407000	-0.031780000	
6	-7.437237000	1.173972000	1.889048000	6	-2.050326000	1.697799000	-1.174078000	
1	-8.152068000	1.988428000	1.930645000	6	-2.004002000	0.525640000	-1.934699000	
1	-7.989425000	0.239541000	1.888684000	6	-2.725396000	-0.645469000	-1.705701000	
1	-6.829199000	1.208233000	2.785441000	7	-3.569942000	-0.780131000	-0.658212000	
6	-7.434349000	1.207150000	-0.648762000	6	-4.523910000	-1.911241000	-0.644888000	
1	-8.125941000	2.041287000	-0.687218000	6	-4.215336000	-3.085019000	0.045727000	
1	-6.810015000	1.234817000	-1.533567000	6	-5.150694000	-4.111179000	0.039724000	
1	-8.010698000	0.289223000	-0.661845000	6	-6.349759000	-3.979878000	-0.625153000	
6	-5.557277000	-2.777373000	0.157050000	6	-6.644221000	-2.808461000	-1.291436000	
1	-5.226694000	-1.813968000	0.508846000	6	-5.746035000	-1.752928000	-1.310279000	
6	-6.946856000	-2.612052000	-0.493930000	6	-1.278737000	2.892063000	-1.649381000	
1	-7.351060000	-3.568339000	-0.806169000	6	-2.843575000	3.092173000	0.668549000	
1	-7.639621000	-2.176722000	0.219612000	6	-1.882583000	3.425778000	1.627550000	
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6	-5.642467000	-3.740794000	1.360850000	6	-3.021784000	5.525447000	1.955584000	

6	-3.969150000	5.172796000	1.017628000	6	0.639052000	3.194836000	1.919539000
6	-3.904446000	3.953282000	0.361664000	1	1.422161000	2.462515000	2.066148000
1	-1.335833000	0.524499000	-2.786059000	1	0.783571000	3.633528000	0.940051000
1	-4.933025000	-5.019366000	0.562436000	1	0.743831000	3.975364000	2.663956000
1	-7.056973000	-4.785218000	-0.620249000	6	-5.001828000	3.609133000	-0.644497000
1	-7.583362000	-2.712128000	-1.796628000	1	-4.810453000	2.625873000	-1.048442000
1	-0.774146000	2.665282000	-2.588409000	6	-6.380403000	3.580786000	0.053815000
1	-1.942754000	3.746341000	-1.792013000	1	-7.152336000	3.297525000	-0.652018000
1	-0.532835000	3.187155000	-0.907633000	1	-6.384075000	2.872484000	0.874023000
1	-1.270136000	4.934980000	2.994017000	1	-6.629079000	4.556858000	0.450251000
1	-3.087270000	6.472728000	2.452723000	6	-5.021247000	4.606351000	-1.824006000
1	-4.768110000	5.850191000	0.796041000	1	-5.250389000	5.606257000	-1.477390000
6	-2.914803000	-3.272089000	0.817457000	1	-4.064740000	4.634773000	-2.331187000
1	-2.279648000	-2.425551000	0.628341000	1	-5.779709000	4.316446000	-2.543130000
6	-6.143299000	-0.466362000	-2.032498000	6	-2.573871000	-1.785915000	-2.667028000
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6	-2.150347000	-4.537715000	0.370155000	1	-2.339945000	-2.703497000	-2.126785000
1	-2.706267000	-5.436101000	0.611071000	1	-3.505489000	-1.955894000	-3.210660000
1	-1.963441000	-4.527510000	-0.696967000	1	-2.212774000	-0.423449000	2.126365000
1	-1.192812000	-4.585136000	0.874509000	1	-1.506008000	-0.518376000	1.889921000
6	-3.203439000	-3.332084000	2.334696000	7	3.981445000	0.775945000	-0.533279000
1	-2.271526000	-3.392531000	2.884229000	6	2.752952000	1.185870000	-0.949637000
1	-3.741679000	-2.450852000	2.665232000	6	1.576269000	0.642366000	-0.493120000
1	-3.800987000	-4.203495000	2.575783000	6	1.364973000	-0.638290000	0.169110000
6	-6.416420000	-0.715247000	-3.532168000	7	2.451116000	-1.335332000	0.626022000
1	-7.258176000	-1.383354000	-3.664569000	6	2.257078000	-2.696669000	1.062599000
1	-6.648937000	0.221500000	-4.026851000	6	2.344556000	-3.749020000	0.142471000
1	-5.555846000	-1.153706000	-4.021914000	6	2.138094000	-5.049543000	0.577926000
6	-7.386390000	0.159788000	-1.361483000	6	1.866817000	-5.320974000	1.904353000
1	-7.202479000	0.354200000	-0.311426000	6	1.804583000	-4.284610000	2.813052000
1	-7.642978000	1.094416000	-1.847513000	6	1.992481000	-2.969625000	2.410138000
1	-8.238050000	-0.504276000	-1.437212000	6	0.079017000	-1.132484000	0.222825000
6	-0.737545000	2.500418000	2.031355000	6	2.678464000	2.342280000	-1.920454000
1	-0.720171000	1.641621000	1.380406000	6	5.171644000	1.395070000	-1.075684000
6	-0.953717000	2.008664000	3.481725000	6	5.812636000	0.848499000	-2.192455000
1	-0.887437000	2.837828000	4.176389000	6	6.946339000	1.472387000	-2.694101000
1	-1.925592000	1.544734000	3.600545000	6	7.456943000	2.605805000	-2.097897000
1	-0.191581000	1.283021000	3.738461000	6	6.842584000	3.122203000	-0.975506000

6	5.704266000	2.530401000	-0.449444000	1	4.720256000	-4.166505000	-1.188226000
1	0.664367000	1.101772000	-0.857503000	6	1.419984000	-3.733496000	-2.206941000
1	2.199787000	-5.858806000	-0.122513000	1	0.606452000	-3.098294000	-1.881808000
1	1.720643000	-6.333276000	2.228894000	1	1.645364000	-3.511612000	-3.246558000
1	1.615586000	-4.500534000	3.845965000	1	1.108276000	-4.771239000	-2.141222000
1	-0.133691000	-2.095294000	0.660508000	6	1.941499000	-1.847782000	3.441280000
1	-0.731829000	-0.545941000	-0.176723000	1	1.944532000	-0.912445000	2.905899000
1	3.202383000	3.220815000	-1.540564000	6	0.668116000	-1.914463000	4.310227000
1	3.147814000	2.079486000	-2.871362000	1	0.655882000	-2.804849000	4.928681000
1	1.637181000	2.608894000	-2.112143000	1	0.625722000	-1.053364000	4.970554000
1	7.439350000	1.061138000	-3.552606000	1	-0.219132000	-1.913737000	3.688548000
1	8.335886000	3.074982000	-2.495514000	6	3.200747000	-1.890682000	4.335321000
1	7.257395000	3.988333000	-0.499624000	1	4.092624000	-1.783449000	3.731971000
6	5.083212000	3.089468000	0.826892000	1	3.178609000	-1.081075000	5.058667000
1	4.141542000	2.589340000	0.983318000	1	3.256482000	-2.831512000	4.872572000
6	4.832007000	4.610436000	0.745280000	1	3.608291000	0.499664000	1.946324000
1	4.317291000	4.945913000	1.640316000	32	4.210781000	-0.549993000	0.883593000
1	5.762180000	5.161810000	0.671380000	32	-3.859257000	0.467697000	0.727126000
1	4.219902000	4.861097000	-0.114038000				
6	5.990566000	2.760595000	2.033568000				<i>Ge-inter-TS<sub>1,4'</sub></i>
1	6.115975000	1.689596000	2.122786000	1	-0.042551000	-0.198587000	-0.574340000
1	6.966965000	3.217568000	1.914025000	1	1.029026000	0.080855000	-0.512417000
1	5.545417000	3.130055000	2.952359000	7	3.107641000	-1.421900000	-0.306364000
6	5.318436000	-0.438148000	-2.841611000	6	2.917196000	-1.612268000	1.058152000
1	4.447301000	-0.762836000	-2.296451000	6	2.800085000	-0.588360000	1.943813000
6	4.927194000	-0.220844000	-4.319190000	6	3.048033000	0.849219000	1.753389000
1	5.786153000	0.081673000	-4.907604000	7	3.133126000	1.322097000	0.436616000
1	4.536908000	-1.141752000	-4.741543000	6	3.456465000	2.726284000	0.256980000
1	4.166053000	0.545464000	-4.411272000	6	4.787344000	3.136885000	0.115758000
6	6.394737000	-1.539737000	-2.724927000	6	5.067987000	4.491141000	-0.003583000
1	7.301398000	-1.251086000	-3.244739000	6	4.060673000	5.431421000	-0.007685000
1	6.632281000	-1.717310000	-1.683660000	6	2.748763000	5.022406000	0.101716000
1	6.034732000	-2.465640000	-3.160084000	6	2.432107000	3.679689000	0.239661000
6	2.661757000	-3.483776000	-1.323452000	6	3.183956000	1.634092000	2.853204000
1	2.936297000	-2.444686000	-1.401946000	6	2.776157000	-3.032530000	1.557428000
6	3.850046000	-4.339678000	-1.809121000	6	3.710691000	-2.490230000	-1.082709000
1	3.611175000	-5.396875000	-1.783568000	6	5.072771000	-2.794981000	-0.926575000
1	4.099921000	-4.079932000	-2.832946000	6	5.621435000	-3.845066000	-1.647241000

6	4.864225000	-4.574003000	-2.539234000	1	7.328921000	3.340347000	-1.085477000
6	3.537844000	-4.250752000	-2.720821000	1	7.631440000	1.618589000	-1.159325000
6	2.946074000	-3.223230000	-2.000677000	1	6.279690000	2.309941000	-2.048533000
1	2.606633000	-0.867063000	2.975037000	6	6.750918000	2.221376000	1.405138000
1	6.085428000	4.812884000	-0.096527000	1	6.110293000	2.028387000	2.255585000
1	4.295602000	6.473613000	-0.103883000	1	7.551680000	1.487632000	1.399270000
1	1.965589000	5.753316000	0.077535000	1	7.193614000	3.205490000	1.516839000
1	3.371162000	2.695786000	2.784930000	6	0.972619000	3.258778000	0.305803000
1	3.144484000	1.181555000	3.836506000	1	0.943044000	2.221507000	0.595540000
1	2.064937000	-3.596276000	0.947076000	6	0.168355000	4.073344000	1.338463000
1	3.723233000	-3.571340000	1.504501000	1	0.113921000	5.120568000	1.065379000
1	2.436353000	-3.036200000	2.595662000	1	-0.848502000	3.694792000	1.395586000
1	6.658204000	-4.084412000	-1.520912000	1	0.622077000	3.995525000	2.319408000
1	5.306880000	-5.377439000	-3.094643000	6	0.350079000	3.393138000	-1.099767000
1	2.952699000	-4.805557000	-3.426934000	1	0.902138000	2.792954000	-1.811868000
6	1.476629000	-2.915205000	-2.241862000	1	-0.677398000	3.054081000	-1.101037000
1	1.202012000	-2.149867000	-1.537337000	1	0.377643000	4.426277000	-1.428462000
6	0.586789000	-4.155948000	-2.005600000	7	-2.569359000	-0.763647000	1.311292000
1	-0.463369000	-3.892943000	-2.100085000	6	-1.514896000	-1.157839000	0.595592000
1	0.797633000	-4.928117000	-2.735179000	6	-1.234650000	-0.711379000	-0.728752000
1	0.752978000	-4.573661000	-1.018893000	6	-2.096905000	0.193279000	-1.541803000
6	1.257288000	-2.359739000	-3.666356000	7	-3.374931000	0.504662000	-1.015450000
1	1.853562000	-1.468930000	-3.816891000	6	-4.364649000	1.091318000	-1.924552000
1	1.540280000	-3.094660000	-4.411099000	6	-5.117359000	0.237139000	-2.739298000
1	0.212024000	-2.106674000	-3.820997000	6	-6.091668000	0.788843000	-3.555207000
6	5.990845000	-1.970095000	-0.029977000	6	-6.321126000	2.150015000	-3.563745000
1	5.405370000	-1.189861000	0.427274000	6	-5.572293000	2.980476000	-2.758419000
6	6.638066000	-2.817461000	1.087117000	6	-4.579225000	2.470930000	-1.931923000
1	7.267361000	-3.594554000	0.668265000	6	-1.649702000	0.652641000	-2.720175000
1	7.256065000	-2.186280000	1.717154000	6	-0.445014000	-1.984032000	1.212124000
1	5.889234000	-3.285739000	1.712488000	6	-2.775633000	-1.208675000	2.696005000
6	7.094993000	-1.308441000	-0.883526000	6	-3.475294000	-2.396773000	2.930717000
1	7.733843000	-2.058005000	-1.335813000	6	-3.707236000	-2.767039000	4.246635000
1	6.659599000	-0.708941000	-1.672763000	6	-3.271664000	-1.979811000	5.292799000
1	7.712253000	-0.668815000	-0.262700000	6	-2.597921000	-0.803778000	5.040340000
6	5.937414000	2.139777000	0.094979000	6	-2.337731000	-0.394526000	3.739999000
1	5.506683000	1.155004000	0.022096000	1	-0.832245000	-1.526074000	-1.329667000
6	6.850889000	2.369173000	-1.129134000	1	-6.678935000	0.151244000	-4.184583000

1	-7.082405000	2.560944000	-4.196911000	1	-2.301952000	-4.654872000	1.821006000
1	-5.758564000	4.034785000	-2.771565000	1	-3.666658000	-5.203313000	2.780308000
1	-2.249831000	1.288753000	-3.355788000	6	-1.617758000	0.927650000	3.494657000
1	-0.644862000	0.399074000	-3.039699000	1	-1.365255000	0.995428000	2.447212000
1	-0.779920000	-2.576594000	2.059669000	6	-2.557483000	2.106020000	3.837757000
1	0.028684000	-2.619401000	0.463607000	1	-2.059857000	3.049209000	3.644998000
1	0.339934000	-1.287322000	1.556670000	1	-3.464438000	2.066945000	3.243418000
1	-4.236514000	-3.674392000	4.454758000	1	-2.839829000	2.074147000	4.883434000
1	-3.462081000	-2.281126000	6.303634000	6	-0.306447000	1.023714000	4.301802000
1	-2.270814000	-0.196466000	5.858719000	1	-0.505790000	1.098736000	5.364329000
6	-4.903331000	-1.273916000	-2.744984000	1	0.319811000	0.158692000	4.126000000
1	-4.097097000	-1.502320000	-2.066591000	1	0.253044000	1.897588000	3.995417000
6	-3.772098000	3.421278000	-1.054024000	32	-4.096967000	0.126096000	0.609253000
1	-2.961186000	2.862178000	-0.613988000	32	2.688969000	0.290297000	-1.096575000
6	-4.492916000	-1.774454000	-4.145743000				
1	-5.277860000	-1.591481000	-4.869698000	Ge-inter-IM <sub>1,4'</sub>			
1	-3.592282000	-1.272490000	-4.475645000	1	-1.024498000	0.872077000	-0.643566000
1	-4.302276000	-2.842373000	-4.118080000	1	1.372470000	0.283277000	-0.669466000
6	-6.169642000	-2.005770000	-2.247543000	7	3.165878000	-1.437507000	-0.477391000
1	-5.994718000	-3.076221000	-2.211231000	6	2.935440000	-1.694234000	0.856929000
1	-6.445111000	-1.667187000	-1.254443000	6	2.857544000	-0.717533000	1.810668000
1	-7.007535000	-1.823183000	-2.909235000	6	3.262149000	0.694971000	1.739313000
6	-3.159291000	4.574343000	-1.876915000	7	3.453736000	1.245340000	0.477885000
1	-3.929832000	5.215216000	-2.288009000	6	3.826378000	2.638273000	0.390091000
1	-2.523208000	5.179828000	-1.241405000	6	5.165582000	3.006856000	0.217826000
1	-2.557929000	4.189380000	-2.690697000	6	5.494708000	4.352967000	0.143104000
6	-4.654666000	3.987428000	0.081461000	6	4.524600000	5.330058000	0.217382000
1	-5.078459000	3.190724000	0.682859000	6	3.202698000	4.965773000	0.365375000
1	-4.068085000	4.631687000	0.727957000	6	2.839589000	3.630854000	0.456670000
1	-5.473123000	4.568429000	-0.327422000	6	3.445983000	1.364897000	2.912573000
6	-4.002600000	-3.285042000	1.804436000	6	2.663009000	-3.125388000	1.264994000
1	-3.727316000	-2.846802000	0.856254000	6	3.683096000	-2.496497000	-1.314234000
6	-5.545075000	-3.370552000	1.854129000	6	5.014580000	-2.920832000	-1.181741000
1	-5.874200000	-3.845941000	2.769814000	6	5.475945000	-3.969376000	-1.962929000
1	-5.988919000	-2.383144000	1.806634000	6	4.660493000	-4.581253000	-2.891963000
1	-5.912608000	-3.954996000	1.017614000	6	3.367757000	-4.133111000	-3.056407000
6	-3.383296000	-4.698609000	1.864906000	6	2.865287000	-3.099227000	-2.279764000
1	-3.735689000	-5.293289000	1.029208000	1	2.626261000	-1.056066000	2.815686000

1	6.519862000	4.640287000	0.023304000	1	6.407867000	1.676621000	2.271298000
1	4.795868000	6.366095000	0.154373000	1	7.830214000	1.129562000	1.387229000
1	2.448328000	5.726719000	0.408720000	1	7.554536000	2.850881000	1.628218000
1	3.761757000	2.397863000	2.941248000	6	1.367631000	3.263537000	0.598750000
1	3.329141000	0.837943000	3.851657000	1	1.316150000	2.202261000	0.774541000
1	1.876654000	-3.564633000	0.642156000	6	0.705563000	3.990226000	1.787325000
1	3.544299000	-3.756128000	1.139713000	1	0.692508000	5.063713000	1.639039000
1	2.357384000	-3.170929000	2.312960000	1	-0.324587000	3.660018000	1.903005000
1	6.489855000	-4.299927000	-1.855159000	1	1.243160000	3.772427000	2.701467000
1	5.034485000	-5.387380000	-3.492457000	6	0.619621000	3.571605000	-0.716439000
1	2.741991000	-4.591760000	-3.796522000	1	1.052516000	3.006380000	-1.532304000
6	1.438944000	-2.623227000	-2.517674000	1	-0.431670000	3.305664000	-0.629279000
1	1.235606000	-1.870199000	-1.774642000	1	0.680457000	4.627319000	-0.956271000
6	0.416462000	-3.772021000	-2.369785000	7	-2.525564000	-0.647340000	1.244096000
1	-0.598478000	-3.392947000	-2.464150000	6	-1.493636000	-0.829616000	0.464427000
1	0.559656000	-4.519759000	-3.140414000	6	-1.434846000	-0.130800000	-0.859201000
1	0.517144000	-4.263019000	-1.407733000	6	-2.719048000	-0.011164000	-1.636835000
6	1.311644000	-1.965751000	-3.909583000	7	-3.801466000	0.544863000	-0.921916000
1	1.994171000	-1.130063000	-3.990441000	6	-4.884096000	1.187994000	-1.671100000
1	1.538162000	-2.678959000	-4.693787000	6	-6.048316000	0.475534000	-1.972406000
1	0.300265000	-1.600676000	-4.068864000	6	-7.063632000	1.130785000	-2.656498000
6	5.988083000	-2.212000000	-0.245758000	6	-6.929560000	2.449437000	-3.033033000
1	5.454732000	-1.419232000	0.252133000	6	-5.773109000	3.139671000	-2.731749000
6	6.573671000	-3.161120000	0.821682000	6	-4.733531000	2.526656000	-2.051101000
1	7.146870000	-3.957548000	0.360026000	6	-2.772936000	-0.346705000	-2.930525000
1	7.233851000	-2.610353000	1.483686000	6	-0.313327000	-1.613912000	0.833150000
1	5.791417000	-3.607732000	1.422501000	6	-2.640708000	-1.291264000	2.565786000
6	7.131334000	-1.575953000	-1.066866000	6	-3.274800000	-2.532743000	2.647846000
1	7.715970000	-2.337427000	-1.570575000	6	-3.411749000	-3.106239000	3.902683000
1	6.730736000	-0.900563000	-1.812202000	6	-2.954428000	-2.458267000	5.031891000
1	7.793068000	-1.017526000	-0.413568000	6	-2.353224000	-1.221842000	4.927807000
6	6.262186000	1.955545000	0.124043000	6	-2.183486000	-0.609933000	3.693836000
1	5.774053000	1.006097000	-0.019579000	1	-0.671155000	-0.610125000	-1.470467000
6	7.198350000	2.212303000	-1.075819000	1	-7.965021000	0.604218000	-2.895275000
1	7.748874000	3.138418000	-0.956936000	1	-7.723926000	2.939480000	-3.560124000
1	7.920496000	1.408351000	-1.161775000	1	-5.678272000	4.164421000	-3.027683000
1	6.630233000	2.264240000	-1.997301000	1	-3.667136000	-0.191485000	-3.519846000
6	7.066072000	1.899868000	1.441636000	1	-1.894921000	-0.744417000	-3.423511000

1	-0.375187000	-2.082433000	1.812050000	6	-2.349309000	1.822266000	4.363799000
1	-0.113483000	-2.353890000	0.052485000	1	-1.878130000	2.793588000	4.265343000
1	0.565945000	-0.933693000	0.789085000	1	-3.354006000	1.882499000	3.960376000
1	-3.880294000	-4.063968000	3.997755000	1	-2.421097000	1.587601000	5.418810000
1	-3.069505000	-2.916718000	5.993683000	6	-0.077799000	0.696428000	4.198841000
1	-2.006230000	-0.727009000	5.811053000	1	-0.101070000	0.475662000	5.259571000
6	-6.248841000	-0.983763000	-1.573596000	1	0.512341000	-0.058439000	3.698658000
1	-5.340853000	-1.337376000	-1.108704000	1	0.424391000	1.643690000	4.056007000
6	-3.473033000	3.324502000	-1.736682000	32	2.913558000	0.383982000	-1.163062000
1	-2.777756000	2.673602000	-1.233091000	32	-4.046122000	0.506171000	0.878487000
6	-6.518209000	-1.875594000	-2.804995000				
1	-7.442937000	-1.595118000	-3.293879000				
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1	-6.601864000	-2.912920000	-2.498564000				
6	-7.405311000	-1.109488000	-0.556061000				
1	-7.532549000	-2.143086000	-0.254688000				
1	-7.211628000	-0.512828000	0.328749000				
1	-8.335892000	-0.767868000	-0.992134000				
6	-2.795576000	3.827568000	-3.029255000				
1	-3.437082000	4.521347000	-3.559371000				
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1	-2.565812000	2.997909000	-3.686285000				
6	-3.791278000	4.500833000	-0.787346000				
1	-4.254152000	4.146062000	0.127529000				
1	-2.878855000	5.027098000	-0.529508000				
1	-4.467886000	5.204847000	-1.256592000				
6	-3.803797000	-3.271635000	1.420566000				
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6	-5.291346000	-3.648917000	1.592770000				
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6	-2.959553000	-4.533852000	1.136234000				
1	-3.322446000	-5.032933000	0.244480000				
1	-1.916500000	-4.284361000	0.987665000				
1	-3.027233000	-5.227322000	1.965820000				
6	-1.508929000	0.757838000	3.623213000				
1	-1.431233000	1.058518000	2.588033000				