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Supporting Information

Reciprocity of C=O…π Interactions with the Dominant Anion−π on Fullerene (C_{60}) -Amine- Based Organocatalysts: A Mechanistic Elucidation for Addition vs. Decarboxylation Reaction

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Table. S1 Relative free energies of all the possible intermediates (in kcal/mol) at decarboxylation pathway.

Catalysts	Functionals/Basis sets	$^{D}F_{R}$	$^{D}F_{INT1}$	$^{D}F_{INT2}$	$^{D}F_{p}$
F1	B3LYP/6-31G(d)//B3LYP/6-311+G(d,p)	0	3.98	10.10	-11.99
	B3LYP-D3/6-31G(d)//B3LYP-D3/6-311+G(d,p)	0	3.79	13.49	-7.83
F2	B3LYP/6-31G(d)//B3LYP/6-311+G(d,p)	0	-5.74	8.23	-15.41
	B3LYP-D3/6-31G(d)//B3LYP-D3/6-311+G(d,p)	0	-4.34	9.90	-10.23

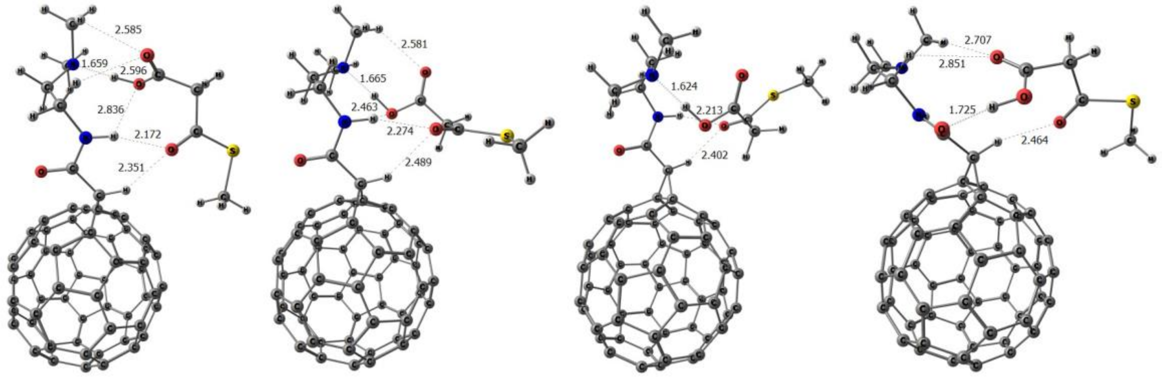
Table. S2 Relative free energies of all the possible intermediates (in kcal/mol) at addition pathway.

Catalysts	Functionals/Basis sets	$^{A}F_{R}$	$^{A}F_{INT1}$	$^{A}F_{INT2}$	$^{A}F_{INT3}$	$^{A}F_{INT4}$	$^{A}F_{p}$
F1	B3LYP/6-31G(d)//B3LYP/6-311+G(d,p)	0	-1.46	15.56	4.94	11.33	-11.82
	B3LYP-D3/6-31G(d)//B3LYP-D3/6-311+G(d,p)	0	-2.84	1.01	-12.36	0.47	-18.04
F2	B3LYP/6-31G(d)//B3LYP/6-311+G(d,p)	0	-6.31	12.72	7.94	5.43	-16.28
	B3LYP-D3/6-31G(d)//B3LYP-D3/6-311+G(d,p)	0	-5.45	1.65	-11.59	-1.00	-20.00

Table S3. Relative free energy differences between ‘without’ and ‘with’ diffuse basis sets involving anionic intermediates (in kcal/mol) for both the pathways.

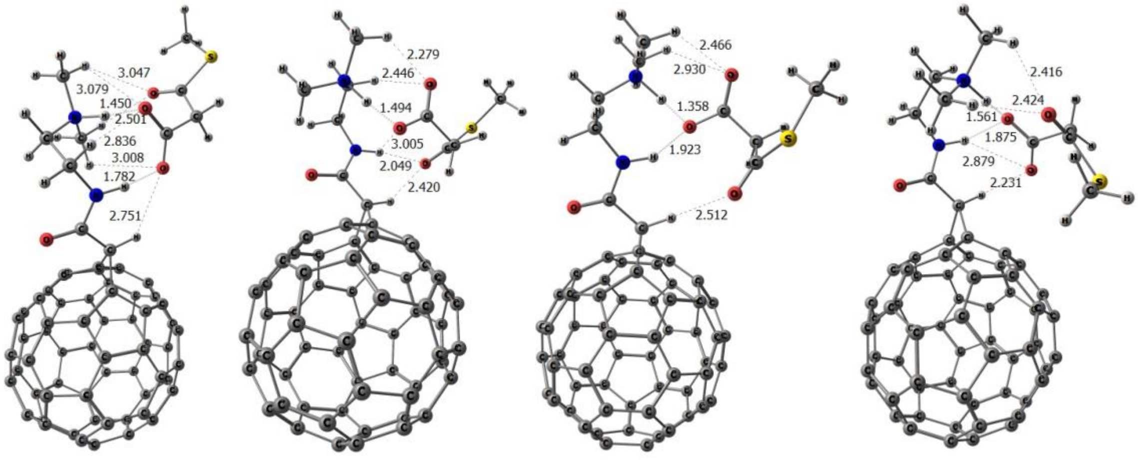
Anionic Species	**Basis Sets**		**Diffuse Basis Set (along with Dispersion-D3)**	
	6-31G(d)	6-31+G(d)	6-31G(d)-D3	6-31+G(d)-D3
${}^{D}F1_{INT1}$	0	-4.91	0	-2.82
${}^{D}F2_{INT1}$	0	-2.73	0	-3.15
${}^{A}F1_{INT1}$	0	-3.66	0	-2.82
${}^{A}F1_{INT1}$	0	-4.02	0	-2.59

All possible conformers (Con) of the reactant species


2.585
1.659
2.596
2.836
2.172
2.351
2.581
1.665
2.463
2.274
2.489
1.624
2.213
2.402
2.707
2.851
1.725
2.464

${}^{D}F1_{R\ (CON\text{-}1)}$	${}^{D}F1_{R\ (CON\text{-}2)}$	${}^{D}F1_{R\ (CON\text{-}3)}$	${}^{D}F1_{R\ (CON\text{-}4)}$
E=-3486.69766615 A.U	**E= -3486.69654116 A.U**	**E= -3486.69174474 A.U**	**E= -3486.68937109 A.U**
0	**0.70 kcal/mol**	**3.71 kcal/mol**	**5.20 kcal/mol**

All possible conformers (Con) of the anionic intermediate (Int1) species


3.047
3.079
1.450
2.501
2.836
3.008
1.782
2.751
2.279
2.446
1.494
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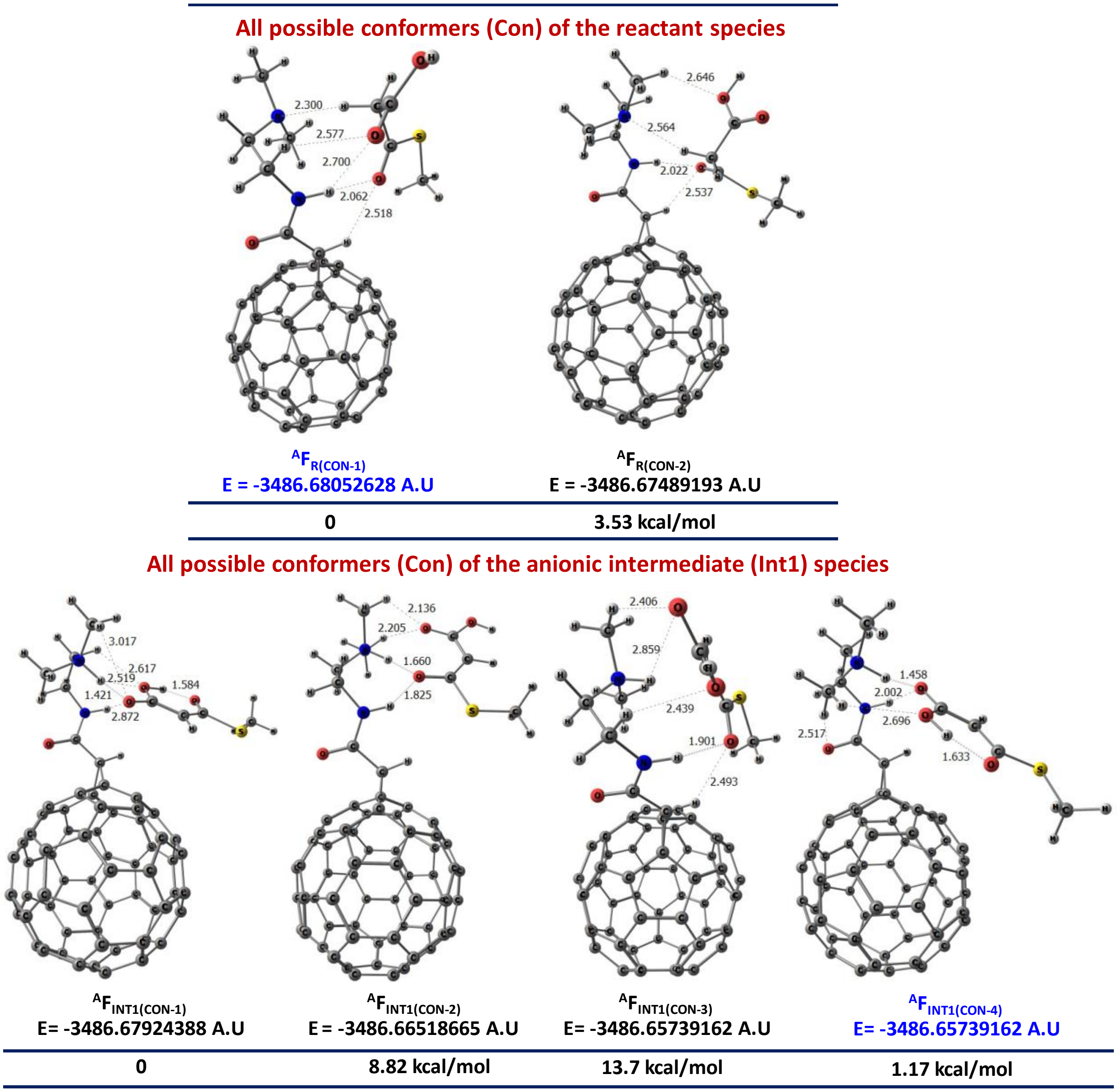
2.049
2.420
2.466
2.930
1.358
1.923
2.512
2.416
2.424
1.561
1.875
2.879
2.231

${}^{D}F1_{INT1(CON\text{-}1)}$	${}^{D}F1_{INT1(CON\text{-}2)}$	${}^{D}F1_{INT1(CON\text{-}3)}$	${}^{D}F1_{INT1(CON\text{-}4)}$
E = -3486.69247478 A.U	**E= -3486.69085576 A.U**	**E = -3486.68744052 A.U**	**E = -3486.68713979 A.U**
0	**1.01 kcal/mol**	**3.15 kcal/mol**	**3.34 kcal/mol**

Figure S1. All possible conformers of the reactant and intermediates (anionic) species along with their energies in Hartree and relative energies in kcal/mol.


2.300
2.577
2.700
2.062
2.518
2.646
2.564
2.022
2.537
3.017
2.617
2.519
1.584
1.421
2.872
2.136
2.205
1.660
1.825
2.406
2.859
2.439
1.901
2.493
1.458
2.002
2.696
2.517
1.633

All possible conformers (Con) of the reactant species

$^{A}F_{R(CON-1)}$ E = -3486.68052628 A.U	$^{A}F_{R(CON-2)}$ E = -3486.67489193 A.U
0	3.53 kcal/mol

All possible conformers (Con) of the anionic intermediate (Int1) species

$^{A}F_{INT1(CON-1)}$ E= -3486.67924388 A.U	$^{A}F_{INT1(CON-2)}$ E = -3486.66518665 A.U	$^{A}F_{INT1(CON-3)}$ E= -3486.65739162 A.U	$^{A}F_{INT1(CON-4)}$ E= -3486.65739162 A.U
0	8.82 kcal/mol	13.7 kcal/mol	1.17 kcal/mol

Figure S2. All possible conformers of the reactant and intermediates (anionic) species along with their energies in Hartree and relative energies in kcal/mol.

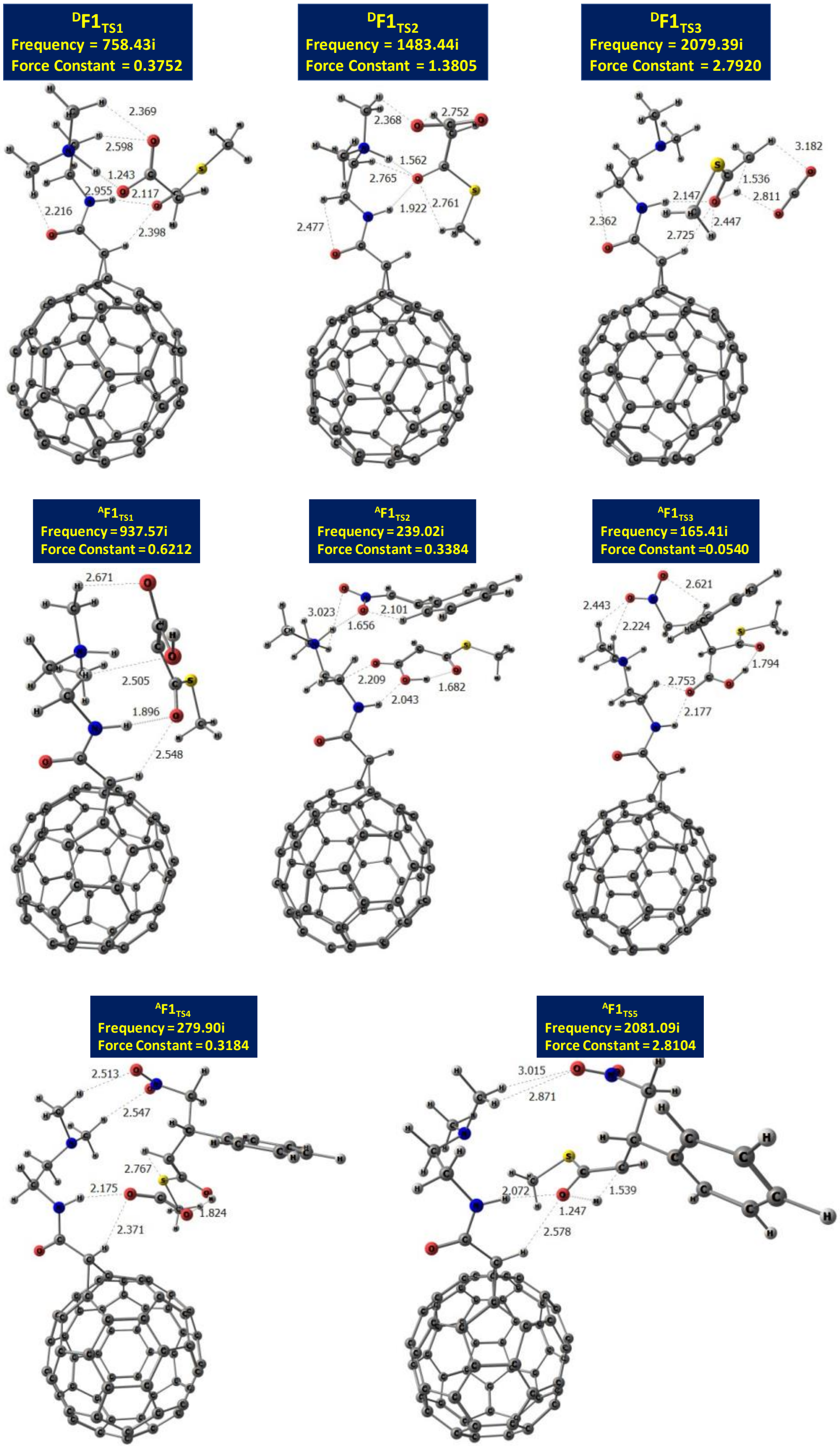

$^{D}F1_{TS1}$
Frequency = 758.43i
Force Constant = 0.3752
2.369
2.598
1.243
2.955
2.117
2.216
2.398
$^{D}F1_{TS2}$
Frequency = 1483.44i
Force Constant = 1.3805
2.752
2.368
1.562
2.765
1.922
2.761
2.477
$^{D}F1_{TS3}$
Frequency = 2079.39i
Force Constant = 2.7920
3.182
1.536
2.147
2.811
2.362
2.447
2.725
$^{A}F1_{TS1}$
Frequency = 937.57i
Force Constant = 0.6212
2.671
2.505
1.896
2.548
$^{A}F1_{TS2}$
Frequency = 239.02i
Force Constant = 0.3384
3.023
2.101
1.656
2.209
1.682
2.043
$^{A}F1_{TS3}$
Frequency = 165.41i
Force Constant =0.0540
2.621
2.443
2.224
1.794
2.753
2.177
$^{A}F1_{TS4}$
Frequency = 279.90i
Force Constant = 0.3184
2.513
2.547
2.767
2.175
1.824
2.371
$^{A}F1_{TS5}$
Frequency = 2081.09i
Force Constant = 2.8104
3.015
2.871
2.072
1.539
1.247
2.578

Figure S3. All possible inter and intramolecular hydrogen bond interactions of the eight transition states in decarboxylation and addition pathways for catalyst F1.

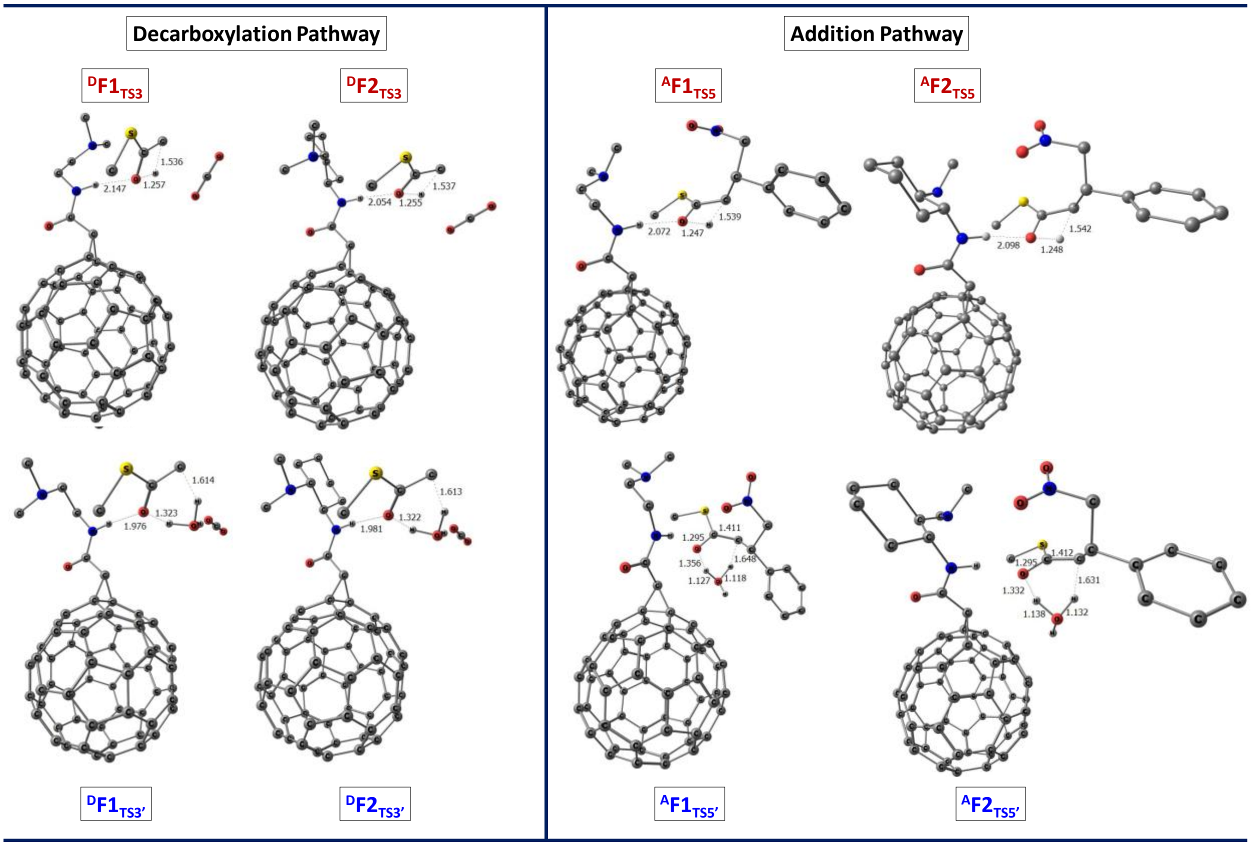


Figure S4. The transition state geometries along with the distances and their H-bonding interactions of the keto–enol tautomerization processes.

1.1 The Nature of Transition States via Bond Order Analysis

The bond order analysis is based on changes in the degree of bonding and computing the percentages of bond forming (BF_i) and bond cleaving (BC_j) at a particular transition state of the reaction path (addition or decarboxylation). More specifically, the bond order analysis exposes the transition state's bond making and breaking processes in the chemical reactions. This could be mainly identified by calculating the average percentage of bond formation cleavage (BFC_{Ave}) in the TS geometries and their percentages are summarized in Table S4. Importantly, the computed BFC_{ave} value indicates an early - "reactant-like" transition state if it ranges between 40-43%. On the other hand, BFC_{ave} values > 60% denote the TS as a late - "product-like" transition state. In the case of the decarboxylation pathway, the rupturing of O–H bond length in $^{D}F1_{TS1}$ was calculated to be around 1.243 Å, which is quite larger compared to the O–H bond length in $^{D}F1_{R}$ (1.032 Å). At the same time, the N–H bond length was estimated to be shorter (1.113 Å) than the same in

$^{D}F1_{TS1}$ transition state (1.272 Å for N–H). Also, the percentage of bond forming (BF_i) (N–H) and bond cleaving (BC_j) (O–H) indices were calculated to be 69.76% and 63.68% respectively. Therefore, the transition state $^{D}F1_{TS1}$ is more of "product-like" which is endorsed by a BFC_{Ave} value (Table S4). The percentages of BF_i, BC_j and BFC_{Ave} of the pertinent bonds in the transition state $^{D}F_{TS2}$ are estimated and listed in Table S4. Again, this transition state for decarboxylation step was highly "product-like" and was endogenic (21.78 kcal/mol) with respect to the reactant $^{D}F_{R}$.

Table S4. Computed Wiberg Bond Formation (BF_i), Bond Cleavage (BC_j) Indices and Bond Formation Cleavage Average (BFC_{Ava}) (in %) of all chosen transition states (TS) across both addition and decarboxylation pathways for both the catalysts F1 and F2.

Pathways	**Transition States**	**BF_i (%)**	**BC_j (%)**	**BFC_{Ave} (%)**
Catalyst (C_{60})-F1				
Decarboxylation	$^{D}F1_{TS1}$	69.76 (N-H)	63.68 (O-H)	66.72
	$^{D}F1_{TS2}$	53.25 (O-H)	78.55 (N-H); 72.61 (C-C)	68.14
	$^{D}F1_{TS3}$	33.53 (C-H)	59.05 (O-H)	46.29
Addition	$^{F}F1_{TS1}$	62.15 (N-H)	40.94 (O-H)	51.54
	$^{F}F1_{TS2}$	41.51 (C-C)	-	41.51
	$^{F}F1_{TS3}$	29.88 (C-H)	95.35 (N-H)	62.62
	$^{F}F1_{TS4}$	86.30 (O-H)	12.81 (O-H); 39.79 (C-C)	46.30
	$^{F}F1_{TS5}$	35.74 (C-H)	50.08 (O-H)	42.92
Catalyst(C_{60})-F2				
Decarboxylation	$^{D}F2_{TS1}$	58.69 (N-H)	72.23 (O-H)	65.46
	$^{D}F2_{TS2}$	11.61 (O-H)	90.66 (N-H); 23.06 (C-C)	41.77
	$^{D}F2_{TS3}$	39.63 (C-H)	57.65 (O-H)	48.64
Addition	$^{F}F2_{TS1}$	75.37 (N-H)	43.65 (O-H)	59.51
	$^{F}F2_{TS2}$	42.93 (C-C)	-	42.93
	$^{F}F2_{TS3}$	39.62 (C-H)	83.21 (N-H)	61.42
	$^{F}F2_{TS4}$	78.07 (O-H)	22.73 (O-H); 47.64 (C-C)	49.48
	$^{F}F2_{TS5}$	35.32 (C-H)	50.21 (O-H)	42.76

Furthermore, a highly exoergic pathway was noticed for the final step of enol-to-keto formation/ the product ($^{D}F1_{P}$). The bond forming (C–H; 1.536 Å) and breaking (O–H; 1.256 Å) were matured by 33.53% and 59.05% respectively, while the total BCF_{Ave} was computed to be

46.29%. This specifies the transition state $^{D}F1_{TS3}$ (enol-to-keto) was "early" in category. From the estimated BC_j, BF_i and BFC_{Ave} components in Table S1, the initial step was associated with the breaking of α-hydrogen (C–H; 1.522 Å) and making of the N–H bond (N–H; 1.237 Å) in the transition state $^{A}F1_{TS1}$ (BFC_{Ave}: 51.54%). This implied the "middle" nature of the transition state, falling neither into 'product-like" nor "reactant-like" categories. Besides, the other BFC_{Ave} values matured in the range between ~41 to 46% for $^{A}F1_{TS2}$, $^{A}F1_{TS4}$ and $^{A}F1_{TS5}$. Among the two pathways, the transition state $^{A}F_{TS3}$ for the addition pathway could be described as "product-like" (BFC_{Ave} = 62.62%). Overall, except $^{A}F1_{TS3}$, all the transition states were "reactant-like" (early TSs), bringing out bond cleavage and bond forming percentages in the addition path. For catalyst F2, $^{D}F2_{TS2}$ witnessed the C-C bond cleavage (23.06 %) to be faster (BFC_{Ave}: 41.77%) than $^{D}F1_{TS2}$ (BFC_{Ave}: 68.14%), as collected in Table S1. In addition, for catalyst F2, BFC_{Ave} were estimated to be matured in the range 42-62% in all the five transition states which undoubtedly ascertains the fact that the key transition states are "early TS" in nature. This detailed analysis distinctly brought out the reaction coordinates and the feasibility of the reaction path, rendering it favourable for addition rather than the decarboxylation pathway.

1.2 Non-covalent Interaction (NCI) Analysis:

The NCI-RDG analysis was carried out on the optimized geometries of all intermediates and the corresponding transition states showing the stabilizing attractive (blue), destabilizing repulsive (red), and weak van der Waals (green) interactions. The RDG and their corresponding isosurfaces were calculated to identify the regions of non-covalent interactions and to analyze the strength of interactions between the substrates and the fullerene (C_{60}) catalyst. Figure 7 displays the RDG scatter plots and their corresponding sign of $(\lambda_2)\rho$ values. In Figure 7, anionic intermediates showed two interactions, the C=O---π surface and the anion-π interactions with the corresponding interaction lengths computed to be 2.691 Å and 3.790 Å for $^{A}F1_{INT1}$ and 2.710 Å and 3.761 Å for $^{A}F2_{INT1}$. At the same time, $^{D}F1_{INT1}$ and $^{D}F2_{INT1}$ showed only the C=O---π surface interaction with a distance of 2.715 Å and 2.641 Å, while the anion-π interaction was absent. This finding agrees with the experimental report where López-Andarias and co-workers mentioned the $^{A}F_{INT1}$ intermediates to exhibit anion-π surface interactions in the addition pathway, whereas, the $^{D}F_{INT1}$ intermediates do not show the same across the decarboxylation pathway. If this were not the case, then $^{A}F_{INT1}$ intermediates would not be exoergic with respect to $^{D}F_{INT1}$ (Figures 1 and 2), and, would have contradicted the experimental observations. Figure 7 also shows the RDG isosurface maps of $^{D}F_{INT1}$ and $^{A}F_{INT1}$ with selected weak interactions such as the intramolecular hydrogen bond (attractive and shown in blue), destabilizing repulsive and weak van der Waals interactions. In NCI analysis, the non-covalent interactions have λ_2 values ranging from large negative magnitudes to zero. On the other side, the positive λ_2 values indicate the destabilizing repulsive interactions. In $^{A}F_{INT1}$, a strong attractive region exists between the anionic substrate and the fullerene catalyst, attributed to anion-π interaction and is depicted as vdW interactions. More importantly, the existence of characteristic C=O---π interaction is seen to be prevalent on the catalyst surfaces.

Comparatively, the non-covalent interaction plots of intermediates $^{A}F1_{INT1}$ and $^{A}F2_{INT1}$ describe the presence of strong attractive interactions of intermolecular hydrogen bonding and vdW interactions. This attractive region is missing between anionic substrate and fullerene catalyst in $^{D}F1_{INT1}$ and $^{D}F2_{INT1}$ as shown in Figure 7. The above computational analysis thus estimated various non-covalent interactions of the type, N-H---O, O-H---O, C=O---π and $C\text{-}O^{-}$---π that stabilized the anionic intermediates. This investigation therefore concretely proves the significant role played by anion-π interactions in stabilizing $^{A}F_{INT1}$ intermediates, but not $^{D}F_{INT1}$ intermediates, further supported by the earlier experimental observations.[1]

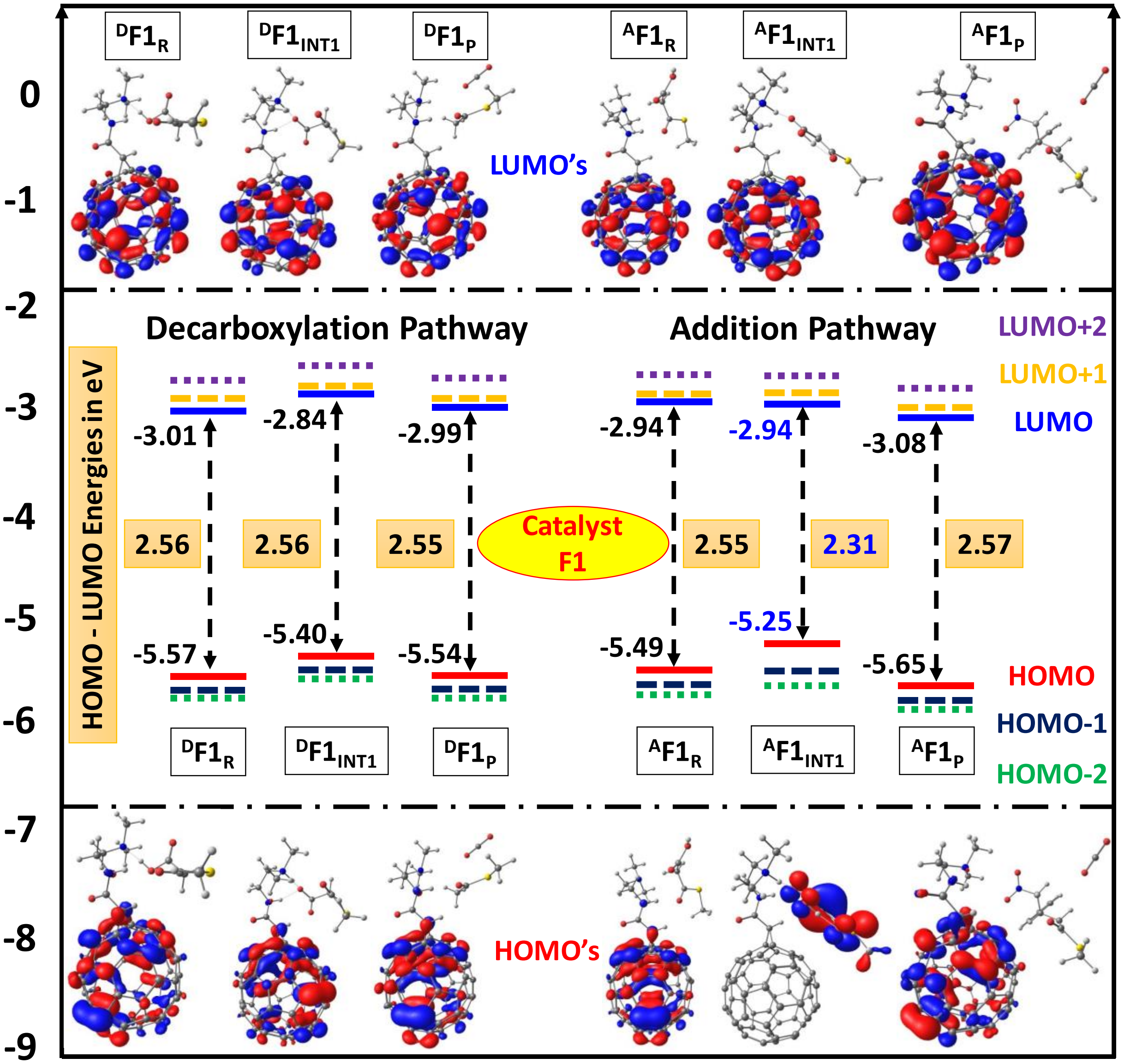
1.3 QTAIM Analysis:

Quantum theory of atoms in molecules (QTAIM) analysis was widely used to study the nature of chemical bonds, hydrogen bonds and various weak interactions present in the reactive species. It is well established that QTAIM analysis is predictable to understanding weak interactions in an anionic intermediate in addition reactions. In the present study, bonding and non-bonding interactions were analysed by assessing the topological properties that indicates the strength of the bond critical points (BCP's) and represents the nature of the bond. Various topological properties such as electron density (ρ(r)), Laplacian of electron density ($\nabla^2 \rho$(r)), Hessian values (λ_1, λ_2), the potential energy density V(r) and and kinetic energy density G(r) values have been calculated and listed in Table 1. As estimated, the molecular graph shows various types of interactions involving in both the anionic intermediates. The computed electron density at the BCPs for these interactions is well located within the hydrogen bond limits (0.002-0.035 a.u) and negative $\nabla^2\rho$ (r) values show these interactions are closed shell in nature.[2,3] It could be noted that

N-H_3---O_3 (1.458 Å) has the higher electron density with 0.091 a.u (for $^{A}F1_{INT1}$) while others range from 0.002 to 0.02 a.u. A similar situation was detected for the $^{A}F2_{INT1}$ intermediate (Figure 8) Furthermore, the calculated electron densities at BCPs of anion-π surface interactions were higher (0.0022 for H1---C1 and 0.0023 for S---C2) in $^{A}F2_{INT1}$ and in $^{A}F1_{INT1,}$ they were 0.0022 for H1---C1 and 0.0022 for S---C2, respectively. Furthermore, other important topological properties like |V|/G ratio values were calculated for both the $^{A}F1_{INT1}$ and $^{A}F2_{INT1}$ intermediates. It is profound to compute the covalency of all the discussed interactions. |V|/G ratio ~1 indicates the shared interactions are of closed shell type. The computed |V|/G ratio of strong intermolecular hydrogen bonding interactions of $^{A}F1_{INT1}$ and $^{A}F2_{INT1}$ were 1.514 and 1.422, implying stronger N-H---O interactions, vide Table 1. On other hand, for the anion-π stacking interactions in $^{A}F1_{INT1}$ and $^{A}F2_{INT1}$ the |V|/G ratio were estimated to be in the range 0.67 to 0.79. Additionally, the C=O---C_{60} surface (intra-molecular) interactions involved in $^{A}F2_{INT1}$ showed |V|/G ratio closer to ~0.80 when compared to $^{A}F2_{INT1}$ intermediate (~0.80 a.u), revealing the importance and the strength of these interactions. Moreover, the $^{A}F1_{INT1}$ shows two C=O---C_{60} surface interactions (C=O_4---C_6 and C=O_4-C_7), that are strong with electron densities ~0.008 a.u and |V|/G ratio ~0.8, which are quite comparable with other inter-molecular hydrogen bonding interactions. Overall, this study not only emphasized the importance of the intermolecular hydrogen bonding interactions, but also established two C=O---C_{60} surface (C=O---$C_{5(C60)}$ and C=O---$C_{6(C60)}$) and four anion---C_{60} interactions (C-H---$C_{1(C60)}$, S---$C_{2(C60)}$, O_1---$C_{3(C60)}$ and C1---$C_{4(C60)}$ respectively, that helps in the stabilization of the anionic intermediates.

1.4 Synergistic Frontier Molecular Orbital (FMO) Energy Levels:

Anion−π interactions relate to the LUMO level of the catalyst. Studies have shown the origin of intrinsic anion−π interactions associated with intrinsic pi-acidity to be synonymous with low LUMO levels. Accordingly, frontier molecular orbital (FMO) analysis for the ground state geometries of reactants, anionic intermediates and products was undertaken and the results are presented in Figure S5(a) and S5(b). For the selected reactive species across both the pathways, HOMO-LUMO energy gaps ranged between 2.27 to 2.57 eV. More specifically, $^{A}F1_{INT1}$ and $^{A}F2_{INT1}$ anionic intermediates possessed the smallest energy gaps of 2.31 eV and 2.27 eV respectively, suggesting them to be consistent with increasing electron sharing through anion-π interactions. Hence, stabilization of anionic intermediates could be facilitated by anion-π interactions on π- acidic surfaces and via electronic communication within this anion-π stack, as reflected in the energy gaps. The small energy gap was caused by favorable electronic communication between the fullerene surfaces and anionic substrates in the stacks. On analyzing the corresponding FMOs, the HOMOs were associated with π-characters and LUMOs with π* characters in fullerene catalysts.



0
-1
-2
-3
-4
-5
-6
-7
-8
-9
HOMO - LUMO Energies in eV
$^{D}F1_{R}$
$^{D}F1_{INT1}$
$^{D}F1_{P}$
$^{A}F1_{R}$
$^{A}F1_{INT1}$
$^{A}F1_{P}$
LUMO's
Decarboxylation Pathway
Addition Pathway
LUMO+2
LUMO+1
LUMO
-3.01
-2.84
-2.99
-2.94
-2.94
-3.08
2.56
2.56
2.55
Catalyst F1
2.55
2.31
2.57
-5.57
-5.40
-5.54
-5.49
-5.25
-5.65
HOMO
HOMO-1
HOMO-2
$^{D}F1_{R}$
$^{D}F1_{INT1}$
$^{D}F1_{P}$
$^{A}F1_{R}$
$^{A}F1_{INT1}$
$^{A}F1_{P}$
HOMO's

Figure S5(a). The energy level diagram of frontier molecular orbitals of fullerene catalyst-F1 in the gas phase obtained at the B3LYP/6-31G(d) level of theory.

Especially, the HOMO's distribution of $^{A}F1_{INT1}$ and $^{A}F2_{INT2}$ intermediates are mainly localized within the anionic substrate species and LUMO's distributions only with fullerene systems. Moreover, the HOMO orbitals of $^{A}F1_{INT1}$ and $^{A}F2_{INT1}$ were computed to be highly stabilized with energies -5.25 eV and -5.17 eV while the other species were relatively less stabilized with energies ranging from -5.65 eV to -5.36 eV.

Analyzing the distribution pattern of HOMOs of reactants, intermediates and products (Figure S5(a) and S5(b)) it is revealed that the molecular orbitals were populated over the entire fullerene molecule with strong π character, while the LUMOs were also delocalized over the entire fullerene molecular skeleton with π* character, except $^{A}F1_{INT1}$ and $^{A}F2_{INT1}$. This also confirms the HOMO to LUMO electronic transitions to be of $\pi \rightarrow \pi^*$ nature. On the other hand, the HOMOs of $^{A}F1_{INT1}$ and $^{A}F2_{INT1}$ were computed to be distributed mainly over the anionic substrates, resembling lone pairs of non-bonding orbitals of C=O and $C\text{-}O^-$ parts and the LUMOs were populated over the entire fullerene molecular geometry with π* orbital nature, thus originating intramolecular charge transfer (ICT) type of interactions. Therefore, a considerable amount of electron density had been delocalized from anionic substrates to fullerene part indicating the prevalence of strong intramolecular charge transfer (ICT). As discussed in the FMO analysis, the HOMO to LUMO transition for the first set of two molecules ($^{A}F1_{INT1}$ and $^{A}F2_{INT1}$) were computed to be purely of ICT nature while all other species exhibited with $\pi \rightarrow \pi^*$ transitions.

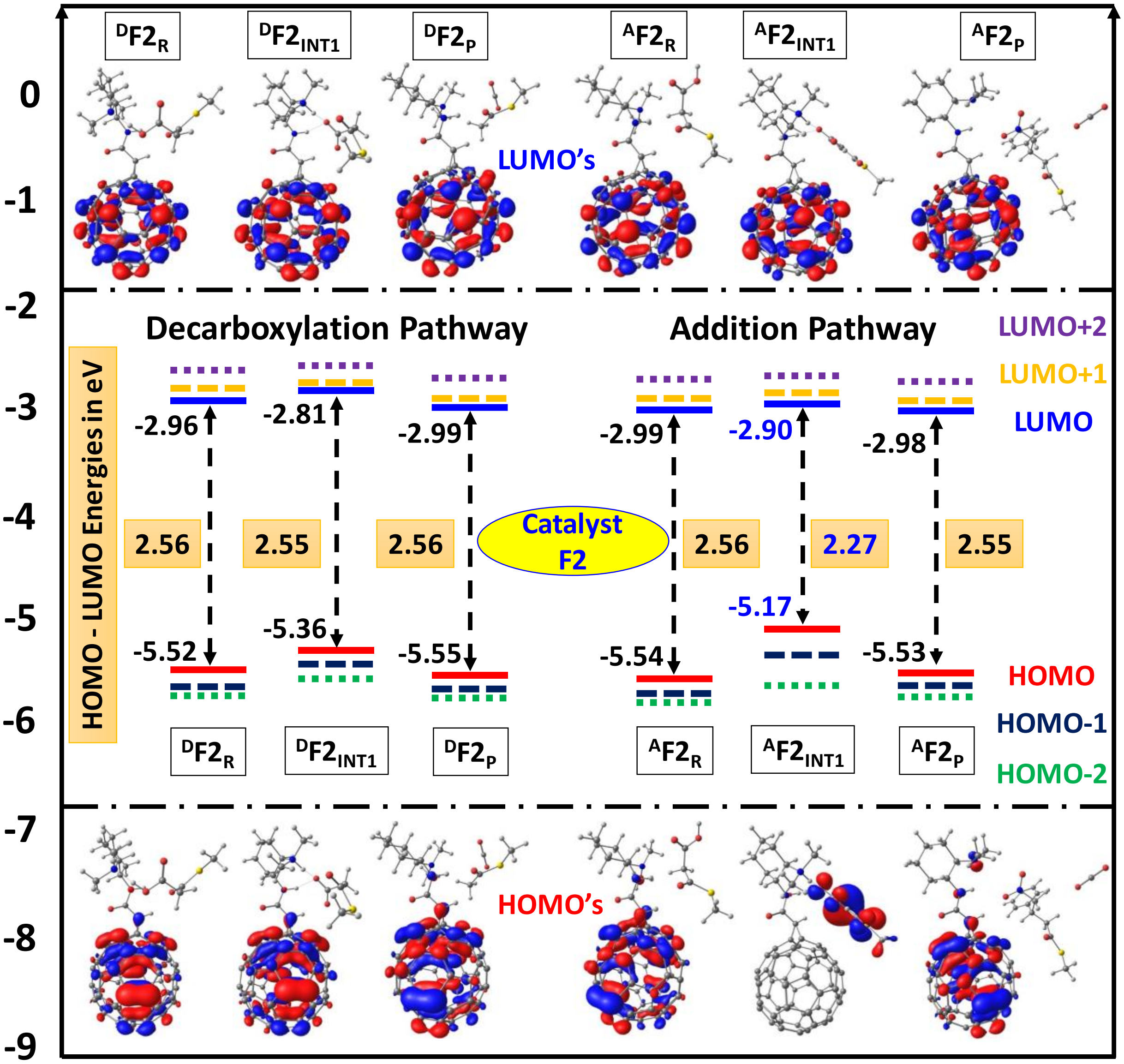

$^{D}F2_{R}$
$^{D}F2_{INT1}$
$^{D}F2_{P}$
$^{A}F2_{R}$
$^{A}F2_{INT1}$
$^{A}F2_{P}$
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
LUMO's
HOMO's
HOMO - LUMO Energies in eV
Decarboxylation Pathway
Addition Pathway
LUMO+2
LUMO+1
LUMO
HOMO
HOMO-1
HOMO-2
-2.96
-2.81
-2.99
-2.99
-2.90
-2.98
2.56
2.55
2.56
2.56
2.27
2.55
Catalyst F2
-5.52
-5.36
-5.55
-5.54
-5.17
-5.53

Figure S5(b). The energy level diagram of frontier molecular orbitals of fullerene catalyst-F2 in the gas phase obtained at the B3LYP/6-31G(d) level of theory.

1.5. Molecular Electrostatic Potential Mapping (MESP)

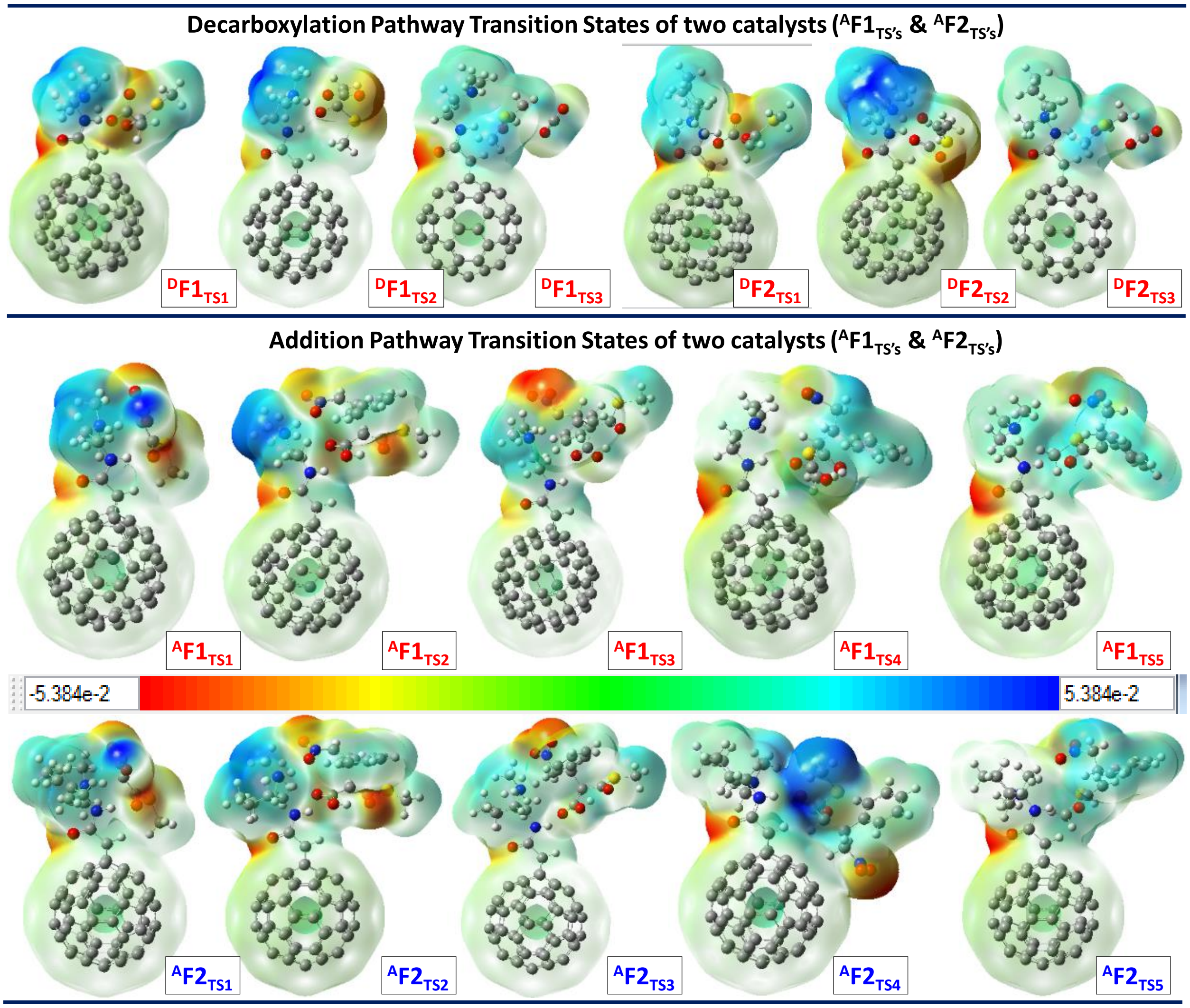

Decarboxylation Pathway Transition States of two catalysts ($^{A}F1_{TS's}$ & $^{A}F2_{TS's}$)
$^{D}F1_{TS1}$
$^{D}F1_{TS2}$
$^{D}F1_{TS3}$
$^{D}F2_{TS1}$
$^{D}F2_{TS2}$
$^{D}F2_{TS3}$
Addition Pathway Transition States of two catalysts ($^{A}F1_{TS's}$ & $^{A}F2_{TS's}$)
$^{A}F1_{TS1}$
$^{A}F1_{TS2}$
$^{A}F1_{TS3}$
$^{A}F1_{TS4}$
$^{A}F1_{TS5}$
-5.384e-2
5.384e-2
$^{A}F2_{TS1}$
$^{A}F2_{TS2}$
$^{A}F2_{TS3}$
$^{A}F2_{TS4}$
$^{A}F2_{TS5}$

Figure S6. All transition states of MESP maps are depicted in decarboxylation and addition pathways.

1.6 Natural Bond Orbital (NBO) Analysis

The possible interactions associated with the transition states for both the pathways were estimated following NBO analysis, employed at the B3LYP/6-31G(d) level of theory, using the optimized geometries. Especially, the second-order perturbation interaction energies between the substituted fullerene C_{60} catalyst and the substrate orbitals could play an extensive role in recognizing their reactivity. In view of this, the calculated second-order perturbation stabilization energy (E^2) for the most prominent interactions in these transition states are collected in Table S5 & S3 and Figure S7(a) & S7(b). In Pathway-I (decarboxylation), $^{D}F1_{TS1}$ is highly stabilized in the lone pairs of nitrogen (N_{71} in fullerene) and oxygen (O_{95}) atoms of substrate (MAHT) species. The orbital interactions arise due to highly stabilized by inter and intramolecular hydrogen bond interactions. The second-order stabilization energies, 207.25 kcal/mol for $N_{71} \rightarrow H_{91}–O_{95}$ and 136.49 kcal/mol for $O_{95} \rightarrow N_{71}–H_{91}$ in Figure S7(a) & S7(b) clearly indicate the prevailing $n \rightarrow \sigma^*$ interactions as well as proton abstraction to take place from the substrate (MAHT) species to fullerene (C_{60}) catalyst via the intermolecular hydrogen bonding interactions.

In $^{D}F1_{TS2}$, three orbital interactions were observed, where nitrogen atom of fullerene (C_{60}) catalyst acted as donor NBO and the σ*(O–H) of substrate acted as an acceptor NBO of which, only one interaction had a very strong stabilization energy of 173.62 kcal/mol. Two other interactions showed 108.68 kcal/mol for $O_{89} \rightarrow N_{71}–H_{95}$ and 44.94 kcal/mol for $O_{82} \rightarrow C_{83}–O_{84}$ respectively (Table S5 & S6). However, the transition state $^{D}F1_{TS3}$ was associated with 95.21 kcal/mol stabilization energy from $O_{84} \rightarrow C_{92}–H_{94}$ interaction and was the lowest perturbed stabilization energy. Consequently, $^{D}F1_{TS1}$ and $^{D}F1_{TS2}$ showed slight significant changes in the second-order stabilization energy, due to the influence of cyclic ring functionalized in catalyst F2. In the addition pathway, intermediates and transition states showed $n \rightarrow \sigma^*$ interactions and their energy ranges were estimated as 50 to 217 kcal/mol, resulting from intermolecular hydrogen bonding interactions (See supporting information Table S5 and S6). On the other hand, $^{D}F2_{TS1}$, $^{D}F2_{TS2}$ and $^{D}F2_{TS3}$ were associated with only $n \rightarrow \sigma^*$ interactions stabilized by 186.95 kcal/mol ($N_{69} \rightarrow H_{89}–O_{93}$), 15.91 kcal/mol ($O_{83} \rightarrow H_{89}–N_{69}$) and 50.24 kcal/mol ($O_{82} \rightarrow H_{92}–C_{90}$), respectively, which could be the major reason for the higher reactivity of the transition states. Overall, $^{A}F1_{TS4}$ showed relatively higher stabilization energy (by 372.86 kcal/mol) compared to all the other $n \rightarrow \sigma^*$ interactions. The overall orbital interactions are shown in Figure S7(a) & S7(b). Overall, a good correlation between the NBO stabilization energies (n−σ*) were visualized for all the transition states. It is interesting to observe the NBO analysis to help explain the higher reactivity of $^{A}F2_{R}$, stabilized by lower energies (2.36 kcal/mol and 4.68 kcal/mol) than all other reactant species of both the pathways (Table S6). To gain more insight into this stabilization, various interactions existing between fullerene (C_{60}) and substrates need to be explained and examined. Overall, the presence of strong hydrogen bonding interactions gripped the key to the variance in the reactivity of the species.

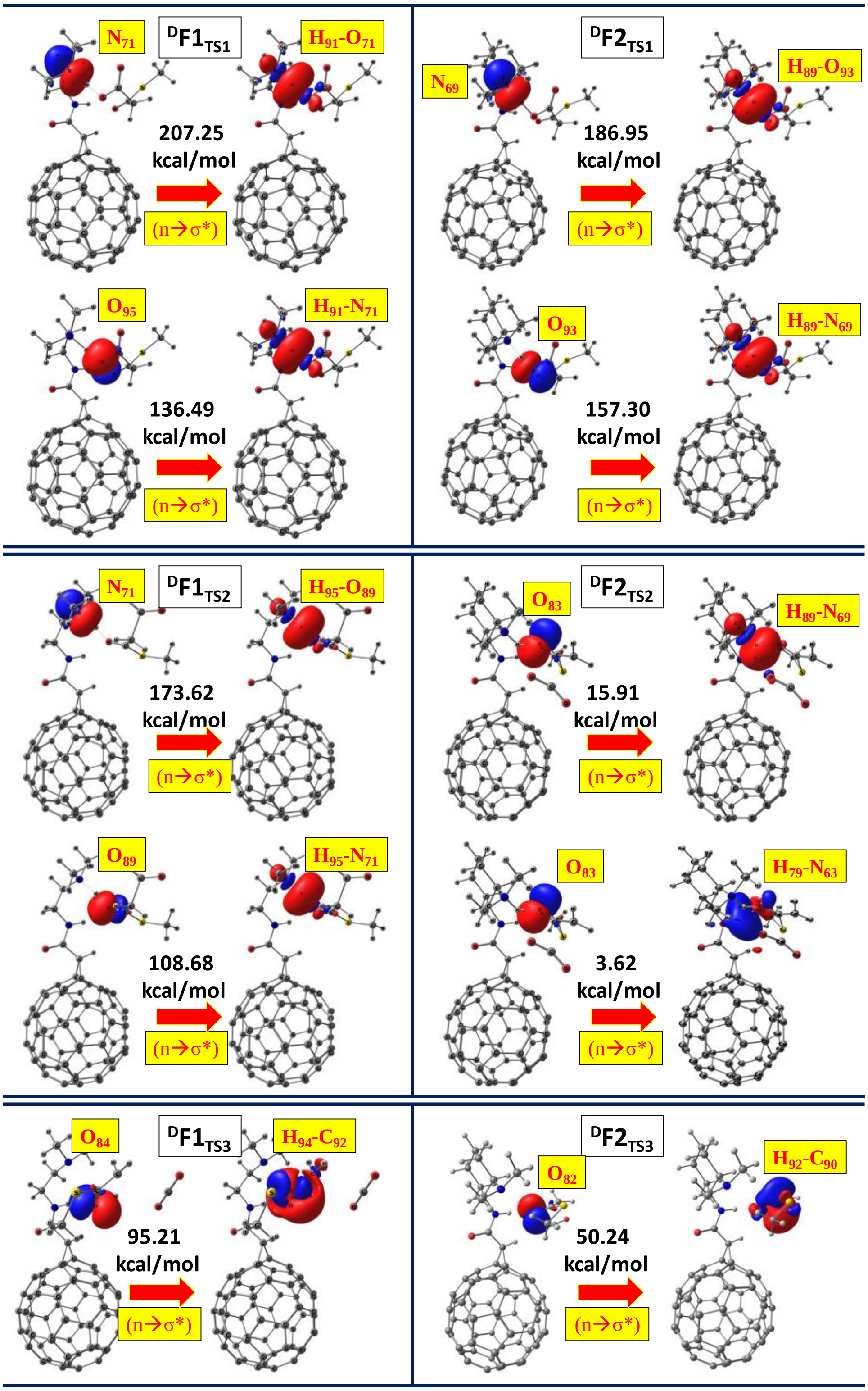

N_{71}
$^{D}F1_{TS1}$
H_{91}-O_{71}
207.25 kcal/mol
(n→σ*)
N_{69}
$^{D}F2_{TS1}$
H_{89}-O_{93}
186.95 kcal/mol
(n→σ*)
O_{95}
H_{91}-N_{71}
136.49 kcal/mol
(n→σ*)
O_{93}
H_{89}-N_{69}
157.30 kcal/mol
(n→σ*)
N_{71}
$^{D}F1_{TS2}$
H_{95}-O_{89}
173.62 kcal/mol
(n→σ*)
O_{83}
$^{D}F2_{TS2}$
H_{89}-N_{69}
15.91 kcal/mol
(n→σ*)
O_{89}
H_{95}-N_{71}
108.68 kcal/mol
(n→σ*)
O_{83}
H_{79}-N_{63}
3.62 kcal/mol
(n→σ*)
O_{84}
$^{D}F1_{TS3}$
H_{94}-C_{92}
95.21 kcal/mol
(n→σ*)
$^{D}F2_{TS3}$
O_{82}
H_{92}-C_{90}
50.24 kcal/mol
(n→σ*)

Figure S7(a). Natural bond orbitals of strong hydrogen bonding interactions in the respective transition states involved in decarboxylation pathways. Second-order stabilization energies are given in kcal/ mol.

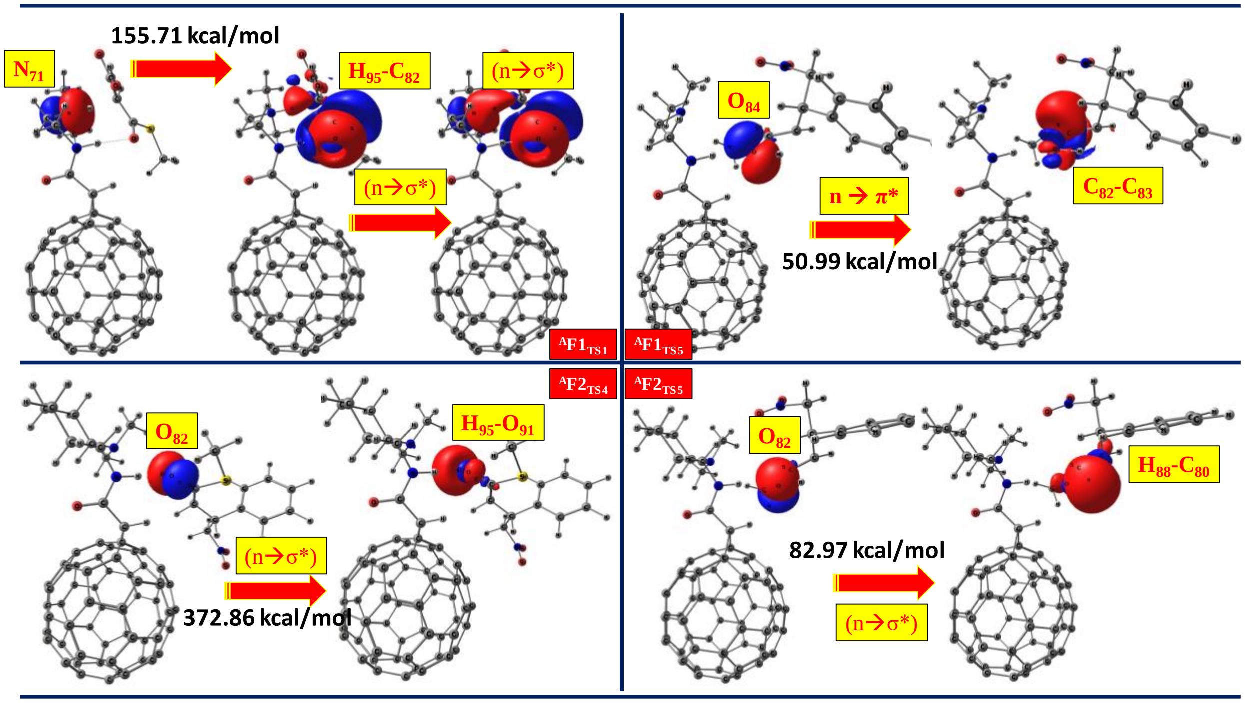

155.71 kcal/mol
N71
H95-C82
(n→σ*)
(n→σ*)
O84
n → π*
C82-C83
50.99 kcal/mol
AF1TS1
AF1TS5
AF2TS4
AF2TS5
O82
H95-O91
(n→σ*)
372.86 kcal/mol
O82
H88-C80
82.97 kcal/mol
(n→σ*)

Figure S7(b). Natural bond orbitals of showing strong hydrogen bonding interactions in the respective transition states involved in addition pathway. Second-order stabilization energies are given in kcal/ mol.

Table. S5 Computed natural bond analysis (NBO) of all chosen for the transition states (TS's) at both addition and decarboxylation pathways in both the catalysts F1 and F2.

Pathways	**Transition States (TS's)**	**Possible Interactions**	**Second-Order Stabilization Energy (E_2) in kcal/mol**
Catalyst-F1			
Decarboxylation	$^{D}F1_{TS1}$	$N_{71} \rightarrow H_{91}$	207.25
		$O_{95} \rightarrow N_{71}–H_{91}$	136.49
	$^{D}F1_{TS2}$	$N_{71} \rightarrow H_{95}$	173.62
		$O_{89} \rightarrow N_{71}–H_{95}$	108.68
		$O_{82} \rightarrow C_{83}–O_{84}$	44.94
	$^{D}F1_{TS3}$	$O_{84} \rightarrow C_{92}–H_{94}$	95.21
Addition	$^{A}F1_{TS1}$	$N_{71} \rightarrow C_{82}–H_{95}$	155.71
		$C_{82}\text{-}H_{95} \rightarrow C_{83}\text{-}O_{84}$	29.51
	$^{A}F1_{TS2}$	$C_{82}–C_{95} \rightarrow C_{83}–O_{84}$	34.08
	$^{A}F1_{TS3}$	$N_{71} \rightarrow C_{97}–H_{109}$	216.34
	$^{A}F1_{TS4}$	$O_{91} \rightarrow C_{82}–C_{90}$	61.25
	$^{A}F1_{TS5}$	$O_{84} \rightarrow C_{82}–C_{83}$	50.99
		$O_{84} \rightarrow H_{90}$	122.79
		C82–C83 $\rightarrow H_{90}$	114.52
Catalyst-F2			
Decarboxylation	$^{D}F2_{TS1}$	$N_{69} \rightarrow H_{89}$	186.95
		$O_{93} \rightarrow H_{89}$	157.30
	$^{D}F2_{TS2}$	$O_{83} \rightarrow H_{89}$	15.91
		$O_{83} \rightarrow N_{63}–H_{79}$	3.62
	$^{D}F2_{TS3}$	$O_{82} \rightarrow C_{90}–H_{92}$	50.24
Addition	$^{A}F2_{TS1}$	$N_{69} \rightarrow C_{80}–H_{93}$	137.56
	$^{A}F2_{TS2}$	$O_{109} \rightarrow N_{69}–H_{107}$	12.61
		$O_{89} \rightarrow N_{63}–H_{79}$	11.61
		$O_{82} \rightarrow O_{89}–H_{91}$	24.42
	$^{A}F2_{TS3}$	$N_{69} \rightarrow C_{95}–H_{107}$	162.88
		$O_{90} \rightarrow C_{63}–H_{79}$	6.55
	$^{A}F2_{TS4}$	$O_{82} \rightarrow H_{91}$	372.86
	$^{A}F2_{TS5}$	$O_{82} \rightarrow H_{88}$	82.97

Table. S6 Computed natural bond analysis (NBO) of all chosen for the reactive species at both addition and decarboxylation pathways in both the catalysts F1 and F2.

Pathways	**Intermediates**	**Possible Interactions**	**Second-Order Stabilization Energy (E_2) in kcal/mol**
Catalyst-F1			
Decarboxylation	$^{D}F1_{R}$	$N_{71} \rightarrow H_{95}$	64.49
		$O_{82} \rightarrow H_{95}$	377.28
	$^{D}F1_{INT1}$	$N_{71} \rightarrow H_{91}$	322.28
	$^{D}F1_{INT2}$	$N_{71} \rightarrow O_{84}–H_{95}$	31.46
	$^{D}F1_{P}$	$N_{71} \rightarrow O_{92}–H_{95}$	3.52
		$O_{84} \rightarrow N_{63}–H_{81}$	7.16
Addition	$^{A}F1_{R}$	$N_{71} \rightarrow C_{82}–H_{95}$	5.80
	$^{A}F1_{INT1}$	$N_{71} \rightarrow H_{90}$	296.46
		$O_{93} \rightarrow H_{90}$	121.38
	$^{A}F1_{INT2}$	$O_{102} \rightarrow H_{91}$	87.49
		$O_{101} \rightarrow N_{63}–H_{81}$	14.61
	$^{D}F1_{INT3}$	$N_{71} \rightarrow H_{93}$	93.47
Catalyst-F2			
Decarboxylation	$^{D}F2_{R}$	$N_{69} \rightarrow H_{89}$	79.72
		$O_{93} \rightarrow H_{89}$	348.08
	$^{D}F2_{INT1}$	$N_{69} \rightarrow H_{84}$	357.31
		$O_{83} \rightarrow H_{84}$	50.19
	$^{D}F2_{INT2}$	$N_{69} \rightarrow O_{82}–H_{93}$	24.41
	$^{D}F2_{P}$	$N_{69} \rightarrow C_{90}–H_{93}$	2.31
		$O_{82} \rightarrow N_{63}–H_{79}$	6.79
Addition	$^{A}F2_{R}$	$N_{69} \rightarrow C_{80}–H_{93}$	2.36
		$O_{69} \rightarrow N_{63}–H_{79}$	4.68
	$^{A}F2_{INT1}$	$O_{91} \rightarrow N_{63}–H_{79}$	5.03
		$O_{91} \rightarrow H_{88}$	91.44
		$O_{82} \rightarrow O_{90}–H_{88}$	30.51
	$^{A}F2_{INT2}$	$O_{100} \rightarrow H_{89}$	44.87
		$O_{99} \rightarrow N_{63}–H_{79}$	13.13
	$^{A}F2_{INT3}$	$N_{69} \rightarrow H_{91}$	81.00

1.7 IRC Analysis

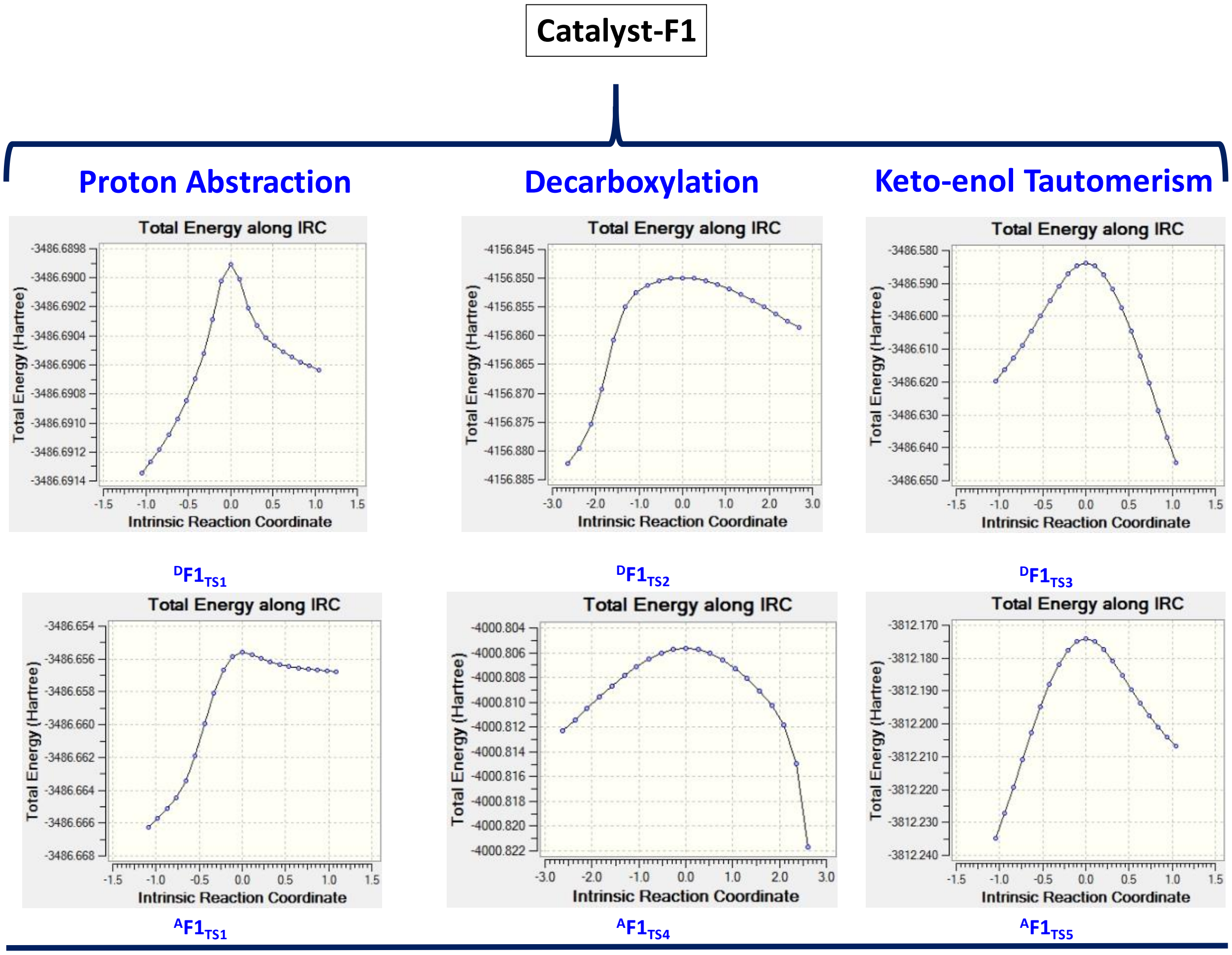


Figure S8. Selected Intrinsic reaction coordinate (IRC) analysis involved at catalyst F1 in decarboxylation and addition pathways.

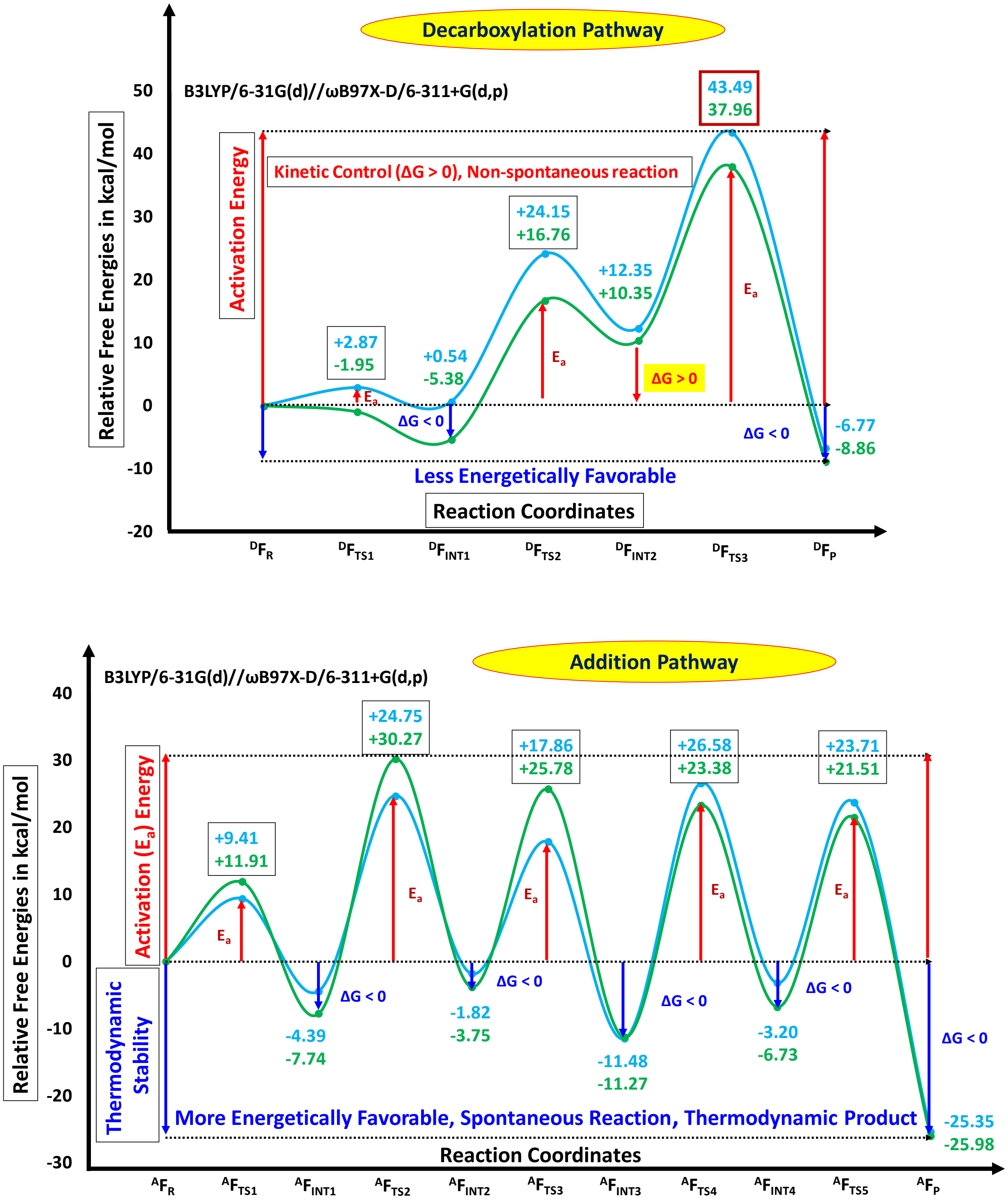


Figure S9. Energetic favorability (under thermodynamic vs kinetic controls) for the decarboxylation and addition pathways at B3LYP/6-31G(d)//ωB97X-D/6-311+G(d,p). The horizontal axis is a reaction coordinate, and the vertical axis represents Gibbs energy in kcal/mol.

References

1 López-Andarias, J.; Frontera, A.; and Matile, S.; *J. Am. Chem. Soc.* **2017**, *139*, 13296−13299.

2 Panneerselvam, M.; Deepankumar, Madhu.; Jaccob, Madhavan.; Solomon, R. V. *ChemistrySelect* **2018**, *3*, 1321–1334.

3 Deepankumar, Madhu.; Jaccob, Madhavan., *Phys. Chem. Chem. Phys.*, **2021**, *23*, 7386-7397.

Cartesian Coordinates of Ground State Optimized Structures

^{D}F1$_{R}$

6	-1.943777000	-1.092882000	-3.321891000
6	-3.102852000	-0.216103000	-3.367823000
6	-2.945290000	1.160532000	-3.213934000
6	-1.619878000	1.718281000	-3.003502000
6	-0.507572000	0.873982000	-2.947726000
6	-0.668822000	-0.559128000	-3.109453000
6	-2.322650000	-2.309730000	-2.645907000
6	-3.720160000	-2.196399000	-2.264917000
6	-4.203833000	-0.900374000	-2.712587000
6	-5.101462000	-0.178136000	-1.923574000
6	-3.877948000	1.913623000	-2.394335000
6	-1.728441000	2.810289000	-2.065200000
6	-0.718713000	3.006724000	-1.116467000
6	0.443941000	2.141419000	-1.086428000
6	0.556512000	1.108882000	-2.004829000
6	1.203695000	-0.198052000	-1.687877000
6	0.297878000	-1.233045000	-2.274806000
6	-0.081740000	-2.381184000	-1.597877000
6	-1.407977000	-2.929337000	-1.788132000
6	-4.155247000	-2.718050000	-1.046064000
6	-3.208736000	-3.375605000	-0.158763000
6	-1.865583000	-3.473567000	-0.521756000
6	-0.822260000	-3.253529000	0.464356000
6	0.286536000	-2.584122000	-0.185718000
6	1.018814000	-1.629879000	0.504219000
6	1.598862000	-0.416375000	-0.146171000
6	1.278450000	0.711313000	0.774806000
6	0.811779000	1.939381000	0.330181000
6	-3.124545000	2.934619000	-1.683378000
6	-1.975066000	2.299661000	2.743316000
6	-2.875434000	2.934929000	1.887194000
6	-4.200459000	2.379524000	1.683270000
6	-4.574540000	1.205269000	2.339754000
6	-3.638534000	0.541336000	3.230003000
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6	-0.578275000	2.175322000	2.364166000
6	-0.133308000	2.684201000	1.138788000
6	-1.073684000	3.344687000	0.250742000
6	-2.414061000	3.472764000	0.617276000
6	-4.562857000	2.579861000	0.288526000
6	-5.284315000	1.597397000	-0.392736000
6	-5.668756000	0.373449000	0.290432000
6	-5.321585000	0.181557000	1.628150000
6	-4.843921000	-1.115848000	2.076972000
6	-3.804689000	-0.894146000	3.066981000
6	-2.691196000	-1.735740000	3.109487000
6	-1.367229000	-1.174502000	3.313816000
6	0.780546000	0.163207000	2.011402000
6	0.617895000	-1.269057000	1.844644000
6	-0.433727000	-1.926171000	2.490314000
6	-1.171649000	-2.945062000	1.783107000
6	-2.569960000	-2.831412000	2.161492000
6	-3.568807000	-3.041418000	1.210074000
6	-4.727828000	-2.169242000	1.167780000
6	-5.090257000	-1.969174000	-0.227229000
6	-5.554116000	-0.723772000	-0.656038000
6	-3.461489000	3.258973000	-0.368552000
6	-4.934971000	1.257370000	-1.760857000
6	-2.365444000	1.078384000	3.429776000
6	2.636815000	-0.334438000	-1.241392000
6	3.468794000	-1.542336000	-1.594458000
7	4.805677000	-1.283328000	-1.652272000
8	2.990200000	-2.653199000	-1.805807000
6	5.760955000	-2.362916000	-1.850425000
1	5.390375000	-2.995651000	-2.662526000
1	6.704354000	-1.920474000	-2.183038000
6	5.957125000	-3.270347000	-0.624853000
1	6.575257000	-4.135531000	-0.924041000
1	4.974080000	-3.654840000	-0.339465000
7	6.548576000	-2.606383000	0.555226000
1	3.183810000	0.604881000	-1.237626000
6	7.967960000	-2.269434000	0.359861000
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1	8.319857000	-1.698116000	1.221185000
6	6.391236000	-3.443351000	1.754809000
1	6.794270000	-2.909450000	2.620521000
1	5.329280000	-3.640732000	1.927896000
1	6.917897000	-4.406918000	1.658966000
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8	5.213504000	-0.340927000	1.142354000
6	6.008098000	0.622567000	1.594146000
8	7.151095000	0.474120000	1.982301000
6	5.327806000	1.986250000	1.515090000
1	4.262306000	1.883031000	1.754234000
1	5.791892000	2.674545000	2.224332000
6	5.410265000	2.535467000	0.092294000
8	5.315808000	1.845612000	-0.906576000
16	5.636103000	4.309567000	0.051534000
6	5.583609000	4.626004000	-1.747313000
1	6.490516000	5.157189000	-2.041712000
1	5.532590000	3.657827000	-2.251061000
1	4.703042000	5.223843000	-1.989606000
1	5.747481000	-1.209109000	0.976657000

^{D}F1$_{INT1}$

6	-0.082108000	0.969318000	-2.765443000
6	-0.996364000	2.095185000	-2.660484000
6	-0.915244000	2.961825000	-1.571164000
6	0.084109000	2.739145000	-0.539350000
6	0.955512000	1.649262000	-0.633752000
6	0.871859000	0.745518000	-1.767057000
6	-0.804639000	-0.151308000	-3.317436000
6	-2.174330000	0.270572000	-3.556846000
6	-2.293162000	1.661469000	-3.150531000
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6	-0.499720000	3.069009000	0.739073000
6	-0.184479000	2.292427000	1.859691000
6	0.741620000	1.183448000	1.754358000
6	1.321677000	0.885701000	0.532306000
6	1.643087000	-0.507128000	0.103261000
6	1.191637000	-0.590419000	-1.319840000
6	0.470799000	-1.660664000	-1.826781000

6	-0.538489000	-1.439317000	-2.841366000
6	-3.227199000	-0.614891000	-3.322592000
6	-2.952025000	-1.959680000	-2.841283000
6	-1.637129000	-2.358640000	-2.602148000
6	-1.313281000	-3.148783000	-1.427197000
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6	0.236820000	-2.696231000	0.422287000
6	1.115715000	-1.672569000	1.066879000
6	0.364180000	-1.221784000	2.275373000
6	0.254337000	0.109934000	2.642334000
6	-1.868942000	3.496238000	0.508458000
6	-3.392602000	0.138039000	3.287331000
6	-3.648202000	1.430875000	2.828364000
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6	-5.356569000	0.573425000	1.269106000
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6	-0.960602000	0.582461000	3.275376000
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6	-2.544658000	2.345896000	2.584033000
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6	-4.416436000	2.646827000	-0.446660000
6	-5.147529000	1.519343000	-1.000632000
6	-5.607649000	0.504471000	-0.160821000
6	-5.494404000	-0.885944000	-0.569566000
6	-5.176422000	-1.675705000	0.607124000
6	-4.296559000	-2.755322000	0.505215000
6	-3.295826000	-2.974328000	1.535004000
6	-0.751370000	-2.111038000	2.477068000
6	-0.831974000	-3.011363000	1.341709000
6	-2.081908000	-3.439669000	0.883622000
6	-2.328684000	-3.511280000	-0.536459000
6	-3.697445000	-3.087484000	-0.777177000
6	-4.003822000	-2.326693000	-1.906226000
6	-4.920168000	-1.206528000	-1.801386000
6	-4.440008000	-0.148115000	-2.677128000
6	-4.554108000	1.187431000	-2.285447000
6	-2.871793000	3.142314000	1.412046000
6	-3.373894000	3.013052000	-1.389172000
6	-4.130416000	-0.986639000	2.734326000
6	2.590815000	-1.416022000	0.856467000
6	3.449983000	-2.400062000	0.109462000
7	4.701035000	-2.548655000	0.643497000
8	3.074160000	-3.005060000	-0.893648000
6	5.690514000	-3.358806000	-0.040573000
1	5.898594000	-4.285411000	0.513416000
1	5.262470000	-3.656720000	-1.001063000
6	7.039890000	-2.649435000	-0.209274000
1	7.687363000	-3.236695000	-0.869694000
1	7.536609000	-2.536751000	0.757771000
7	6.946654000	-1.253048000	-0.762545000
1	3.077839000	-0.917058000	1.694728000
6	6.154182000	-1.140270000	-2.021837000
1	6.665182000	-1.690130000	-2.817468000
1	5.156007000	-1.551067000	-1.871804000
1	6.082124000	-0.081973000	-2.271900000
6	8.303127000	-0.652270000	-0.921730000
1	8.172577000	0.395974000	-1.189121000
1	8.823935000	-0.721198000	0.034757000
1	8.856603000	-1.191579000	-1.694897000
1	5.044612000	-1.850502000	1.316503000
6	6.086482000	2.076583000	1.584976000
1	5.686810000	2.829265000	2.266847000
6	5.457275000	0.685946000	1.933123000
8	6.125028000	-0.330636000	1.508795000
1	6.490561000	-0.678346000	0.031684000
1	7.174155000	2.011567000	1.686314000
6	5.770897000	2.415616000	0.146917000
8	6.273651000	1.841131000	-0.808913000
16	4.542019000	3.706163000	-0.017113000
6	4.316230000	3.750500000	-1.828187000
1	3.362270000	3.289633000	-2.093426000
1	4.332632000	4.790604000	-2.159239000
1	5.140867000	3.195570000	-2.281467000
8	4.393912000	0.667582000	2.551244000

^{D}F1$_{INT2}$

6	-1.343444000	-0.673313000	-3.312353000
6	-2.348314000	0.351719000	-3.545084000
6	-2.108591000	1.668075000	-3.153023000
6	-0.853026000	2.014154000	-2.508506000
6	0.107632000	1.026426000	-2.275570000
6	-0.139119000	-0.344251000	-2.683371000
6	-2.018661000	-1.896832000	-2.951640000
6	-3.448635000	-1.639110000	-2.956555000
6	-3.652941000	-0.247308000	-3.324079000
6	-4.665433000	0.495767000	-2.713643000
6	-3.160344000	2.442841000	-2.518449000
6	-1.121227000	2.997170000	-1.485088000
6	-0.415388000	2.946908000	-0.277775000
6	0.598137000	1.933968000	-0.057694000
6	0.870168000	1.007790000	-1.052958000
6	1.259670000	-0.401695000	-0.761777000
6	0.472274000	-1.233008000	-1.722015000
6	-0.194681000	-2.390849000	-1.351257000
6	-1.456787000	-2.729380000	-1.978496000
6	-4.266716000	-2.231462000	-1.993832000
6	-3.687197000	-3.107879000	-0.988314000
6	-2.312871000	-3.345320000	-0.979974000
6	-1.584262000	-3.380733000	0.275815000
6	-0.276302000	-2.799348000	0.062161000
6	0.316864000	-2.040378000	1.057978000
6	1.180320000	-0.851930000	0.775819000
6	0.715873000	0.200494000	1.728218000
6	0.518704000	1.521895000	1.358727000
6	-2.549023000	3.265161000	-1.486332000
6	-2.797182000	1.981632000	2.942194000
6	-3.344965000	2.826344000	1.976020000
6	-4.601790000	2.482276000	1.337598000
6	-5.263043000	1.302959000	1.686405000
6	-4.694557000	0.421662000	2.691184000
6	-2.483838000	-0.269940000	3.536813000
6	-1.179021000	0.328400000	3.308915000
6	-1.369635000	1.712771000	2.945909000
6	-0.541704000	2.291815000	1.977971000
6	-1.115714000	3.171157000	0.974497000
6	-2.485471000	3.437054000	0.974608000
6	-4.523463000	2.886345000	-0.057830000
6	-5.109532000	2.094640000	-1.047514000
6	-5.793257000	0.864761000	-0.683664000
6	-5.868330000	0.477201000	0.654665000
6	-5.670738000	-0.915462000	1.021349000

6	-4.946203000	-0.950195000	2.279553000
6	-3.980572000	-1.934238000	2.501150000
6	-2.723890000	-1.584697000	3.140148000
6	-0.170059000	-0.411446000	2.686102000
6	-0.417381000	-1.780736000	2.273583000
6	-1.670425000	-2.358108000	2.502732000
6	-2.268266000	-3.180637000	1.479329000
6	-3.697979000	-2.921855000	1.472204000
6	-4.393985000	-2.885466000	0.263330000
6	-5.399803000	-1.865041000	0.033980000
6	-5.321276000	-1.460782000	-1.361674000
6	-5.516694000	-0.123547000	-1.712979000
6	-3.218169000	3.479808000	-0.280824000
6	-4.414028000	1.867815000	-2.302246000
6	-3.487161000	0.754800000	3.308171000
6	2.488711000	-0.789032000	0.032267000
6	3.265895000	-2.035948000	-0.315469000
7	4.581820000	-1.789899000	-0.589171000
8	2.761341000	-3.151784000	-0.358361000
6	5.509922000	-2.856140000	-0.923685000
1	4.918879000	-3.772982000	-0.986059000
1	5.941703000	-2.677702000	-1.916274000
6	6.607226000	-3.049740000	0.129503000
1	7.164920000	-3.975748000	-0.098156000
1	6.124396000	-3.189816000	1.102098000
7	7.544001000	-1.911159000	0.252231000
1	3.103230000	0.061576000	0.321164000
6	8.449185000	-1.821525000	-0.904867000
1	9.059328000	-2.733158000	-1.018026000
1	7.878781000	-1.668648000	-1.824506000
1	9.116402000	-0.966507000	-0.771239000
6	8.331239000	-2.016169000	1.490650000
1	8.981596000	-1.141432000	1.580594000
1	7.660438000	-2.039993000	2.354208000
1	8.956147000	-2.924519000	1.508101000
1	4.932101000	-0.838102000	-0.566703000
8	8.323320000	2.769765000	-1.724048000
6	5.845133000	1.204960000	1.050745000
8	6.409473000	0.573969000	-0.019756000
16	5.612684000	2.959371000	0.812619000
6	4.915843000	3.014103000	-0.881579000
1	5.576647000	2.504610000	-1.583687000
1	3.910973000	2.583987000	-0.911635000
1	4.857910000	4.072420000	-1.147849000
6	8.832635000	2.181017000	-0.853104000
8	9.381822000	1.593365000	-0.002853000
6	5.536465000	0.625703000	2.221313000
1	5.053153000	1.192085000	3.006948000
1	5.785683000	-0.411789000	2.423742000
1	6.781571000	-0.335866000	0.233792000

^{D}F1$_{P}$

6	2.358725000	1.873274000	-2.874729000
6	3.472429000	0.978111000	-3.144278000
6	3.240728000	-0.376430000	-3.379197000
6	1.882976000	-0.893848000	-3.349820000
6	0.814016000	-0.035297000	-3.078765000
6	1.052498000	1.375428000	-2.836118000
6	2.779108000	2.833633000	-1.883558000
6	4.157231000	2.540259000	-1.528796000
6	4.587082000	1.391778000	-2.309880000
6	5.423128000	0.430393000	-1.738313000
6	4.109276000	-1.377913000	-2.786152000
6	1.908060000	-2.206215000	-2.748190000
6	0.862246000	-2.598052000	-1.905139000
6	-0.255064000	-1.709484000	-1.653779000
6	-0.287562000	-0.459436000	-2.252339000
6	-0.876460000	0.744383000	-1.595656000
6	0.097118000	1.848078000	-1.861555000
6	0.514540000	2.742268000	-0.888545000
6	1.872339000	3.244652000	-0.901254000
6	4.582173000	2.680784000	-0.207142000
6	3.644691000	3.122038000	0.813632000
6	2.319663000	3.392224000	0.472534000
6	1.237949000	2.969111000	1.344389000
6	0.116453000	2.569114000	0.519346000
6	-0.684272000	1.506236000	0.908202000
6	-1.305925000	0.553308000	-0.061314000
6	-1.070030000	-0.801008000	0.517527000
6	-0.653154000	-1.883749000	-0.241997000
6	3.284103000	-2.510098000	-2.395466000
6	2.038358000	-3.052397000	2.017702000
6	2.930081000	-3.477894000	1.032318000
6	4.287188000	-2.964676000	1.008739000
6	4.701101000	-2.039538000	1.969312000
6	3.774279000	-1.593646000	2.994825000
6	1.358697000	-1.195460000	3.287316000
6	0.246481000	-1.606491000	2.447072000
6	0.661468000	-2.748904000	1.667602000
6	0.227590000	-2.875057000	0.342964000
6	1.158965000	-3.318659000	-0.679467000
6	2.479585000	-3.618477000	-0.343307000
6	4.679677000	-2.793881000	-0.381829000
6	5.470074000	-1.704986000	-0.754964000
6	5.896124000	-0.740134000	0.245164000
6	5.520036000	-0.903975000	1.578832000
6	5.096131000	0.245057000	2.361722000
6	4.018158000	-0.180604000	3.237066000
6	2.948161000	0.679031000	3.494324000
6	1.591740000	0.159869000	3.516619000
6	-0.581788000	-0.643102000	1.864433000
6	-0.341860000	0.768389000	2.102199000
6	0.722526000	1.161253000	2.919535000
6	1.531988000	2.291080000	2.531875000
6	2.910949000	1.998195000	2.884206000
6	3.946704000	2.404198000	2.042010000
6	5.060503000	1.512668000	1.777080000
6	5.453128000	1.683455000	0.386325000
6	5.865339000	0.579647000	-0.363038000
6	3.565091000	-3.202020000	-1.216568000
6	5.179291000	-0.982646000	-1.980998000
6	2.470075000	-2.091309000	3.020215000
6	-2.315149000	0.835491000	-1.152205000
6	-3.073262000	2.142314000	-1.177403000
7	-4.401697000	1.989925000	-1.424323000
8	-2.534262000	3.229811000	-0.990240000
6	-5.303904000	3.130198000	-1.408240000
1	-4.764536000	3.987280000	-1.820848000
1	-6.139756000	2.910044000	-2.079841000
6	-5.794501000	3.513312000	-0.004796000
1	-6.375694000	4.454439000	-0.083583000
1	-4.910486000	3.732572000	0.602558000
7	-6.563191000	2.466295000	0.675057000
1	-2.905144000	-0.037128000	-1.424195000

6	-7.878307000	2.256821000	0.075088000
1	-8.517199000	3.160438000	0.117357000
1	-7.780516000	1.959966000	-0.973409000
1	-8.393694000	1.448553000	0.603911000
6	-6.697024000	2.762197000	2.100024000
1	-7.224946000	1.941634000	2.597674000
1	-5.704925000	2.858224000	2.552854000
1	-7.256384000	3.697143000	2.295974000
1	-4.793886000	1.052692000	-1.465765000
8	-10.318220000	-2.581263000	0.83726900
6	-5.738783000	-1.400787000	-0.419858000
8	-5.398953000	-0.869580000	-1.466054000
16	-6.689084000	-2.916785000	-0.40641600
6	-6.835388000	-3.215334000	-2.201870000
1	-7.271491000	-2.343497000	-2.691937000
1	-5.853803000	-3.423040000	-2.631239000
1	-7.488358000	-4.081949000	-2.323942000
6	-9.614422000	-1.810831000	1.361339000
8	-8.919819000	-1.032806000	1.893124000
6	-5.396881000	-0.854667000	0.943896000
1	-5.931571000	-1.366170000	1.747599000
1	-4.317817000	-0.971009000	1.104148000
1	-5.633922000	0.218071000	0.953939000

$^{D}\mathrm{F2}_{R}$

6	0.939238000	-0.714472000	3.026833000
6	2.002559000	0.162262000	3.491008000
6	1.996976000	1.512713000	3.144413000
6	0.927424000	2.042725000	2.315407000
6	-0.088131000	1.197122000	1.860569000
6	-0.084842000	-0.208564000	2.220305000
6	1.515766000	-2.000089000	2.714741000
6	2.942418000	-1.929808000	2.981169000
6	3.244002000	-0.591295000	3.462118000
6	4.431323000	0.037568000	3.081443000
6	3.230720000	2.168713000	2.748588000
6	1.490737000	3.021367000	1.415189000
6	1.011028000	3.108831000	0.103466000
6	-0.061752000	2.245190000	-0.348921000
6	-0.617595000	1.323757000	0.525967000
6	-1.118525000	-0.010774000	0.087850000
6	-0.618118000	-0.972483000	1.115956000
6	-0.038791000	-2.191180000	0.796980000
6	1.040758000	-2.713763000	1.609645000
6	3.841762000	-2.585458000	2.139525000
6	3.349597000	-3.340018000	0.997699000
6	1.980432000	-3.396807000	0.738047000
6	1.488371000	-3.289392000	-0.624148000
6	0.242384000	-2.552544000	-0.603452000
6	-0.067559000	-1.684512000	-1.638538000
6	-0.817522000	-0.406194000	-1.438457000
6	-0.065864000	0.612115000	-2.229616000
6	0.219002000	1.882248000	-1.753002000
6	2.917104000	3.102443000	1.678564000
6	3.795461000	1.969940000	-2.710930000
6	4.259721000	2.698674000	-1.615125000
6	5.331504000	2.170391000	-0.791895000
6	5.897361000	0.929811000	-1.092646000
6	5.415353000	0.168987000	-2.231997000
6	3.324223000	-0.197644000	-3.486328000
6	2.081604000	0.555230000	-3.450700000
6	2.369703000	1.888337000	-2.977021000
6	1.458087000	2.531412000	-2.132430000
6	1.945555000	3.289506000	-0.993434000
6	3.315244000	3.376127000	-0.741385000
6	5.054877000	2.527211000	0.591222000
6	5.355044000	1.628644000	1.617073000
6	5.939456000	0.335628000	1.302256000
6	6.204814000	-0.006502000	-0.024265000
6	5.909418000	-1.346649000	-0.503470000
6	5.422425000	-1.238844000	-1.867496000
6	4.400186000	-2.080320000	-2.311334000
6	3.329169000	-1.546759000	-3.134878000
6	0.896173000	-0.071414000	-3.056486000
6	0.898502000	-1.475993000	-2.691705000
6	2.093398000	-2.201308000	-2.736470000
6	2.395415000	-3.133237000	-1.677274000
6	3.821495000	-3.061908000	-1.408251000
6	4.289861000	-3.162579000	-0.097686000
6	5.354139000	-2.290535000	0.362982000
6	5.077204000	-1.933735000	1.746292000
6	5.366638000	-0.647606000	2.206658000
6	3.811822000	3.275310000	0.621729000
6	4.424580000	1.445421000	2.717180000
6	4.386690000	0.679097000	-3.026388000
6	-2.221912000	-0.195600000	-0.928295000
6	-3.193601000	-1.339246000	-0.791008000
7	-4.498008000	-0.969418000	-0.931514000
8	-2.835180000	-2.491327000	-0.551930000
6	-5.602762000	-1.918479000	-0.864123000
1	-5.131878000	-2.903075000	-0.793400000
6	-6.541997000	-1.714986000	0.360622000
1	-7.025269000	-0.733812000	0.250252000
7	-5.812296000	-1.620956000	1.664060000
1	-2.665843000	0.744495000	-1.246520000
6	-4.957970000	-2.777830000	1.994914000
1	-4.216069000	-2.949657000	1.213697000
1	-4.425739000	-2.553107000	2.924603000
1	-5.543556000	-3.695622000	2.154426000
6	-6.720600000	-1.324690000	2.789423000
1	-6.113589000	-1.072135000	3.665025000
1	-7.335169000	-0.456987000	2.541828000
1	-7.360972000	-2.176762000	3.055434000
1	-4.697576000	0.001185000	-1.149660000
6	-4.529334000	2.898603000	0.823908000
1	-3.446646000	2.756728000	0.841847000
6	-4.957759000	2.997138000	-0.640340000
8	-4.487299000	2.257420000	-1.488886000
16	-6.204018000	4.163756000	-1.15838800
6	-6.883205000	4.871734000	0.389653000
1	-7.153220000	4.069925000	1.079263000
1	-6.189895000	5.577758000	0.853269000
1	-7.785862000	5.410457000	0.089883000
1	-4.974606000	-0.261479000	1.638960000
1	-4.800768000	3.781402000	1.402603000
6	-5.244980000	1.669224000	1.392914000
8	-6.455570000	1.669736000	1.572813000
8	-4.436950000	0.642901000	1.560442000
6	-6.418374000	-1.859737000	-2.173004000
1	-6.837469000	-0.848902000	-2.289080000
1	-5.731598000	-2.014236000	-3.012776000
6	-7.646944000	-2.796049000	0.327076000
1	-7.191151000	-3.790590000	0.430063000
1	-8.321952000	-2.667776000	1.179489000

6	-8.458749000	-2.743693000	-0.976066000
1	-9.225655000	-3.527787000	-0.966902000
1	-8.993067000	-1.784159000	-1.030912000
6	-7.550959000	-2.892794000	-2.201297000
1	-8.130215000	-2.787370000	-3.126591000
1	-7.119081000	-3.903748000	-2.215077000

^{D}F2$_{\mathrm{INT1}}$

6	0.699053000	0.853495000	2.896833000
6	1.763763000	1.843892000	2.879318000
6	1.798365000	2.814774000	1.879116000
6	0.768916000	2.836877000	0.852947000
6	-0.248284000	1.876868000	0.862841000
6	-0.284912000	0.864518000	1.902966000
6	1.258571000	-0.406146000	3.324332000
6	2.676316000	-0.207223000	3.572789000
6	2.989232000	1.185727000	3.297558000
6	4.202052000	1.523703000	2.693354000
6	3.058810000	3.168550000	1.250221000
6	1.383608000	3.202554000	-0.401212000
6	0.951774000	2.589988000	-1.583061000
6	-0.122268000	1.618282000	-1.563289000
6	-0.728264000	1.288703000	-0.362225000
6	-1.241411000	-0.079053000	-0.060431000
6	-0.795515000	-0.363198000	1.337798000
6	-0.231836000	-1.569199000	1.725869000
6	0.807142000	-1.591508000	2.734741000
6	3.590162000	-1.205692000	3.233070000
6	3.121912000	-2.445030000	2.632691000
6	1.761610000	-2.629124000	2.385633000
6	1.318886000	-3.248185000	1.148522000
6	0.088590000	-2.608124000	0.731924000
6	-0.166033000	-2.404934000	-0.615493000
6	-0.896721000	-1.210984000	-1.141518000
6	-0.097163000	-0.754881000	-2.317356000
6	0.199171000	0.577245000	-2.558872000
6	2.801651000	3.407493000	-0.161147000
6	3.807493000	0.152251000	-3.277646000
6	4.249000000	1.345508000	-2.704371000
6	5.280178000	1.323833000	-1.683751000
6	5.830206000	0.108451000	-1.270903000
6	5.371710000	-1.134825000	-1.865349000
6	3.317218000	-2.101347000	-2.828348000
6	2.090484000	-1.440644000	-3.241609000
6	2.390356000	-0.056232000	-3.520246000
6	1.463958000	0.932379000	-3.170606000
6	1.927822000	2.172997000	-2.574487000
6	3.289365000	2.379312000	-2.350546000
6	4.963067000	2.349437000	-0.701490000
6	5.209341000	2.117960000	0.653430000
6	5.776760000	0.850381000	1.082251000
6	6.080586000	-0.133275000	0.140314000
6	5.773447000	-1.526782000	0.418014000
6	5.336395000	-2.146116000	-0.820891000
6	4.312138000	-3.095200000	-0.802416000
6	3.281969000	-3.069853000	-1.826111000
6	0.878925000	-1.768762000	-2.626483000
6	0.839744000	-2.776850000	-1.583274000
6	2.019453000	-3.420024000	-1.195344000
6	2.264994000	-3.663040000	0.205679000
6	3.682096000	-3.461899000	0.455525000
6	4.103029000	-2.864807000	1.644482000
6	5.169039000	-1.880583000	1.626149000
6	4.851870000	-0.854688000	2.608270000
6	5.152308000	0.482886000	2.342435000
6	3.736320000	3.004468000	-1.115910000
6	4.237502000	2.534925000	1.648872000
6	4.381747000	-1.113483000	-2.849772000
6	-2.315702000	-0.769031000	-0.875319000
6	-3.305575000	-1.676451000	-0.194152000
7	-4.591990000	-1.497517000	-0.616419000
8	-2.999457000	-2.484418000	0.681848000
6	-5.674684000	-2.231034000	0.019500000
1	-5.330856000	-2.490137000	1.027903000
6	-6.965676000	-1.389406000	0.116372000
1	-7.321173000	-1.178747000	-0.899375000
7	-6.702066000	0.007838000	0.675003000
1	-2.732710000	-0.126947000	-1.652300000
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1	-5.002367000	-0.473786000	1.853364000
1	-5.745143000	1.110076000	2.177755000
6	-7.933501000	0.852199000	0.746721000
1	-7.603599000	1.883521000	0.875427000
1	-8.476331000	0.755943000	-0.195044000
1	-8.561782000	0.539715000	1.582087000
1	-4.828452000	-0.733156000	-1.265100000
6	-5.299228000	3.251223000	-1.599078000
1	-4.789885000	3.937146000	-2.278450000
6	-4.851500000	1.786448000	-1.923998000
8	-5.680303000	0.872818000	-1.555227000
1	-6.131104000	0.490135000	-0.097074000
1	-6.383684000	3.332911000	-1.716608000
6	-4.957388000	3.552155000	-0.158573000
8	-5.571173000	3.088812000	0.792609000
16	-3.520119000	4.604839000	0.015031000
6	-3.317251000	4.632268000	1.829213000
1	-2.426978000	4.064127000	2.107355000
1	-3.217744000	5.667563000	2.160948000
1	-4.208104000	4.178266000	2.269785000
8	-3.761073000	1.623478000	-2.470789000
6	-8.049357000	-2.159591000	0.884456000
1	-8.970649000	-1.571016000	0.947491000
1	-7.713068000	-2.347844000	1.913174000
6	-5.986284000	-3.558811000	-0.703730000
1	-6.285929000	-3.342464000	-1.738578000
1	-5.057159000	-4.135170000	-0.751004000
6	-8.351525000	-3.501785000	0.192225000
1	-8.798372000	-3.302439000	-0.792112000
1	-9.106030000	-4.044647000	0.773290000
6	-7.085201000	-4.349442000	0.017472000
1	-7.317477000	-5.266194000	-0.536899000
1	-6.717657000	-4.665581000	1.004061000

^{D}F2$_{\mathrm{INT2}}$

6	2.012752000	2.591409000	-2.345775000
6	3.261994000	2.035846000	-2.841236000
6	3.286597000	0.758891000	-3.400234000
6	2.061438000	-0.018181000	-3.484573000
6	0.863178000	0.511978000	-2.998130000
6	0.834694000	1.841407000	-2.416658000
6	2.296821000	3.351616000	-1.152618000
6	3.725051000	3.271833000	-0.897603000
6	4.322889000	2.457568000	-1.943197000

6	5.364983000	1.580168000	-1.636323000
6	4.369837000	-0.154973000	-3.082971000
6	2.380860000	-1.402309000	-3.225744000
6	1.486658000	-2.191185000	-2.493462000
6	0.234814000	-1.637376000	-2.017170000
6	-0.079677000	-0.315297000	-2.289601000
6	-0.847773000	0.546714000	-1.344410000
6	-0.132102000	1.859826000	-1.343529000
6	0.160513000	2.561388000	-0.184395000
6	1.389586000	3.321398000	-0.088682000
6	4.194762000	3.175916000	0.412815000
6	3.253972000	3.157917000	1.521867000
6	1.883230000	3.224394000	1.273810000
6	0.961794000	2.391769000	2.026800000
6	-0.107614000	1.978487000	1.141946000
6	-0.660234000	0.713389000	1.265877000
6	-1.140718000	-0.086065000	0.096633000
6	-0.607865000	-1.461912000	0.320024000
6	-0.035231000	-2.222274000	-0.687373000
6	3.808928000	-1.492470000	-2.974952000
6	2.967655000	-3.319408000	1.181410000
6	3.863557000	-3.304708000	0.111518000
6	5.089117000	-2.532738000	0.199928000
6	5.371882000	-1.799925000	1.354380000
6	4.440427000	-1.812679000	2.468733000
6	2.016253000	-2.000696000	2.877832000
6	0.956775000	-2.417728000	1.974809000
6	1.539249000	-3.230856000	0.933160000
6	1.057973000	-3.122028000	-0.376043000
6	1.993453000	-3.107082000	-1.486735000
6	3.365547000	-3.201164000	-1.250659000
6	5.354231000	-1.957067000	-1.109751000
6	5.890998000	-0.671980000	-1.211412000
6	6.180037000	0.091563000	-0.009021000
6	5.925932000	-0.460573000	1.246916000
6	5.333955000	0.355202000	2.294252000
6	4.416794000	-0.479757000	3.049786000
6	3.216866000	0.054537000	3.523791000
6	1.992674000	-0.721908000	3.432778000
6	-0.078993000	-1.534673000	1.658024000
6	-0.106408000	-0.203421000	2.235226000
6	0.908762000	0.192645000	3.111651000
6	1.455564000	1.523946000	3.006149000
6	2.884212000	1.444817000	3.259103000
6	3.766147000	2.244601000	2.531337000
6	5.014632000	1.690838000	2.041452000
6	5.279684000	2.266668000	0.731633000
6	5.853311000	1.483317000	-0.271924000
6	4.292035000	-2.373439000	-2.006497000
6	5.388793000	0.247325000	-2.217512000
6	3.263337000	-2.558708000	2.385283000
6	-2.251729000	0.230655000	-0.875404000
6	-3.245571000	1.335502000	-0.608554000
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1	-6.491032000	1.442442000	-1.393275000
6	-6.028469000	2.142578000	0.603658000
1	-5.124446000	2.520528000	1.091022000
7	-6.327921000	0.831827000	1.261680000
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1	-7.936834000	0.351994000	-0.026695000
1	-7.761130000	-0.699976000	1.381626000
6	-6.038642000	0.872128000	2.702353000
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8	-7.617533000	-3.152623000	-1.789084000
6	-4.597463000	-2.399150000	0.742998000
8	-5.393210000	-1.522733000	0.066579000
16	-4.526542000	-4.020903000	-0.00331400
6	-4.141084000	-3.611132000	-1.747145000
1	-4.900581000	-2.948764000	-2.165318000
1	-3.144195000	-3.170560000	-1.835442000
1	-4.158212000	-4.558899000	-2.291352000
6	-7.887290000	-3.190249000	-0.651688000
8	-8.204290000	-3.225697000	0.473081000
6	-3.970149000	-2.155007000	1.902717000
1	-3.325115000	-2.901745000	2.346632000
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6	-5.414215000	3.293480000	-1.615721000
1	-4.481508000	3.722242000	-1.238026000
1	-5.264442000	3.084118000	-2.681620000
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1	-7.477811000	3.924384000	-1.880378000
1	-6.307746000	5.239647000	-1.909809000
6	-7.145293000	3.195531000	0.773646000
1	-8.081625000	2.817966000	0.341856000
1	-7.336414000	3.356803000	1.841931000
6	-6.805831000	4.524132000	0.085038000
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1	-5.910991000	4.966743000	0.544443000

^{D}F2$_{P}$

6	-2.338263000	-2.723827000	-2.106663000
6	-3.572847000	-2.134049000	-2.599065000
6	-3.546947000	-0.908572000	-3.263348000
6	-2.283071000	-0.218454000	-3.459200000
6	-1.098378000	-0.779965000	-2.975097000
6	-1.122441000	-2.056363000	-2.285172000
6	-2.614560000	-3.364556000	-0.843782000
6	-4.023174000	-3.175012000	-0.541770000
6	-4.616992000	-2.413905000	-1.628882000
6	-5.591765000	-1.451406000	-1.357957000
6	-4.559965000	0.093674000	-2.983315000
6	-2.509339000	1.199503000	-3.306900000
6	-1.539438000	1.988717000	-2.678963000
6	-0.302261000	1.399790000	-2.206030000
6	-0.078420000	0.042218000	-2.375097000
6	0.681759000	-0.787189000	-1.395029000
6	-0.112147000	-2.046512000	-1.252827000
6	-0.395409000	-2.630837000	-0.028378000
6	-1.661809000	-3.301961000	0.178218000
6	-4.429459000	-2.942737000	0.772777000
6	-3.442059000	-2.891725000	1.839384000
6	-2.089585000	-3.062781000	1.545333000
6	-1.089229000	-2.229374000	2.188909000
6	-0.036367000	-1.958315000	1.232219000
6	0.594000000	-0.723543000	1.226837000
6	1.071740000	-0.053982000	-0.022051000

6	0.629017000	1.365574000	0.104191000
6	0.057165000	2.074222000	-0.942091000
6	-3.917388000	1.398173000	-3.010217000
6	-2.792624000	3.505584000	0.941596000
6	-3.732711000	3.457606000	-0.088540000
6	-4.996567000	2.773317000	0.111450000
6	-5.271690000	2.156916000	1.333837000
6	-4.294085000	2.203721000	2.406943000
6	-1.847682000	2.274516000	2.706176000
6	-0.805567000	2.549360000	1.731314000
6	-1.383820000	3.307492000	0.647111000
6	-0.966536000	3.062387000	-0.666028000
6	-1.948320000	3.014205000	-1.735222000
6	-3.300934000	3.212005000	-1.455423000
6	-5.351104000	2.109561000	-1.133753000
6	-5.966080000	0.856279000	-1.105666000
6	-6.247329000	0.213546000	0.167334000
6	-5.907669000	0.850248000	1.361558000
6	-5.319650000	0.088258000	2.450822000
6	-4.323296000	0.924119000	3.097352000
6	-3.137293000	0.357307000	3.568682000
6	-1.874818000	1.046406000	3.365478000
6	0.161912000	1.580356000	1.450983000
6	0.136562000	0.301473000	2.136345000
6	-0.861141000	0.043026000	3.081607000
6	-1.488719000	-1.255761000	3.110175000
6	-2.898060000	-1.067882000	3.409891000
6	-3.855876000	-1.868651000	2.786834000
6	-5.089900000	-1.280805000	2.299895000
6	-5.444516000	-1.944867000	1.054578000
6	-6.014209000	-1.212643000	0.010923000
6	-4.306171000	2.384195000	-2.102453000
6	-5.562509000	-0.172002000	-2.048656000
6	-3.080007000	2.866223000	2.215868000
6	2.117248000	-0.520788000	-1.009086000
6	3.061875000	-1.652087000	-0.664107000
7	4.327370000	-1.447116000	-1.111093000
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6	5.445863000	-2.364291000	-0.861500000
1	6.308336000	-1.900997000	-1.357999000
6	5.769561000	-2.511307000	0.650101000
1	4.859947000	-2.906743000	1.113401000
7	6.004643000	-1.193899000	1.283621000
1	2.565366000	0.293697000	-1.573988000
6	7.317472000	-0.607913000	1.031385000
1	8.145700000	-1.114806000	1.557834000
1	7.542895000	-0.616056000	-0.039605000
1	7.317458000	0.438535000	1.358640000
6	5.696557000	-1.190162000	2.710234000
1	5.751065000	-0.163240000	3.091328000
1	4.677535000	-1.556471000	2.868955000
1	6.385174000	-1.805172000	3.319574000
1	4.555225000	-0.524268000	-1.470712000
8	7.070762000	4.257993000	2.229628000
6	5.119987000	2.217367000	-0.992850000
8	4.973651000	1.401848000	-1.890315000
16	5.981558000	3.761153000	-1.263457000
6	6.410152000	3.570552000	-3.028005000
1	7.037253000	2.689064000	-3.170998000
1	5.502681000	3.474906000	-3.626385000
1	6.956545000	4.470735000	-3.317076000
6	7.999149000	3.659335000	1.844804000
8	8.925006000	3.053392000	1.468410000
6	4.589513000	2.023815000	0.407559000
1	4.993313000	2.752702000	1.114754000
1	3.497903000	2.131075000	0.384411000
1	4.824273000	1.001010000	0.730706000
6	5.194132000	-3.732931000	-1.530931000
1	4.259215000	-4.141985000	-1.135094000
1	5.045089000	-3.571060000	-2.605482000
6	6.336920000	-4.724950000	-1.283751000
1	6.094058000	-5.689702000	-1.746139000
1	7.256827000	-4.367837000	-1.771313000
6	6.904724000	-3.538622000	0.865503000
1	7.839680000	-3.153594000	0.434749000
1	7.085098000	-3.661573000	1.941024000
6	6.594950000	-4.895151000	0.218029000
1	7.426052000	-5.590663000	0.390665000
1	5.708290000	-5.338584000	0.692962000

^{A}F1$_{R}$

6	-1.814391000	-1.732233000	-3.024239000
6	-2.952194000	-0.899231000	-3.379295000
6	-2.797516000	0.480777000	-3.503574000
6	-1.496771000	1.086722000	-3.273616000
6	-0.406432000	0.286935000	-2.920419000
6	-0.564513000	-1.149794000	-2.792121000
6	-2.277324000	-2.783659000	-2.151455000
6	-3.706541000	-2.609486000	-1.956248000
6	-4.124934000	-1.443308000	-2.717054000
6	-5.095032000	-0.582098000	-2.200141000
6	-3.805284000	1.378286000	-2.966940000
6	-1.694418000	2.350756000	-2.604349000
6	-0.791323000	2.755300000	-1.614871000
6	0.351641000	1.930335000	-1.277268000
6	0.551386000	0.728697000	-1.938856000
6	1.146072000	-0.472941000	-1.284432000
6	0.298951000	-1.620176000	-1.734077000
6	-0.163471000	-2.604934000	-0.875393000
6	-1.467681000	-3.196953000	-1.088524000
6	-4.276765000	-2.867680000	-0.709165000
6	-3.439138000	-3.311615000	0.393905000
6	-2.065799000	-3.466906000	0.207066000
6	-1.133150000	-3.030430000	1.231339000
6	0.046305000	-2.500326000	0.579084000
6	0.711387000	-1.414265000	1.126674000
6	1.373445000	-0.358518000	0.300725000
6	0.964504000	0.934584000	0.921879000
6	0.562037000	2.035512000	0.181065000
6	-3.122167000	2.535372000	-2.410222000
6	-2.465316000	2.863171000	2.148633000
6	-3.260912000	3.292166000	1.085399000
6	-4.562026000	2.690008000	0.861337000
6	-5.017637000	1.676201000	1.706568000
6	-4.190688000	1.226676000	2.812717000
6	-1.805019000	0.975639000	3.383136000
6	-0.633762000	1.517088000	2.714469000
6	-1.037110000	2.678567000	1.957361000
6	-0.456709000	2.922539000	0.707441000
6	-1.288433000	3.369504000	-0.396239000
6	-2.659128000	3.555518000	-0.211987000
6	-4.769185000	2.586923000	-0.575103000
6	-5.423342000	1.474063000	-1.107542000
6	-5.892792000	0.417206000	-0.226995000

6	-5.694292000	0.516225000	1.150600000
6	-5.282272000	-0.651198000	1.912284000
6	-4.353928000	-0.212761000	2.939554000
6	-3.260717000	-1.012651000	3.278759000
6	-1.960426000	-0.404846000	3.501669000
6	0.329753000	0.653977000	2.184973000
6	0.170919000	-0.783266000	2.308463000
6	-0.951601000	-1.302123000	2.961485000
6	-1.619786000	-2.455937000	2.410111000
6	-3.049545000	-2.282219000	2.602353000
6	-3.941655000	-2.700500000	1.614353000
6	-5.079528000	-1.871100000	1.263766000
6	-5.286802000	-1.974533000	-0.172806000
6	-5.688217000	-0.853556000	-0.902487000
6	-3.595953000	3.125617000	-1.237768000
6	-4.931731000	0.857425000	-2.327201000
6	-2.940852000	1.809403000	3.031071000
6	2.524375000	-0.496427000	-0.670117000
6	3.373075000	-1.747336000	-0.689716000
7	4.698937000	-1.499563000	-0.852465000
8	2.903055000	-2.874766000	-0.559996000
6	5.680159000	-2.572805000	-0.903388000
1	5.233650000	-3.417781000	-1.438286000
1	6.529401000	-2.201125000	-1.481988000
6	6.163005000	-3.078497000	0.464556000
1	6.880257000	-3.883781000	0.266064000
1	5.318465000	-3.532320000	1.005536000
7	6.830879000	-2.051483000	1.292729000
1	3.074335000	0.431286000	-0.808608000
6	7.986075000	-2.597191000	2.006196000
1	7.717900000	-3.401720000	2.716080000
1	8.711108000	-2.998950000	1.291020000
1	8.476195000	-1.798742000	2.574588000
6	5.902449000	-1.428367000	2.240031000
1	6.415438000	-0.627507000	2.785244000
1	5.058674000	-0.992914000	1.702096000
1	5.507943000	-2.147865000	2.981246000
1	5.027692000	-0.544273000	-0.954594000
6	7.710228000	0.929702000	-0.085531000
6	6.435804000	1.748517000	0.086818000
8	5.351639000	1.396221000	-0.337471000
16	6.667114000	3.269634000	0.987117000
6	4.947465000	3.886434000	0.986070000
1	4.639130000	4.144310000	-0.028483000
1	4.276345000	3.127153000	1.390787000
1	4.934411000	4.776170000	1.618817000
6	8.000222000	0.682672000	-1.554565000
8	9.215010000	1.154773000	-1.910371000
8	7.254703000	0.122733000	-2.326945000
1	9.326894000	0.942386000	-2.857180000
1	8.563470000	1.406165000	0.400196000
1	7.520576000	-0.060897000	0.370724000

^{A}F1$_{INT1}$

6	-0.093377000	-0.277039000	2.943370000
6	0.781855000	0.838946000	3.263020000
6	0.662554000	2.040792000	2.566290000
6	-0.337437000	2.178170000	1.521229000
6	-1.172417000	1.102455000	1.207436000
6	-1.048087000	-0.150342000	1.929422000
6	0.671431000	-1.496923000	3.047794000
6	2.028138000	-1.146044000	3.431574000
6	2.096689000	0.300079000	3.564571000
6	3.241681000	0.985905000	3.153872000
6	1.852357000	2.756321000	2.139561000
6	0.224455000	2.974414000	0.455589000
6	-0.073806000	2.654699000	-0.873891000
6	-0.959712000	1.552052000	-1.185260000
6	-1.518343000	0.807992000	-0.159536000
6	-1.783547000	-0.656386000	-0.274677000
6	-1.325069000	-1.240856000	1.023053000
6	-0.565398000	-2.397617000	1.103357000
6	0.444338000	-2.530479000	2.133460000
6	3.107933000	-1.847689000	2.893641000
6	2.873756000	-2.930903000	1.951670000
6	1.570947000	-3.259338000	1.577809000
6	1.264082000	-3.573414000	0.193249000
6	-0.051364000	-3.051840000	-0.112754000
6	-0.315935000	-2.529270000	-1.368824000
6	-1.231635000	-1.367001000	-1.592096000
6	-0.508591000	-0.480557000	-2.552993000
6	-0.444604000	0.895604000	-2.403002000
6	1.581166000	3.332719000	0.832349000
6	3.192302000	1.282468000	-2.978452000
6	3.408145000	2.324368000	-2.075588000
6	4.410420000	2.189038000	-1.035052000
6	5.157409000	1.013699000	-0.932583000
6	4.933134000	-0.072904000	-1.869755000
6	3.095670000	-1.055921000	-3.188251000
6	1.779159000	-0.516274000	-3.484834000
6	1.837338000	0.920872000	-3.357898000
6	0.747463000	1.609701000	-2.814716000
6	0.976414000	2.694309000	-1.876290000
6	2.277188000	3.048552000	-1.517507000
6	3.902854000	2.835288000	0.165678000
6	4.163118000	2.279857000	1.420087000
6	4.935832000	1.053382000	1.524828000
6	5.422935000	0.433692000	0.373391000
6	5.359487000	-1.012660000	0.243009000
6	5.057754000	-1.326078000	-1.142711000
6	4.215680000	-2.397402000	-1.447935000
6	3.213677000	-2.256917000	-2.490207000
6	0.633426000	-1.196515000	-3.062119000
6	0.753792000	-2.447221000	-2.335462000
6	2.021536000	-2.969833000	-2.060217000
6	2.282861000	-3.548603000	-0.764467000
6	3.639037000	-3.196897000	-0.379395000
6	3.929054000	-2.893024000	0.951341000
6	4.806631000	-1.782037000	1.268844000
6	4.299132000	-1.135857000	2.469900000
6	4.364758000	0.253389000	2.595768000
6	2.587530000	3.369954000	-0.133675000
6	3.116930000	2.239060000	2.426731000
6	3.971486000	0.059140000	-2.873401000
6	-2.713798000	-1.260848000	-1.308300000
6	-3.538007000	-2.471933000	-0.972289000
7	-4.836801000	-2.397869000	-1.410077000
8	-3.098731000	-3.434103000	-0.347915000
6	-5.800918000	-3.407490000	-1.007121000
1	-6.191112000	-3.947399000	-1.880138000
1	-5.257397000	-4.133302000	-0.398394000
6	-7.018113000	-2.835943000	-0.261391000
1	-7.583909000	-3.651092000	0.204666000
1	-7.681791000	-2.317372000	-0.960121000

7	-6.672646000	-1.818993000	0.781878000
1	-3.221888000	-0.510551000	-1.909642000
6	-5.703327000	-2.282401000	1.814000000
1	-4.817633000	-2.706302000	1.341224000
1	-5.412217000	-1.412221000	2.403866000
1	-6.178984000	-3.034737000	2.450882000
6	-7.894902000	-1.252039000	1.416067000
1	-7.587353000	-0.425366000	2.058068000
1	-8.551304000	-0.868811000	0.632761000
1	-8.409579000	-2.021690000	1.998282000
1	-5.186670000	-1.480923000	-1.685506000
6	-4.954190000	2.245431000	-0.808582000
6	-4.342976000	3.280039000	-0.059283000
8	-4.175787000	3.268789000	1.182370000
16	-3.784645000	4.701283000	-1.04469400
6	-2.957289000	5.692147000	0.246379000
1	-3.301986000	5.320854000	1.214308000
1	-1.872232000	5.583855000	0.176250000
1	-3.236654000	6.740133000	0.119060000
1	-6.253041000	-0.955956000	0.201282000
6	-5.439805000	1.100432000	-0.167115000
8	-5.340857000	0.988004000	1.178106000
8	-5.984777000	0.105602000	-0.761254000
1	-4.882202000	1.830077000	1.494157000
1	-5.057697000	2.319138000	-1.883218000

^{A}F1$_{INT2}$

6	-3.760380000	1.828817000	2.844205000
6	-4.634647000	0.714166000	3.172288000
6	-4.092360000	-0.533885000	3.475846000
6	-2.651132000	-0.720241000	3.461691000
6	-1.811798000	0.348555000	3.135093000
6	-2.373768000	1.648826000	2.819673000
6	-4.390836000	2.609367000	1.807431000
6	-5.660934000	1.982984000	1.482136000
6	-5.812406000	0.809794000	2.327527000
6	-6.398266000	-0.349950000	1.815803000
6	-4.700428000	-1.741281000	2.945187000
6	-2.366366000	-2.032331000	2.930732000
6	-1.255621000	-2.212928000	2.098951000
6	-0.376892000	-1.102566000	1.789537000
6	-0.638671000	0.150139000	2.322247000
6	-0.347591000	1.420138000	1.595013000
6	-1.552765000	2.278067000	1.811672000
6	-2.164911000	2.996538000	0.796556000
6	-3.602654000	3.167854000	0.795853000
6	-6.102861000	1.948605000	0.158984000
6	-5.291885000	2.541340000	-0.892904000
6	-4.067947000	3.132295000	-0.579596000
6	-2.914692000	2.927572000	-1.438303000
6	-1.733014000	2.845756000	-0.604101000
6	-0.704666000	1.979894000	-0.943247000
6	0.120579000	1.253525000	0.068674000
6	0.209926000	-0.147139000	-0.433804000
6	0.056096000	-1.254151000	0.385503000
6	-3.631909000	-2.668403000	2.607742000
6	-2.279811000	-3.141288000	-1.781720000
6	-3.050317000	-3.710583000	-0.766913000
6	-4.489915000	-3.527922000	-0.757541000
6	-5.106295000	-2.778958000	-1.762030000
6	-4.306439000	-2.184486000	-2.818619000
6	-2.049969000	-1.248178000	-3.154703000
6	-0.874622000	-1.341699000	-2.304928000
6	-1.013028000	-2.506145000	-1.462240000
6	-0.566755000	-2.454087000	-0.137056000
6	-1.371499000	-3.047696000	0.916073000
6	-2.583736000	-3.667241000	0.609640000
6	-4.916016000	-3.379026000	0.625669000
6	-5.941073000	-2.487121000	0.947963000
6	-6.578130000	-1.704179000	-0.097920000
6	-6.169328000	-1.847003000	-1.424413000
6	-6.023829000	-0.674640000	-2.271304000
6	-4.873759000	-0.883008000	-3.133416000
6	-4.033841000	0.187893000	-3.446238000
6	-2.593514000	0.000344000	-3.454574000
6	-0.296973000	-0.181554000	-1.781930000
6	-0.860781000	1.118816000	-2.092765000
6	-1.984822000	1.207789000	-2.919730000
6	-3.037896000	2.136189000	-2.584917000
6	-4.308774000	1.510187000	-2.907700000
6	-5.413630000	1.707625000	-2.078399000
6	-6.288479000	0.595821000	-1.755675000
6	-6.714488000	0.744779000	-0.372263000
6	-6.858907000	-0.382768000	0.438808000
6	-3.739325000	-3.469335000	1.470079000
6	-5.830926000	-1.651402000	2.130723000
6	-2.921764000	-2.363305000	-2.829499000
6	1.031328000	1.822314000	1.128842000
6	1.458414000	3.265724000	1.079188000
7	2.781459000	3.447057000	1.363507000
8	0.693676000	4.190875000	0.815112000
6	3.374086000	4.754183000	1.167469000
1	2.686339000	5.511227000	1.554828000
1	4.297712000	4.812960000	1.750061000
6	3.614687000	5.095233000	-0.310016000
1	4.058995000	6.093182000	-0.410680000
1	2.652566000	5.084953000	-0.827711000
7	4.506397000	4.120726000	-1.024917000
1	1.815245000	1.133367000	1.433614000
6	5.893571000	4.074415000	-0.474973000
1	6.352635000	5.063361000	-0.571430000
1	5.853752000	3.764988000	0.567368000
1	6.469582000	3.327200000	-1.024075000
6	4.527097000	4.390005000	-2.489326000
1	5.121827000	3.613660000	-2.972969000
1	3.504776000	4.351670000	-2.869651000
1	4.962719000	5.374417000	-2.682972000
1	3.412855000	2.636134000	1.294075000
6	7.128269000	-0.276051000	0.053322000
1	6.891283000	0.633558000	0.610619000
6	8.141858000	-1.096290000	0.848117000
8	8.991555000	-1.816716000	0.380691000
16	7.928485000	-0.898887000	2.635182000
6	9.185692000	-2.101553000	3.189631000
1	8.953148000	-3.094717000	2.801438000
1	10.175035000	-1.799694000	2.842025000
1	9.156173000	-2.107435000	4.281383000
1	4.069387000	3.094875000	-0.946809000
6	7.656070000	0.206735000	-1.285468000
8	8.116743000	-0.766558000	-2.090015000
8	7.647336000	1.374850000	-1.630658000
1	8.423354000	-0.321598000	-2.903616000
6	5.714064000	-1.024213000	-0.049676000
6	4.771937000	-0.185933000	-0.859291000

1	5.361448000	-1.006732000	0.987612000
1	4.432838000	-0.446414000	-1.850697000
7	4.341804000	0.962594000	-0.395986000
8	4.683389000	1.402210000	0.778957000
8	3.547019000	1.718050000	-1.131011000
6	5.764643000	-2.474601000	-0.503368000
6	5.709019000	-3.487553000	0.464381000
6	5.832730000	-2.849785000	-1.852386000
6	5.730564000	-4.834229000	0.100356000
1	5.641128000	-3.216155000	1.515152000
6	5.850514000	-4.194836000	-2.220089000
1	5.883217000	-2.090159000	-2.625403000
6	5.800927000	-5.192792000	-1.245682000
1	5.683444000	-5.601080000	0.869045000
1	5.902404000	-4.462986000	-3.272072000
1	5.812829000	-6.240410000	-1.534195000

^{A}**F1**$_{\mathbf{INT3}}$

6	3.352934000	1.354324000	-3.103227000
6	4.204776000	0.218780000	-3.418312000
6	3.678002000	-1.072026000	-3.417415000
6	2.275740000	-1.281834000	-3.098348000
6	1.460035000	-0.191091000	-2.784126000
6	2.006000000	1.153653000	-2.785487000
6	4.126614000	2.302929000	-2.339091000
6	5.464530000	1.761339000	-2.172075000
6	5.513357000	0.471259000	-2.840715000
6	6.241126000	-0.580105000	-2.279548000
6	4.433585000	-2.167171000	-2.835227000
6	2.160616000	-2.497504000	-2.327884000
6	1.234669000	-2.565029000	-1.280870000
6	0.375653000	-1.436808000	-0.982181000
6	0.471249000	-0.280718000	-1.740079000
6	0.260962000	1.082885000	-1.170663000
6	1.358421000	1.919968000	-1.746402000
6	2.112479000	2.803947000	-0.990655000
6	3.514996000	3.001381000	-1.293115000
6	6.146727000	1.947533000	-0.969129000
6	5.518262000	2.685271000	0.115421000
6	4.229926000	3.195014000	-0.043799000
6	3.268818000	3.107508000	1.041559000
6	1.958340000	2.870412000	0.473021000
6	1.054545000	2.051745000	1.131830000
6	0.092353000	1.156262000	0.417830000
6	0.167006000	-0.149084000	1.138667000
6	0.220947000	-1.369631000	0.484645000
6	3.494226000	-3.048886000	-2.160580000
6	3.010310000	-2.839681000	2.426979000
6	3.604965000	-3.548386000	1.382274000
6	5.006588000	-3.341928000	1.068630000
6	5.761651000	-2.430038000	1.808996000
6	5.144694000	-1.690006000	2.895793000
6	2.947154000	-0.755891000	3.510974000
6	1.640107000	-1.006858000	2.927160000
6	1.676456000	-2.288035000	2.262440000
6	0.988364000	-2.458090000	1.055933000
6	1.610513000	-3.197445000	-0.028484000
6	2.888069000	-3.735079000	0.130845000
6	5.159082000	-3.407976000	-0.376808000
6	6.060257000	-2.559294000	-1.022856000
6	6.841809000	-1.607036000	-0.251502000
6	6.695577000	-1.543763000	1.134685000
6	6.652967000	-0.254150000	1.803965000
6	5.695689000	-0.344213000	2.892503000
6	4.877010000	0.746447000	3.192896000
6	3.474459000	0.534659000	3.505768000
6	0.917852000	0.043323000	2.353246000
6	1.464470000	1.387938000	2.347388000
6	2.717694000	1.629177000	2.919395000
6	3.642567000	2.512058000	2.250593000
6	4.980808000	1.970545000	2.415396000
6	5.900214000	2.054265000	1.369054000
6	6.753254000	0.922306000	1.058466000
6	6.905685000	0.856308000	-0.387209000
6	6.951704000	-0.383384000	-1.028259000
6	3.851551000	-3.654982000	-0.955467000
6	5.690154000	-1.925960000	-2.276385000
6	3.797003000	-1.891719000	3.199905000
6	-1.031622000	1.530116000	-0.523057000
6	-1.501589000	2.957930000	-0.640824000
7	-2.848779000	3.072428000	-0.851532000
8	-0.750998000	3.924768000	-0.571158000
6	-3.496211000	4.373730000	-0.898153000
1	-2.742482000	5.090420000	-1.232952000
1	-4.289729000	4.347224000	-1.652951000
6	-4.033481000	4.853822000	0.459726000
1	-4.289189000	5.924227000	0.393137000
1	-3.228023000	4.756011000	1.193399000
7	-5.203525000	4.090239000	0.959519000
1	-1.815493000	0.775972000	-0.571009000
6	-6.450387000	4.462200000	0.266741000
1	-6.725506000	5.509105000	0.466083000
1	-6.335927000	4.328986000	-0.811953000
1	-7.253731000	3.805514000	0.610699000
6	-5.368267000	4.242580000	2.416583000
1	-6.189644000	3.601268000	2.746971000
1	-4.451085000	3.925535000	2.920774000
1	-5.584879000	5.284500000	2.697059000
1	-3.430457000	2.248309000	-0.760648000
6	-5.634591000	-0.711342000	0.507848000
6	-4.826303000	-0.807822000	-0.802732000
8	-3.624727000	-0.990259000	-0.780247000
16	-5.715378000	-0.578487000	-2.33942100
6	-4.288898000	-0.629956000	-3.480759000
1	-3.629774000	0.224817000	-3.316004000
1	-3.726992000	-1.553877000	-3.337506000
1	-4.701676000	-0.593061000	-4.491236000
6	-5.909303000	0.761464000	0.856814000
8	-4.943942000	1.552633000	0.416684000
8	-6.852678000	1.145528000	1.530047000
1	-5.081840000	2.567548000	0.703116000
1	-4.883999000	-1.012566000	1.252504000
6	-6.820242000	-1.713250000	0.657541000
1	-6.367627000	-2.696635000	0.493262000
6	-7.298690000	-1.729941000	2.121523000
6	-7.999279000	-1.602102000	-0.307075000
6	-8.821497000	-0.466436000	-0.380236000
6	-8.317529000	-2.709500000	-1.106818000
6	-9.913453000	-0.437469000	-1.248614000
1	-8.611146000	0.393762000	0.245218000
6	-9.411862000	-2.682072000	-1.970559000
1	-7.703271000	-3.604012000	-1.047757000
6	-10.212002000	-1.541939000	-2.04768000
1	-10.537486000	0.451311000	-1.29356600

1	-9.638611000	-3.552648000	-2.579940000
1	-11.065954000	-1.516738000	-2.71929200
1	-7.950149000	-0.899711000	2.376682000
7	-8.080395000	-2.991367000	2.424902000
8	-7.642159000	-4.053679000	1.989350000
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1	-6.454339000	-1.758784000	2.818692000

^{A}F1$_{\mathrm{INT4}}$

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6	4.921394000	1.890630000	-2.145067000
6	4.441629000	0.926772000	-3.030581000
6	3.034153000	0.913474000	-3.391702000
6	2.163830000	1.861641000	-2.846790000
6	2.661336000	2.867263000	-1.926500000
6	4.401897000	3.127770000	-0.218607000
6	5.545319000	2.284393000	0.084961000
6	5.868425000	1.519124000	-1.108299000
6	6.293524000	0.193864000	-0.995720000
6	4.882477000	-0.452141000	-2.915409000
6	2.605664000	-0.460659000	-3.505450000
6	1.326278000	-0.821025000	-3.068601000
6	0.422100000	0.176514000	-2.531865000
6	0.827572000	1.499877000	-2.445931000
6	0.395729000	2.420855000	-1.353333000
6	1.638006000	3.148717000	-0.947536000
6	2.008490000	3.343661000	0.373568000
6	3.407615000	3.336331000	0.742911000
6	5.661977000	1.692678000	1.343196000
6	4.637288000	1.920827000	2.349675000
6	3.534341000	2.720957000	2.052249000
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6	1.254333000	2.715068000	1.472402000
6	0.158191000	1.906151000	1.213763000
6	-0.419189000	1.724545000	-0.150918000
6	-0.648736000	0.259376000	-0.283964000
6	-0.328932000	-0.455960000	-1.428383000
6	3.745801000	-1.310644000	-3.208843000
6	1.386685000	-3.286669000	0.234786000
6	2.363574000	-3.501055000	-0.739082000
6	3.767809000	-3.493725000	-0.374587000
6	4.144128000	-3.264259000	0.950491000
6	3.130125000	-3.037838000	1.965046000
6	0.877949000	-2.058279000	2.173335000
6	-0.067401000	-1.683306000	1.132943000
6	0.245728000	-2.438475000	-0.060417000
6	0.126935000	-1.828535000	-1.314379000
6	1.143582000	-2.055762000	-2.325492000
6	2.236471000	-2.877440000	-2.046750000
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6	5.600450000	-2.045929000	-1.175166000
6	5.988348000	-1.804545000	0.204748000
6	5.276167000	-2.401488000	1.245459000
6	4.958809000	-1.638557000	2.441033000
6	3.633391000	-2.031723000	2.886371000
6	2.765765000	-1.077001000	3.420698000
6	1.361358000	-1.089707000	3.051674000
6	-0.478318000	-0.350556000	1.011742000
6	0.020910000	0.657947000	1.928158000
6	0.920783000	0.291596000	2.932985000
6	2.040614000	1.152393000	3.227282000
6	3.186247000	0.310808000	3.528435000
6	4.458885000	0.686382000	3.097763000
6	5.362426000	-0.306024000	2.545692000
6	6.105974000	0.316250000	1.460776000
6	6.415551000	-0.419602000	0.315013000
6	3.566116000	-2.495910000	-2.494426000
6	5.790082000	-0.812087000	-1.917401000
6	1.778122000	-3.050922000	1.615442000
6	-1.039756000	2.760871000	-1.057996000
6	-1.443240000	4.111497000	-0.503199000
7	-2.763740000	4.384821000	-0.664118000
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1	-3.591433000	6.307232000	-0.867352000
6	-4.665882000	5.183620000	0.661432000
1	-5.108523000	6.091475000	1.116948000
1	-4.394421000	4.508279000	1.479922000
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1	-5.592828000	5.919477000	-1.740249000
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6	-3.935934000	-3.689858000	1.005945000
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16	-4.291786000	-5.431260000	0.95901300
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1	-1.931026000	-5.794080000	1.442144000
1	-2.738663000	-7.221261000	0.740830000
6	-6.438906000	-3.620793000	-3.614816000
8	-6.404421000	-2.695840000	-2.897311000
8	-6.474361000	-4.540222000	-4.332099000
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6	-6.061934000	-0.761082000	1.085148000
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1	-7.176036000	-1.303172000	-0.689259000
6	-7.377525000	0.306355000	2.828927000
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1	-7.431091000	0.753124000	3.818114000
1	-9.472805000	0.596463000	2.402504000
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7	-4.042615000	0.829205000	-0.632500000
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1	-2.501935000	-2.512646000	1.560541000

^{A}F1$_{\mathrm{P}}$

6	-4.919786000	2.096698000	0.906312000
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6	-4.258357000	0.250090000	2.970141000
6	-3.486185000	1.399334000	2.785908000
6	-3.821878000	2.341019000	1.734715000
6	-4.810268000	2.357670000	-0.509196000
6	-5.538170000	1.316579000	-1.213693000
6	-6.100702000	0.411717000	-0.223555000
6	-6.142573000	-0.961088000	-0.474702000
6	-5.437791000	-1.436778000	1.843156000
6	-3.602682000	-1.005337000	3.250232000
6	-2.206454000	-1.049690000	3.331652000
6	-1.416315000	0.155227000	3.166018000
6	-2.051277000	1.364578000	2.926130000
6	-1.471146000	2.436077000	2.068355000
6	-2.599240000	2.902558000	1.212075000
6	-2.482402000	3.124011000	-0.151556000
6	-3.606037000	2.847782000	-1.025544000
6	-5.043441000	0.810665000	-2.416331000
6	-3.798587000	1.326601000	-2.961810000
6	-3.095039000	2.318670000	-2.277341000
6	-1.647665000	2.255593000	-2.183148000
6	-1.253141000	2.750492000	-0.878483000
6	-0.180193000	2.169045000	-0.218586000
6	-0.110906000	2.023521000	1.265061000
6	0.373329000	0.633020000	1.495819000
6	-0.184724000	-0.216464000	2.439163000
6	-4.328561000	-2.053423000	2.554001000
6	-0.481241000	-3.214712000	0.280325000
6	-1.673572000	-3.705542000	0.813798000
6	-2.805484000	-3.969506000	-0.055160000
6	-2.705257000	-3.726457000	-1.426527000
6	-1.466289000	-3.213226000	-1.984091000
6	0.419486000	-1.764014000	-1.334131000
6	0.800321000	-1.276866000	-0.017588000
6	0.248704000	-2.168563000	0.975346000
6	-0.245639000	-1.641934000	2.175465000
6	-1.487614000	-2.156267000	2.726039000
6	-2.183924000	-3.169377000	2.065126000
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6	-5.079941000	-3.009612000	-0.022823000
6	-4.972320000	-2.752337000	-1.449305000
6	-3.809952000	-3.103582000	-2.136728000
6	-3.252726000	-2.202195000	-3.131363000
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6	-1.039596000	-1.116025000	-3.215384000
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6	0.489720000	1.037561000	-0.813362000
6	0.134528000	0.570603000	-2.080800000
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6	-1.691618000	0.155323000	-3.487419000
6	-3.082628000	0.218790000	-3.573959000
6	-3.878029000	-0.981926000	-3.395259000
6	-5.090334000	-0.615920000	-2.679109000
6	-5.627609000	-1.485172000	-1.727562000
6	-3.633868000	-3.114648000	1.972607000
6	-5.804032000	-1.904087000	0.579578000
6	-0.375452000	-2.965145000	-1.148594000
6	-0.164253000	3.121464000	2.289956000
6	-0.009215000	4.597786000	1.926727000
7	1.102154000	4.872084000	1.202441000
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1	0.535162000	6.816623000	0.744493000
1	2.186393000	6.669546000	1.346620000
6	1.942518000	6.069089000	-0.741247000
1	2.287366000	7.057384000	-1.100888000
1	1.100764000	5.766970000	-1.374077000
7	2.974907000	5.036969000	-0.856676000
1	0.314539000	2.874254000	3.237424000
6	4.269392000	5.470738000	-0.336468000
1	4.689851000	6.325171000	-0.901382000
1	4.180477000	5.770484000	0.712823000
1	4.977271000	4.638867000	-0.394099000
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16	3.947131000	-3.769495000	2.814817000
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1	2.008129000	-2.735404000	3.843878000
1	2.737051000	-4.024706000	4.849469000
6	9.605933000	-0.641462000	1.901557000
8	8.585588000	-0.997541000	1.449841000
8	10.622305000	-0.288413000	2.352144000
1	4.963042000	-3.348610000	0.289069000
6	4.850105000	-1.279517000	-0.363098000
1	3.768275000	-1.189207000	-0.493893000
6	5.360284000	0.084379000	0.120276000
6	5.462529000	-1.692300000	-1.695669000
6	6.843921000	-1.892702000	-1.835570000
6	4.640116000	-1.888637000	-2.811992000
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1	3.568969000	-1.727820000	-2.720685000
6	6.556276000	-2.476883000	-4.165898000
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1	4.526703000	-2.424076000	-4.893161000
1	6.979234000	-2.779197000	-5.120055000
1	6.443722000	0.128971000	0.228337000
7	5.002580000	1.206543000	-0.821852000
8	3.925075000	1.148596000	-1.406812000
8	5.802623000	2.135959000	-0.905029000
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$^{A}F2_{R}$

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6	-2.183820000	-3.341916000	-1.273616000
6	-3.606702000	-3.314960000	-0.980779000
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6	-1.570831000	2.269497000	-2.416046000
6	-0.290904000	1.736943000	-1.993175000
6	0.056005000	0.435798000	-2.322525000
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6	0.195687000	-1.769933000	-1.464649000
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6	-1.251216000	-3.322607000	-0.231507000
6	-4.045962000	-3.283918000	0.343267000
6	-3.078148000	-3.279241000	1.429031000
6	-1.712791000	-3.293350000	1.145160000
6	-0.797213000	-2.462672000	1.907369000
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6	0.755436000	-0.708013000	1.172811000
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6	0.614185000	1.497545000	0.315617000
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6	-5.345431000	1.614423000	1.505720000
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6	-1.568933000	3.176276000	1.048488000
6	-1.117540000	3.132677000	-0.275475000
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6	-5.862416000	0.263875000	1.359791000
6	-5.220310000	-0.572840000	2.359943000
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6	-3.082418000	-0.255090000	3.548635000
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6	-2.715354000	-1.623430000	3.222210000
6	-3.591412000	-2.421201000	2.485304000
6	-4.867741000	-1.887363000	2.047543000
6	-5.148693000	-2.420725000	0.723122000
6	-5.770561000	-1.617461000	-0.235033000
6	-4.368147000	2.348529000	-1.855366000
6	-5.391863000	-0.294466000	-2.141670000
6	-3.235147000	2.397644000	2.514775000
6	2.278179000	-0.097401000	-0.989140000
6	3.311847000	-1.177992000	-0.754184000
7	4.589146000	-0.777722000	-0.976529000
8	2.988256000	-2.308327000	-0.387283000
6	5.764431000	-1.651106000	-0.823801000
1	6.625358000	-1.000047000	-1.012370000
6	5.883534000	-2.224843000	0.614997000
1	4.949075000	-2.760147000	0.799944000
7	5.943582000	-1.136287000	1.624023000
1	2.659018000	0.819821000	-1.429544000
6	7.285057000	-0.674450000	1.966373000
1	7.872356000	-1.397053000	2.560837000
1	7.850165000	-0.440620000	1.059503000
1	7.207594000	0.244548000	2.560913000
6	5.173781000	-1.443475000	2.826585000
1	5.156138000	-0.565083000	3.482998000
1	4.142391000	-1.684771000	2.552951000
1	5.584335000	-2.287331000	3.413327000
1	4.752990000	0.193522000	-1.221500000
6	5.860746000	2.325386000	0.715401000
6	4.817149000	2.903372000	-0.237453000
8	4.422418000	2.304344000	-1.220942000
16	4.253759000	4.530823000	0.204244000
6	3.064877000	4.827423000	-1.150169000
1	3.548994000	4.653732000	-2.112417000
1	2.200276000	4.169646000	-1.043787000
1	2.753062000	5.870596000	-1.067293000
6	7.200953000	2.233288000	0.003690000
8	8.101515000	3.095828000	0.522558000
8	7.447430000	1.492070000	-0.921023000
1	8.923950000	2.980674000	0.008432000
1	5.950622000	2.925857000	1.622246000
1	5.552474000	1.299460000	0.966403000
6	5.736201000	-2.766283000	-1.893223000
1	4.785664000	-3.303087000	-1.801398000
1	5.747394000	-2.297799000	-2.885013000
6	7.034264000	-3.251075000	0.712365000
1	8.000716000	-2.748000000	0.572604000
1	7.048900000	-3.680421000	1.722655000
6	6.917698000	-4.362158000	-0.339478000
1	5.996483000	-4.938307000	-0.173227000
1	7.753682000	-5.065188000	-0.232809000
6	6.895452000	-3.758806000	-1.748437000
1	7.852317000	-3.250379000	-1.940621000
1	6.803366000	-4.547056000	-2.506087000

$^{A}\text{F2}_{\text{INT1}}$

6	0.459545000	0.104184000	3.010683000
6	1.550733000	1.040780000	3.224669000
6	1.638882000	2.197616000	2.451330000
6	0.639232000	2.467777000	1.432232000
6	-0.404105000	1.562751000	1.219893000
6	-0.496361000	0.356647000	2.021755000
6	0.973331000	-1.234995000	3.173804000
6	2.388480000	-1.138750000	3.488665000
6	2.746086000	0.270090000	3.519910000
6	3.983855000	0.687760000	3.026445000
6	2.925673000	2.634603000	1.938487000
6	1.297952000	3.069912000	0.296958000
6	0.882878000	2.735353000	-0.997020000
6	-0.215829000	1.814489000	-1.203335000
6	-0.863137000	1.260501000	-0.111621000
6	-1.416694000	-0.125596000	-0.117258000
6	-1.023276000	-0.709828000	1.201547000
6	-0.503389000	-1.987836000	1.336539000
6	0.506127000	-2.256216000	2.340297000
6	3.283787000	-2.072878000	2.965745000
6	2.798702000	-3.142794000	2.108111000
6	1.441169000	-3.227247000	1.799875000
6	1.016284000	-3.557469000	0.450673000
6	-0.183177000	-2.803754000	0.152125000
6	-0.396514000	-2.316333000	-1.127622000
6	-1.075481000	-1.011190000	-1.401213000

6	-0.235487000	-0.346447000	-2.442300000
6	0.104504000	0.995936000	-2.389252000
6	2.714320000	3.173027000	0.604234000
6	3.716799000	0.614750000	-3.106854000
6	4.174041000	1.645788000	-2.285106000
6	5.176038000	1.376933000	-1.270543000
6	5.681075000	0.084746000	-1.111851000
6	5.205450000	-0.990373000	-1.964685000
6	3.152751000	-1.665904000	-3.152561000
6	1.956160000	-0.893785000	-3.442862000
6	2.301467000	0.507955000	-3.416764000
6	1.393965000	1.431702000	-2.887157000
6	1.874043000	2.503816000	-2.033030000
6	3.233984000	2.613374000	-1.741815000
6	4.860245000	2.183154000	-0.101165000
6	5.062693000	1.664387000	1.179355000
6	5.582949000	0.317135000	1.342918000
6	5.885863000	-0.456022000	0.221547000
6	5.533421000	-1.865921000	0.192778000
6	5.113645000	-2.196664000	-1.157733000
6	4.064435000	-3.095323000	-1.361483000
6	3.063580000	-2.821642000	-2.378021000
6	0.719375000	-1.305046000	-2.937669000
6	0.623982000	-2.508062000	-2.131258000
6	1.775171000	-3.255424000	-1.862032000
6	1.975801000	-3.794832000	-0.538762000
6	3.390693000	-3.697563000	-0.222596000
6	3.794555000	-3.376952000	1.074100000
6	4.886934000	-2.445829000	1.286225000
6	4.571349000	-1.639772000	2.455960000
6	4.914392000	-0.286399000	2.483867000
6	3.663708000	2.950075000	-0.393995000
6	4.075431000	1.894129000	2.219585000
6	4.244108000	-0.730607000	-2.943354000
6	-2.492545000	-0.594592000	-1.076806000
6	-3.523904000	-1.595775000	-0.633958000
7	-4.803246000	-1.276480000	-1.007905000
8	-3.250317000	-2.599416000	0.020531000
6	-5.929630000	-2.065681000	-0.526618000
1	-5.509199000	-2.768439000	0.200138000
6	-7.013183000	-1.200782000	0.160038000
1	-7.472865000	-0.557650000	-0.601947000
7	-6.412203000	-0.198949000	1.129394000
1	-2.870017000	0.205078000	-1.709898000
6	-5.515498000	-0.753553000	2.184461000
1	-4.763354000	-1.404658000	1.740426000
1	-5.017567000	0.092395000	2.660582000
1	-6.104061000	-1.309475000	2.918581000
6	-7.423835000	0.720272000	1.728582000
1	-6.879986000	1.561877000	2.160321000
1	-8.079585000	1.087416000	0.937092000
1	-8.005752000	0.206969000	2.496152000
1	-4.977342000	-0.326100000	-1.336525000
6	-3.966115000	3.311637000	-0.849413000
6	-3.128137000	4.247923000	-0.198149000
8	-2.911865000	4.288520000	1.035635000
16	-2.338597000	5.457053000	-1.30340800
6	-1.277804000	6.346093000	-0.112855000
1	-1.652161000	6.122076000	0.888771000
1	-0.240481000	6.013820000	-0.199978000
1	-1.344398000	7.417469000	-0.313655000
1	-5.841876000	0.478842000	0.475128000
6	-4.646870000	2.334435000	-0.111473000
8	-4.511324000	2.298292000	1.236999000
8	-5.406498000	1.436907000	-0.610985000
1	-3.879172000	3.049033000	1.473659000
1	-4.099364000	3.332902000	-1.923141000
6	-6.588364000	-2.897108000	-1.645993000
1	-6.985299000	-2.220802000	-2.416342000
1	-5.810076000	-3.501235000	-2.123522000
6	-8.098165000	-2.097491000	0.772389000
1	-8.868401000	-1.492106000	1.262424000
1	-7.654119000	-2.743123000	1.542112000
6	-8.749257000	-2.967937000	-0.318603000
1	-9.496381000	-3.625760000	0.140027000
1	-9.293389000	-2.316047000	-1.016704000
6	-7.707800000	-3.789202000	-1.090741000
1	-7.269356000	-4.543240000	-0.421894000
1	-8.190580000	-4.339425000	-1.906653000

^{A}F2$_{INT2}$

6	-3.856765000	2.177560000	2.511245000
6	-4.848862000	1.196684000	2.921320000
6	-4.443844000	-0.038066000	3.426382000
6	-3.027864000	-0.344923000	3.540414000
6	-2.074644000	0.593817000	3.135674000
6	-2.493717000	1.880106000	2.610243000
6	-4.349230000	2.856080000	1.337085000
6	-5.650304000	2.299364000	1.007911000
6	-5.960302000	1.272273000	1.989153000
6	-6.619928000	0.105971000	1.595865000
6	-5.129015000	-1.252212000	3.019328000
6	-2.835373000	-1.737234000	3.210864000
6	-1.698790000	-2.124149000	2.492035000
6	-0.703889000	-1.145390000	2.101100000
6	-0.878261000	0.186845000	2.443102000
6	-0.427328000	1.314917000	1.575850000
6	-1.558998000	2.292155000	1.589156000
6	-2.040952000	2.910420000	0.445848000
6	-3.453673000	3.199908000	0.319088000
6	-6.014189000	2.118650000	-0.327068000
6	-5.090399000	2.488926000	-1.387767000
6	-3.837630000	3.012821000	-1.069166000
6	-2.659399000	2.594691000	-1.808132000
6	-1.542166000	2.530446000	-0.887642000
6	-0.580280000	1.542271000	-1.033845000
6	0.110280000	0.896170000	0.122356000
6	0.099724000	-0.562132000	-0.181974000
6	-0.204097000	-1.527274000	0.764464000
6	-4.133115000	-2.303677000	2.885818000
6	-2.572128000	-3.494552000	-1.293318000
6	-3.451246000	-3.850428000	-0.269497000
6	-4.865638000	-3.547988000	-0.387709000
6	-5.348983000	-2.897051000	-1.524597000
6	-4.435798000	-2.524523000	-2.590864000
6	-2.086067000	-1.837132000	-2.886487000
6	-0.977028000	-1.909858000	-1.949899000
6	-1.273142000	-2.929932000	-0.971531000
6	-0.903586000	-2.731635000	0.363415000
6	-1.821237000	-3.102945000	1.425868000
6	-3.065386000	-3.655137000	1.118758000
6	-5.357455000	-3.172690000	0.929196000
6	-6.312453000	-2.161751000	1.055523000
6	-6.810650000	-1.481343000	-0.128257000

6	-6.338993000	-1.841279000	-1.391248000
6	-6.035054000	-0.814498000	-2.374304000
6	-4.859914000	-1.236532000	-3.116156000
6	-3.906858000	-0.293980000	-3.507939000
6	-2.492296000	-0.601277000	-3.388351000
6	-0.325774000	-0.741087000	-1.546494000
6	-0.746751000	0.546042000	-2.067270000
6	-1.806636000	0.613350000	-2.976842000
6	-2.787085000	1.664516000	-2.844858000
6	-4.089198000	1.108676000	-3.171522000
6	-5.218363000	1.511598000	-2.457208000
6	-6.210497000	0.533033000	-2.052699000
6	-6.702326000	0.908286000	-0.735585000
6	-6.998896000	-0.079283000	0.206089000
6	-4.246637000	-3.243114000	1.860177000
6	-6.195914000	-1.182010000	2.121347000
6	-3.075573000	-2.819060000	-2.478964000
6	1.008274000	1.526365000	1.155938000
6	1.577906000	2.904196000	0.931457000
7	2.913438000	2.981860000	1.198551000
8	0.890963000	3.850015000	0.543570000
6	3.708912000	4.171418000	0.903006000
1	4.734868000	3.914689000	1.193646000
6	3.696651000	4.529890000	-0.605281000
1	2.650514000	4.688089000	-0.880853000
7	4.145241000	3.344575000	-1.456059000
1	1.701970000	0.818990000	1.602999000
6	5.616485000	3.070769000	-1.441030000
1	6.145872000	3.852100000	-1.988944000
1	5.961937000	3.019804000	-0.409963000
1	5.796303000	2.099772000	-1.904261000
6	3.643007000	3.434422000	-2.859081000
1	3.879704000	2.494115000	-3.358368000
1	2.559665000	3.563705000	-2.834904000
1	4.113426000	4.270335000	-3.380421000
1	3.446362000	2.099564000	1.193630000
6	6.752669000	-1.195750000	-0.185587000
1	6.671009000	-0.185461000	0.222984000
6	7.812155000	-1.964963000	0.598430000
8	8.522789000	-2.839367000	0.162806000
16	7.894957000	-1.438946000	2.330824000
6	9.130762000	-2.648022000	2.918349000
1	8.765378000	-3.665034000	2.765381000
1	10.071078000	-2.517241000	2.380304000
1	9.277285000	-2.456992000	3.983694000
1	3.689094000	2.419794000	-1.100651000
6	7.099367000	-1.002796000	-1.650248000
8	7.372562000	-2.138654000	-2.316903000
8	7.108690000	0.083539000	-2.199652000
1	7.575188000	-1.869224000	-3.233546000
6	5.287886000	-1.803993000	0.049319000
6	4.287278000	-1.012801000	-0.736999000
1	5.113234000	-1.592577000	1.110295000
1	3.764066000	-1.391896000	-1.601933000
7	4.023116000	0.231513000	-0.413182000
8	4.598499000	0.808152000	0.602481000
8	3.166707000	0.934806000	-1.121748000
6	5.157694000	-3.304729000	-0.157081000
6	5.191558000	-4.147221000	0.963050000
6	4.973459000	-3.887438000	-1.418745000
6	5.055609000	-5.529395000	0.830262000
1	5.319578000	-3.712522000	1.951571000

6	4.833158000	-5.268181000	-1.555020000
1	4.948816000	-3.263665000	-2.306215000
6	4.874910000	-6.095340000	-0.431641000
1	5.082682000	-6.161052000	1.714314000
1	4.689937000	-5.698221000	-2.542886000
1	4.763525000	-7.170944000	-0.539466000
6	3.266994000	5.383757000	1.751402000
1	2.204847000	5.566572000	1.564593000
1	3.366627000	5.106752000	2.806795000
6	4.508473000	5.798918000	-0.902587000
1	5.567326000	5.629561000	-0.668131000
1	4.452280000	6.048164000	-1.969360000
6	4.078800000	6.645630000	1.436739000
1	3.702723000	7.484734000	2.033762000
1	5.130119000	6.501447000	1.727352000
6	4.008326000	6.981564000	-0.057787000
1	4.610212000	7.868910000	-0.286346000
1	2.972282000	7.220905000	-0.333916000

^{A}F2$_{INT3}$

6	3.776614000	2.729360000	-1.868086000
6	4.819138000	1.862005000	-2.392688000
6	4.482771000	0.762156000	-3.180523000
6	3.087413000	0.481758000	-3.474506000
6	2.084990000	1.309335000	-2.960850000
6	2.432742000	2.455471000	-2.141503000
6	4.158478000	3.144083000	-0.539968000
6	5.440263000	2.534523000	-0.229194000
6	5.850052000	1.741278000	-1.376539000
6	6.500277000	0.520277000	-1.185979000
6	5.158483000	-0.508385000	-2.984723000
6	2.898742000	-0.949723000	-3.465785000
6	1.716296000	-1.485285000	-2.943902000
6	0.672446000	-0.615675000	-2.439215000
6	0.846176000	0.758895000	-2.472208000
6	0.301756000	1.674871000	-1.426047000
6	1.410538000	2.636999000	-1.137377000
6	1.785528000	2.999408000	0.146722000
6	3.177027000	3.260380000	0.449449000
6	5.698672000	2.074539000	1.062610000
6	4.684557000	2.207158000	2.096748000
6	3.451327000	2.783165000	1.793399000
6	2.226249000	2.212641000	2.325617000
6	1.189155000	2.342692000	1.322887000
6	0.238174000	1.344080000	1.175802000
6	-0.342944000	0.958358000	-0.146883000
6	-0.326396000	-0.534010000	-0.158843000
6	0.077243000	-1.274467000	-1.259923000
6	4.177712000	-1.567600000	-3.160891000
6	2.310159000	-3.627916000	0.525880000
6	3.275999000	-3.752876000	-0.473332000
6	4.669429000	-3.478420000	-0.176346000
6	5.045076000	-3.082993000	1.109053000
6	4.041255000	-2.949975000	2.150236000
6	1.661791000	-2.349722000	2.388270000
6	0.633955000	-2.224672000	1.367924000
6	1.030675000	-3.010425000	0.223079000
6	0.766033000	-2.534390000	-1.065823000
6	1.773232000	-2.668490000	-2.103458000
6	2.999701000	-3.267979000	-1.816403000
6	5.258105000	-2.829550000	-1.337985000
6	6.198423000	-1.811609000	-1.166773000

6	6.584595000	-1.397409000	0.171862000
6	6.020276000	-2.019882000	1.285872000
6	5.616100000	-1.227352000	2.435330000
6	4.394011000	-1.801900000	2.969983000
6	3.393072000	-0.967840000	3.472344000
6	1.999836000	-1.247272000	3.171535000
6	-0.007673000	-0.997997000	1.168781000
6	0.341963000	0.150960000	1.984157000
6	1.324302000	0.025143000	2.971299000
6	2.289365000	1.083121000	3.148007000
6	3.572265000	0.474800000	3.457438000
6	4.746255000	1.024574000	2.941380000
6	5.788394000	0.158245000	2.422792000
6	6.377015000	0.807393000	1.261074000
6	6.769712000	0.044315000	0.159466000
6	4.228115000	-2.703824000	-2.352333000
6	6.147321000	-0.627508000	-2.006262000
6	2.701150000	-3.218807000	1.865361000
6	-1.168753000	1.794286000	-1.102485000
6	-1.767368000	3.101432000	-0.640110000
7	-3.066391000	3.274122000	-1.025200000
8	-1.134543000	3.918755000	0.024802000
6	-3.924377000	4.370527000	-0.548923000
1	-4.913724000	4.173886000	-0.982842000
6	-4.057596000	4.389502000	0.999285000
1	-3.037055000	4.460054000	1.384531000
7	-4.601379000	3.094423000	1.533706000
1	-1.803589000	1.187788000	-1.745032000
6	-6.074292000	3.002342000	1.559131000
1	-6.529648000	3.665027000	2.306892000
1	-6.483835000	3.247338000	0.574831000
1	-6.349077000	1.971034000	1.798954000
6	-4.049778000	2.778757000	2.866368000
1	-4.385649000	1.780206000	3.157794000
1	-2.957586000	2.776804000	2.812760000
1	-4.366857000	3.502329000	3.632092000
1	-3.532927000	2.457298000	-1.396071000
6	-4.115722000	-1.372700000	-0.352613000
6	-4.384055000	-0.964971000	-1.815039000
8	-3.490036000	-0.534408000	-2.518582000
16	-6.064545000	-1.093750000	-2.41647400
6	-5.802780000	-0.386024000	-4.080668000
1	-5.462305000	0.648754000	-4.010872000
1	-5.064212000	-0.973022000	-4.628634000
1	-6.768784000	-0.429643000	-4.588580000
6	-4.458966000	-0.211089000	0.595926000
8	-4.257047000	0.959664000	0.012638000
8	-4.788247000	-0.352282000	1.762699000
1	-4.335313000	1.783040000	0.667092000
1	-3.016692000	-1.393929000	-0.327985000
6	-4.581180000	-2.799712000	0.067806000
1	-4.118104000	-3.464302000	-0.668906000
6	-3.928007000	-3.174048000	1.412379000
6	-6.075212000	-3.119054000	0.072657000
6	-6.999516000	-2.444388000	0.886179000
6	-6.534791000	-4.182346000	-0.718677000
6	-8.345879000	-2.811425000	0.883765000
1	-6.665720000	-1.635738000	1.526252000
6	-7.879221000	-4.552182000	-0.716787000
1	-5.829257000	-4.728675000	-1.338788000
6	-8.791774000	-3.863344000	0.082522000
1	-9.046964000	-2.275607000	1.518430000
1	-8.210686000	-5.379713000	-1.338169000
1	-9.840400000	-4.148670000	0.087091000
1	-4.432128000	-2.747571000	2.274337000
7	-3.930117000	-4.674144000	1.621181000
8	-3.646429000	-5.386565000	0.660630000
8	-4.176962000	-5.074651000	2.752460000
1	-2.868308000	-2.896820000	1.436083000
6	-3.413752000	5.720704000	-1.099889000
1	-2.365572000	5.830970000	-0.805212000
1	-3.436576000	5.672674000	-2.194978000
6	-4.840160000	5.628450000	1.481007000
1	-5.883522000	5.566956000	1.144160000
1	-4.864461000	5.640207000	2.577948000
6	-4.218602000	6.919408000	-0.586644000
1	-5.250757000	6.873976000	-0.965738000
1	-3.783879000	7.847334000	-0.977292000
6	-4.242315000	6.936397000	0.945654000
1	-4.827871000	7.787074000	1.315144000
1	-3.220240000	7.064726000	1.328189000

^{A}F2$_{INT4}$

6	3.890484000	-2.957449000	1.809609000
6	4.937646000	-2.050785000	2.251563000
6	4.623719000	-0.962975000	3.065085000
6	3.246280000	-0.734019000	3.467489000
6	2.238677000	-1.599450000	3.033999000
6	2.563817000	-2.733130000	2.188842000
6	4.180627000	-3.360672000	0.455218000
6	5.409306000	-2.703351000	0.044836000
6	5.879568000	-1.893401000	1.157392000
6	6.467394000	-0.649791000	0.917933000
6	5.233698000	0.331482000	2.817704000
6	3.003704000	0.689261000	3.474538000
6	1.764383000	1.178273000	3.047414000
6	0.716226000	0.268815000	2.627588000
6	0.942694000	-1.099548000	2.646646000
6	0.351884000	-2.043407000	1.654216000
6	1.472412000	-2.953468000	1.270370000
6	1.755550000	-3.305255000	-0.040182000
6	3.127538000	-3.512827000	-0.453156000
6	5.549259000	-2.236795000	-1.262702000
6	4.462051000	-2.407535000	-2.212851000
6	3.277763000	-3.027778000	-1.813599000
6	1.995126000	-2.504603000	-2.248202000
6	1.044025000	-2.671732000	-1.165873000
6	0.075922000	-1.703009000	-0.946051000
6	-0.421594000	-1.339502000	0.411700000
6	-0.452878000	0.148120000	0.428742000
6	0.007325000	0.903609000	1.497423000
6	4.230730000	1.353891000	3.071022000
6	2.005266000	3.338973000	-0.454929000
6	3.041635000	3.500073000	0.466169000
6	4.416652000	3.277245000	0.060398000
6	4.704412000	2.893269000	-1.251031000
6	3.627953000	2.721582000	-2.210434000
6	1.261194000	2.036361000	-2.264675000
6	0.318894000	1.876151000	-1.167349000
6	0.777334000	2.676481000	-0.052918000
6	0.633184000	2.189869000	1.251385000
6	1.712167000	2.361744000	2.207117000
6	2.889539000	3.006809000	1.825655000
6	5.118276000	2.652740000	1.171592000

6	6.078305000	1.669282000	0.925445000
6	6.373472000	1.267241000	-0.439878000
6	5.701877000	1.866990000	-1.505690000
6	5.238606000	1.058191000	-2.620758000
6	3.957739000	1.586220000	-3.057006000
6	2.952137000	0.715092000	-3.480529000
6	1.577940000	0.944670000	-3.071823000
6	-0.256211000	0.624442000	-0.919236000
6	0.070867000	-0.511125000	-1.761499000
6	0.967642000	-0.351560000	-2.820790000
6	1.952770000	-1.375475000	-3.073171000
6	3.184041000	-0.720655000	-3.480593000
6	4.414074000	-1.225558000	-3.058611000
6	5.461345000	-0.320218000	-2.622739000
6	6.162595000	-0.945389000	-1.511845000
6	6.612649000	-0.166412000	-0.443876000
6	4.176237000	2.490528000	2.263319000
6	6.137535000	0.485571000	1.764833000
6	2.304842000	2.942558000	-1.821828000
6	-1.109569000	-2.233943000	1.408680000
6	-1.658052000	-3.590831000	0.973924000
7	-2.912664000	-3.514499000	0.471471000
8	-1.006157000	-4.625846000	1.078106000
6	-3.705642000	-4.693668000	0.132100000
1	-3.690656000	-5.380032000	0.991997000
6	-5.157877000	-4.244926000	-0.152228000
1	-5.118007000	-3.641797000	-1.071614000
7	-5.648465000	-3.323073000	0.882864000
1	-1.763428000	-1.695156000	2.093183000
6	-5.889660000	-3.911851000	2.194187000
1	-6.772825000	-4.575728000	2.231425000
1	-5.017716000	-4.485931000	2.520978000
1	-6.046351000	-3.106351000	2.920169000
6	-6.761844000	-2.489993000	0.450951000
1	-6.940972000	-1.712384000	1.202101000
1	-6.512011000	-1.991723000	-0.491278000
1	-7.710499000	-3.042119000	0.310627000
1	-3.431689000	-2.643955000	0.564512000
6	-4.137115000	3.703637000	-0.612836000
6	-3.230880000	4.362736000	-1.358336000
8	-2.209549000	3.812900000	-2.077601000
16	-3.367367000	6.118878000	-1.60044200
6	-1.615846000	6.643152000	-1.466351000
1	-1.237118000	6.504712000	-0.450597000
1	-1.000021000	6.090932000	-2.176843000
1	-1.598520000	7.706790000	-1.716797000
6	-5.495781000	5.367187000	3.259665000
8	-5.634365000	4.345734000	2.703816000
8	-5.358933000	6.383366000	3.816219000
6	-4.290865000	2.197153000	-0.539073000
1	-3.607791000	1.721716000	-1.250555000
6	-3.878636000	1.727780000	0.865078000
6	-5.708888000	1.760122000	-0.905550000
6	-6.810355000	2.122079000	-0.117083000
6	-5.931200000	0.996140000	-2.057173000
6	-8.100465000	1.726493000	-0.472389000
1	-6.668860000	2.723181000	0.777885000
6	-7.221286000	0.602704000	-2.416786000
1	-5.086695000	0.704688000	-2.676401000
6	-8.310886000	0.965499000	-1.623722000
1	-8.942395000	2.016777000	0.150539000
1	-7.373069000	0.012939000	-3.316927000
1	-9.315979000	0.659823000	-1.901128000
1	-4.539729000	2.083805000	1.654875000
7	-3.841724000	0.223555000	1.015041000
8	-3.638444000	-0.453881000	0.008387000
8	-3.953132000	-0.225619000	2.151091000
1	-2.856794000	2.039625000	1.103605000
1	-4.849682000	4.299015000	-0.052611000
1	-1.969194000	2.939424000	-1.721857000
6	-3.143759000	-5.460574000	-1.080073000
1	-3.106705000	-4.777600000	-1.940751000
1	-2.116768000	-5.763519000	-0.860053000
6	-6.034982000	-5.481306000	-0.449447000
1	-6.074854000	-6.127038000	0.438722000
1	-7.064849000	-5.163069000	-0.653943000
6	-5.481663000	-6.284027000	-1.638445000
1	-5.555353000	-5.673433000	-2.550494000
1	-6.098242000	-7.175364000	-1.810716000
6	-4.015462000	-6.680526000	-1.412357000
1	-3.958162000	-7.402457000	-0.584577000
1	-3.618110000	-7.193121000	-2.297083000

$^{A}F2_{P}$

6	2.276707000	0.799402000	-3.317156000
6	2.993938000	-0.453036000	-3.492769000
6	2.432606000	-1.649460000	-3.048270000
6	1.129965000	-1.642126000	-2.404270000
6	0.446156000	-0.436487000	-2.224312000
6	1.027902000	0.809524000	-2.687548000
6	3.235798000	1.830034000	-3.002320000
6	4.556220000	1.224156000	-2.978108000
6	4.406810000	-0.189662000	-3.282502000
6	5.201516000	-1.133813000	-2.628992000
6	3.257572000	-2.632720000	-2.369007000
6	1.142771000	-2.616231000	-1.338176000
6	0.471285000	-2.336464000	-0.141519000
6	-0.259286000	-1.094731000	0.022052000
6	-0.289603000	-0.172437000	-1.013752000
6	-0.323161000	1.303040000	-0.792528000
6	0.654842000	1.864670000	-1.774979000
6	1.591869000	2.831406000	-1.446324000
6	2.897975000	2.816388000	-2.070117000
6	5.495371000	1.636074000	-2.031842000
6	5.151555000	2.672844000	-1.071363000
6	3.879641000	3.244496000	-1.089167000
6	3.181114000	3.516969000	0.154721000
6	1.768687000	3.270987000	-0.051415000
6	1.004404000	2.726726000	0.969058000
6	-0.126689000	1.778848000	0.729480000
6	0.061341000	0.689965000	1.730467000
6	-0.080334000	-0.654900000	1.422005000
6	2.459680000	-3.230348000	-1.309918000
6	3.016578000	-1.855218000	3.062735000
6	3.337170000	-2.851544000	2.139721000
6	4.640733000	-2.860409000	1.502383000
6	5.574587000	-1.868361000	1.808127000
6	5.242871000	-0.829502000	2.767374000
6	3.274222000	0.427707000	3.557121000
6	1.861967000	0.163759000	3.338758000
6	1.701200000	-1.239337000	3.038221000
6	0.755616000	-1.636145000	2.085953000
6	1.093298000	-2.672853000	1.126860000
6	2.353570000	-3.271840000	1.154798000

6	4.465388000	-3.293814000	0.124579000
6	5.230965000	-2.717404000	-0.890996000
6	6.199670000	-1.681713000	-0.571860000
6	6.367790000	-1.266061000	0.749494000
6	6.523454000	0.146720000	1.053931000
6	5.829233000	0.416811000	2.300716000
6	5.139124000	1.619177000	2.468157000
6	3.834279000	1.622329000	3.106571000
6	1.070474000	1.103379000	2.672353000
6	1.650791000	2.348162000	2.204187000
6	3.007631000	2.604884000	2.424166000
6	3.792730000	3.206247000	1.373539000
6	5.112742000	2.599362000	1.394715000
6	5.778885000	2.336926000	0.197040000
6	6.498606000	1.088966000	0.023624000
6	6.323162000	0.655521000	-1.354392000
6	6.179641000	-0.702536000	-1.645836000
6	3.053400000	-3.552180000	-0.088385000
6	4.615176000	-2.380028000	-2.162449000
6	3.990384000	-0.823813000	3.384132000
6	-1.413775000	2.014107000	-0.029362000
6	-1.836903000	3.420993000	-0.393912000
7	-3.142237000	3.686107000	-0.121972000
8	-1.046878000	4.241592000	-0.854057000
6	-3.786208000	4.942317000	-0.506554000
1	-3.644461000	5.094382000	-1.587889000
6	-5.295892000	4.819788000	-0.190498000
1	-5.375562000	4.790889000	0.906451000
7	-5.827426000	3.526246000	-0.640413000
1	-2.219545000	1.352922000	0.279181000
6	-5.945472000	3.351769000	-2.084748000
1	-6.757665000	3.948627000	-2.537861000
1	-5.007564000	3.623147000	-2.578901000
1	-6.141765000	2.295306000	-2.290808000
6	-7.042456000	3.110475000	0.048987000
1	-7.242571000	2.061952000	-0.190767000
1	-6.899130000	3.192462000	1.132079000
1	-7.935722000	3.703033000	-0.224494000
1	-3.800748000	2.914321000	-0.018270000
6	-3.750332000	-3.968284000	0.337844000
6	-2.794907000	-4.328616000	-0.794381000
8	-2.630886000	-3.659878000	-1.795440000
16	-1.930256000	-5.879557000	-0.52881600
6	-0.987037000	-5.960258000	-2.090771000
1	-1.666797000	-5.940103000	-2.944170000
1	-0.295317000	-5.118377000	-2.151113000
1	-0.433574000	-6.901492000	-2.072848000
6	-8.219103000	-5.219276000	-1.350228000
8	-7.286732000	-4.750194000	-0.818535000
8	-9.147312000	-5.687804000	-1.878816000
1	-3.331002000	-4.324072000	1.284958000
6	-4.059041000	-2.453748000	0.457655000
1	-3.108872000	-1.913547000	0.413846000
6	-4.896802000	-1.999164000	-0.744666000
6	-4.726675000	-2.148743000	1.793177000
6	-6.007849000	-2.630860000	2.099321000
6	-4.048677000	-1.390033000	2.755457000
6	-6.594558000	-2.358097000	3.335500000
1	-6.555867000	-3.226684000	1.373187000
6	-4.632965000	-1.118278000	3.993414000
1	-3.055304000	-1.008238000	2.532471000
6	-5.908808000	-1.600778000	4.286871000
1	-7.588571000	-2.738639000	3.555311000
1	-4.090782000	-0.526619000	4.726094000
1	-6.366274000	-1.388442000	5.249317000
1	-5.869528000	-2.486217000	-0.805792000
7	-5.192452000	-0.521519000	-0.729664000
8	-4.325917000	0.239341000	-0.304970000
8	-6.275505000	-0.171460000	-1.190533000
1	-4.343364000	-2.171557000	-1.671297000
1	-4.676185000	-4.539472000	0.183158000
6	-3.204713000	6.172461000	0.213460000
1	-3.309112000	6.027292000	1.298233000
1	-2.136845000	6.243365000	-0.005283000
6	-6.032904000	6.087335000	-0.672040000
1	-5.940995000	6.176698000	-1.763286000
1	-7.104120000	5.999534000	-0.451623000
6	-5.454090000	7.345834000	-0.003698000
1	-5.959045000	8.242105000	-0.385810000
1	-5.663099000	7.307147000	1.075569000
6	-3.937176000	7.451345000	-0.221341000
1	-3.735696000	7.637136000	-1.286481000
1	-3.534053000	8.313862000	0.323547000

Cartesian coordinates of all transition states in both the pathways

^{D}F1$_{TS1}$

6	0.362637000	-1.272973000	2.758325000
6	1.311526000	-0.412859000	3.447255000
6	1.211359000	0.972921000	3.331197000
6	0.158023000	1.556897000	2.517895000
6	-0.746633000	0.729258000	1.847296000
6	-0.644942000	-0.713127000	1.966884000
6	1.069124000	-2.438783000	2.284524000
6	2.462956000	-2.309244000	2.674026000
6	2.613155000	-1.055220000	3.394193000
6	3.764058000	-0.283300000	3.221932000
6	2.406953000	1.777707000	3.152238000
6	0.693110000	2.715638000	1.842482000
6	0.297267000	2.992453000	0.529103000
6	-0.662639000	2.142219000	-0.146713000
6	-1.193599000	1.044861000	0.513969000
6	-1.544996000	-0.227638000	-0.180018000
6	-1.033443000	-1.312394000	0.711144000
6	-0.329687000	-2.410980000	0.241865000
6	0.734076000	-2.984372000	1.041000000
6	3.470959000	-2.740588000	1.810843000
6	3.124778000	-3.320917000	0.523001000
6	1.786511000	-3.434366000	0.147053000
6	1.379921000	-3.130520000	-1.213782000
6	0.075837000	-2.502890000	-1.171707000
6	-0.238040000	-1.494618000	-2.069466000
6	-1.107747000	-0.329423000	-1.719751000
6	-0.397388000	0.863536000	-2.267753000
6	-0.257257000	2.049567000	-1.563989000
6	2.085891000	2.856318000	2.230931000
6	3.354268000	2.568301000	-2.199712000
6	3.677989000	3.129285000	-0.963631000
6	4.733961000	2.548219000	-0.155438000
6	5.424931000	1.423861000	-0.611721000
6	5.089154000	0.837542000	-1.897387000
6	3.127467000	0.538169000	-3.361151000
6	1.824351000	1.178702000	-3.301859000

6	1.962267000	2.427666000	-2.590795000
6	0.943100000	2.845217000	-1.727778000
6	1.284439000	3.429037000	-0.442449000
6	2.621075000	3.573144000	-0.068980000
6	4.334228000	2.638792000	1.240587000
6	4.641840000	1.601421000	2.123326000
6	5.356854000	0.429514000	1.645964000
6	5.740018000	0.342593000	0.307055000
6	5.595641000	-0.912763000	-0.411286000
6	5.194252000	-0.607552000	-1.773229000
6	4.281898000	-1.433565000	-2.432904000
6	3.226557000	-0.847235000	-3.240560000
6	0.674149000	0.406770000	-3.115956000
6	0.774665000	-1.035651000	-2.991380000
6	2.028627000	-1.651171000	-3.058899000
6	2.338764000	-2.726947000	-2.148678000
6	3.731768000	-2.596912000	-1.756383000
6	4.117707000	-2.887313000	-0.447244000
6	5.068269000	-2.031126000	0.237528000
6	4.668546000	-1.940495000	1.633803000
6	4.812567000	-0.735244000	2.324171000
6	3.031431000	3.275683000	1.294175000
6	3.658843000	1.161852000	3.098050000
6	4.075860000	1.399066000	-2.676585000
6	-2.557674000	-0.315605000	-1.298173000
6	-3.431059000	-1.533197000	-1.430726000
7	-4.741390000	-1.246733000	-1.677109000
8	-3.000268000	-2.680329000	-1.317164000
6	-5.748190000	-2.287434000	-1.768552000
1	-6.363858000	-2.118505000	-2.661056000
1	-5.214617000	-3.228278000	-1.915555000
6	-6.727105000	-2.378831000	-0.584176000
1	-7.429289000	-3.199126000	-0.793752000
1	-7.306066000	-1.454253000	-0.498038000
7	-6.120389000	-2.600730000	0.762227000
1	-3.062579000	0.627692000	-1.491056000
6	-5.209099000	-3.768396000	0.826029000
1	-4.366450000	-3.628312000	0.147037000
1	-4.830646000	-3.851527000	1.847869000
1	-5.749034000	-4.689718000	0.570589000
6	-7.197073000	-2.713781000	1.778482000
1	-6.736681000	-2.852012000	2.760004000
1	-7.765426000	-1.782505000	1.782665000
1	-7.846114000	-3.570547000	1.559726000
1	-5.023911000	-0.270874000	-1.700369000
6	-5.236809000	1.928511000	0.905395000
1	-4.145820000	1.882633000	0.912131000
6	-5.678464000	2.305270000	-0.501692000
8	-5.135637000	1.832697000	-1.490816000
16	-7.045365000	3.418231000	-0.77745200
6	-7.794591000	3.682777000	0.873545000
1	-7.957400000	2.718546000	1.358683000
1	-7.186163000	4.344563000	1.494896000
1	-8.757536000	4.163935000	0.683120000
1	-5.513757000	-1.522785000	1.059523000
1	-5.582149000	2.640026000	1.656391000
6	-5.836957000	0.536222000	1.197523000
8	-7.066519000	0.424391000	1.279921000
8	-4.970781000	-0.421482000	1.250171000

$^{D}F1_{TS2}$

6	-1.139509000	1.528850000	2.953975000
6	-2.113736000	0.615505000	3.529294000
6	-1.887420000	-0.759723000	3.496383000
6	-0.676803000	-1.279902000	2.883266000
6	0.254480000	-0.402343000	2.321041000
6	0.021305000	1.029800000	2.354801000
6	-1.852539000	2.612488000	2.321909000
6	-3.275640000	2.378235000	2.498605000
6	-3.437580000	1.142199000	3.246642000
6	-4.482305000	0.269119000	2.936547000
6	-2.972890000	-1.669622000	3.175385000
6	-1.006103000	-2.503434000	2.190900000
6	-0.388462000	-2.792146000	0.969104000
6	0.594807000	-1.886713000	0.408719000
6	0.927532000	-0.725834000	1.088867000
6	1.280673000	0.548377000	0.395317000
6	0.553064000	1.617183000	1.147315000
6	-0.153711000	2.632601000	0.522876000
6	-1.370797000	3.141248000	1.120069000
6	-4.166265000	2.691416000	1.471087000
6	-3.669048000	3.253723000	0.225145000
6	-2.301713000	3.468287000	0.054279000
6	-1.663788000	3.152395000	-1.211673000
6	-0.336794000	2.639854000	-0.939052000
6	0.191758000	1.630698000	-1.728666000
6	1.080453000	0.554868000	-1.190433000
6	0.565456000	-0.712467000	-1.787455000
6	0.410327000	-1.879990000	-1.056892000
6	-2.427111000	-2.748453000	2.367106000
6	-3.003380000	-2.726574000	-2.214425000
6	-3.471514000	-3.268786000	-1.016873000
6	-4.683638000	-2.751809000	-0.409293000
6	-5.380834000	-1.707411000	-1.019846000
6	-4.894662000	-1.140256000	-2.265420000
6	-2.757496000	-0.726488000	-3.423221000
6	-1.433502000	-1.251130000	-3.133965000
6	-1.582674000	-2.481513000	-2.393065000
6	-0.682096000	-2.781233000	-1.364954000
6	-1.173309000	-3.345974000	-0.120261000
6	-2.536569000	-3.589330000	0.049882000
6	-4.502138000	-2.758755000	1.034234000
6	-5.025439000	-1.721126000	1.808314000
6	-5.746648000	-0.632076000	1.170912000
6	-5.920634000	-0.625380000	-0.213493000
6	-5.764735000	0.611627000	-0.960647000
6	-5.131668000	0.294049000	-2.228632000
6	-4.194997000	1.171209000	-2.779269000
6	-2.983026000	0.648784000	-3.385887000
6	-0.391152000	-0.377720000	-2.811351000
6	-0.623194000	1.054487000	-2.772882000
6	-1.895514000	1.557851000	-3.061133000
6	-2.428647000	2.634550000	-2.261649000
6	-3.851527000	2.400350000	-2.082989000
6	-4.459783000	2.702600000	-0.864085000
6	-5.435451000	1.792982000	-0.293042000
6	-5.253905000	1.786081000	1.150694000
6	-5.409191000	0.598056000	1.867909000
6	-3.177847000	-3.279761000	1.317747000
6	-4.245276000	-1.165201000	2.900005000
6	-3.730738000	-1.640544000	-2.851938000
6	2.448127000	0.687164000	-0.556316000
6	3.227695000	1.969363000	-0.652420000
7	4.566194000	1.800982000	-0.873631000

8	2.719519000	3.079497000	-0.533158000
6	5.404271000	2.984385000	-0.961722000
1	5.245914000	3.511345000	-1.913644000
1	5.094737000	3.686269000	-0.181028000
6	6.895506000	2.680215000	-0.873448000
1	7.445641000	3.626442000	-0.849834000
1	7.227788000	2.103549000	-1.741126000
7	7.319298000	1.863959000	0.320815000
1	3.046811000	-0.215997000	-0.633494000
6	6.676922000	2.256096000	1.609145000
1	6.932578000	3.292767000	1.845459000
1	5.597525000	2.143460000	1.516605000
1	7.045819000	1.580141000	2.379425000
6	8.806417000	1.870584000	0.445662000
1	9.083371000	1.152766000	1.216684000
1	9.241076000	1.573857000	-0.510653000
1	9.141367000	2.877406000	0.709682000
1	4.984599000	0.876552000	-0.997175000
6	8.389632000	-1.684719000	-0.389082000
1	8.841979000	-2.654479000	-0.561919000
6	7.086424000	-1.460618000	-0.810208000
8	6.439391000	-0.354396000	-0.748786000
16	6.257163000	-2.925818000	-1.48249000
6	4.504190000	-2.435144000	-1.433560000
1	4.174515000	-2.248066000	-0.408384000
1	4.325903000	-1.556204000	-2.056749000
1	3.937974000	-3.277516000	-1.839143000
1	7.021750000	0.846251000	0.063407000
1	9.069439000	-0.841145000	-0.318697000
6	8.045981000	-1.786777000	1.851379000
8	7.836862000	-0.639251000	2.133872000
8	8.204031000	-2.931956000	2.107891000

^{D}F1$_{TS3}$

6	1.414973000	-1.741382000	2.895856000
6	2.397012000	-0.807415000	3.423337000
6	2.102632000	0.553757000	3.490721000
6	0.812802000	1.038805000	3.029066000
6	-0.126297000	0.142079000	2.511716000
6	0.177185000	-1.275430000	2.441546000
6	2.112072000	-2.751306000	2.136870000
6	3.532734000	-2.450272000	2.186144000
6	3.709472000	-1.247112000	2.982872000
6	4.674254000	-0.304437000	2.621557000
6	3.104790000	1.535786000	3.115822000
6	1.010865000	2.311848000	2.377022000
6	0.259762000	2.628678000	1.239490000
6	-0.730669000	1.702138000	0.727992000
6	-0.936282000	0.491162000	1.371677000
6	-1.297609000	-0.762231000	0.647225000
6	-0.445597000	-1.826864000	1.260319000
6	0.242522000	-2.770803000	0.513827000
6	1.537391000	-3.242007000	0.959977000
6	4.329456000	-2.662066000	1.060420000
6	3.737117000	-3.185897000	-0.160307000
6	2.371308000	-3.463701000	-0.208247000
6	1.594606000	-3.118377000	-1.385816000
6	0.278504000	-2.693595000	-0.956943000
6	-0.375642000	-1.675551000	-1.632563000
6	-1.261403000	-0.679675000	-0.953712000
6	-0.865418000	0.642643000	-1.521584000
6	-0.695212000	1.779174000	-0.746565000
6	2.428917000	2.623530000	2.426704000
6	2.540608000	2.866032000	-2.183043000
6	3.100530000	3.371280000	-1.008917000
6	4.391369000	2.890091000	-0.553087000
6	5.073210000	1.917065000	-1.286628000
6	4.492124000	1.388852000	-2.508456000
6	2.271570000	0.920401000	-3.473033000
6	0.959679000	1.357291000	-3.025688000
6	1.122720000	2.554522000	-2.235319000
6	0.316531000	2.751748000	-1.108827000
6	0.903142000	3.278400000	0.111016000
6	2.263283000	3.585842000	0.160417000
6	4.356295000	2.813723000	0.899508000
6	5.004230000	1.767198000	1.559092000
6	5.709532000	0.752399000	0.794023000
6	5.743071000	0.825723000	-0.598963000
6	5.572978000	-0.378150000	-1.395619000
6	4.800756000	-0.030677000	-2.575505000
6	3.856874000	-0.927632000	-3.079990000
6	2.566076000	-0.440942000	-3.534825000
6	-0.000832000	0.413657000	-2.651277000
6	0.302696000	-1.003894000	-2.716468000
6	1.562225000	-1.422653000	-3.156667000
6	2.224426000	-2.508425000	-2.475440000
6	3.644961000	-2.207480000	-2.423629000
6	4.386881000	-2.538529000	-1.289157000
6	5.369775000	-1.608014000	-0.766246000
6	5.334378000	-1.684448000	0.686441000
6	5.503686000	-0.528010000	1.450515000
6	3.043411000	3.247221000	1.340135000
6	4.365756000	1.115085000	2.688960000
6	3.252070000	1.855054000	-2.949290000
6	-2.545642000	-0.913054000	-0.195154000
6	-3.271121000	-2.235873000	-0.265330000
7	-4.627135000	-2.119797000	-0.181209000
8	-2.683980000	-3.307993000	-0.371288000
6	-5.504425000	-3.275062000	-0.295037000
1	-4.889185000	-4.116330000	-0.622889000
1	-5.912315000	-3.541149000	0.689542000
6	-6.630106000	-3.027061000	-1.300966000
1	-7.215330000	-3.959890000	-1.423146000
1	-6.174661000	-2.803301000	-2.272104000
7	-7.487221000	-1.893484000	-0.935549000
1	-3.190193000	-0.038334000	-0.159140000
6	-8.392547000	-2.217909000	0.164592000
1	-9.103496000	-3.027567000	-0.090764000
1	-7.828323000	-2.528469000	1.048530000
1	-8.970292000	-1.328621000	0.436834000
6	-8.240344000	-1.410358000	-2.089780000
1	-8.839571000	-0.539725000	-1.800772000
1	-7.550244000	-1.101973000	-2.881841000
1	-8.929229000	-2.169332000	-2.508051000
1	-5.058856000	-1.200414000	-0.142996000
8	-5.710880000	4.015266000	-1.886936000
6	-6.382933000	1.124884000	1.163048000
8	-5.411190000	0.864254000	0.329442000
16	-6.334397000	0.660839000	2.824734000
6	-4.587042000	0.153404000	3.051678000
1	-4.419737000	0.095351000	4.129701000
1	-4.411302000	-0.821360000	2.595041000
1	-3.922352000	0.899132000	2.611595000
6	-6.718807000	4.451841000	-1.484195000

8	-7.724620000	4.904795000	-1.098050000
6	-7.383794000	1.883112000	0.492942000
1	-8.026899000	2.568626000	1.040945000
1	-6.077265000	1.724780000	-0.299321000
1	-7.913528000	1.288743000	-0.256469000

^{D}F2$_{TS1}$

6	0.927299000	-0.713922000	3.014173000
6	1.991460000	0.156615000	3.487966000
6	1.992914000	1.508484000	3.146896000
6	0.929867000	2.046288000	2.314552000
6	-0.086436000	1.206668000	1.850575000
6	-0.090371000	-0.200465000	2.204359000
6	1.500623000	-2.000471000	2.699593000
6	2.926062000	-1.936879000	2.974038000
6	3.230120000	-0.601600000	3.462366000
6	4.421928000	0.024242000	3.090839000
6	3.231339000	2.161378000	2.760623000
6	1.501826000	3.026599000	1.421673000
6	1.029619000	3.121356000	0.107782000
6	-0.043935000	2.263815000	-0.354032000
6	-0.607953000	1.340984000	0.513768000
6	-1.111561000	0.010392000	0.067234000
6	-0.620487000	-0.957606000	1.093800000
6	-0.044274000	-2.177303000	0.772730000
6	1.028846000	-2.707743000	1.588996000
6	3.827440000	-2.592427000	2.134431000
6	3.338565000	-3.340168000	0.986738000
6	1.970575000	-3.390600000	0.719485000
6	1.486330000	-3.275386000	-0.644887000
6	0.243170000	-2.533718000	-0.627768000
6	-0.057825000	-1.659979000	-1.660727000
6	-0.803986000	-0.379677000	-1.459039000
6	-0.044397000	0.639106000	-2.242099000
6	0.243062000	1.905821000	-1.758068000
6	2.927057000	3.100895000	1.692959000
6	3.824883000	1.983927000	-2.696510000
6	4.285975000	2.706113000	-1.595048000
6	5.351240000	2.170121000	-0.768340000
6	5.914024000	0.928693000	-1.071413000
6	5.435242000	0.174647000	-2.216622000
6	3.349454000	-0.178477000	-3.483690000
6	2.109582000	0.579081000	-3.451647000
6	2.400266000	1.908976000	-2.970650000
6	1.486620000	2.551837000	-2.128105000
6	1.970800000	3.303127000	-0.983217000
6	3.339431000	3.383518000	-0.723487000
6	5.068493000	2.522079000	0.614794000
6	5.359737000	1.618016000	1.638385000
6	5.940800000	0.324100000	1.321098000
6	6.212037000	-0.013376000	-0.005434000
6	5.914057000	-1.350301000	-0.491993000
6	5.434875000	-1.234749000	-1.858155000
6	4.411848000	-2.070355000	-2.311177000
6	3.347387000	-1.529138000	-3.138208000
6	0.919568000	-0.044589000	-3.066586000
6	0.914629000	-1.450729000	-2.707827000
6	2.106946000	-2.180529000	-2.749237000
6	2.399655000	-3.118146000	-1.692433000
6	3.824530000	-3.053550000	-1.415439000
6	4.285416000	-3.161682000	-0.102801000
6	5.350561000	-2.295781000	0.367382000
6	5.067516000	-1.943850000	1.750704000
6	5.359287000	-0.660792000	2.218127000
6	3.828215000	3.274930000	0.641808000
6	4.422596000	1.433667000	2.732631000
6	4.412818000	0.692156000	-3.014282000
6	-2.210265000	-0.165719000	-0.955230000
6	-3.186474000	-1.304779000	-0.825520000
7	-4.488506000	-0.927497000	-0.962338000
8	-2.835237000	-2.461684000	-0.593864000
6	-5.596367000	-1.868984000	-0.882336000
1	-5.133268000	-2.858411000	-0.826987000
6	-6.516505000	-1.667173000	0.356989000
1	-6.987544000	-0.679173000	0.274045000
7	-5.758756000	-1.588831000	1.660328000
1	-2.651633000	0.776367000	-1.271095000
6	-4.870597000	-2.739443000	1.954610000
1	-4.143887000	-2.881679000	1.153961000
1	-4.329266000	-2.517358000	2.878441000
1	-5.449296000	-3.659114000	2.103400000
6	-6.654427000	-1.326947000	2.815794000
1	-6.026300000	-1.077754000	3.675628000
1	-7.280577000	-0.463247000	2.588713000
1	-7.263065000	-2.201335000	3.066601000
1	-4.683961000	0.050730000	-1.154688000
6	-4.571284000	2.820635000	0.812766000
1	-3.486782000	2.692732000	0.812544000
6	-5.027640000	2.917186000	-0.636794000
8	-4.559814000	2.192475000	-1.503046000
16	-6.310594000	4.056571000	-1.12931600
6	-6.982001000	4.733695000	0.435554000
1	-7.204031000	3.915149000	1.122815000
1	-6.303610000	5.461068000	0.888236000
1	-7.910130000	5.240953000	0.159345000
1	-5.064847000	-0.481873000	1.627572000
1	-4.843023000	3.699339000	1.398222000
6	-5.261383000	1.570776000	1.397162000
8	-6.485964000	1.580179000	1.555831000
8	-4.463863000	0.567383000	1.589008000
6	-6.439932000	-1.795680000	-2.172875000
1	-6.854480000	-0.781710000	-2.272942000
1	-5.770187000	-1.947782000	-3.026380000
6	-7.577086000	-2.823770000	-2.184036000
1	-8.175647000	-2.709663000	-3.095683000
1	-7.150615000	-3.836687000	-2.213485000
6	-7.623987000	-2.740751000	0.348465000
1	-7.172374000	-3.738431000	0.439471000
1	-8.284481000	-2.609611000	1.211333000
6	-8.459469000	-2.678186000	-0.940081000
1	-9.227807000	-3.460257000	-0.917645000
1	-8.991511000	-1.716939000	-0.978023000

^{D}F2$_{TS2}$

6	-0.934411000	0.085291000	3.164049000
6	-2.053825000	-0.810964000	3.404522000
6	-2.092395000	-2.060568000	2.787549000
6	-1.012985000	-2.466987000	1.903707000
6	0.057695000	-1.601372000	1.664628000
6	0.099559000	-0.299579000	2.304562000
6	-1.440320000	1.435606000	3.103020000
6	-2.878695000	1.386744000	3.302580000
6	-3.258702000	-0.004032000	3.489446000
6	-4.455485000	-0.480065000	2.949829000

6	-3.336383000	-2.558039000	2.226662000
6	-1.580214000	-3.212628000	0.805416000
6	-1.049855000	-3.056792000	-0.479767000
6	0.077105000	-2.175974000	-0.710482000
6	0.635766000	-1.482050000	0.350415000
6	1.212207000	-0.111768000	0.210401000
6	0.711556000	0.645022000	1.399168000
6	0.200131000	1.930821000	1.317854000
6	-0.888032000	2.333934000	2.184260000
6	-3.711791000	2.245452000	2.584175000
6	-3.138805000	3.189501000	1.637516000
6	-1.758617000	3.227407000	1.440313000
6	-1.214106000	3.373240000	0.101673000
6	-0.004095000	2.582519000	0.012351000
6	0.310059000	1.926359000	-1.167625000
6	0.990147000	0.594950000	-1.205810000
6	0.233539000	-0.199910000	-2.217976000
6	-0.128505000	-1.522460000	-2.018198000
6	-3.018764000	-3.270552000	0.999332000
6	-3.660259000	-1.228849000	-3.092019000
6	-4.201798000	-2.139329000	-2.183630000
6	-5.283283000	-1.733968000	-1.305092000
6	-5.781016000	-0.430578000	-1.364265000
6	-5.217769000	0.519389000	-2.307546000
6	-3.060748000	1.023520000	-3.391085000
6	-1.855257000	0.215601000	-3.470635000
6	-2.222087000	-1.168936000	-3.288838000
6	-1.376964000	-2.016194000	-2.563770000
6	-1.944707000	-2.962971000	-1.619912000
6	-3.326284000	-3.028548000	-1.436620000
6	-5.081370000	-2.377634000	-0.015902000
6	-5.385484000	-1.691502000	1.161719000
6	-5.898075000	-0.332869000	1.098830000
6	-6.091762000	0.284318000	-0.137553000
6	-5.717058000	1.676530000	-0.322509000
6	-5.177933000	1.822467000	-1.663178000
6	-4.101697000	2.682351000	-1.892040000
6	-3.021379000	2.272098000	-2.772033000
6	-0.660782000	0.686598000	-2.918095000
6	-0.617304000	1.986248000	-2.273416000
6	-1.775854000	2.766731000	-2.207690000
6	-2.081421000	3.479021000	-0.990441000
6	-3.519566000	3.429360000	-0.788927000
6	-4.038328000	3.286378000	0.498632000
6	-5.158643000	2.395441000	0.736366000
6	-4.956837000	1.751973000	2.025872000
6	-5.321420000	0.415720000	2.203533000
6	-3.875271000	-3.180392000	-0.098682000
6	-4.495065000	-1.783197000	2.305515000
6	-4.179719000	0.128026000	-3.155342000
6	2.369252000	0.218695000	-0.706204000
6	3.370081000	1.276822000	-0.333672000
7	4.653462000	0.980091000	-0.704772000
8	3.067692000	2.314799000	0.253985000
6	5.751986000	1.867858000	-0.356792000
1	5.324168000	2.639338000	0.291358000
6	6.879399000	1.121470000	0.391966000
1	7.322202000	0.389187000	-0.290137000
7	6.307269000	0.237153000	1.498426000
1	2.786078000	-0.656604000	-1.203135000
6	5.478829000	0.949832000	2.521255000
1	6.116784000	1.638417000	3.078555000
1	4.668909000	1.492000000	2.034230000
1	5.054412000	0.199019000	3.185680000
6	7.344331000	-0.621004000	2.148516000
1	6.822702000	-1.350265000	2.769123000
1	7.896097000	-1.141043000	1.365426000
1	8.008148000	-0.010705000	2.761505000
1	4.898299000	0.024411000	-0.989485000
6	5.410266000	-3.645732000	0.382586000
1	5.064431000	-4.650138000	0.175434000
6	5.364557000	-2.674687000	-0.597869000
8	5.882144000	-1.511232000	-0.552945000
16	4.287261000	-3.081988000	-2.04632300
6	5.180961000	-2.193826000	-3.373528000
1	4.456015000	-1.898707000	-4.135766000
1	5.653388000	-1.303872000	-2.951929000
1	5.944022000	-2.831511000	-3.828149000
1	5.719011000	-0.456733000	0.977643000
1	6.110353000	-3.519858000	1.204680000
6	3.733563000	-2.801911000	1.755720000
8	4.131659000	-1.694868000	1.980383000
8	3.001289000	-3.722947000	1.863223000
6	6.357223000	2.574086000	-1.586906000
1	5.551756000	3.101424000	-2.108437000
1	6.748407000	1.818627000	-2.282754000
6	7.955853000	2.104048000	0.866975000
1	7.521424000	2.834699000	1.562171000
1	8.755970000	1.580863000	1.402126000
6	8.553884000	2.844593000	-0.345098000
1	9.088791000	2.120770000	-0.975788000
1	9.300740000	3.566221000	0.005057000
6	7.471484000	3.547543000	-1.175996000
1	7.035851000	4.367662000	-0.587836000
1	7.918644000	4.005708000	-2.065766000

^{D}F2$_{TS3}$

6	1.208466000	-2.071800000	2.565681000
6	2.290578000	-1.407918000	3.274976000
6	2.222077000	-0.039636000	3.533630000
6	1.067904000	0.723633000	3.089496000
6	0.033476000	0.087051000	2.398049000
6	0.101563000	-1.337340000	2.128525000
6	1.781884000	-3.070985000	1.697086000
6	3.225393000	-3.033254000	1.859506000
6	3.540562000	-2.004085000	2.836818000
6	4.672219000	-1.203315000	2.669027000
6	3.398018000	0.794818000	3.360568000
6	1.521754000	2.021313000	2.647852000
6	0.918883000	2.622286000	1.537077000
6	-0.171307000	1.964633000	0.844222000
6	-0.621675000	0.729812000	1.286551000
6	-1.132288000	-0.326047000	0.364134000
6	-0.516218000	-1.599204000	0.849119000
6	0.059018000	-2.533878000	0.002077000
6	1.221444000	-3.282573000	0.433221000
6	4.056111000	-3.220189000	0.754124000
6	3.476074000	-3.455041000	-0.558855000
6	2.090298000	-3.479983000	-0.713770000
6	1.469983000	-2.841776000	-1.861425000
6	0.214844000	-2.257883000	-1.436695000
6	-0.209897000	-1.056235000	-1.980980000
6	-0.964938000	-0.026553000	-1.202355000
6	-0.314640000	1.272639000	-1.543699000

6	-0.015679000	2.241275000	-0.598285000
6	2.964287000	2.070199000	2.812450000
6	3.451932000	2.936785000	-1.696727000
6	4.000458000	3.165746000	-0.434166000
6	5.156551000	2.406599000	0.004943000
6	5.719474000	1.442659000	-0.833971000
6	5.149896000	1.201916000	-2.148224000
6	2.958878000	1.269674000	-3.277670000
6	1.708514000	1.861987000	-2.833098000
6	2.009662000	2.888759000	-1.863631000
6	1.167176000	3.063140000	-0.760153000
6	1.742053000	3.301894000	0.552131000
6	3.127062000	3.356528000	0.712672000
6	5.002828000	2.133452000	1.425732000
6	5.418059000	0.907427000	1.949484000
6	5.999461000	-0.096933000	1.074403000
6	6.146691000	0.165029000	-0.288175000
6	5.837747000	-0.865958000	-1.265125000
6	5.222539000	-0.225947000	-2.414521000
6	4.182354000	-0.863715000	-3.093566000
6	3.027037000	-0.099613000	-3.530819000
6	0.579981000	1.057664000	-2.652486000
6	0.647940000	-0.367586000	-2.916973000
6	1.849227000	-0.933954000	-3.354638000
6	2.270376000	-2.203902000	-2.814623000
6	3.713429000	-2.166230000	-2.649453000
6	4.305154000	-2.778746000	-1.544167000
6	5.387922000	-2.117645000	-0.839870000
6	5.234016000	-2.390683000	0.581107000
6	5.536592000	-1.401202000	1.518786000
6	3.751593000	2.723693000	1.863574000
6	4.599419000	0.224403000	2.935742000
6	4.039828000	1.935051000	-2.572017000
6	-2.322245000	-0.135439000	-0.549739000
6	-3.254211000	-1.284660000	-0.852990000
7	-4.567452000	-0.933697000	-0.851069000
8	-2.844308000	-2.422370000	-1.076585000
6	-5.633581000	-1.890895000	-1.114808000
1	-5.131383000	-2.848121000	-1.279958000
6	-6.621173000	-2.022576000	0.073433000
1	-7.134428000	-1.052407000	0.171365000
7	-5.934857000	-2.222340000	1.363235000
1	-2.810853000	0.827578000	-0.419338000
6	-5.135173000	-3.443100000	1.472965000
1	-5.736132000	-4.370257000	1.458068000
1	-4.391419000	-3.491658000	0.674287000
1	-4.594261000	-3.419375000	2.425651000
6	-6.829100000	-2.077138000	2.506653000
1	-6.233842000	-2.031699000	3.426237000
1	-7.394632000	-1.142228000	2.421831000
1	-7.551988000	-2.904879000	2.625427000
1	-4.824637000	0.014496000	-0.590105000
8	-4.093902000	5.014909000	-2.028044000
6	-5.745221000	2.554807000	0.997885000
8	-5.095788000	1.952777000	0.031821000
16	-5.754618000	1.988722000	2.624522000
6	-4.406122000	0.744833000	2.653942000
1	-4.243080000	0.512297000	3.709464000
1	-4.701595000	-0.158985000	2.113093000
1	-3.495676000	1.177398000	2.234236000
6	-4.704417000	5.852897000	-1.485657000
8	-5.306768000	6.704522000	-0.958964000
6	-6.341490000	3.741107000	0.484311000
1	-6.530675000	4.593576000	1.133315000
1	-5.340895000	3.074680000	-0.473249000
1	-7.161376000	3.534810000	-0.209496000
6	-7.698982000	-3.077278000	-0.280085000
1	-7.221469000	-4.058522000	-0.408084000
1	-8.406004000	-3.178563000	0.551599000
6	-6.390654000	-1.514598000	-2.405458000
1	-6.832789000	-0.514215000	-2.282705000
1	-5.667333000	-1.440556000	-3.225549000
6	-7.492329000	-2.528138000	-2.743321000
1	-7.030016000	-3.495225000	-2.988049000
1	-8.035607000	-2.206330000	-3.640407000
6	-8.456738000	-2.711263000	-1.565135000
1	-9.015754000	-1.777601000	-1.403192000
1	-9.201637000	-3.483116000	-1.795500000

^{A}F1$_{TS1}$

6	-1.792762000	-2.382368000	-2.562469000
6	-3.006732000	-1.728847000	-3.024514000
6	-2.963628000	-0.408947000	-3.471361000
6	-1.703153000	0.314362000	-3.471982000
6	-0.538742000	-0.310661000	-3.017374000
6	-0.580928000	-1.684844000	-2.552888000
6	-2.131267000	-3.228351000	-1.443588000
6	-3.558507000	-3.103839000	-1.201207000
6	-4.100917000	-2.175947000	-2.180282000
6	-5.107052000	-1.280288000	-1.812307000
6	-4.009572000	0.523968000	-3.090634000
6	-1.963767000	1.684662000	-3.099017000
6	-1.047148000	2.365107000	-2.290041000
6	0.170200000	1.714924000	-1.847250000
6	0.429027000	0.407690000	-2.227909000
6	1.142770000	-0.568130000	-1.352896000
6	0.365503000	-1.840229000	-1.472845000
6	0.022265000	-2.625026000	-0.383116000
6	-1.241794000	-3.331905000	-0.369345000
6	-4.045671000	-3.098717000	0.106343000
6	-3.124018000	-3.219674000	1.224865000
6	-1.753739000	-3.328834000	0.989825000
6	-0.808549000	-2.607275000	1.823816000
6	0.293229000	-2.170415000	0.991813000
6	0.900355000	-0.947274000	1.231486000
6	1.437893000	-0.074567000	0.142333000
6	0.965220000	1.301119000	0.477059000
6	0.442021000	2.169683000	-0.468847000
6	-3.390264000	1.819458000	-2.859954000
6	-2.538596000	3.242552000	1.449533000
6	-3.415347000	3.360837000	0.370426000
6	-4.676253000	2.642609000	0.375682000
6	-5.011715000	1.827568000	1.458742000
6	-4.099992000	1.701387000	2.582277000
6	-1.677052000	1.740285000	3.037805000
6	-0.584260000	2.183354000	2.188209000
6	-1.111505000	3.108239000	1.212904000
6	-0.613545000	3.089671000	-0.094674000
6	-1.529475000	3.214099000	-1.214911000
6	-2.899446000	3.351560000	-0.989310000
6	-4.944552000	2.194264000	-0.982195000
6	-5.537423000	0.949249000	-1.201515000
6	-5.881540000	0.099829000	-0.073398000
6	-5.624351000	0.529775000	1.228863000

6	-5.087896000	-0.399543000	2.209413000
6	-4.146770000	0.323944000	3.046221000
6	-2.980600000	-0.304390000	3.488103000
6	-1.721030000	0.419058000	3.480618000
6	0.415803000	1.283287000	1.809498000
6	0.372498000	-0.092482000	2.269610000
6	-0.674396000	-0.514245000	3.095510000
6	-1.279142000	-1.804355000	2.867936000
6	-2.706826000	-1.680784000	3.108383000
6	-3.611413000	-2.373344000	2.302800000
6	-4.825125000	-1.722108000	1.846406000
6	-5.093355000	-2.170375000	0.488302000
6	-5.613622000	-1.277972000	-0.451203000
6	-3.849635000	2.636011000	-1.825804000
6	-5.060327000	0.097095000	-2.276507000
6	-2.888898000	2.396033000	2.578928000
6	2.549925000	-0.362904000	-0.842717000
6	3.482591000	-1.529180000	-0.633802000
7	4.772662000	-1.263648000	-0.973667000
8	3.122120000	-2.614559000	-0.180797000
6	5.801809000	-2.278185000	-0.852197000
1	5.429283000	-3.223906000	-1.261888000
1	6.649843000	-1.956098000	-1.458411000
6	6.244902000	-2.577640000	0.589263000
1	7.081537000	-3.281081000	0.552297000
1	5.421842000	-3.054119000	1.127774000
7	6.684136000	-1.369722000	1.374042000
1	3.029682000	0.535927000	-1.224041000
6	7.989503000	-1.591407000	2.050537000
1	7.933758000	-2.460500000	2.714330000
1	8.757429000	-1.731797000	1.287626000
1	8.237561000	-0.702819000	2.635650000
6	5.647374000	-0.926551000	2.340926000
1	5.935916000	0.046039000	2.747141000
1	4.692920000	-0.830748000	1.824030000
1	5.549395000	-1.655506000	3.152646000
1	5.038454000	-0.332136000	-1.303726000
6	7.398251000	0.870072000	-0.047243000
6	6.239474000	1.704505000	-0.317086000
8	5.376000000	1.529284000	-1.177145000
16	6.076791000	3.087136000	0.861232000
6	4.450333000	3.742013000	0.353006000
1	4.337431000	4.715268000	0.836076000
1	4.427570000	3.857939000	-0.731520000
1	3.638710000	3.080763000	0.664637000
6	8.183912000	0.230706000	-1.102597000
8	7.593512000	0.192403000	-2.335095000
8	9.265167000	-0.316765000	-0.920087000
1	8.243502000	-0.264187000	-2.901884000
1	8.058755000	1.254441000	0.730683000
1	6.900415000	-0.385189000	0.656510000

^{A}F1$_{TS2}$

6	-3.116994000	0.659664000	3.351340000
6	-4.201643000	-0.292577000	3.528056000
6	-4.008289000	-1.638071000	3.218548000
6	-2.721017000	-2.087593000	2.715509000
6	-1.682114000	-1.170130000	2.535359000
6	-1.880712000	0.230880000	2.857936000
6	-3.677269000	1.900892000	2.874445000
6	-5.114444000	1.727277000	2.749560000
6	-5.439483000	0.369427000	3.154813000
6	-6.433766000	-0.342375000	2.480464000
6	-5.041486000	-2.380488000	2.518108000
6	-2.952098000	-3.102381000	1.714745000
6	-2.132843000	-3.152430000	0.581617000
6	-1.042093000	-2.212025000	0.418754000
6	-0.807075000	-1.255592000	1.393836000
6	-0.301639000	0.114230000	1.082729000
6	-1.125740000	1.034999000	1.925644000
6	-1.682879000	2.208135000	1.441770000
6	-2.974231000	2.650082000	1.925464000
6	-5.798215000	2.318516000	1.686585000
6	-5.071378000	3.109120000	0.705778000
6	-3.690520000	3.265776000	0.822151000
6	-2.844259000	3.197727000	-0.356248000
6	-1.601328000	2.551336000	0.011202000
6	-0.965606000	1.710224000	-0.888591000
6	-0.214430000	0.486347000	-0.470724000
6	-0.647420000	-0.580357000	-1.420377000
6	-0.960421000	-1.868115000	-1.015291000
6	-4.387427000	-3.286585000	1.587433000
6	-4.131896000	-2.210721000	-2.895779000
6	-4.821072000	-2.973374000	-1.951961000
6	-6.109022000	-2.525654000	-1.455418000
6	-6.658604000	-1.328212000	-1.918005000
6	-5.942517000	-0.531963000	-2.899169000
6	-3.622357000	-0.012899000	-3.552818000
6	-2.385464000	-0.674492000	-3.172903000
6	-2.696409000	-2.026016000	-2.770980000
6	-2.002744000	-2.604453000	-1.702297000
6	-2.723633000	-3.397670000	-0.722349000
6	-4.101011000	-3.583183000	-0.845426000
6	-6.189393000	-2.864526000	-0.042726000
6	-6.816364000	-1.992517000	0.849601000
6	-7.383579000	-0.744150000	0.367480000
6	-7.306345000	-0.418997000	-0.987246000
6	-6.987462000	0.940039000	-1.392430000
6	-6.145602000	0.870823000	-2.573917000
6	-5.103254000	1.784756000	-2.741743000
6	-3.815913000	1.331627000	-3.239048000
6	-1.396119000	0.034950000	-2.486383000
6	-1.594925000	1.434867000	-2.159274000
6	-2.781450000	2.072355000	-2.534917000
6	-3.421507000	2.977365000	-1.610951000
6	-4.858794000	2.803241000	-1.733538000
6	-5.667820000	2.866823000	-0.598455000
6	-6.753066000	1.919450000	-0.425109000
6	-6.833767000	1.580463000	0.987684000
6	-7.145396000	0.275688000	1.375505000
6	-4.951216000	-3.521474000	0.332732000
6	-6.230594000	-1.745121000	2.155387000
6	-4.705323000	-0.965003000	-3.379923000
6	1.019329000	0.386037000	0.399153000
6	1.835161000	1.609224000	0.730613000
7	3.180330000	1.388773000	0.729152000
8	1.336937000	2.700588000	0.991529000
6	4.114475000	2.478719000	0.937336000
1	3.688964000	3.150303000	1.686294000
1	5.045819000	2.052645000	1.318034000
6	4.381370000	3.202060000	-0.393808000
1	3.570495000	3.892601000	-0.644072000
1	4.496822000	2.449126000	-1.174447000
7	5.676032000	3.971310000	-0.393767000

1	1.600561000	-0.515536000	0.215609000
6	5.678722000	5.141689000	0.527633000
1	4.939631000	5.872313000	0.189755000
1	5.436499000	4.807030000	1.536911000
1	6.678599000	5.578845000	0.521133000
6	6.051438000	4.363530000	-1.788102000
1	7.013675000	4.872055000	-1.757937000
1	6.141539000	3.451002000	-2.377547000
1	5.271038000	5.013728000	-2.192304000
1	3.581549000	0.535267000	0.346310000
6	7.165113000	-1.078510000	-1.595133000
6	7.035985000	-2.465565000	-1.225645000
8	6.250740000	-2.897742000	-0.365219000
16	8.183143000	-3.585981000	-2.04872300
6	7.765836000	-5.131413000	-1.170108000
1	8.438599000	-5.900853000	-1.555780000
1	7.912267000	-5.003783000	-0.096394000
1	6.728842000	-5.409450000	-1.364537000
6	6.058787000	-0.153756000	-1.331289000
8	5.151621000	-0.542994000	-0.393351000
8	5.944670000	0.936828000	-1.878939000
1	5.382529000	-1.477905000	-0.121139000
1	7.707335000	-0.853130000	-2.506313000
6	8.775707000	-0.317676000	-0.274875000
1	9.472859000	-0.950611000	-0.818618000
6	8.993807000	1.019809000	-0.673657000
6	8.482715000	-0.919744000	1.049508000
6	7.573775000	-0.431403000	2.005331000
6	9.200277000	-2.093799000	1.361420000
6	7.406527000	-1.087034000	3.223737000
1	7.016442000	0.466009000	1.786359000
6	9.036226000	-2.742040000	2.582731000
1	9.903679000	-2.494147000	0.636141000
6	8.134663000	-2.239820000	3.521947000
1	6.699601000	-0.690366000	3.947905000
1	9.613378000	-3.636899000	2.799786000
1	7.999533000	-2.742619000	4.475851000
1	6.427106000	3.306931000	-0.032243000
7	8.372581000	2.163428000	-0.275897000
8	7.429887000	2.150842000	0.600595000
8	8.708477000	3.259844000	-0.793205000
1	9.658270000	1.210178000	-1.505105000

^{A}F1$_{TS3}$

6	3.107012000	-0.819606000	3.248547000
6	4.247930000	0.031386000	3.546071000
6	4.176071000	1.404083000	3.313294000
6	2.959281000	1.983469000	2.769378000
6	1.866874000	1.163583000	2.473221000
6	1.938909000	-0.265455000	2.715806000
6	3.599433000	-2.070612000	2.724620000
6	5.050514000	-2.004527000	2.691237000
6	5.452287000	-0.703309000	3.200200000
6	6.536450000	-0.033629000	2.629348000
6	5.302845000	2.102701000	2.720440000
6	3.326331000	3.034861000	1.850329000
6	2.583013000	3.217476000	0.678971000
6	1.436022000	2.377847000	0.395760000
6	1.071534000	1.386227000	1.292726000
6	0.484090000	0.081834000	0.866555000
6	1.183124000	-0.950188000	1.693287000
6	1.677644000	-2.132878000	1.166740000
6	2.900428000	-2.703562000	1.691916000
6	5.750553000	-2.583788000	1.632238000
6	5.026463000	-3.254351000	0.563774000
6	3.633198000	-3.307468000	0.592965000
6	2.867146000	-3.102141000	-0.623757000
6	1.656764000	-2.382479000	-0.285209000
6	1.141721000	-1.441538000	-1.163076000
6	0.461696000	-0.188854000	-0.709497000
6	1.030529000	0.895032000	-1.563567000
6	1.415282000	2.127484000	-1.059823000
6	4.776568000	3.111728000	1.814928000
6	4.711342000	2.328804000	-2.735290000
6	5.397843000	2.976430000	-1.707503000
6	6.615981000	2.399518000	-1.170086000
6	7.100262000	1.192066000	-1.677376000
6	6.386484000	0.515107000	-2.745911000
6	4.077504000	0.221602000	-3.559607000
6	2.873586000	0.955285000	-3.206891000
6	3.261060000	2.251547000	-2.702468000
6	2.549804000	2.818789000	-1.639266000
6	3.268183000	3.492565000	-0.571785000
6	4.660640000	3.574722000	-0.605954000
6	6.636504000	2.646229000	0.263623000
6	7.140376000	1.675325000	1.131499000
6	7.639681000	0.416986000	0.602517000
6	7.620071000	0.180425000	-0.772472000
6	7.224244000	-1.122408000	-1.281181000
6	6.462809000	-0.916259000	-2.500614000
6	5.366368000	-1.733059000	-2.784411000
6	4.149359000	-1.150314000	-3.322154000
6	1.793615000	0.286806000	-2.623567000
6	1.865499000	-1.141620000	-2.376565000
6	3.021149000	-1.847432000	-2.725671000
6	3.534010000	-2.853932000	-1.827758000
6	4.985203000	-2.787538000	-1.859063000
6	5.717056000	-2.982474000	-0.687105000
6	6.858481000	-2.136158000	-0.393274000
6	6.879134000	-1.889569000	1.040707000
6	7.264559000	-0.639099000	1.528185000
6	5.431162000	3.375609000	0.611132000
6	6.460166000	1.397791000	2.384342000
6	5.217006000	1.072820000	-3.266053000
6	-0.810887000	-0.042809000	0.095723000
6	-1.735223000	-1.214173000	0.308499000
7	-3.057586000	-0.884484000	0.264630000
8	-1.336616000	-2.356019000	0.514835000
6	-4.097625000	-1.885650000	0.397933000
1	-3.710322000	-2.685522000	1.031953000
1	-4.949136000	-1.415612000	0.893246000
6	-4.511067000	-2.415070000	-0.984726000
1	-3.788907000	-3.158974000	-1.339994000
1	-4.534992000	-1.578546000	-1.684075000
7	-5.877753000	-3.023891000	-1.027940000
1	-1.308632000	0.912710000	-0.058468000
6	-6.074703000	-4.126228000	-0.044892000
1	-5.334617000	-4.913676000	-0.219711000
1	-5.960955000	-3.734724000	0.967013000
1	-7.088312000	-4.507867000	-0.171242000
6	-6.175357000	-3.496617000	-2.412011000
1	-7.225746000	-3.785087000	-2.445616000
1	-5.994895000	-2.672940000	-3.106231000
1	-5.517129000	-4.334477000	-2.660926000

1	-3.374122000	0.031686000	-0.037285000
6	-7.589687000	1.202550000	-0.946639000
6	-8.300138000	2.546238000	-0.856722000
8	-8.145904000	3.323988000	0.075472000
16	-9.399117000	2.861858000	-2.22354100
6	-10.144228000	4.450096000	-1.70961600
1	-11.173901000	4.289192000	-1.38498800
1	-9.548704000	4.850883000	-0.886553000
1	-10.121566000	5.131748000	-2.56160500
6	-6.141676000	1.270769000	-0.448114000
8	-5.871428000	2.068691000	0.580524000
8	-5.263568000	0.596487000	-0.959336000
1	-6.674821000	2.599831000	0.802701000
1	-7.534658000	0.907479000	-1.997715000
6	-8.447973000	0.077730000	-0.200434000
1	-9.490688000	0.308091000	-0.466483000
6	-8.085946000	-1.279252000	-0.810702000
6	-8.366091000	0.192201000	1.320412000
6	-7.466283000	-0.562024000	2.081283000
6	-9.214425000	1.079833000	1.997130000
6	-7.392673000	-0.420022000	3.466471000
1	-6.844164000	-1.295401000	1.581272000
6	-9.145452000	1.229259000	3.382498000
1	-9.950038000	1.651325000	1.437622000
6	-8.228176000	0.483727000	4.123772000
1	-6.688392000	-1.023048000	4.033856000
1	-9.817626000	1.921527000	3.882559000
1	-8.175315000	0.594782000	5.203377000
1	-6.673254000	-2.213538000	-0.795079000
7	-9.041391000	-2.291062000	-0.510469000
8	-9.844305000	-2.131567000	0.422685000
8	-9.000254000	-3.363924000	-1.172784000
1	-8.006991000	-1.229439000	-1.899305000

^{A}F1$_{TS4}$

6	3.727908000	2.076306000	-2.697179000
6	4.678514000	1.021224000	-3.009299000
6	4.223377000	-0.237942000	-3.397857000
6	2.795883000	-0.495906000	-3.487063000
6	1.882588000	0.514906000	-3.175276000
6	2.353831000	1.826749000	-2.772218000
6	4.248033000	2.842139000	-1.590893000
6	5.524976000	2.265925000	-1.205652000
6	5.792329000	1.138764000	-2.084299000
6	6.403901000	-0.011144000	-1.580715000
6	4.857959000	-1.435150000	-2.875285000
6	2.546305000	-1.842020000	-3.028494000
6	1.394567000	-2.112945000	-2.281616000
6	0.440169000	-1.062027000	-1.989138000
6	0.670635000	0.224427000	-2.451558000
6	0.264122000	1.448520000	-1.700046000
6	1.436957000	2.371124000	-1.798535000
6	1.943991000	3.074631000	-0.717718000
6	3.367128000	3.316003000	-0.613268000
6	5.881535000	2.197316000	0.141684000
6	4.973527000	2.703241000	1.159085000
6	3.743290000	3.245287000	0.787686000
6	2.548768000	2.947106000	1.558114000
6	1.429748000	2.843406000	0.643292000
6	0.428208000	1.913452000	0.878642000
6	-0.290670000	1.190244000	-0.213469000
6	-0.337830000	-0.233286000	0.225969000
6	-0.073256000	-1.295485000	-0.624262000
6	3.819619000	-2.427439000	-2.646493000
6	2.212440000	-3.155643000	1.620540000
6	3.075933000	-3.640642000	0.637417000
6	4.501496000	-3.387053000	0.731721000
6	5.011182000	-2.651900000	1.803982000
6	4.114455000	-2.143817000	2.827174000
6	1.795296000	-1.336852000	3.049174000
6	0.684120000	-1.452469000	2.118981000
6	0.937664000	-2.570979000	1.241379000
6	0.576424000	-2.483683000	-0.108034000
6	1.477429000	-2.991182000	-1.127741000
6	2.698046000	-3.561641000	-0.764780000
6	5.008073000	-3.158438000	-0.612982000
6	6.003418000	-2.203445000	-0.830293000
6	6.529207000	-1.435204000	0.286003000
6	6.043904000	-1.654892000	1.575602000
6	5.782455000	-0.528497000	2.456195000
6	4.590982000	-0.830240000	3.229980000
6	3.677903000	0.183460000	3.527972000
6	2.252046000	-0.076076000	3.431449000
6	0.081359000	-0.299834000	1.603895000
6	0.555065000	1.013785000	2.002032000
6	1.616907000	1.121911000	2.905105000
6	2.638957000	2.114933000	2.678611000
6	3.917099000	1.539518000	3.061260000
6	5.061370000	1.826567000	2.316251000
6	6.012409000	0.774349000	2.009484000
6	6.519166000	1.003473000	0.664805000
6	6.775081000	-0.079860000	-0.178346000
6	3.895178000	-3.270832000	-1.537276000
6	5.926911000	-1.324471000	-1.983954000
6	2.743247000	-2.392465000	2.739043000
6	-1.158107000	1.759800000	-1.314175000
6	-1.662985000	3.182530000	-1.233807000
7	-3.008830000	3.291340000	-1.408824000
8	-0.916936000	4.136478000	-1.032826000
6	-3.685344000	4.576577000	-1.322980000
1	-2.909664000	5.342860000	-1.385407000
1	-4.338902000	4.692650000	-2.195148000
6	-4.467308000	4.766772000	-0.019371000
1	-4.808416000	5.821331000	0.034508000
1	-3.771550000	4.613697000	0.813317000
7	-5.587307000	3.836503000	0.147494000
1	-1.876963000	1.044101000	-1.704363000
6	-6.700325000	4.152493000	-0.747747000
1	-7.105777000	5.169481000	-0.576882000
1	-6.384310000	4.086636000	-1.793185000
1	-7.506884000	3.429376000	-0.600170000
6	-6.045689000	3.837029000	1.535870000
1	-6.876978000	3.135040000	1.650054000
1	-5.230078000	3.520174000	2.194987000
1	-6.392126000	4.833829000	1.873240000
1	-3.575748000	2.451875000	-1.454545000
6	-5.687828000	-0.456143000	0.256877000
6	-5.033427000	-0.952621000	1.392746000
8	-4.573079000	-2.192439000	1.476403000
16	-4.678834000	0.094526000	2.741537000
6	-3.348723000	-0.813004000	3.614103000
1	-3.700939000	-1.789364000	3.947429000
1	-2.471025000	-0.921673000	2.974485000
1	-3.098163000	-0.194695000	4.479285000

6	-4.186659000	-0.666088000	-1.098999000
8	-3.749150000	-1.790101000	-0.997012000
8	-4.150142000	0.369174000	-1.708430000
1	-4.406601000	-2.503740000	0.547965000
1	-5.822918000	0.624399000	0.278832000
6	-6.849124000	-1.163767000	-0.482184000
6	-6.761441000	-2.665533000	-0.738805000
6	-8.193815000	-0.872127000	0.233198000
6	-6.953366000	-3.614558000	0.277128000
6	-6.546608000	-3.123493000	-2.046122000
1	-8.215744000	-1.229389000	1.261370000
7	-8.451734000	0.608279000	0.301679000
6	-6.918568000	-4.980722000	-0.006820000
1	-7.121481000	-3.295787000	1.301849000
6	-6.510306000	-4.487760000	-2.332058000
1	-6.401417000	-2.403382000	-2.847550000
8	-8.629121000	1.186810000	-0.767572000
8	-8.441512000	1.139207000	1.409184000
6	-6.696470000	-5.421628000	-1.311932000
1	-7.067056000	-5.699053000	0.794661000
1	-6.337194000	-4.819014000	-3.352040000
1	-6.669938000	-6.485091000	-1.532162000
1	-6.924027000	-0.668493000	-1.456121000
1	-9.021573000	-1.292462000	-0.341648000

^{A}F1$_{TS5}$

6	-2.646340000	0.816176000	-3.387403000
6	-3.565490000	1.891526000	-3.050910000
6	-3.150385000	2.933578000	-2.222963000
6	-1.797359000	2.941168000	-1.692588000
6	-0.918049000	1.901278000	-2.006760000
6	-1.347030000	0.816578000	-2.870134000
6	-3.390352000	-0.419157000	-3.429546000
6	-4.777412000	-0.119871000	-3.117042000
6	-4.886405000	1.310969000	-2.883382000
6	-5.738225000	1.794254000	-1.888011000
6	-4.034862000	3.437879000	-1.187322000
6	-1.839901000	3.449786000	-0.341873000
6	-1.000193000	2.895002000	0.630250000
6	-0.072352000	1.835819000	0.286092000
6	-0.017301000	1.366554000	-1.017252000
6	0.269648000	-0.057441000	-1.359875000
6	-0.712464000	-0.404979000	-2.433035000
6	-1.442654000	-1.582802000	-2.440213000
6	-2.798350000	-1.591345000	-2.948286000
6	-5.526085000	-1.009498000	-2.345674000
6	-4.916936000	-2.236162000	-1.856177000
6	-3.582210000	-2.515760000	-2.148089000
6	-2.711922000	-3.076940000	-1.129845000
6	-1.388104000	-2.514137000	-1.299879000
6	-0.606505000	-2.236194000	-0.189100000
6	0.325395000	-1.069563000	-0.116576000
6	0.089534000	-0.464947000	1.226631000
6	-0.018665000	0.902529000	1.429821000
6	-3.223535000	3.756962000	-0.023269000
6	-3.054351000	0.838022000	3.550552000
6	-3.629729000	2.018626000	3.079000000
6	-4.983191000	2.009754000	2.555800000
6	-5.709996000	0.818012000	2.518346000
6	-5.112660000	-0.412519000	3.006786000
6	-2.894702000	-1.476372000	3.175610000
6	-1.575018000	-0.893059000	3.001720000
6	-1.670648000	0.528928000	3.233833000
6	-0.913993000	1.408468000	2.451228000
6	-1.516627000	2.636360000	1.962877000
6	-2.843074000	2.938689000	2.272935000
6	-5.036468000	2.929584000	1.429741000
6	-5.814484000	2.620188000	0.312283000
6	-6.566621000	1.377059000	0.272585000
6	-6.515631000	0.494931000	1.352488000
6	-6.413073000	-0.936083000	1.118966000
6	-5.547059000	-1.497277000	2.141002000
6	-4.663486000	-2.528848000	1.816604000
6	-3.309808000	-2.514857000	2.343102000
6	-0.728249000	-1.368320000	1.996473000
6	-1.157477000	-2.449904000	1.129203000
6	-2.423728000	-3.016586000	1.304824000
6	-3.220470000	-3.339931000	0.146193000
6	-4.607868000	-3.039346000	0.456424000
6	-5.439373000	-2.497220000	-0.524155000
6	-6.360092000	-1.427614000	-0.186954000
6	-6.413406000	-0.507638000	-1.313126000
6	-6.517651000	0.866425000	-1.087472000
6	-3.716070000	3.506348000	1.258079000
6	-5.303723000	2.879125000	-1.022464000
6	-3.812101000	-0.402773000	3.514589000
6	1.539407000	-0.772634000	-0.968733000
6	2.145897000	-1.844552000	-1.843759000
7	3.504191000	-1.891990000	-1.783669000
8	1.469631000	-2.595760000	-2.540783000
6	4.254109000	-2.905520000	-2.509907000
1	3.733904000	-3.089579000	-3.453798000
1	5.238824000	-2.491730000	-2.747890000
6	4.372095000	-4.242448000	-1.765710000
1	4.866530000	-4.971047000	-2.440048000
1	3.356343000	-4.609817000	-1.585864000
7	5.060045000	-4.156844000	-0.474585000
1	2.259946000	-0.126522000	-0.472252000
6	6.488453000	-3.876139000	-0.619067000
1	7.018847000	-4.661193000	-1.192165000
1	6.648585000	-2.919260000	-1.121991000
1	6.952676000	-3.798185000	0.368089000
6	4.860255000	-5.383098000	0.294489000
1	5.337752000	-5.284569000	1.275400000
1	3.789802000	-5.556251000	0.447415000
1	5.285292000	-6.277115000	-0.200984000
1	3.994798000	-1.308405000	-1.113487000
6	6.326146000	1.295677000	1.234706000
6	5.544638000	0.096545000	1.252505000
8	4.733703000	0.096343000	0.217692000
16	5.501849000	-1.108726000	2.474881000
6	3.952593000	-2.016642000	2.105999000
1	4.092256000	-2.639403000	1.217237000
1	3.759099000	-2.643871000	2.980004000
1	3.130042000	-1.310553000	1.973257000
1	5.137065000	1.275827000	0.257293000
6	7.415785000	1.449523000	0.160800000
6	7.551622000	2.866571000	-0.397632000
6	8.807240000	1.021735000	0.694338000
6	8.217068000	3.059066000	-1.617637000
6	7.054280000	3.988058000	0.275297000
1	9.104245000	1.594850000	1.572430000
7	8.787119000	-0.422769000	1.110864000
6	8.383807000	4.336516000	-2.150364000

1	8.597920000	2.197660000	-2.163665000
6	7.223425000	5.269594000	-0.253667000
1	6.512919000	3.860703000	1.207349000
8	8.970107000	-0.684236000	2.295380000
8	8.553749000	-1.247394000	0.227324000
6	7.889257000	5.448874000	-1.465989000
1	8.893079000	4.462106000	-3.102090000
1	6.827354000	6.127784000	0.282650000
1	8.016006000	6.445827000	-1.878905000
1	7.186335000	0.776736000	-0.673452000
1	9.569266000	1.095029000	-0.084971000
1	6.600078000	1.712835000	2.205172000

$^{A}F2_{TS1}$

6	-1.812158000	-2.724461000	-2.138356000
6	-3.075135000	-2.299430000	-2.720263000
6	-3.166573000	-1.069740000	-3.370773000
6	-1.997667000	-0.211369000	-3.464198000
6	-0.786909000	-0.615610000	-2.895141000
6	-0.689029000	-1.895509000	-2.218267000
6	-2.092527000	-3.419437000	-0.905109000
6	-3.532534000	-3.428496000	-0.711319000
6	-4.141134000	-2.735520000	-1.835230000
6	-5.255541000	-1.918839000	-1.632696000
6	-4.325170000	-0.219182000	-3.162263000
6	-2.426129000	1.159780000	-3.319036000
6	-1.622993000	2.061678000	-2.612434000
6	-0.356437000	1.637186000	-2.050035000
6	0.063070000	0.326461000	-2.212739000
6	0.850867000	-0.408688000	-1.180689000
6	0.229127000	-1.766861000	-1.110307000
6	-0.061638000	-2.407285000	0.084318000
6	-1.236700000	-3.248243000	0.187586000
6	-4.064382000	-3.277076000	0.569818000
6	-3.176311000	-3.112352000	1.709772000
6	-1.794847000	-3.093666000	1.519481000
6	-0.969171000	-2.143802000	2.244472000
6	0.104939000	-1.714773000	1.373880000
6	0.560543000	-0.406585000	1.426409000
6	1.036478000	0.342792000	0.222195000
6	0.396110000	1.687811000	0.324462000
6	-0.188214000	2.330178000	-0.756888000
6	-3.866455000	1.160546000	-3.129980000
6	-3.339554000	3.329104000	0.912407000
6	-4.184387000	3.173150000	-0.187162000
6	-5.354561000	2.320519000	-0.090070000
6	-5.634089000	1.650605000	1.102811000
6	-4.755330000	1.810026000	2.248116000
6	-2.370720000	2.205804000	2.734816000
6	-1.305382000	2.636723000	1.845084000
6	-1.898831000	3.329109000	0.725746000
6	-1.354739000	3.165817000	-0.553012000
6	-2.237634000	3.005060000	-1.695020000
6	-3.621713000	3.012923000	-1.518608000
6	-5.520533000	1.637190000	-1.363793000
6	-5.959318000	0.311933000	-1.392592000
6	-6.245143000	-0.385689000	-0.149888000
6	-6.086164000	0.269571000	1.071674000
6	-5.483211000	-0.425211000	2.197166000
6	-4.661716000	0.526186000	2.924699000
6	-3.448371000	0.116912000	3.481638000
6	-2.279994000	0.974110000	3.381472000
6	-0.196019000	1.813402000	1.632640000
6	-0.099048000	0.531014000	2.305114000
6	-1.120550000	0.122584000	3.168829000
6	-1.565686000	-1.249472000	3.139233000
6	-3.005959000	-1.259688000	3.331090000
6	-3.795930000	-2.171670000	2.630237000
6	-5.058368000	-1.747686000	2.054125000
6	-5.224319000	-2.431135000	0.780247000
6	-5.808128000	-1.764016000	-0.298602000
6	-4.453164000	2.068267000	-2.247310000
6	-5.349281000	-0.635019000	-2.309388000
6	-3.631913000	2.633831000	2.155780000
6	2.207653000	0.040094000	-0.684336000
6	3.257673000	-0.971150000	-0.290787000
7	4.501486000	-0.665946000	-0.742372000
8	3.002629000	-1.962235000	0.395834000
6	5.673141000	-1.528734000	-0.586079000
1	6.457468000	-1.026419000	-1.159237000
6	6.193794000	-1.682302000	0.874055000
1	5.456512000	-2.261632000	1.439904000
7	6.299030000	-0.331030000	1.577247000
1	2.592721000	0.917758000	-1.198778000
6	7.523174000	-0.112712000	2.394434000
1	7.598723000	-0.846828000	3.202004000
1	8.404695000	-0.139267000	1.755193000
1	7.447760000	0.885178000	2.833685000
6	5.105775000	-0.058510000	2.422705000
1	5.044965000	1.017693000	2.608847000
1	4.201843000	-0.398480000	1.923888000
1	5.196397000	-0.588030000	3.378309000
1	4.642019000	0.222677000	-1.227595000
6	6.754071000	1.847446000	-0.020037000
6	5.534005000	2.508981000	-0.465532000
8	4.770689000	2.135386000	-1.355066000
16	5.138167000	3.988487000	0.520456000
6	3.498905000	4.404146000	-0.166831000
1	3.523702000	4.275497000	-1.250050000
1	2.715838000	3.771840000	0.257579000
1	3.303282000	5.449287000	0.082963000
6	7.704525000	1.240316000	-0.955547000
8	7.248815000	1.066250000	-2.230289000
8	8.815034000	0.829742000	-0.635709000
1	7.993164000	0.645547000	-2.700662000
1	7.296528000	2.392158000	0.753741000
1	6.384841000	0.634409000	0.752833000
6	5.457574000	-2.918905000	-1.222105000
1	4.666356000	-3.442957000	-0.676618000
1	5.097514000	-2.769775000	-2.246577000
6	7.517627000	-2.467997000	0.840070000
1	8.265351000	-1.900956000	0.269500000
1	7.911881000	-2.597914000	1.852662000
6	7.320807000	-3.852675000	0.200490000
1	6.638818000	-4.446586000	0.825364000
1	8.280252000	-4.383349000	0.191373000
6	6.749913000	-3.743367000	-1.217098000
1	7.494489000	-3.269242000	-1.873066000
1	6.559084000	-4.741056000	-1.630161000

$^{A}F2_{TS2}$

6	-3.283686000	1.528094000	3.040749000
6	-4.363943000	0.625596000	3.405755000
6	-4.130777000	-0.746377000	3.489424000

6	-2.806226000	-1.274209000	3.208732000
6	-1.771185000	-0.407488000	2.847051000
6	-2.011065000	1.021127000	2.760000000
6	-3.828510000	2.573355000	2.208272000
6	-5.251394000	2.325757000	2.048666000
6	-5.583194000	1.120189000	2.790395000
6	-6.519454000	0.219583000	2.278125000
6	-5.103462000	-1.684826000	2.958019000
6	-2.954295000	-2.530539000	2.512680000
6	-2.059843000	-2.860829000	1.488507000
6	-0.974444000	-1.965762000	1.140550000
6	-0.820233000	-0.772575000	1.828249000
6	-0.314085000	0.475062000	1.185135000
6	-1.206237000	1.563950000	1.690097000
6	-1.746280000	2.542561000	0.869996000
6	-3.074117000	3.057283000	1.134716000
6	-5.870539000	2.582042000	0.824670000
6	-5.090896000	3.098329000	-0.289305000
6	-3.723345000	3.325135000	-0.136544000
6	-2.798738000	2.965504000	-1.197262000
6	-1.574333000	2.484733000	-0.592190000
6	-0.866349000	1.451464000	-1.185641000
6	-0.124502000	0.414220000	-0.403918000
6	-0.479456000	-0.885007000	-1.047855000
6	-0.800865000	-2.022935000	-0.325002000
6	-4.374995000	-2.788892000	2.353485000
6	-3.833033000	-2.968841000	-2.228835000
6	-4.573124000	-3.466807000	-1.155712000
6	-5.897993000	-2.942810000	-0.880433000
6	-6.432651000	-1.935621000	-1.686345000
6	-5.663726000	-1.414490000	-2.802875000
6	-3.312448000	-1.018322000	-3.431343000
6	-2.094405000	-1.510564000	-2.809840000
6	-2.412003000	-2.710540000	-2.072419000
6	-1.783716000	-2.952165000	-0.845743000
6	-2.557549000	-3.471344000	0.268313000
6	-3.920652000	-3.728096000	0.117314000
6	-6.068683000	-2.886037000	0.563350000
6	-6.767010000	-1.824396000	1.142220000
6	-7.318580000	-0.774058000	0.302573000
6	-7.154833000	-0.828507000	-1.082046000
6	-6.829259000	0.378036000	-1.824452000
6	-5.908710000	0.016424000	-2.888057000
6	-4.870854000	0.883215000	-3.236469000
6	-3.546381000	0.353752000	-3.510827000
6	-1.163918000	-0.609073000	-2.285320000
6	-1.404970000	0.819645000	-2.367536000
6	-2.572711000	1.291617000	-2.975341000
6	-3.286768000	2.393193000	-2.376440000
6	-4.709898000	2.145665000	-2.533612000
6	-5.594528000	2.490306000	-1.510913000
6	-6.674952000	1.591315000	-1.150594000
6	-6.845708000	1.648069000	0.293411000
6	-7.163738000	0.489270000	1.004665000
6	-4.849294000	-3.375220000	1.179347000
6	-6.274487000	-1.211357000	2.363312000
6	-4.390696000	-1.921805000	-3.070168000
6	1.046996000	0.589927000	0.534652000
6	1.823926000	1.884141000	0.582254000
7	3.142049000	1.704131000	0.862220000
8	1.289630000	2.976746000	0.398146000
6	4.179079000	2.746321000	0.827169000
1	5.090463000	2.173162000	1.015234000
6	4.311304000	3.349698000	-0.615323000
1	3.849094000	2.623184000	-1.282512000
7	5.778100000	3.302617000	-1.069301000
1	1.649475000	-0.309919000	0.636338000
6	6.685952000	4.361149000	-0.529883000
1	6.576295000	4.410889000	0.552723000
1	7.702795000	4.054152000	-0.776820000
1	6.439264000	5.323384000	-0.979699000
6	5.894950000	3.214024000	-2.561489000
1	5.480267000	4.116809000	-3.013224000
1	6.952187000	3.105239000	-2.802328000
1	5.355623000	2.324987000	-2.885771000
1	3.506566000	0.756514000	0.779270000
6	5.895251000	-1.872222000	-1.397679000
6	5.546403000	-3.190698000	-0.927312000
8	4.916677000	-3.423986000	0.117654000
16	6.174483000	-4.550559000	-1.92994600
6	5.603942000	-5.956125000	-0.913133000
1	5.984684000	-5.863143000	0.105027000
1	4.513515000	-5.990072000	-0.890185000
1	5.996381000	-6.860571000	-1.383508000
6	5.091096000	-0.725350000	-0.962372000
8	4.401672000	-0.880348000	0.200422000
8	5.039689000	0.344002000	-1.558506000
1	4.491989000	-1.834501000	0.488849000
1	6.247474000	-1.788375000	-2.419606000
6	7.860160000	-1.482845000	-0.491341000
1	8.253006000	-2.336206000	-1.039302000
6	8.342388000	-0.305172000	-1.112981000
6	7.694843000	-1.841323000	0.938957000
6	7.299990000	-0.972498000	1.973266000
6	8.002267000	-3.175704000	1.279928000
6	7.228621000	-1.425940000	3.289234000
1	7.068384000	0.054357000	1.733028000
6	7.932584000	-3.623934000	2.595757000
1	8.311119000	-3.864744000	0.497884000
6	7.542860000	-2.747762000	3.609478000
1	6.926163000	-0.736006000	4.072864000
1	8.184584000	-4.655024000	2.828472000
1	7.485267000	-3.091513000	4.638844000
1	6.189319000	2.413249000	-0.690965000
7	8.082017000	0.998636000	-0.826008000
8	7.304302000	1.336573000	0.138070000
8	8.594126000	1.895659000	-1.552328000
1	8.893345000	-0.398400000	-2.038825000
6	4.068584000	3.788545000	1.968800000
1	3.672044000	3.275411000	2.851384000
1	5.091664000	4.095316000	2.231029000
6	3.650703000	4.725776000	-0.826490000
1	2.592578000	4.514980000	-1.004384000
6	3.252023000	5.049334000	1.655506000
1	3.350442000	5.753862000	2.490864000
6	3.738665000	5.704487000	0.357741000
1	4.034246000	5.191896000	-1.743241000
1	4.763414000	6.076084000	0.491710000
1	2.194922000	4.791600000	1.558735000
1	3.124599000	6.582528000	0.124312000

^{A}F2$_{TS3}$

6	3.447135000	-1.306652000	3.107813000
6	4.579030000	-0.459021000	3.446577000

6	4.436437000	0.927781000	3.455085000
6	3.154537000	1.525865000	3.121601000
6	2.070094000	0.710961000	2.784949000
6	2.215524000	-0.732926000	2.776736000
6	3.934333000	-2.427963000	2.341505000
6	5.372868000	-2.283228000	2.196840000
6	5.772323000	-1.064416000	2.881414000
6	6.774545000	-0.255593000	2.341758000
6	5.477814000	1.770882000	2.894890000
6	3.397147000	2.731152000	2.364553000
6	2.542979000	3.065253000	1.307768000
6	1.405756000	2.226350000	0.985659000
6	1.161798000	1.083336000	1.730496000
6	0.582802000	-0.161034000	1.143784000
6	1.393452000	-1.277688000	1.721477000
6	1.881030000	-2.330689000	0.963571000
6	3.166654000	-2.916855000	1.279692000
6	5.992907000	-2.643866000	0.999930000
6	5.198447000	-3.165933000	-0.100876000
6	3.816572000	-3.294016000	0.036843000
6	2.934783000	-2.931231000	-1.058692000
6	1.735210000	-2.339748000	-0.502492000
6	1.107706000	-1.294549000	-1.162512000
6	0.426174000	-0.170130000	-0.449840000
6	0.876144000	1.066500000	-1.153636000
6	1.260442000	2.217627000	-0.484283000
6	4.834201000	2.886787000	2.219815000
6	4.378923000	2.860139000	-2.375204000
6	5.133176000	3.364206000	-1.314897000
6	6.415525000	2.769475000	-0.987213000
6	6.894652000	1.688286000	-1.729645000
6	6.110663000	1.160596000	-2.832554000
6	3.748730000	0.887212000	-3.485358000
6	2.556603000	1.490566000	-2.913724000
6	2.941515000	2.704515000	-2.233268000
6	2.311189000	3.051519000	-1.033104000
6	3.099801000	3.576696000	0.067674000
6	4.479297000	3.734836000	-0.069970000
6	6.559261000	2.778322000	0.460571000
6	7.175633000	1.704889000	1.106862000
6	7.669245000	0.577715000	0.333385000
6	7.531789000	0.569592000	-1.055105000
6	7.138233000	-0.650422000	-1.740273000
6	6.260895000	-0.285857000	-2.838752000
6	5.173406000	-1.099933000	-3.162174000
6	3.891739000	-0.499614000	-3.489168000
6	1.559927000	0.681001000	-2.361670000
6	1.706037000	-0.762916000	-2.365217000
6	2.849244000	-1.341893000	-2.924941000
6	3.478702000	-2.454779000	-2.255805000
6	4.917454000	-2.310054000	-2.398214000
6	5.760765000	-2.657461000	-1.342143000
6	6.893000000	-1.813757000	-1.007894000
6	7.036327000	-1.805201000	0.440194000
6	7.419516000	-0.633848000	1.096664000
6	5.365343000	3.378310000	1.026658000
6	6.624097000	1.190859000	2.348228000
6	4.878803000	1.735698000	-3.150412000
6	-0.770883000	-0.218782000	0.474184000
6	-1.637421000	-1.455356000	0.564010000
7	-2.962444000	-1.157209000	0.650841000
8	-1.154039000	-2.584978000	0.569409000
6	-4.112856000	-2.078975000	0.611709000
1	-4.952704000	-1.395186000	0.736871000
6	-4.260636000	-2.714811000	-0.809190000
1	-3.745772000	-2.029256000	-1.484663000
7	-5.695929000	-2.670462000	-1.337550000
1	-1.308400000	0.725945000	0.522125000
6	-6.607060000	-3.724979000	-0.808318000
1	-6.248605000	-4.717487000	-1.088522000
1	-6.664240000	-3.649102000	0.278244000
1	-7.594927000	-3.561034000	-1.238437000
6	-5.678715000	-2.726095000	-2.830786000
1	-6.703064000	-2.601525000	-3.182095000
1	-5.060704000	-1.905194000	-3.201566000
1	-5.267634000	-3.677975000	-3.177236000
1	-3.229982000	-0.211694000	0.385673000
6	-6.571345000	1.893549000	-0.824611000
6	-7.009600000	3.288796000	-0.398401000
8	-6.800062000	3.747873000	0.717697000
16	-7.881584000	4.199828000	-1.64898800
6	-8.279992000	5.711023000	-0.702762000
1	-7.363385000	6.175612000	-0.336465000
1	-8.792044000	6.381714000	-1.395706000
1	-8.933045000	5.470840000	0.137782000
6	-5.232207000	1.486541000	-0.214669000
8	-4.956192000	1.890978000	1.022871000
8	-4.454775000	0.770309000	-0.823080000
1	-5.643815000	2.541684000	1.313964000
1	-6.427794000	1.886383000	-1.908419000
6	-7.711969000	0.821795000	-0.519988000
1	-8.616201000	1.278738000	-0.946002000
6	-7.422962000	-0.456319000	-1.329619000
6	-7.996377000	0.653562000	0.970404000
6	-7.428267000	-0.367444000	1.739096000
6	-8.871093000	1.544345000	1.609751000
6	-7.696514000	-0.482442000	3.103420000
1	-6.796715000	-1.102320000	1.254988000
6	-9.144772000	1.436766000	2.972642000
1	-9.362061000	2.321694000	1.029423000
6	-8.551599000	0.424854000	3.728807000
1	-7.243361000	-1.288211000	3.675119000
1	-9.830550000	2.137841000	3.440831000
1	-8.765312000	0.335790000	4.790412000
1	-6.325015000	-1.619317000	-1.119929000
7	-8.649628000	-1.173546000	-1.569144000
8	-9.616337000	-1.003118000	-0.812912000
8	-8.687786000	-1.997362000	-2.515517000
1	-7.022284000	-0.210279000	-2.316016000
6	-4.171018000	-3.075242000	1.792587000
1	-3.825591000	-2.551900000	2.690965000
1	-5.231918000	-3.307892000	1.965472000
6	-3.583000000	-4.101988000	-0.923900000
1	-2.510976000	-3.898572000	-1.007902000
1	-3.878612000	-4.593727000	-1.858458000
6	-3.407975000	-4.393158000	1.600463000
1	-2.334085000	-4.200651000	1.622888000
6	-3.778939000	-5.057755000	0.269240000
1	-4.810623000	-5.426945000	0.316853000
1	-3.148815000	-5.940437000	0.105501000
1	-3.645668000	-5.067104000	2.433200000

$^{A}F2_{TS4}$

6	-3.422779000	2.289830000	2.597940000

6	-4.376223000	1.272802000	3.011589000
6	-3.925474000	0.034238000	3.465921000
6	-2.499520000	-0.240693000	3.520813000
6	-1.583905000	0.733222000	3.113042000
6	-2.050532000	2.023906000	2.641515000
6	-3.972012000	2.990120000	1.462413000
6	-5.270293000	2.411281000	1.161487000
6	-5.521302000	1.348474000	2.121174000
6	-6.166177000	0.178170000	1.715801000
6	-4.595461000	-1.184085000	3.046468000
6	-2.285851000	-1.618267000	3.144113000
6	-1.166053000	-1.957662000	2.377161000
6	-0.209169000	-0.942676000	1.982865000
6	-0.404585000	0.375004000	2.366640000
6	-0.010011000	1.539110000	1.518810000
6	-1.162781000	2.489147000	1.601718000
6	-1.698647000	3.127699000	0.494853000
6	-3.121374000	3.385995000	0.425291000
6	-5.675837000	2.260606000	-0.165055000
6	-4.798671000	2.684605000	-1.245009000
6	-3.548799000	3.230237000	-0.953941000
6	-2.387353000	2.862831000	-1.744782000
6	-1.237740000	2.799975000	-0.865625000
6	-0.257157000	1.842371000	-1.075750000
6	0.486820000	1.178883000	0.038793000
6	0.499876000	-0.271586000	-0.309993000
6	0.249605000	-1.272579000	0.618239000
6	-3.580371000	-2.206374000	2.847052000
6	-2.139369000	-3.236511000	-1.418081000
6	-2.972685000	-3.641995000	-0.375204000
6	-4.396891000	-3.371753000	-0.435659000
6	-4.934628000	-2.699647000	-1.535145000
6	-4.068734000	-2.274038000	-2.620545000
6	-1.748588000	-1.520965000	-2.976302000
6	-0.607298000	-1.592562000	-2.079389000
6	-0.844480000	-2.648073000	-1.122130000
6	-0.431996000	-2.483226000	0.205316000
6	-1.301964000	-2.908136000	1.287472000
6	-2.543055000	-3.478469000	1.004915000
6	-4.851008000	-3.047392000	0.907977000
6	-5.824370000	-2.064494000	1.097338000
6	-6.379636000	-1.362115000	-0.047704000
6	-5.944328000	-1.673125000	-1.336339000
6	-5.699203000	-0.610900000	-2.297653000
6	-4.540825000	-0.981830000	-3.091492000
6	-3.625119000	-0.004810000	-3.487411000
6	-2.200557000	-0.280642000	-3.424403000
6	0.030517000	-0.419469000	-1.664918000
6	-0.436494000	0.872792000	-2.131844000
6	-1.529774000	0.938545000	-3.000846000
6	-2.529207000	1.960395000	-2.803838000
6	-3.828477000	1.382315000	-3.102746000
6	-4.940745000	1.735978000	-2.338363000
6	-5.894799000	0.721808000	-1.929793000
6	-6.348939000	1.046092000	-0.585984000
6	-6.589231000	0.024356000	0.335022000
6	-3.707136000	-3.117731000	1.797913000
6	-5.693877000	-1.113793000	2.187558000
6	-2.698986000	-2.538751000	-2.564523000
6	1.405684000	1.802514000	1.067193000
6	1.933969000	3.207267000	0.875626000
7	3.273528000	3.316816000	1.118548000
8	1.201731000	4.135860000	0.548385000
6	4.065105000	4.513616000	0.785996000
1	5.086579000	4.273541000	1.110827000
6	4.089780000	4.779225000	-0.742711000
1	3.046351000	4.938735000	-1.035557000
7	4.538315000	3.573573000	-1.473880000
1	2.120256000	1.094157000	1.480443000
6	5.985804000	3.378436000	-1.525164000
1	6.513139000	4.102651000	-2.171671000
1	6.418556000	3.449653000	-0.520940000
1	6.194503000	2.375825000	-1.911655000
6	3.954551000	3.469166000	-2.809951000
1	4.219783000	2.499711000	-3.242718000
1	2.863181000	3.524393000	-2.740193000
1	4.295673000	4.258080000	-3.506569000
1	3.791184000	2.447247000	1.100692000
6	4.108640000	-1.549356000	-0.389013000
6	4.758504000	-0.679456000	0.516001000
8	4.713529000	0.630223000	0.311008000
16	5.684621000	-1.195959000	1.899753000
6	6.354829000	0.396740000	2.506052000
1	6.929200000	0.895180000	1.724382000
1	5.559258000	1.050977000	2.866265000
1	7.012498000	0.128924000	3.336231000
6	4.865850000	-1.026529000	-2.135322000
8	4.829047000	0.197219000	-2.185788000
8	5.112907000	-2.001494000	-2.789425000
1	4.574848000	0.776426000	-0.685296000
1	3.161534000	-1.105146000	-0.708291000
6	3.935690000	-3.048499000	-0.101653000
1	3.231213000	-3.104874000	0.737742000
6	3.196473000	-3.720162000	-1.276437000
6	5.173041000	-3.850277000	0.299032000
6	6.340803000	-3.875778000	-0.479004000
6	5.121189000	-4.637324000	1.458925000
6	7.432178000	-4.652217000	-0.089736000
1	6.393282000	-3.293269000	-1.392079000
6	6.212480000	-5.416366000	1.845478000
1	4.215284000	-4.644952000	2.059269000
6	7.374180000	-5.422507000	1.073474000
1	8.329717000	-4.658592000	-0.702577000
1	6.150741000	-6.019602000	2.747198000
1	8.225888000	-6.028150000	1.371379000
1	3.841482000	-3.966341000	-2.114596000
7	2.553025000	-5.019465000	-0.842444000
8	1.974157000	-5.038395000	0.242838000
8	2.617540000	-5.958327000	-1.625945000
1	2.358350000	-3.107917000	-1.625954000
6	3.594777000	5.741931000	1.589516000
1	2.535752000	5.913324000	1.376635000
1	3.674686000	5.513508000	2.659609000
6	4.873714000	6.072161000	-1.060982000
1	5.935680000	5.931916000	-0.816224000
1	4.826286000	6.270212000	-2.139242000
6	4.401748000	6.998291000	1.237780000
1	5.450801000	6.870790000	1.545835000
1	4.013434000	7.854361000	1.803139000
6	4.348622000	7.278255000	-0.269608000
1	4.936410000	8.171613000	-0.515661000
1	3.311423000	7.492409000	-0.564046000

^{A}F2$_{TS5}$

6	2.750860000	0.272043000	-3.433243000
6	3.776972000	-0.754791000	-3.518703000
6	3.504838000	-2.053495000	-3.090877000
6	2.193785000	-2.378833000	-2.555009000
6	1.211794000	-1.388728000	-2.462130000
6	1.491963000	-0.036608000	-2.908282000
6	3.383941000	1.515692000	-3.067215000
6	4.808310000	1.269304000	-2.920208000
6	5.052179000	-0.136222000	-3.200524000
6	6.003332000	-0.842139000	-2.460936000
6	4.492695000	-2.789551000	-2.321833000
6	2.364668000	-3.312018000	-1.466503000
6	1.544623000	-3.211028000	-0.337182000
6	0.510846000	-2.197558000	-0.264343000
6	0.333693000	-1.318665000	-1.321809000
6	-0.094739000	0.099410000	-1.141163000
6	0.785104000	0.890750000	-2.055815000
6	1.411798000	2.067413000	-1.676614000
6	2.726964000	2.386055000	-2.191424000
6	5.526974000	1.912297000	-1.911738000
6	4.848927000	2.829311000	-1.008996000
6	3.479440000	3.055154000	-1.144849000
6	2.631320000	3.143122000	0.030861000
6	1.351508000	2.541950000	-0.283211000
6	0.667689000	1.823088000	0.685285000
6	-0.157387000	0.614797000	0.377838000
6	0.215586000	-0.386102000	1.419350000
6	0.451236000	-1.722338000	1.132936000
6	3.786713000	-3.568145000	-1.316506000
6	3.599462000	-2.080978000	3.050914000
6	4.241207000	-2.964461000	2.182030000
6	5.553088000	-2.640356000	1.653290000
6	6.172958000	-1.440721000	2.009160000
6	5.506264000	-0.518648000	2.911835000
6	3.221760000	0.193300000	3.506724000
6	1.947652000	-0.425511000	3.181401000
6	2.177340000	-1.823605000	2.903286000
6	1.449276000	-2.453843000	1.887791000
6	2.121049000	-3.373157000	0.986071000
6	3.485301000	-3.627683000	1.131453000
6	5.612215000	-3.109187000	0.277183000
6	6.288590000	-2.358832000	-0.686834000
6	6.929318000	-1.107958000	-0.316076000
6	6.872882000	-0.658509000	1.003703000
6	6.635224000	0.747845000	1.283874000
6	5.791672000	0.834843000	2.462921000
6	4.805422000	1.820159000	2.543304000
6	3.493931000	1.490197000	3.073314000
6	1.001647000	0.276789000	2.429465000
6	1.282089000	1.627163000	1.978141000
6	2.504539000	2.224617000	2.300968000
6	3.196058000	3.003825000	1.302815000
6	4.620757000	2.757009000	1.446962000
6	5.431104000	2.670262000	0.314370000
6	6.458086000	1.648523000	0.231580000
6	6.517288000	1.179863000	-1.144749000
6	6.751128000	-0.170494000	-1.412625000
6	4.336847000	-3.722826000	-0.043399000
6	5.717698000	-2.195592000	-2.012245000
6	4.246143000	-0.832927000	3.424302000
6	-1.393175000	0.503850000	-0.486540000
6	-2.144054000	1.744271000	-0.922579000
7	-3.492003000	1.616699000	-0.836356000
8	-1.557814000	2.753774000	-1.311396000
6	-4.450098000	2.683654000	-1.160294000
1	-5.434509000	2.262110000	-0.927907000
6	-4.241167000	3.954607000	-0.293413000
1	-3.226829000	4.302296000	-0.510246000
7	-4.260154000	3.638486000	1.152169000
1	-2.019535000	-0.344760000	-0.221918000
6	-5.589207000	3.514071000	1.749431000
1	-6.125584000	4.475279000	1.844234000
1	-6.217037000	2.826507000	1.175968000
1	-5.487796000	3.099176000	2.759226000
6	-3.421s381000	4.543871000	1.931345000
1	-3.371031000	4.190635000	2.968409000
1	-2.405278000	4.549522000	1.524509000
1	-3.791281000	5.586596000	1.957356000
1	-3.862135000	0.759885000	-0.438764000
6	-6.152020000	-2.194185000	1.157046000
6	-5.233612000	-1.138611000	1.453582000
8	-4.337012000	-1.058079000	0.495093000
16	-5.150948000	-0.204422000	2.89322200
6	-3.487617000	0.562326000	2.808920000
1	-3.511916000	1.432298000	2.145161000
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1	-2.759830000	-0.175572000	2.465440000
1	-4.876588000	-2.165039000	0.290607000
6	-7.144497000	-2.031486000	-0.011752000
6	-7.569101000	-3.379152000	-0.583863000
6	-8.414521000	-1.238709000	0.377597000
6	-7.338976000	-3.671424000	-1.933739000
6	-8.205749000	-4.343184000	0.210580000
1	-8.933128000	-1.651869000	1.242086000
7	-8.073685000	0.185138000	0.738878000
6	-7.728883000	-4.896165000	-2.478059000
1	-6.846658000	-2.934726000	-2.564761000
6	-8.598004000	-5.567604000	-0.330564000
1	-8.393658000	-4.144681000	1.263162000
8	-8.475828000	0.622277000	1.809449000
8	-7.403357000	0.817213000	-0.079964000
6	-8.360413000	-5.848324000	-1.677420000
1	-7.537742000	-5.104570000	-3.527269000
1	-9.087922000	-6.303317000	0.301551000
1	-8.664519000	-6.802534000	-2.098605000
1	-6.667782000	-1.457636000	-0.812086000
1	-9.100587000	-1.164174000	-0.471511000
1	-6.564261000	-2.739155000	2.007269000
6	-5.227360000	5.065347000	-0.721755000
1	-6.257222000	4.752200000	-0.502213000
1	-5.040367000	5.966403000	-0.123576000
6	-4.404811000	3.010975000	-2.669273000
1	-3.382151000	3.308415000	-2.925556000
1	-4.623985000	2.094902000	-3.231857000
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6	-5.125050000	5.388445000	-2.218583000
1	-5.840996000	6.177602000	-2.481659000
1	-4.123908000	5.781994000	-2.445532000