

Supporting Information

The catalytic mechanism of aromatic nitration by cytochrome P₄₅₀ TxtE: Involvement of a ferric-peroxynitrite intermediate

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Part I: Experimental data.

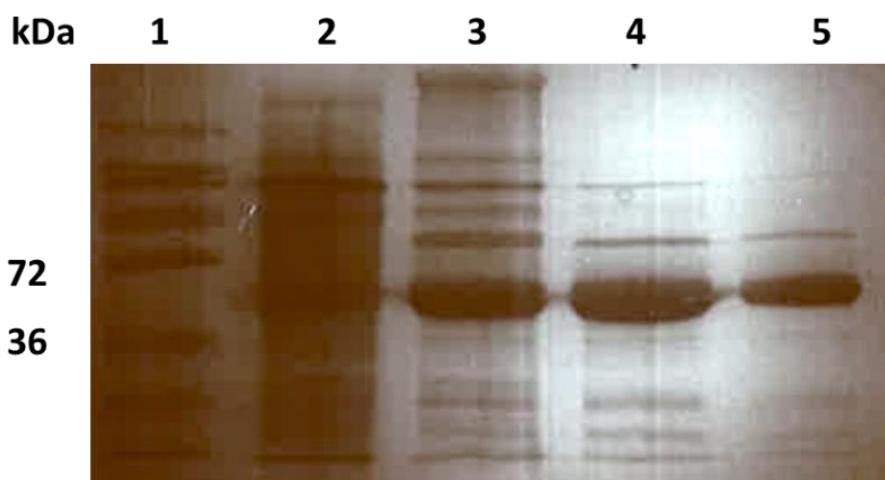


Figure S1: Representative SDS-PAGE of purified TxtE.

Lane 1: molecular size markers;

Lane 2: soluble protein;

Lane 3: after passing the sample through a Ni^{2+} -IDA resin;

Lane 4: after passing the sample through a Ni^{2+} -IDA resin using an FPLC instrument;

Lane 5: after a further gel filtration step using a Superdex 12 column (see Methods section for details).

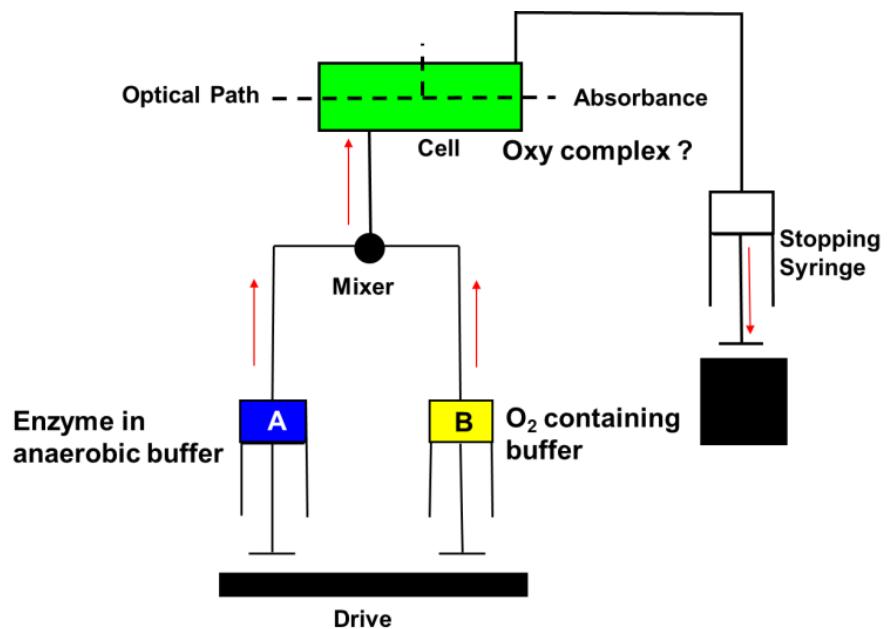


Figure S2: Diagram of stopped-flow apparatus for single mixing experiments. The scheme shows the mixing of enzyme against O₂ but also applies to NO.

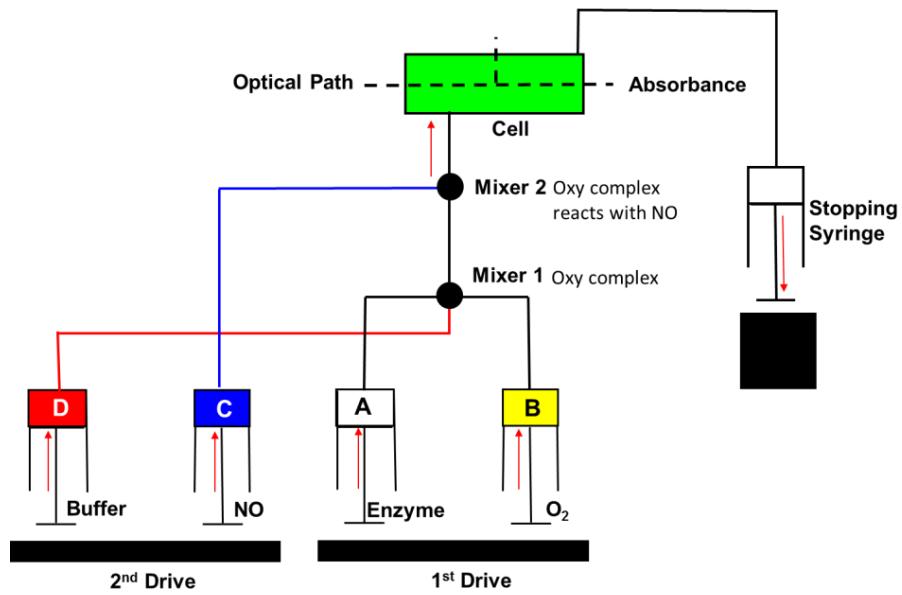


Figure S3: Diagram of stopped-flow apparatus for double mixing experiments. The enzyme is initially mixed against the first gas (in this case O_2 to form the oxy-complex), aged for a defined time delay and then mixed against the second gas (in this case NO). The order of mixing of the two gases can be varied in different stopped-slow experiments.

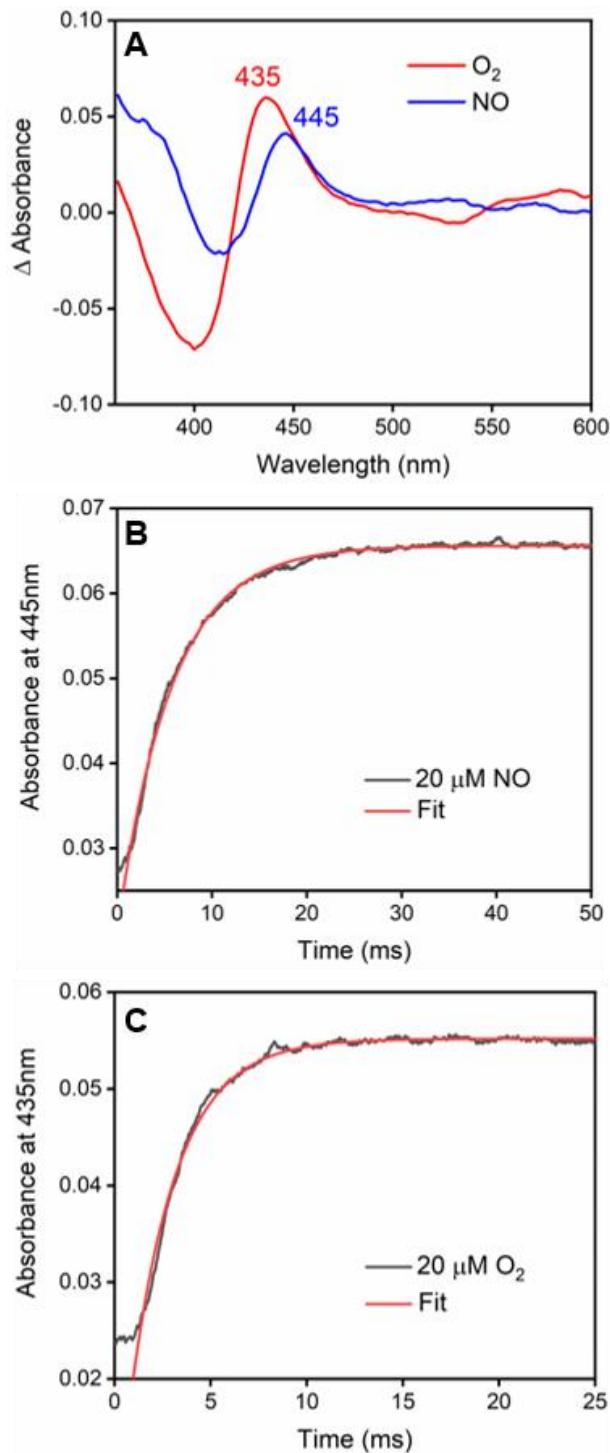


Figure S4: Examples of rapid mixing stopped-flow data to illustrate the rates of NO and O₂ binding to TxtE. A) Absorbance difference spectra measured after 50 ms from stopped-flow photodiode array experiments. A TxtE sample mixed against anaerobic buffer was used as a baseline. The maximum increases in absorbance (435 nm for O₂ and 445 nm for NO) were used to measure the rates of binding. Examples of kinetic transients are shown for binding of 20 μM NO (B) and 20 μM O₂ (C).

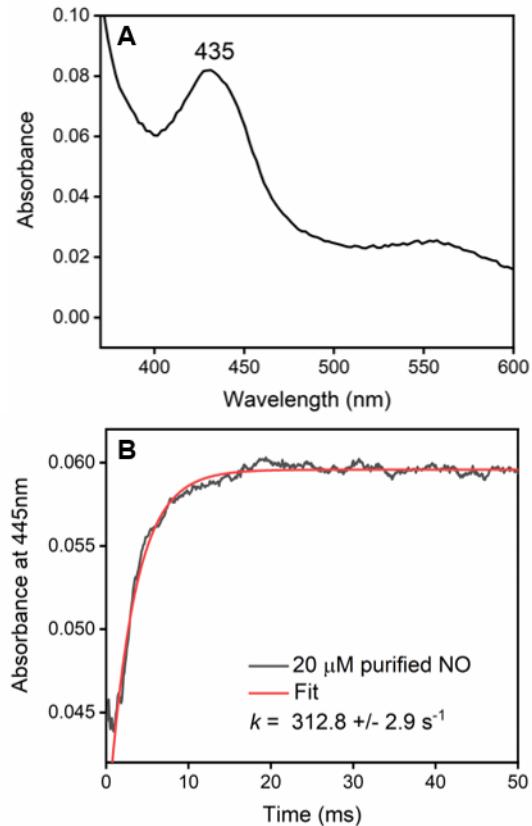


Figure S5: Rapid mixing stopped-flow data to illustrate binding of re-purified NO to TxtE. A) Absorbance spectra measured after 50 ms from stopped-flow photodiode array experiments. B) Example of kinetic transients at 445 nm are shown for binding of 20 μ M NO.

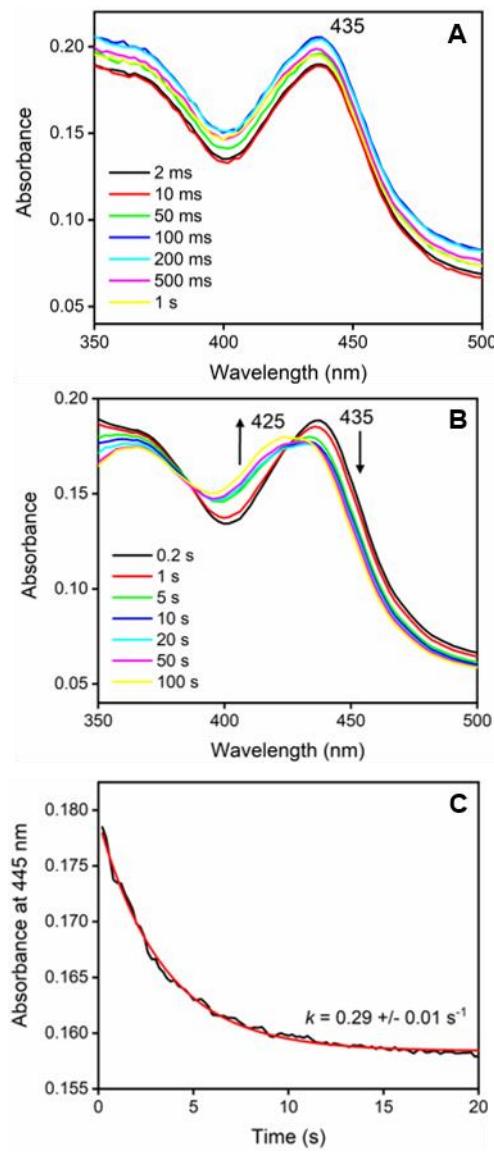


Figure S6: Representative double mixing stopped-flow measurements where TxtE was first mixed with 20 μM NO, aged for 50 ms and then mixed with 20 μM O₂, prior to data collection. A) Spectral changes over 1 s at selected time points show only the formation of the iron(II)-NO species at 435 nm. B) Spectral changes over 100 seconds show gradual disappearance of the iron(II)-NO species at 435 nm and formation of new peak at 425 nm. C) A kinetic transient at 445 nm showing disappearance of the iron(II)-NO species over a period of 20 s.

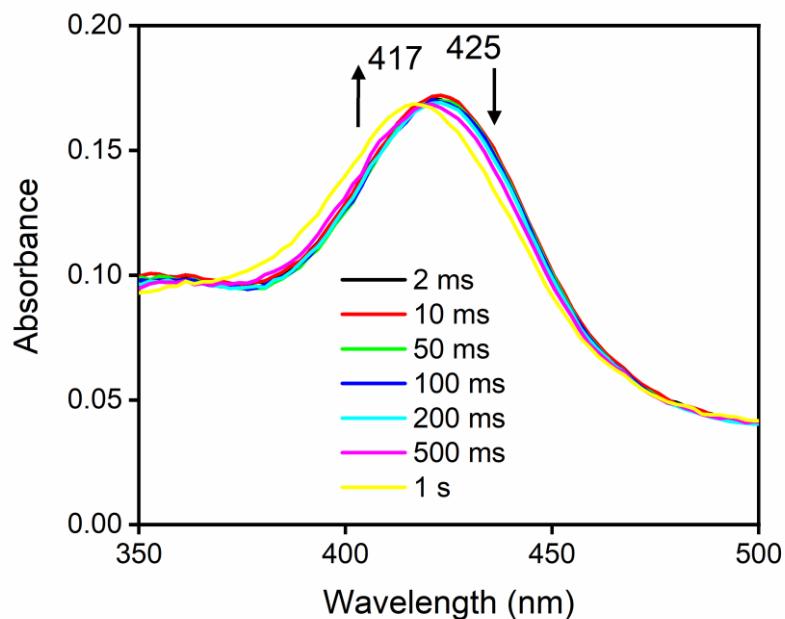


Figure S7: Representative double mixing stopped-flow measurements where TxtE was first mixed with 20 μ M O₂, aged for 50 ms and then mixed with anaerobic buffer, prior to data collection. Spectral changes over 1 s at selected time points show decay of the iron(III)-superoxide species at 425 nm and a simultaneous increase at 417 nm.

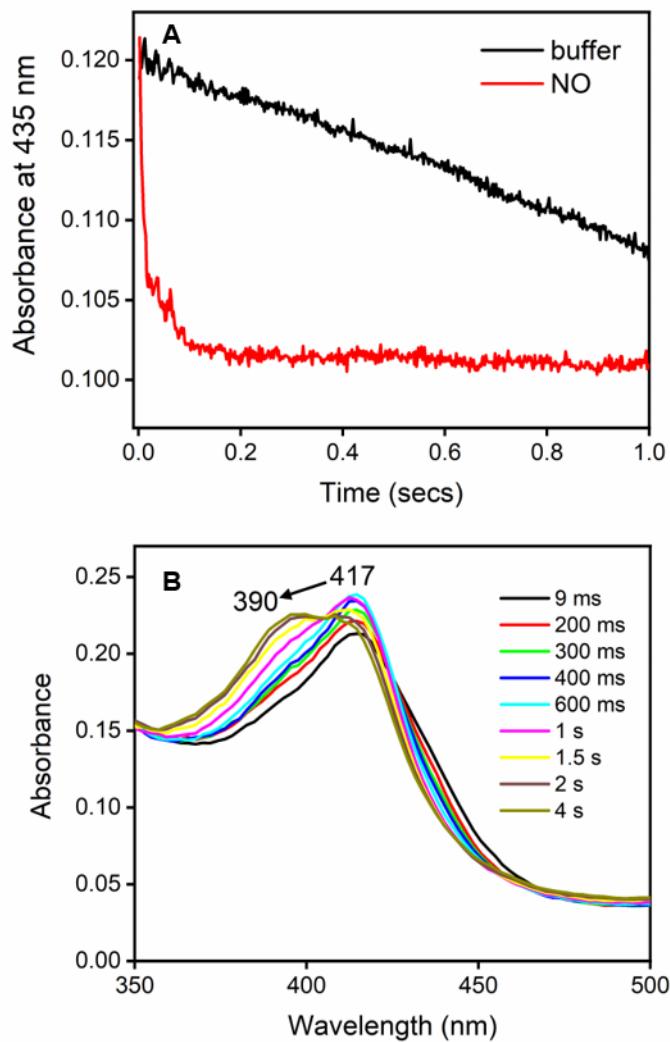


Figure S8: Double mixing stopped-flow measurements where TxtE was first mixed with 20 μM O_2 , aged for 50 ms and then mixed with either anaerobic buffer or 20 μM NO. A) Representative transients at 435 nm from double mixing stopped-flow measurements that show the disappearance of the iron(III)-superoxo species. **B)** Representative double mixing stopped-flow measurements where TxtE was first mixed with 20 μM O_2 , aged for 50 ms and then mixed with 20 μM NO, prior to data collection. Spectral changes over 4 s at selected time points showing slower conversion of 417 nm absorbing species to substrate-bound heme peak at 390 nm.

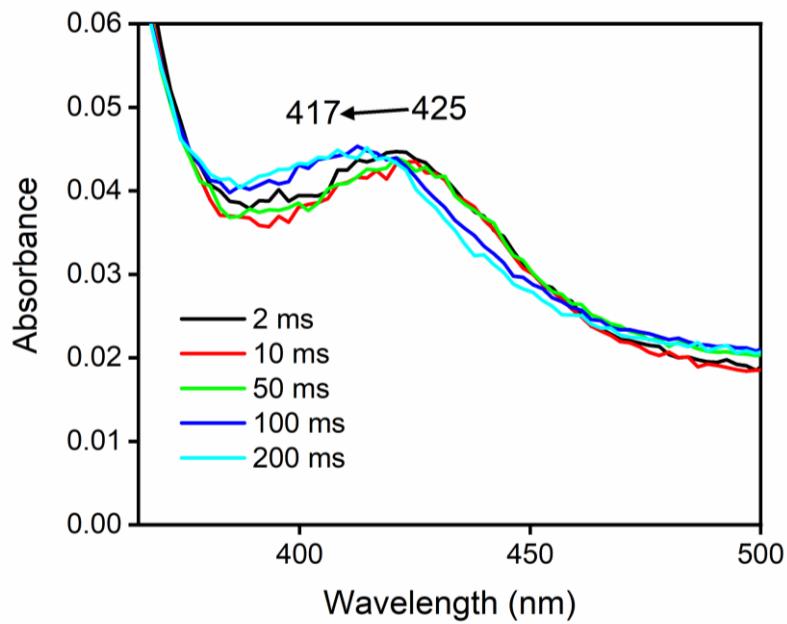


Figure S9: Representative double mixing stopped-flow measurements where 20 μM O_2 was first mixed with 20 μM NO, aged for 50 ms and then mixed with TxtE, prior to data collection. Spectral changes over 200 ms at selected time points show decay of the iron(III)-superoxo species at 425 nm and a simultaneous increase at 417 nm.

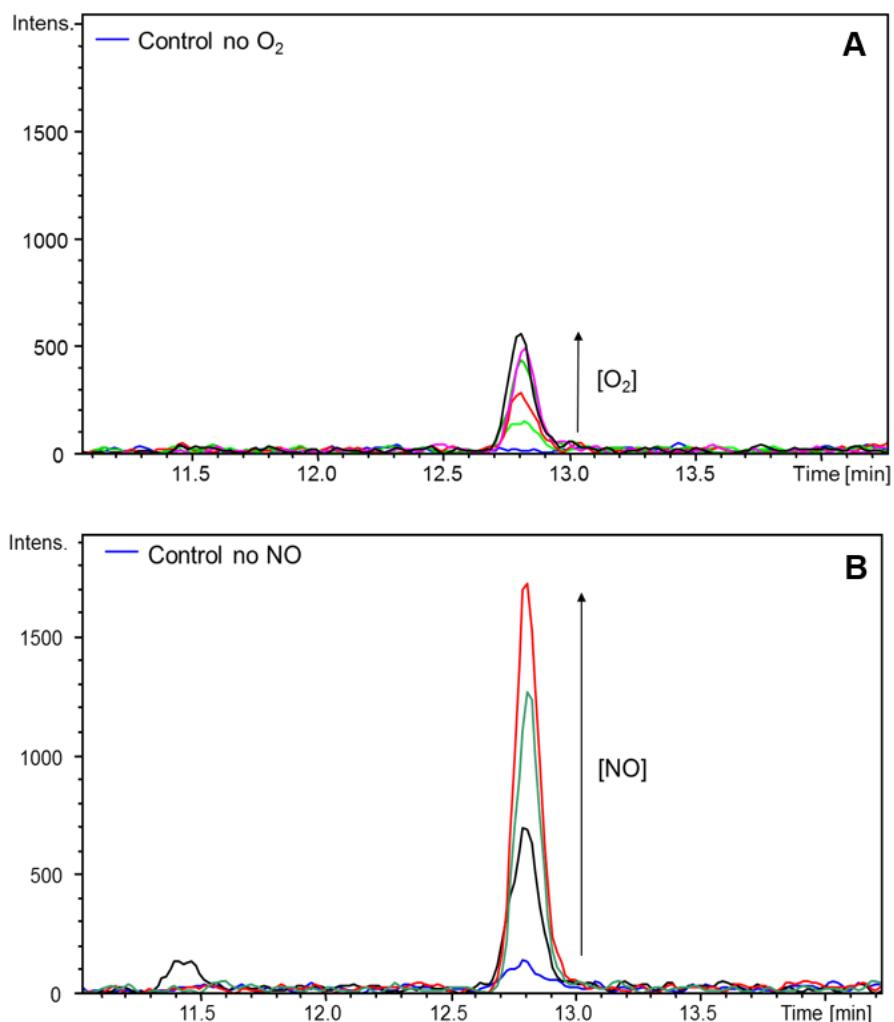
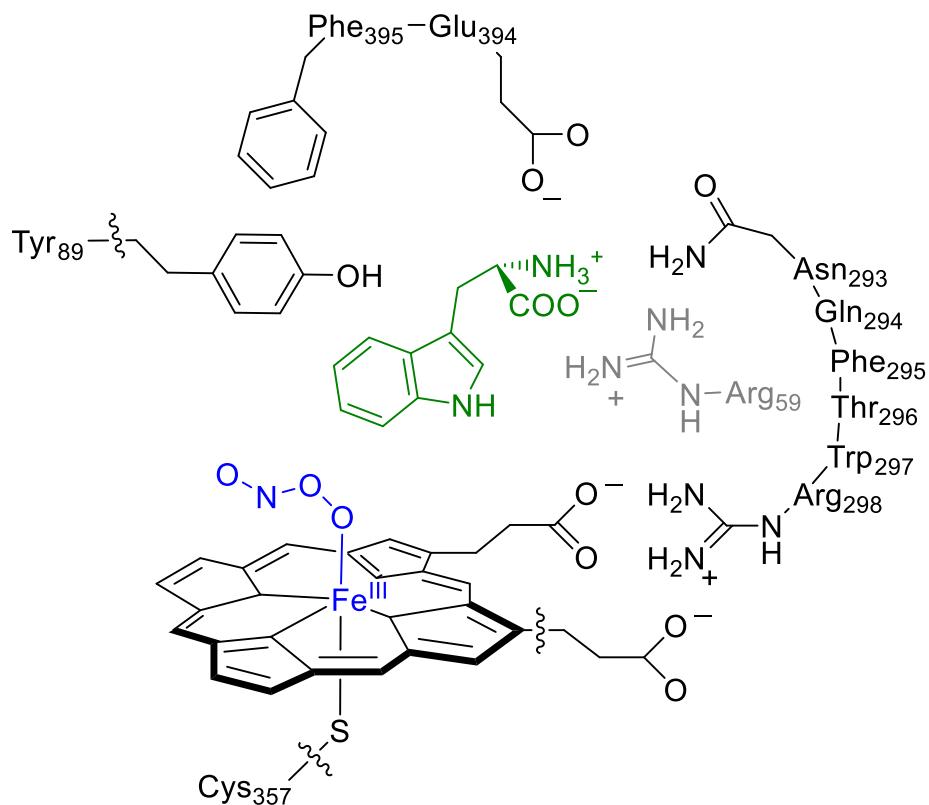
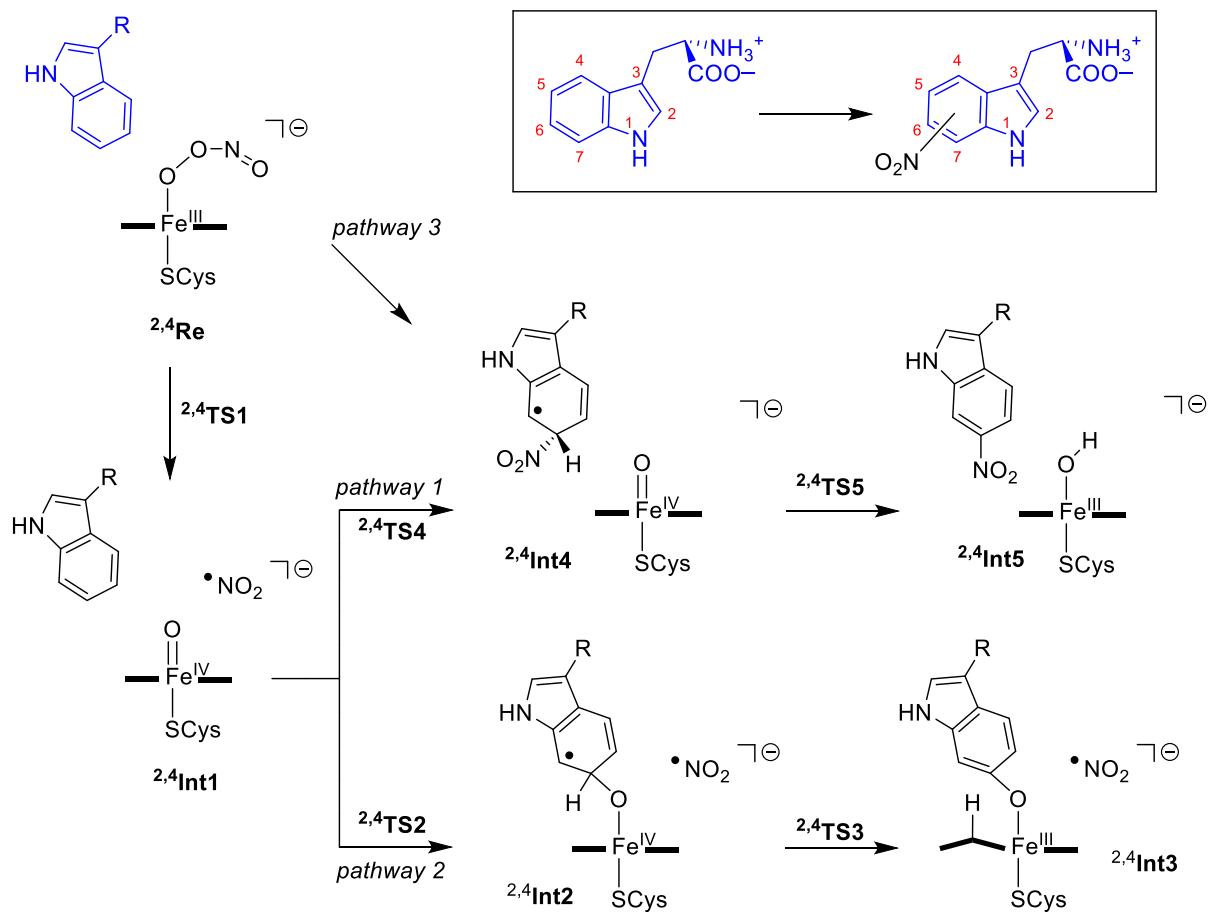


Figure S10: **A)** Representative mass spectral analysis of samples following double mixing experiments of TxtE iron(II)-NO complex reacted with buffers containing increasing concentrations of O_2 (0, 2, 5, 10, 20 and 100 μM). **B)** Representative mass spectral analysis of samples following double mixing experiments of TxtE iron(III)-superoxo complex reacted with buffers containing increasing concentrations of NO (0, 20, 40 and 100 μM). The data are LC-HRMS extracted ion chromatograms at m/z 250.0800 ± 0.05.

Part II: Computational data.



Scheme S1: Models A and B as studied in this work. Labelling taken from the 4TPO pdb file. Model A contains the heme without side chains, SH⁻ as axial ligand, peroxynitrite and Trp substrate. Model B has model A expanded with one propionate side chain of the heme and part of the substrate binding pocket (Arg₅₉ and Tyr₈₉ side chains, the small chain Asn₂₉₃-Gln₂₉₄-Phe₂₉₅-Thr₂₉₆-Trp₂₉₇-Arg₂₉₈, and Glu₃₉₄-Phe₃₉₅, whereby Gln₂₉₄ was abbreviated to Gly). Wiggly lines are where the model was cut from the crystal structure coordinates and where a hydrogen atom was added.



Scheme S2: Reaction mechanisms as studied in this work with labelling of the individual local minima and transition states for C⁶-activation.

Small model A Data.

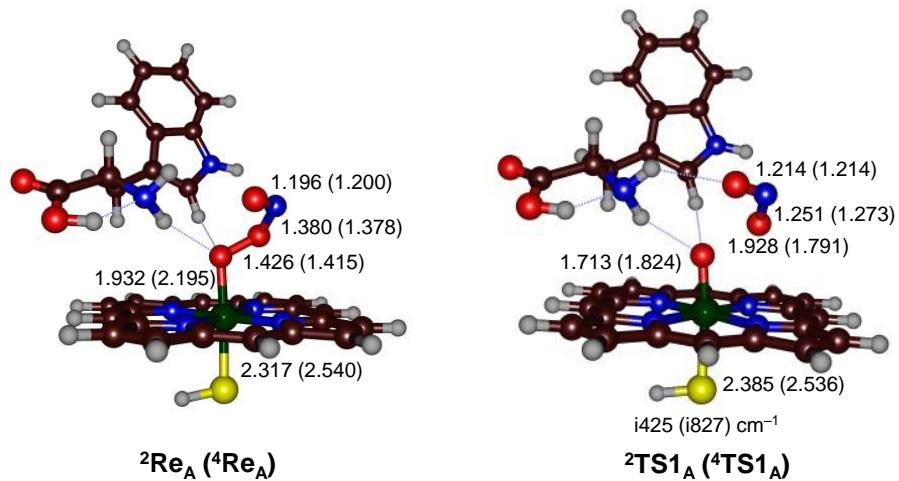


Figure S11: UB3LYP/BS1 optimized geometries of ${}^2,{}^4\text{Re}_\text{A}$ and ${}^2,{}^4\text{TS1}_\text{A}$ as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

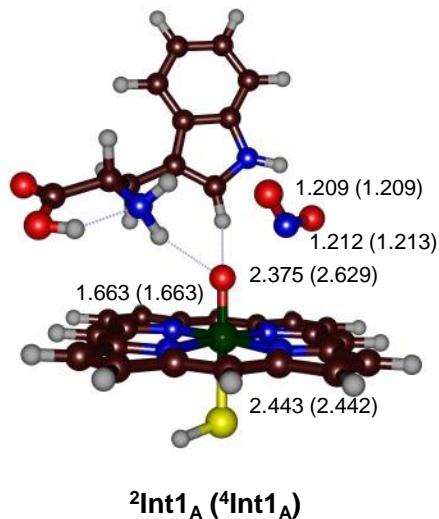


Figure S12: UB3LYP/BS1 optimized geometries of ${}^2,{}^4\text{Int1}_\text{A}$ as obtained in Gaussian-09. Bond lengths are in angstroms.

Table S1: Absolute (free) energies (in au) of local minima and transition states for activation of peroxy nitrite as calculated with B3LYP with model A in Gaussian-09.

	E [BS1,au]	ZPE [BS1,au]	G [BS1,au]	E [BS2,au]
² Re _A	-2477.355600	0.518586	-2476.913189	-2477.977766
² TS1 _A	-2477.334388	0.516799	-2476.893638	-2477.956603
² Int1 _A	-2477.348699	0.517539	-2476.909727	-2477.972255
⁴ Re _A	-2477.335188	0.516706	-2476.897065	-2477.946672
⁴ TS1 _A	-2477.309364	0.515451	-2476.871264	-2477.935138
⁴ Int1 _A	-2477.347933	0.517404	-2476.909656	-2477.971097

Table S2: Relative (free) energies (in kcal mol⁻¹) of local minima and transition states for activation of peroxy nitrite as calculated with B3LYP with model A in Gaussian-09.

	ΔE BS1	ΔE+ZPE BS1	ΔG BS1	ΔE BS2	ΔE+ZPE BS2	ΔG BS2
² Re _A	0.00	0.00	0.00	0.00	0.00	0.00
² TS1 _A	13.31	12.19	12.27	13.28	12.16	12.24
² Int1 _A	4.33	3.67	2.17	3.46	2.80	1.30
⁴ Re _A	12.81	11.63	10.12	19.51	18.33	16.82
⁴ TS1 _A	29.01	27.05	26.31	26.75	24.78	24.04
⁴ Int1 _A	4.81	4.07	2.22	4.18	3.44	1.59

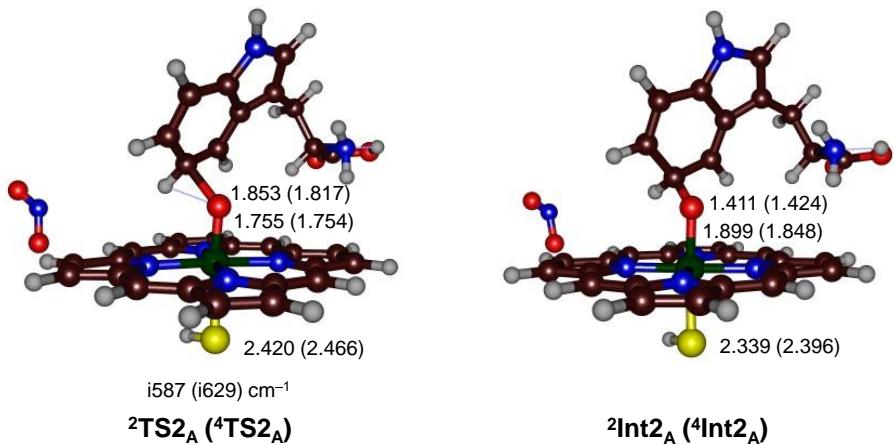


Figure S13: UB3LYP/BS1 optimized geometries of ${}^2,{}^4\text{TS2}_\text{A}$ and ${}^2,{}^4\text{Int2}_\text{A}$ as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

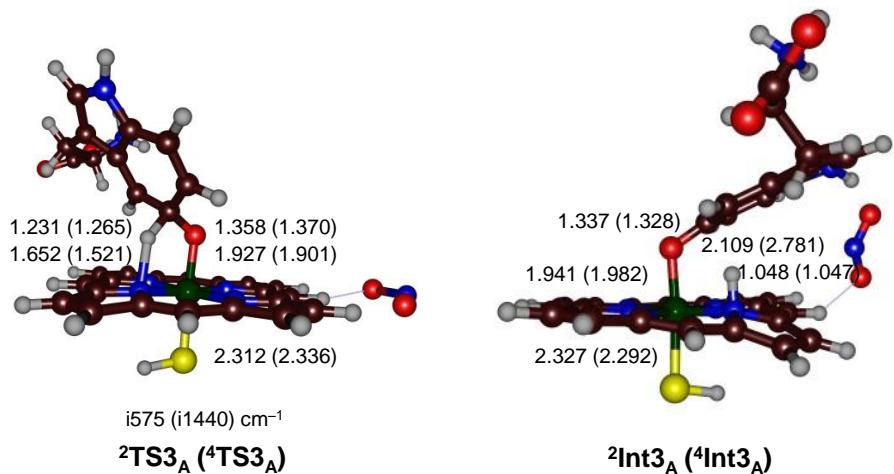


Figure S14: UB3LYP/BS1 optimized geometries of ${}^2,{}^4\text{TS3}_\text{A}$ and ${}^2,{}^4\text{Int3}_\text{A}$ as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

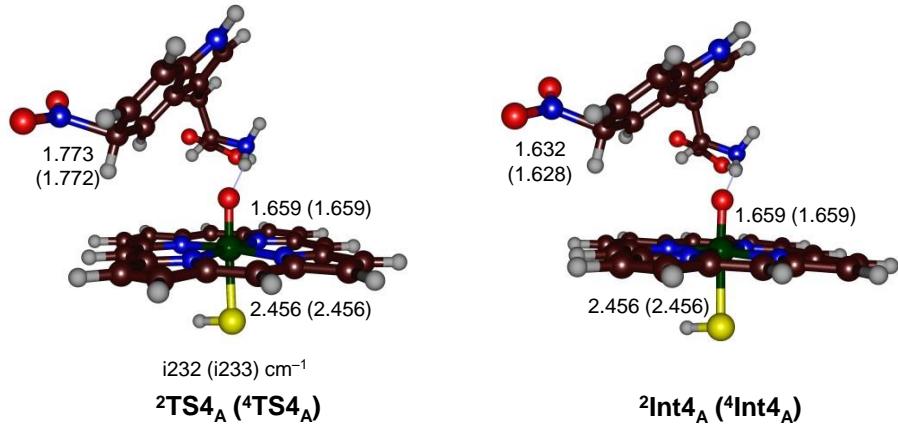


Figure S15: UB3LYP/BS1 optimized geometries of $^{2,4}\text{TS4}_\text{A}$ and $^{2,4}\text{Int4}_\text{A}$ as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

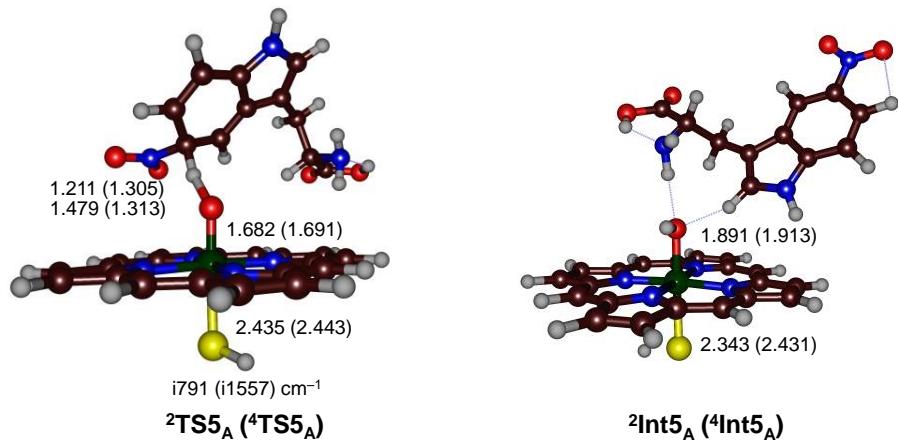


Figure S16: UB3LYP/BS1 optimized geometries of $^{2,4}\text{TS5}_\text{A}$ and $^{2,4}\text{Int5}_\text{A}$ as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

Table S3: Absolute (free) energies (in au) of local minima and transition states for Pathway 1 as calculated with B3LYP with model A in Gaussian-09.

Pathway 1:	E [BS1,au]	ZPE [BS1,au]	G [BS1,au]	E [BS2,au]
² TS _A	-2477.291661	0.515360	-2476.855971	-2477.933385
² Int _A	-2477.313338	0.516972	-2476.875642	-2477.967220
² TS _A	-2477.301674	0.512808	-2476.866745	-2477.968688
² Int _A	-2477.370838	0.519961	-2476.923404	-2478.014560
⁴ TS _A	-2477.289667	0.514911	-2476.855535	-2477.922144
⁴ Int _A	-2477.306212	0.515710	-2476.871496	-2477.937934
⁴ TS _A	-2477.274705	0.510352	-2476.841094	-2477.910412
⁴ Int _A	-2477.337098	0.516594	-2476.898687	-2477.968318

Table S4: Relative (free) energies (in kcal mol⁻¹) of local minima and transition states for Pathway 1 as calculated with B3LYP with model A in Gaussian-09.

	ΔE BS1	ΔE+ZPE BS1	ΔG BS1	ΔE BS2	ΔE+ZPE BS2	ΔG BS2
² TS _A	40.12	38.10	35.90	27.85	25.83	23.63
² Int _A	26.52	25.51	23.56	6.62	5.60	3.66
² TS _A	33.84	30.21	29.14	5.70	2.07	1.00
² Int _A	-9.56	-8.70	-6.41	-23.09	-22.23	-19.94
⁴ TS _A	41.37	39.07	36.18	34.90	32.60	29.71
⁴ Int _A	30.99	29.19	26.16	25.00	23.19	20.17
⁴ TS _A	50.76	45.60	45.24	42.27	37.10	36.74
⁴ Int _A	11.61	10.36	9.10	5.93	4.68	3.42

Table S5: Absolute (free) energies (in au) of local minima and transition states for Pathway 2 as calculated with B3LYP with model A in Gaussian-09.

Pathway 2:	E [BS1,au]	ZPE [BS1,au]	G [BS1,au]	E [BS2,au]
² TS4 _A	-2477.306740	0.517517	-2476.866469	-2477.942997
² Int4 _A	-2477.307151	0.518460	-2476.865556	-2477.942251
² TS5 _A	-2477.297479	0.514492	-2476.856103	-2477.933611
² Int5 _A	-2477.426807	0.521753	-2476.978990	-2478.053632
⁴ TS4 _A	-2477.306644	0.517495	-2476.867422	-2477.942978
⁴ Int4 _A	-2477.307049	0.518143	-2476.865821	-2477.942325
⁴ TS5 _A	-2477.290360	0.513241	-2476.851355	-2477.927986
⁴ Int5 _A	-2477.405500	0.519056	-2476.962580	-2478.033157

Table S6: Relative (free) energies (in kcal mol⁻¹) of local minima and transition states for Pathway 2 as calculated with B3LYP with model A in Gaussian-09.

	ΔE BS1	ΔE+ZPE BS1	ΔG BS1	ΔE BS2	ΔE+ZPE BS2	ΔG BS2
² TS4 _A	30.66	29.99	29.32	21.82	21.15	20.47
² Int4 _A	30.40	30.32	29.89	22.29	22.21	21.77
² TS5 _A	36.47	33.90	35.82	27.71	25.14	27.06
² Int5 _A	-44.68	-42.70	-41.29	-47.61	-45.62	-44.21
⁴ TS4 _A	30.72	30.04	28.72	21.83	21.15	19.83
⁴ Int4 _A	30.47	30.19	29.72	22.24	21.96	21.50
⁴ TS5 _A	40.94	37.58	38.80	31.24	27.88	29.10
⁴ Int5 _A	-31.31	-31.02	-30.99	-34.76	-34.46	-34.44

Table S7: Group spin densities and charges of local minima and transition states for activation of peroxy nitrite as calculated with B3LYP with model A in Gaussian-09.

Spin Densities:

	Fe	O38	NO2	Por	SH	Trp	Total
² Re _A	1.01	0.04	0.00	-0.07	0.03	0.00	1.00
² TS1 _A	1.14	0.44	-0.49	-0.09	0.00	0.00	1.00
² Int1 _A	1.37	0.62	-0.86	-0.10	-0.03	0.01	1.00
⁴ Re _A	2.58	0.11	0.01	-0.06	0.35	0.00	3.00
⁴ TS1 _A	2.17	0.27	0.30	-0.08	0.33	0.01	3.00
⁴ Int1 _A	1.28	0.80	0.87	-0.05	0.09	0.01	3.00

Charges:

	Fe	O38	NO2	Por	SH	Trp	Total
² Re _A	0.34	-0.41	-0.14	-0.60	-0.13	-0.07	-1.00
² TS1 _A	0.40	-0.46	-0.18	-0.52	-0.18	-0.07	-1.00
² Int1 _A	0.44	-0.55	-0.10	-0.49	-0.23	-0.08	-1.00
⁴ Re _A	0.50	-0.40	-0.19	-0.52	-0.29	-0.10	-1.00
⁴ TS1 _A	0.51	-0.46	-0.22	-0.49	-0.25	-0.09	-1.00
⁴ Int1 _A	0.43	-0.54	-0.10	-0.49	-0.21	-0.08	-1.00

Table S8: Group spin densities and charges of local minima and transition states for Pathway 1 as calculated with B3LYP with model A in Gaussian-09.

Spin densities:

	Fe	O38	NO2	Por	SH	Trp	Total
² TS _A	1.05	0.57	-0.63	-0.18	-0.06	0.25	1.00
² Int _A	1.00	0.08	-0.58	-0.09	0.03	0.56	1.00
² TS _A	0.98	0.05	-0.23	-0.05	0.05	0.20	1.00
² Int _A	0.99	0.06	0.00	-0.07	0.03	-0.01	1.00
⁴ TS _A	0.95	0.64	0.69	0.00	0.26	0.46	3.00
⁴ Int _A	0.94	0.17	0.73	0.05	0.18	0.93	3.00
⁴ TS _A	0.98	0.07	0.70	0.80	0.06	0.40	3.00
⁴ Int _A	1.04	0.03	0.84	1.03	0.03	0.03	3.00

Charges:

	Fe	O38	NO2	Por	SH	Trp	Total
² TS _A	0.35	-0.49	-0.34	-0.49	-0.20	0.17	-1.00
² Int _A	0.27	-0.56	-0.38	-0.58	-0.14	0.38	-1.00
² TS _A	0.25	-0.57	-0.64	-0.49	-0.11	0.57	-1.00
² Int _A	0.26	-0.58	-0.75	-0.31	-0.13	0.53	-1.00
⁴ TS _A	0.38	-0.50	-0.28	-0.54	-0.17	0.10	-1.00
⁴ Int _A	0.32	-0.56	-0.24	-0.52	-0.14	0.14	-1.00
⁴ TS _A	0.27	-0.58	-0.27	-0.71	-0.15	0.44	-1.00
⁴ Int _A	0.27	-0.66	-0.16	-0.91	-0.11	0.56	-1.00

Table S9: Group spin densities and charges of local minima and transition states for Pathway 2 as calculated with B3LYP with model A in Gaussian-09.

Spin densities:

	Fe	O38	NO2	Por	SH	Trp	Total
² TS4 _A	1.27	0.81	-0.23	-0.08	-0.01	-0.75	1.00
² Int4 _A	1.27	0.81	-0.11	-0.08	-0.01	-0.88	1.00
² TS5 _A	1.24	0.69	-0.05	-0.08	0.00	-0.79	1.00
² Int5 _A	0.97	0.06	0.00	-0.08	0.05	0.00	1.00
⁴ TS4 _A	1.27	0.81	0.23	-0.08	0.00	0.77	3.00
⁴ Int4 _A	1.27	0.81	0.11	-0.08	0.00	0.90	3.00
⁴ TS5 _A	1.58	0.60	0.11	-0.10	0.01	0.80	3.00
⁴ Int5 _A	2.83	0.12	0.00	0.06	-0.01	0.01	3.00

Charges:

	Fe	O38	NO2	Por	SH	Trp	Total
² TS4 _A	0.39	-0.52	-0.31	-0.53	-0.27	0.23	-1.00
² Int4 _A	0.39	-0.52	-0.31	-0.52	-0.27	0.23	-1.00
² TS5 _A	0.39	-0.54	-0.30	-0.52	-0.25	0.22	-1.00
² Int5 _A	0.28	-0.75	-0.45	-0.61	-0.17	0.69	-1.00
⁴ TS4 _A	0.39	-0.52	-0.31	-0.53	-0.27	0.23	-1.00
⁴ Int4 _A	0.39	-0.52	-0.31	-0.53	-0.27	0.24	-1.00
⁴ TS5 _A	0.45	-0.60	-0.37	-0.45	-0.22	0.20	-1.00
⁴ Int5 _A	0.43	-0.78	-0.45	-0.71	-0.21	0.71	-1.00

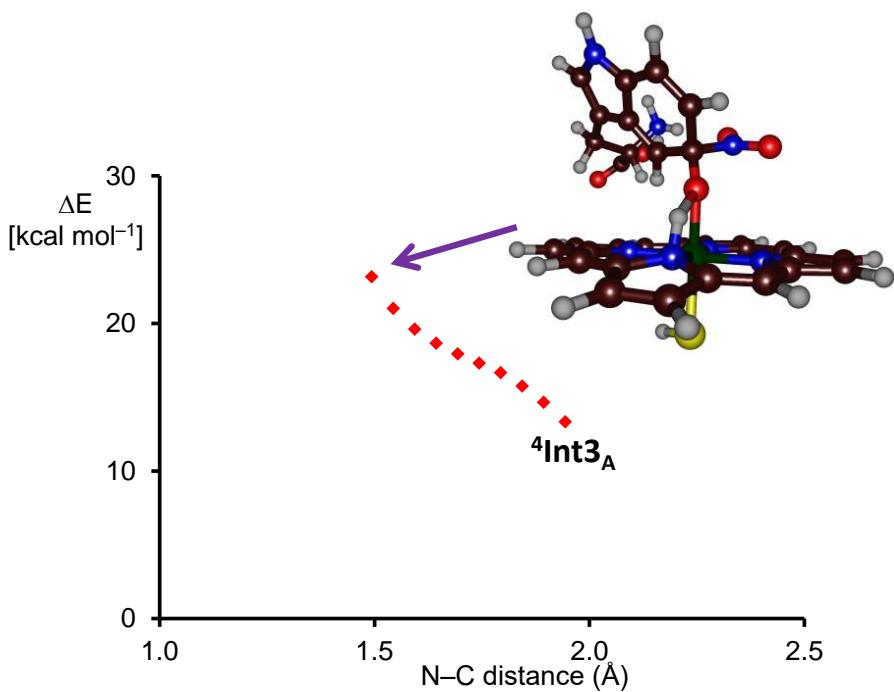


Figure S17: UB3LYP/BS1 geometry scan for NO_2 attack on the *ipso*-carbon atom of the substrate in ${}^4\text{Int3}_\text{A}$ as obtained in Gaussian-09. All points refer to a full geometry optimization with fixed C–N distance. Energies are relative to ${}^4\text{Re}_\text{A}$.

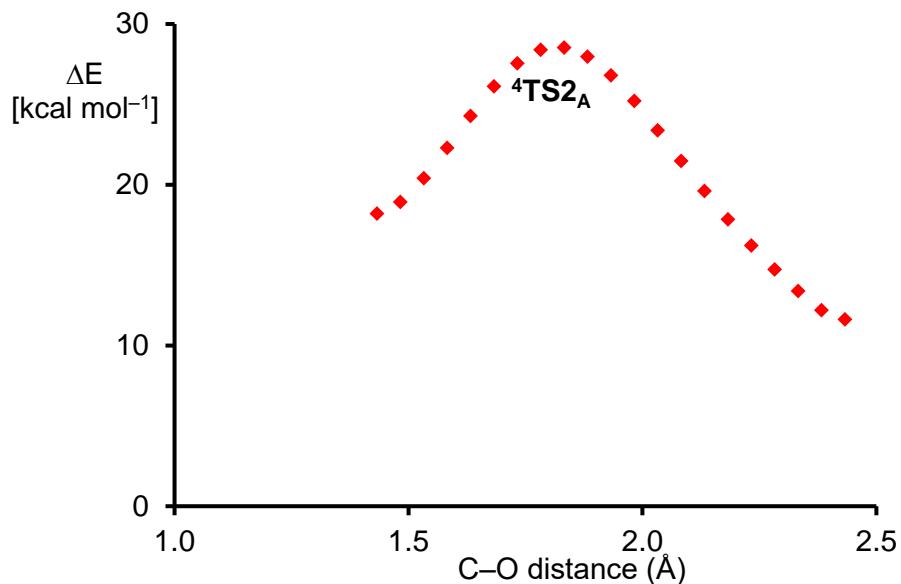


Figure S18: UB3LYP/BS1 geometry scan for electrophilic attack on the exo atom of the substrate starting from ${}^4\text{Int1}_\text{A}$ as obtained in Gaussian-09. All points refer to a full geometry optimization with fixed C–O distance. Energies are relative to ${}^4\text{Re}_\text{A}$.

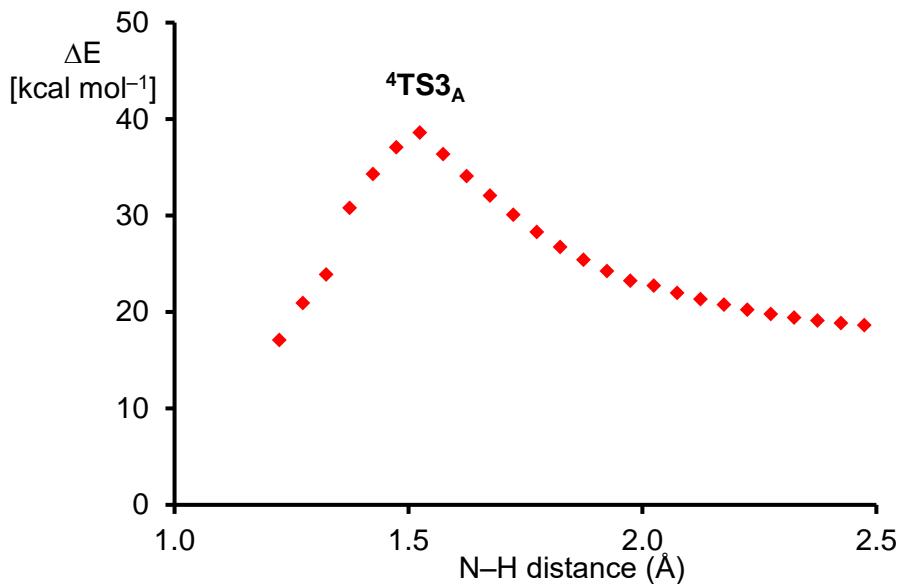


Figure S19: UB3LYP/BS1 geometry scan for proton transfer from the *ipso*-C–H bond of substrate in ${}^4\text{Int2}_\text{A}$ as obtained in Gaussian-09. All points refer to a full geometry optimization with fixed H–N distance. Energies are relative to ${}^4\text{Re}_\text{A}$.

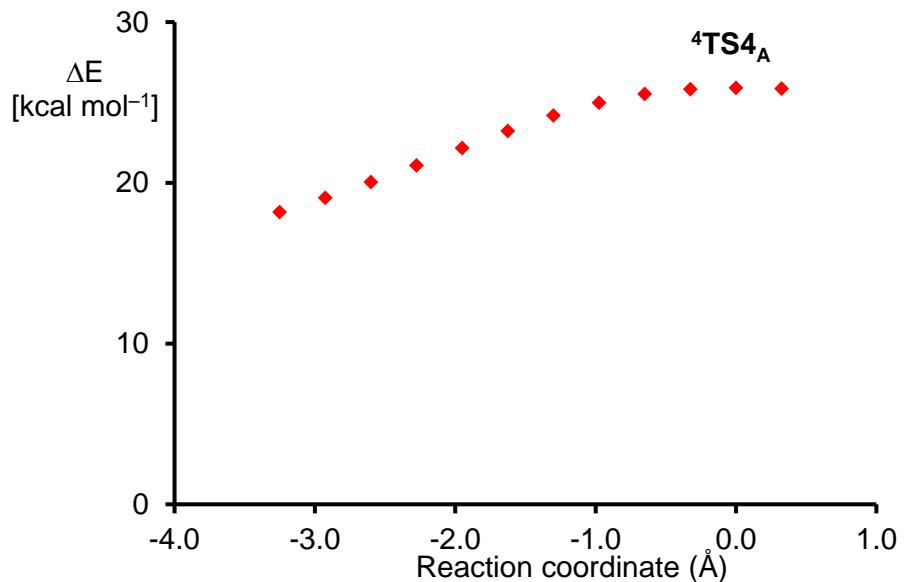


Figure S20: UB3LYP/BS1 calculated intrinsic reaction coordinate scan for NO_2 transfer to substrate in ${}^4\text{Int1}_\text{A}$ around ${}^4\text{TS4}_\text{A}$ as obtained in Gaussian-09. Energies are relative to ${}^4\text{Int1}_\text{A}$.

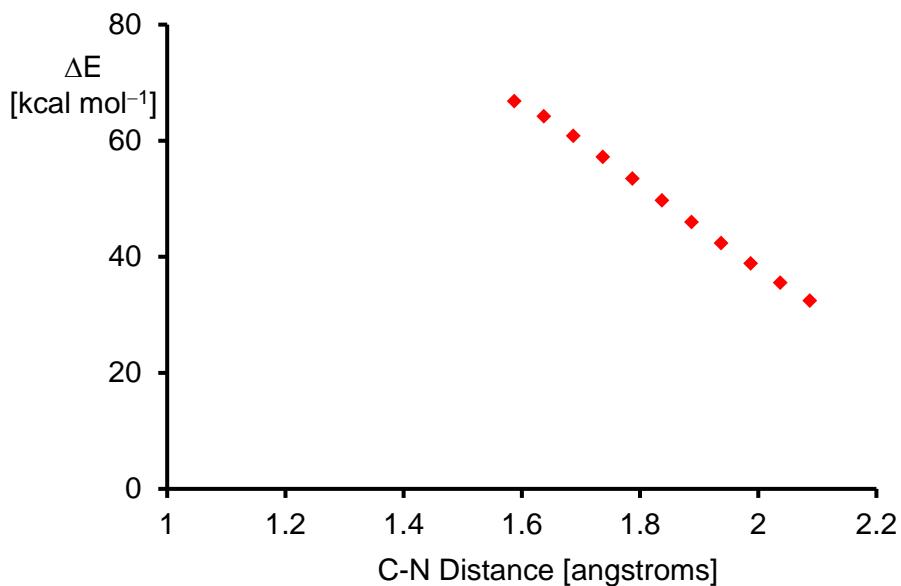
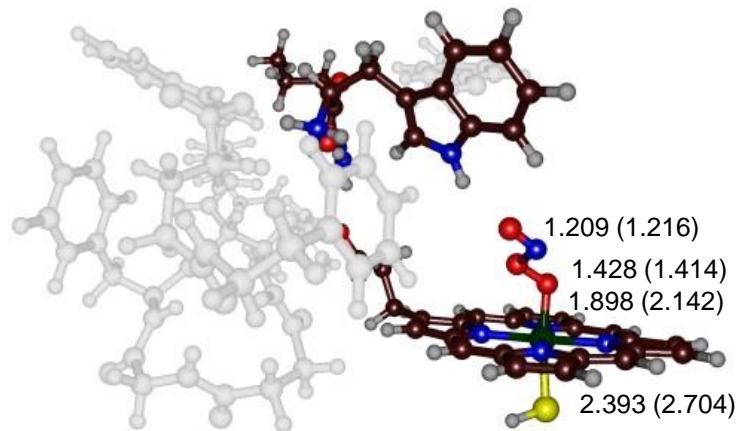


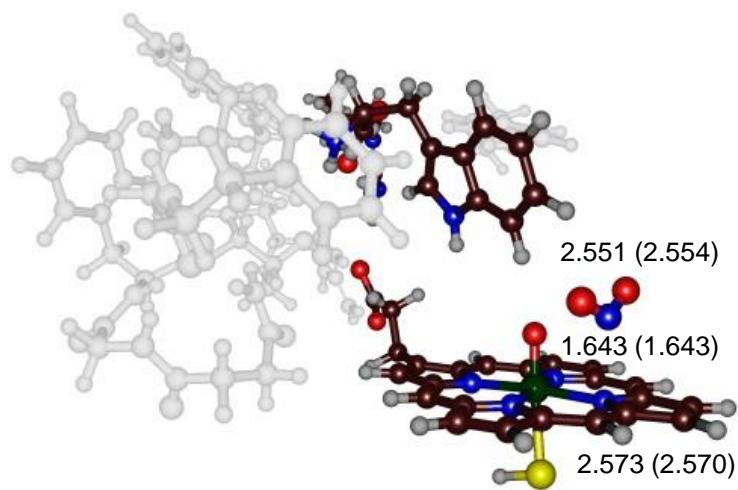
Figure S21: UB3LYP/BS1 calculated constraint geometry scan for direct attack of peroxyxinitrite on the substrate in ${}^4\text{Re}_\text{A}$ as obtained in Gaussian-09. Energies are relative to ${}^4\text{Re}_\text{A}$.

Large model B Data.



${}^2\text{Re}_\text{B}$ (${}^4\text{Re}_\text{B}$)

Figure S22: UB3LYP/BS1 optimized geometries of ${}^{2,4}\text{Re}_\text{B}$ as obtained in Gaussian-09.
Bond lengths are in angstroms.



${}^2\text{Int1}_\text{B}$ (${}^4\text{Int1}_\text{B}$)

Figure S23: UB3LYP/BS1 optimized geometries of ${}^{2,4}\text{Int1}_\text{B}$ as obtained in Gaussian-09.
Bond lengths are in angstroms.

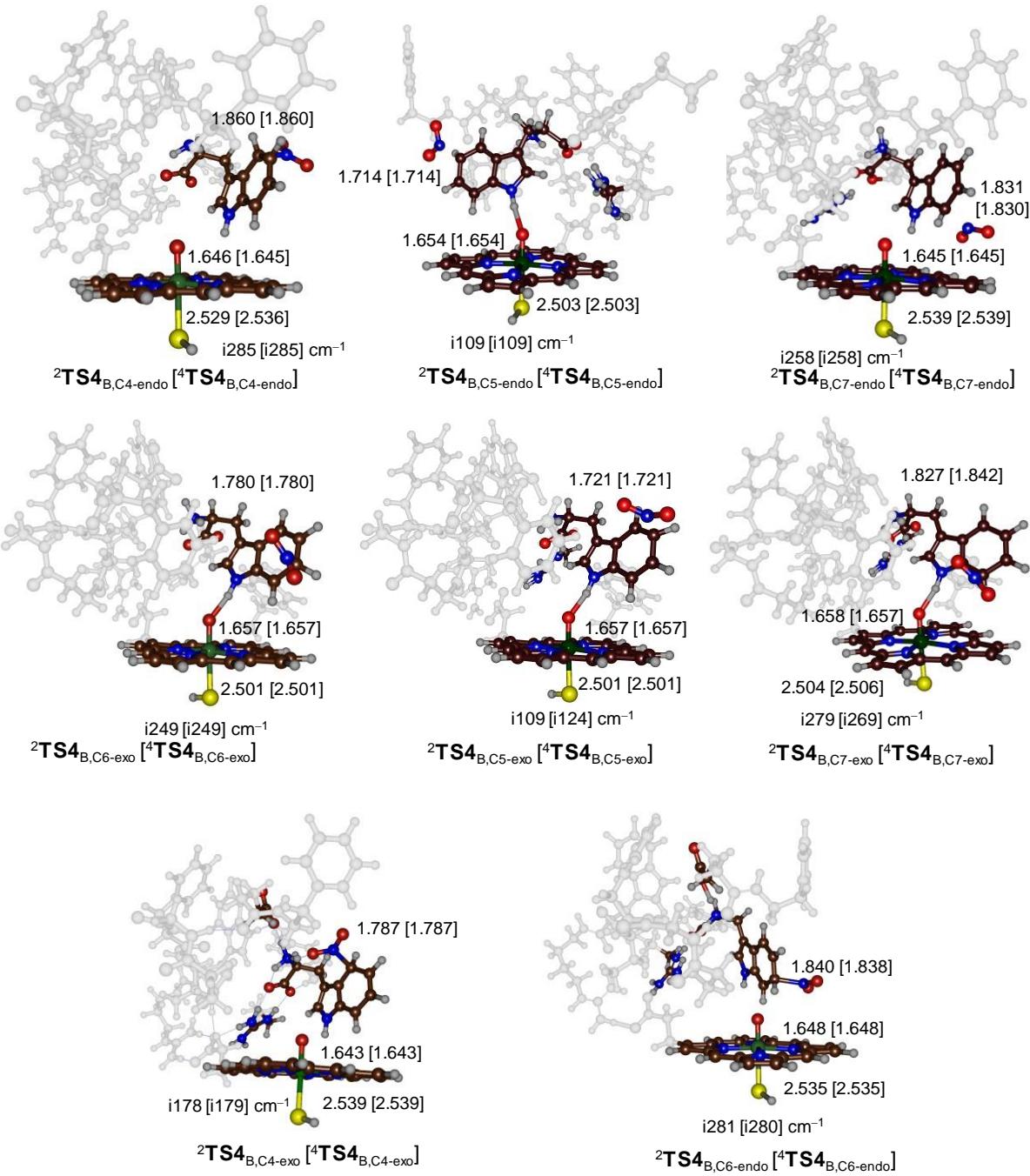


Figure S24: UB3LYP/BS1 optimized transition state geometries for NO_2 attack on L-Trp substrate via $^{2,4}\text{TS4}_\text{B}$. N–C bond formation barriers calculated for attack on the C^4 , C^5 , C^6 and C^7 -positions.

Bond lengths are in angstroms and the imaginary frequency in the transition state in cm^{-1} .

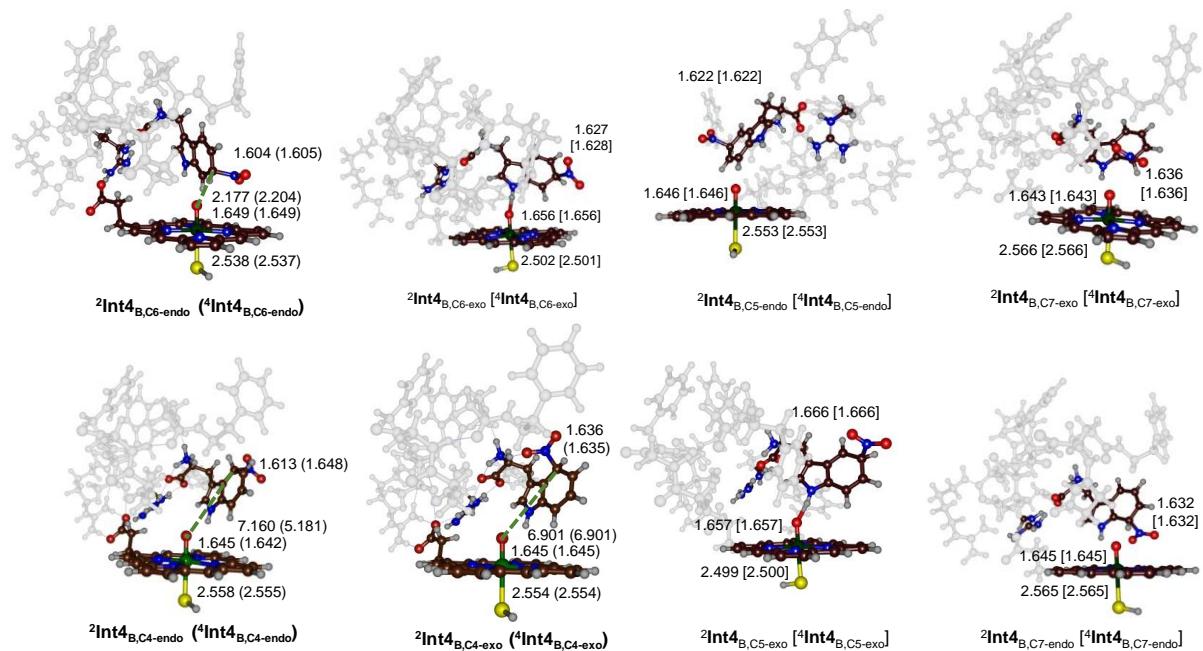


Figure S25: UB3LYP/BS1 optimized transition state geometries for NO_2 attack on L-Trp substrate via ${}^{2,4}\text{Int4}_\text{B}$. N–C bond formation calculated for attack on the C^4 , C^5 , C^6 and C^7 -positions. Bond lengths are in angstroms.

Table S10: Absolute (free) energies (in au) of local minima and transition states for Pathway 2-C4 as calculated with B3LYP with model B in Gaussian-09.

Model B-C4	E [au]	ZPE [au]	G [au]	E [au]	E _{disp} [au]
	[BS1,au]	[BS1,au]	[BS1,au]	[BS2,au]	[BS2,au]
ver1:					
² R_{eB}	-6677.060921	2.049469	-6675.212340	-6678.806670	0.375488
² TS_{1B}	-6677.052201	2.049078	-6675.204844	-6678.800153	0.374037
² Int_{1B}	-6677.056943	2.047748	-6675.215182	-6678.805779	0.379619
⁴ R_{eB}	-6677.045210	2.047408	-6675.202362	-6678.795184	0.375934
⁴ TS_{1B}	-6677.030813	2.047526	-6675.185986	-6678.779820	0.371348
⁴ Int_{1B}	-6677.056916	2.047740	-6675.216449	-6678.805556	0.379652
Pathway C4-endo:					
² TS_{4B,C4-endo}	-6677.049204	2.049851	-6675.202993	-6678.796562	0.376604
² Int_{4B,C4-endo}	-6677.049140	2.050807	-6675.202181	-6678.797819	0.370501
² TS_{5B,C4-endo}	-6677.045271	2.047227	-6675.195421	-6678.786938	0.412531
² Int_{5B,C4-endo}	-6677.148981	2.053599	-6675.292449	-6678.889153	0.408725
⁴ TS_{4B,C4-endo}	-6677.063982	2.049926	-6675.218339	-6678.811947	0.376650
⁴ Int_{4B,C4-endo}	-6677.066903	2.050787	-6675.216600	-6678.810851	0.374258
⁴ Int_{5B,C4-endo}	-6677.091156	2.049539	-6675.239285	-6678.830437	0.409153
Pathway C4-oxo:					
² TS_{4B,C4-oxo}	-6677.071584	2.050842	-6675.221058	-6678.815380	0.377088
² Int_{4B,C4-oxo}	-6677.070616	2.051379	-6675.219694	-6678.814071	0.376689
² Int_{5B,C4-oxo}	-6677.158908	2.052011	-6675.308455	-6678.901643	0.401059
⁴ TS_{4B,C4-oxo}	-6677.071572	2.050842	-6675.221707	-6678.815366	0.377051
⁴ Int_{4B,C4-oxo}	-6677.070613	2.051357	-6675.220457	-6678.814071	0.376705
⁴ Int_{5B,C4-oxo}	-6677.100416	2.048103	-6675.251439		

Table S11: Relative (free) energies (in kcal mol⁻¹) of local minima and transition states for Pathway 2-C4 as calculated with B3LYP with model B in Gaussian-09.

Model B	ΔE	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$	ΔG
	BS1	BS1	BS1	BS2	BS2	BS2
Pathway C4-endo:						
² Re_B	0.00	0.00	0.00	0.00	0.00	0.00
² TS1_B	5.47	5.23	4.70	4.09	3.84	3.32
² Int1_B	2.50	1.42	-1.78	0.56	-0.52	-3.72
⁴ Re_B	9.86	8.57	6.26	7.21	5.91	3.61
⁴ TS1_B	18.89	17.67	16.54	16.85	15.63	14.49
⁴ Int1_B	2.51	1.43	-2.58	0.70	-0.39	-4.39
Pathway C4-exo:						
² TS4_{B,C4-endo}	7.35	7.59	5.87	6.34	6.58	4.86
² Int4_{B,C4-endo}	7.39	8.23	6.37	5.55	6.39	4.54
² TS5_{B,C4-endo}	9.82	8.41	10.62	12.38	10.98	13.18
² Int5_{B,C4-endo}	-55.26	-52.67	-50.27	-51.76	-49.17	-46.77
⁴ TS4_{B,C4-endo}	-1.92	-1.63	-3.76	-3.31	-3.02	-5.15
⁴ Int4_{B,C4-endo}	-1.90	-1.02	-3.30	-2.22	-1.35	-3.63
⁴ Int5_{B,C4-endo}	-18.97	-18.93	-16.91	-14.91	-14.87	-12.85
Pathway C4-oxo:						
² TS4_{B,C4-oxo}	-6.69	-5.83	-5.47	-5.47	-4.60	-4.25
² Int4_{B,C4-oxo}	-6.08	-4.88	-4.61	-4.64	-3.45	-3.18
² Int5_{B,C4-oxo}	-61.49	-59.89	-60.31	-59.60	-58.00	-58.2
⁴ TS4_{B,C4-oxo}	-6.68	-5.82	-5.88	-5.46	-4.60	-4.65
⁴ Int4_{B,C4-oxo}	-6.08	-4.90	-5.09	-4.64	-3.46	-3.66
⁴ Int5_{B,C4-oxo}	-24.78	-25.64	-24.54		-23.20	-22.2

Table S12: Absolute (free) energies (in au) of local minima and transition states for Pathway 2-C6 as calculated with B3LYP with model B in Gaussian-09.

Model B-C6	E [au]	ZPE [au]	G [au]	E [au]	E _{disp} [au]
	[BS1,au]	[BS1,au]	[BS1,au]	[BS2,au]	[BS2,au]
Pathway C6-endo:					
² TS4_{B,C6-endo}	-6677.056044	2.048825	-6675.210684	-6678.804549	0.379386
² Int4_{B,C6-endo}	-6677.057783	2.049977	-6675.207802	-6678.810546	0.373479
² TS5_{B,C6-endo}	-6677.051281	2.046036	-6675.201298	-6678.796693	0.388985
² INT5_{B,C6-endo}	-6677.139864	2.052567	-6675.282522	-6678.886511	0.384782
⁴ TS4_{B,C6-endo}	-6677.055965	2.048818	-6675.211416	-6678.804439	0.379344
⁴ Int4_{B,C6-out}	-6677.057634	2.050036	-6675.211911	-6678.804382	0.360495
² Int4_{B,C6-endo}	-6677.057634	2.050014	-6675.213090	-6678.805395	0.378394
⁴ TS5_{B,C6-endo}	-6677.043256	2.044794	-6675.197786	-6678.792313	0.385831
⁴ INT5_{B,C6-endo}	-6677.119941	2.049671	-6675.268069	-6678.871938	0.386353
Pathway C6-exo:					
² TS4_{B,C6-exo}	-6677.054336	2.048996	-6675.205872	-6678.807116	0.389643
² Int4_{B,C6-exo}	-6677.054872	2.049949	-6675.206157	-6678.809986	0.386087
² TS5_{B,C6-exo}	-6677.053882	2.045997	-6675.202529	-6678.797774	0.385222
² INT5_{B,C6-exo}	-6677.158110	2.051059	-6675.308964	-6678.904025	0.371072
⁴ TS4_{B,C6-exo}	-6677.054339	2.049028	-6675.206351	-6678.807116	0.389642
⁴ Int4_{B,C6-exo}	-6677.054862	2.049839	-6675.204363	-6678.807745	0.388363
⁴ TS5_{B,C6-exo}	-6677.045041	2.044307	-6675.197234	-6678.792720	0.383390
⁴ INT5_{B,C6-exo}	-6677.135053	2.048678	-6675.290130	-6678.895719	0.358053
Pathway C6-HAT:					
² TS6_B	-6677.012161	2.039512	-6675.178016	-6678.760755	0.389879
⁴ TS6_B	-6677.012052	2.039407	-6675.179073	-6678.760560	0.389735
⁴ Int6_B	-6677.018236	2.045007	-6675.175445	-6678.769099	0.383061

Table S13: Relative (free) energies (in kcal mol⁻¹) of local minima and transition states for Pathway 2-C6 as calculated with B3LYP with model B in Gaussian-09.

Model B-C6	ΔE	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$	ΔG
	BS1	BS1	BS1	BS2	BS2	BS2
Pathway C6-endo:						
² TS4 _{B,C6-endo}	3.06	2.66	1.04	1.33	0.93	-0.69
² Int4 _{B,C6-endo}	1.97	2.29	2.85	-2.43	-2.11	-1.55
² TS5 _{B,C6-endo}	6.05	3.90	6.93	6.26	4.11	7.14
² INT5 _{B,C6-endo}	-49.54	-47.59	-44.04	-50.10	-48.16	-44.60
⁴ TS4 _{B,C6-endo}	3.11	2.70	0.58	1.40	0.99	-1.13
⁴ Int4 _{B,C6-endo}	2.06	2.40	-0.47	0.80	-0.14	-1.73
⁴ TS5 _{B,C6-endo}	11.08	8.15	9.13	9.01	6.08	7.06
⁴ INT5 _{B,C6-endo}	-37.04	-36.91	-34.97	-40.96	-40.83	-38.89
Pathway C6-exo:						
² TS4 _{B,C6-exo}	4.13	3.84	4.06	-0.28	-0.58	-0.35
² Int4 _{B,C6-exo}	3.80	4.10	3.88	-2.08	-1.78	-2.00
² TS5 _{B,C6-exo}	4.42	2.24	6.16	5.58	3.40	7.32
² INT5 _{B,C6-exo}	-60.99	-59.99	-60.63	-61.09	-60.09	-60.74
⁴ TS4 _{B,C6-exo}	4.13	3.85	3.76	-0.28	-0.56	-0.65
⁴ Int4 _{B,C6-exo}	3.80	4.03	5.01	-0.67	-0.44	0.53
⁴ TS5 _{B,C6-exo}	9.96	6.73	9.48	8.75	5.51	8.27
⁴ INT5 _{B,C6-exo}	-46.52	-47.01	-48.81	-55.88	-56.38	-58.17
Pathway C6-HAT:						
² TS6_B	30.60	24.35	21.54	28.81	22.56	19.75
⁴ TS6_B	30.67	24.35	20.88	28.93	22.62	19.14
⁴ Int6_B	26.79	23.99	23.15	23.58	20.78	19.94

Table S14: Group spin densities and charges of local minima and transition states for Pathway 2-C6 as calculated with B3LYP/BS1 with model B in Gaussian-09.

Spin densities:

Species	pFe	pPorp	pSH	pO	pOH	pNO2	pSubs	pSubs(NO ₂)	pLig1	pArg	pPheGlu	pTyr	pTotal
ver1:													
² Re_B	1.34	-0.12	-0.20	-0.03		0.00	0.00		0.00	0.00	0.00	0.00	1.00
² TS1_B	1.23	-0.07	-0.16	0.00		0.00	0.00		0.00	0.00	0.00	0.00	1.00
² Int1_B	1.27	-0.28	-0.05	0.82		-0.75	-0.01		0.00	0.00	0.00	0.00	1.00
⁴ Re_B	2.64	-0.02	0.29	0.09		0.00	0.00		0.00	0.00	0.00	0.00	3.00
⁴ TS1_B	2.20	-0.04	0.24	0.38		0.23	0.00		0.00	0.00	0.00	0.00	3.00
⁴ Int1_B	1.25	0.12	-0.01	0.83		0.80	0.01		0.00	0.00	0.00	0.00	3.00
Pathway C6-endo:													
² TS4_{B,C6-endo}	1.29	-0.07	-0.02	0.80		0.00	-0.99		0.00	0.00	0.00	0.00	1.00
² Int4_{B,C6-endo}	1.29	-0.07	-0.02	0.80				-0.99	0.00	0.00	0.00	0.00	1.00
² TS5_{B,C6-endo}	1.02	-0.06	-0.04		0.36	0.00		-0.28	0.00	0.00	0.00	0.00	1.00
² INT5_{B,C6-endo}	1.13	-0.06	-0.08		0.02	0.00		0.00	0.00	0.00	0.00	0.00	1.00
⁴ TS4_{B,C6-endo}	1.29	-0.07	-0.02	0.80		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ Int4_{B,C6-endo}	1.29	-0.07	-0.02	0.80				1.00	0.00	0.00	0.00	0.00	3.00
⁴ TS5_{B,C6-endo}	1.92	-0.10	0.00		0.47	0.00		0.70	0.00	0.00	0.00	0.00	3.00
⁴ INT5_{B,C6-endo}	2.63	-0.06	0.11		0.31			0.00	0.00	0.00	0.00	0.00	3.00
Pathway C6-exo:													
² TS4_{B,C6-exo}	1.38	-0.08	-0.03	0.72		-0.50	-0.50		0.00	0.00	0.00	0.00	1.00
² Int4_{B,C6-exo}	1.38	-0.08	-0.03	0.72		0.00	-1.00		0.00	0.00	0.00	0.00	1.00
² TS5_{B,C6-exo}	1.20	-0.07	-0.01		0.58			-0.69	0.00	0.00	0.00	0.00	1.00
² INT5_{B,C6-exo}	0.92	-0.05	0.00		0.14			0.00	0.00	0.00	0.00	0.00	1.00

⁴ TS4 _{B,C6-exo}	1.38	-0.08	-0.03	0.72		0.24	0.76		0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C6-exo}	1.38	-0.08	-0.03	0.72		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C6-exo}	1.45	-0.08	-0.02		0.69			0.97	0.00	0.00	0.00	0.00	3.00
⁴ INT5 _{B,C6-exo}	2.76	0.22	-0.08		0.10			0.00	0.00	0.00	0.00	0.00	3.00
Pathway C6-HAT:													
² TS6 _{B,HAT}	1.21	-0.07	-0.02		0.57	-0.96	0.27		0.00	0.00	0.00	0.00	1.00
⁴ TS6 _{B,HAT}	1.20	-0.05	0.00		0.61	0.96	0.28		0.00	0.00	0.00	0.00	3.00
⁴ Int6 _{B,HAT}	0.99	-0.04	0.02		0.25	0.96	0.82		0.00	0.00	0.00	0.00	3.00

Charges:

Species	Fe	Porp	SH	O	OH	NO2	Subs	Subs(NO ₂)	Lig1	Arg	PheGlu	Tyr	Total
ver1:													
² Re _B	0.33	-1.08	-0.23	-0.35		-0.28	0.11		0.51	0.71	-0.65	-0.06	-1.00
² TS1 _B	0.40	-1.01	-0.34	-0.32		-0.28	0.02		0.52	0.69	-0.63	-0.06	-1.00
² Int1 _B	0.43	-0.90	-0.46	-0.49		-0.19	0.08		0.51	0.72	-0.65	-0.06	-1.00
⁴ Re _B	0.47	-1.01	-0.40	-0.38		-0.29	0.11		0.51	0.71	-0.65	-0.06	-1.00
⁴ TS1 _B	0.49	-0.94	-0.37	-0.40		-0.32	0.02		0.52	0.69	-0.63	-0.06	-1.00
⁴ Int1 _B	0.43	-0.94	-0.48	-0.48		-0.14	0.05		0.53	0.70	-0.65	-0.02	-1.00
Pathway C6-endo:													
² TS4 _{B,C6-endo}	0.42	-1.05	-0.44	-0.51		0.00	0.06		0.49	0.70	-0.61	-0.06	-1.00
² Int4 _{B,C6-endo}	0.42	-1.05	-0.44	-0.51				0.06	0.49	0.70	-0.61	-0.06	-1.00
² TS5 _{B,C6-endo}	0.40	-1.15	-0.43		-0.29			-0.02	0.51	0.71	-0.62	-0.10	-1.00
² INT5 _{B,C6-endo}	0.44	-1.11	-0.55		-0.33			0.06	0.46	0.74	-0.65	-0.05	-1.00
⁴ TS4 _{B,C6-endo}	0.42	-1.05	-0.44	-0.51		0.00	0.06		0.49	0.70	-0.61	-0.06	-1.00
⁴ Int4 _{B,C6-endo}	0.42	-1.05	-0.44	-0.51				0.06	0.49	0.70	-0.61	-0.06	-1.00
⁴ TS5 _{B,C6-endo}	0.48	-1.01	-0.38		-0.28			-0.31	0.51	0.71	-0.62	-0.10	-1.00
⁴ INT5 _{B,C6-endo}	0.55	-1.10	-0.68		-0.41			0.09	0.52	0.74	-0.68	-0.02	-1.00
Pathway C6-exo:													
² TS4 _{B,C6-exo}	0.44	-1.01	-0.39	-0.56		-0.30	0.31		0.51	0.69	-0.65	-0.04	-1.00
² Int4 _{B,C6-exo}	0.44	-1.01	-0.39	-0.56		0.00	0.02		0.51	0.69	-0.65	-0.04	-1.00
² TS5 _{B,C6-exo}	0.41	-1.09	-0.41		-0.22			-0.27	0.59	0.69	-0.61	-0.08	-1.00
² INT5 _{B,C6-exo}	0.30	-1.17	-0.46		-0.26			0.00	0.59	0.69	-0.60	-0.08	-1.00
⁴ TS4 _{B,C6-exo}	0.44	-1.01	-0.39	-0.56		-0.33	0.34		0.51	0.69	-0.65	-0.04	-1.00
⁴ Int4 _{B,C6-exo}	0.44	-1.01	-0.39	-0.56		0.00	0.00		0.51	0.70	-0.65	-0.03	-1.00
⁴ TS5 _{B,C6-exo}	0.44	-1.01	-0.38		-0.21			-0.42	0.58	0.69	-0.61	-0.08	-1.00

⁴ INT5 _{B,C6-exo}	0.42	-1.38	-0.39		-0.25		0.01	0.59	0.69	-0.60	-0.08	-1.00	
Pathway C6-HAT:													
² TS6 _{B,HAT}	0.41	-1.07	-0.37		-0.26	-0.03	-0.18		0.50	0.69	-0.64	-0.06	-1.00
⁴ TS6 _{B,HAT}	0.41	-1.07	-0.37		-0.26	-0.03	-0.18		0.50	0.69	-0.64	-0.06	-1.00
⁴ Int6 _{B,HAT}	0.28	-1.14	-0.33		-0.30	-0.05	0.04		0.50	0.69	-0.64	-0.05	-1.00

Table S15: Group spin densities and charges of local minima and transition states for Pathway 2-C6 as calculated with B3LYP/BS2 with model B in Gaussian-09.

Spin densities:

Species	ρ_{Fe}	ρ_{Porp}	ρ_{SH}	ρ_{O}	ρ_{OH}	ρ_{NO_2}	ρ_{Subs}	$\rho_{\text{Subs(No}_2)}$	ρ_{Lig1}	ρ_{Arg}	ρ_{PheGlu}	ρ_{Tyr}	ρ_{Total}
ver1:													
² Re_B	1.16	-0.19	-0.01	0.04		0.00	0.00		0.00	0.00	0.00	0.00	1.00
² TS1_B	1.54	-0.23	-0.03	0.06		-0.34	0.00		0.00	0.00	0.00	0.00	1.00
² Int1_B	1.41	-0.21	-0.03	0.83		-0.98	-0.02		0.00	0.00	0.00	0.00	1.00
⁴ Re_B	3.01	-0.32	0.20	0.10		0.02	0.00		0.00	0.00	0.00	0.00	3.00
⁴ TS1_B	2.40	-0.26	0.21	0.37		0.28	0.00		0.00	0.00	0.00	0.00	3.00
⁴ Int1_B	1.33	0.09	0.01	0.85		0.70	0.01		0.00	0.00	0.00	0.00	3.00
Pathway C6-endo:													
² TS4_{B,C6-endo}	1.44	-0.23	-0.04	0.82		0.00	-1.00		0.00	0.00	0.00	0.00	1.00
² Int4_{B,C6-endo}	1.45	-0.24	-0.04	0.82				-1.00	0.00	0.00	0.00	0.00	1.00
² TS5_{B,C6-endo}	1.48	-0.25	-0.04		0.59	0.00		-0.77	0.00	0.00	0.00	0.00	1.00
² INT5_{B,C6-endo}	1.13	-0.20	-0.01		0.08	0.00		0.00	0.00	0.00	0.00	0.00	1.00
⁴ TS4_{B,C6-endo}	1.44	-0.22	-0.04	0.83		0.00	0.99		0.00	0.00	0.00	0.00	3.00
⁴ Int4_{B,C6-endo}	1.45	-0.22	-0.04	0.82				0.99	0.00	0.00	0.00	0.00	3.00
⁴ TS5_{B,C6-endo}	1.90	-0.27	-0.04		0.57	0.00		0.84	0.00	0.00	0.01	0.00	3.00
⁴ INT5_{B,C6-endo}	2.94	-0.30	0.10		0.26			0.00	0.00	0.00	0.00	0.00	3.00
Pathway C6-exo:													
² TS4_{B,C6-exo}	1.56	-0.28	-0.04	0.77		-0.22	-0.79		0.00	0.00	0.00	0.00	1.00
² Int4_{B,C6-exo}	1.56	-0.28	-0.04	0.77				-1.01	0.00	0.00	0.00	0.00	1.00
² TS5_{B,C6-exo}	1.40	-0.21	-0.03		0.61			-0.76	0.00	-0.01	0.00	0.00	1.00
² INT5_{B,C6-exo}	1.07	-0.16	0.00		0.08			0.00	0.00	0.00	0.00	0.00	1.00

⁴ TS4 _{B,C6-exo}	1.56	-0.27	-0.04	0.77		0.22	0.77		0.00	0.00	-0.01	0.00	3.00
⁴ Int4 _{B,C6-exo}	1.55	-0.27	-0.04	0.77				0.99	0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C6-exo}	1.87	-0.24	-0.04		0.58			0.83	0.00	0.01	0.00	0.00	3.00
⁴ INT5 _{B,C6-exo}	3.09	-0.03	-0.08		0.02			0.00	0.00	0.00	0.00	0.00	3.00
Pathway C6-HAT:													
² TS6 _{B,HAT}	1.18	-0.18	-0.02		0.29	-0.95	0.68		0.00	0.00	0.00	0.00	1.00
⁴ TS6 _{B,HAT}	1.24	-0.18	0.00		0.35	0.95	0.65		0.00	0.00	0.00	0.00	3.00
⁴ Int6 _{B,HAT}	1.17	-0.20	0.00		0.11	0.95	0.98		0.00	0.00	0.00	0.00	3.00

Charges:

Species	Fe	Porp	SH	O	OH	NO2	Subs	Subs(NO ₂)	Lig1	Arg	PheGlu	Tyr	Total
ver1:													
² Re _B	-1.41	0.08	-0.36	-0.22		-0.01	-0.30		1.07	0.93	-0.89	0.12	-1.00
² TS1 _B	-1.79	0.60	-0.33	0.01		-0.40	-0.31		1.09	0.92	-0.93	0.14	-1.00
² Int1 _B	-2.70	1.37	-0.49	0.13		-0.18	-0.40		1.05	0.94	-0.87	0.15	-1.00
⁴ Re _B	-1.01	0.16	-0.70	-0.29		-0.07	-0.29		1.07	0.93	-0.90	0.12	-1.00
⁴ TS1 _B	-2.13	0.74	-0.42	0.17		-0.26	-0.30		1.08	0.93	-0.93	0.13	-1.00
⁴ Int1 _B	-2.68	1.38	-0.50	0.13		-0.17	-0.39		1.02	0.94	-0.86	0.14	-1.00
Pathway C6-endo:													
² TS4 _{B,C6-endo}	-3.69	1.97	-0.41	0.14		0.00	-0.34		1.05	1.06	-0.80	0.03	-1.00
² Int4 _{B,C6-endo}	-3.66	1.94	-0.43	0.16				-0.35	1.05	1.06	-0.80	0.03	-1.00
² TS5 _{B,C6-endo}	-3.97	2.43	-0.27		0.83			-1.04	0.90	0.95	-0.84	0.01	-1.00
² INT5 _{B,C6-endo}	-2.80	1.17	-0.38		0.14			-0.14	0.85	0.97	-0.86	0.05	-1.00
⁴ TS4 _{B,C6-endo}	-3.67	1.96	-0.41	0.13		0.00	-0.34		1.05	1.06	-0.80	0.03	-1.00
⁴ Int4 _{B,C6-endo}	-3.63	1.93	-0.43	0.15				-0.35	1.05	1.06	-0.80	0.03	-1.00
⁴ TS5 _{B,C6-endo}	-2.76	1.44	-0.53		1.11			-1.27	0.89	0.94	-0.84	0.01	-1.00
⁴ INT5 _{B,C6-endo}	-2.44	1.36	-0.82		0.09			-0.19	0.85	0.96	-0.86	0.05	-1.00
Pathway C6-exo:													
² TS4 _{B,C6-exo}	-4.76	2.94	-0.21	0.28		-0.21	-0.12		1.01	0.91	-0.97	0.13	-1.00
² Int4 _{B,C6-exo}	-4.70	2.89	-0.22	0.27				-0.32	1.01	0.92	-0.97	0.11	-1.00
² TS5 _{B,C6-exo}	-2.67	1.30	-0.50		0.74			-0.72	0.76	0.91	-0.86	0.04	-1.00
² INT5 _{B,C6-exo}	-0.75	-0.35	-0.53		-0.29			-0.12	0.99	0.92	-0.88	0.00	-1.00
⁴ TS4 _{B,C6-exo}	-4.76	2.94	-0.21	0.28		-0.21	-0.12		1.01	0.91	-0.97	0.13	-1.00
⁴ Int4 _{B,C6-exo}	-4.56	2.79	-0.23	0.25				-0.34	1.02	0.89	-0.96	0.13	-1.00
⁴ TS5 _{B,C6-exo}	-2.35	1.03	-0.63		1.02			-0.89	0.74	0.91	-0.85	0.02	-1.00

⁴ INT5 _{B,C6-exo}	-0.96	-0.23	-0.43		-0.29		0.00	-0.12	0.99	0.92	-0.88	-1.00	
Pathway C6-HAT:													
² TS6 _{B,HAT}	-3.77	1.92	-0.27		0.54	0.02	-0.72		1.08	0.97	-0.91	0.13	-1.00
⁴ TS6 _{B,HAT}	-3.68	1.85	-0.28		0.53	0.03	-0.73		1.09	0.97	-0.90	0.13	-1.00
⁴ Int6 _{B,HAT}	-3.42	1.53	-0.27		0.25	0.07	-0.43		1.01	1.00	-0.90	0.14	-1.00

Table S16: Absolute (free) energies (in au) of local minima and transition states for Pathway2-C7 as calculated with B3LYP with model B in Gaussian-09.

Model B-C7	E [au]	ZPE [au]	G [au]	E [au]	E _{disp} [au]
	[BS1,au]	[BS1,au]	[BS1,au]	[BS2,au]	[BS2,au]
Pathway C7-endo:					
² TS4 _{B,C7-endo}	-6677.062341	2.049647	-6675.215334	-6678.808421	0.378834
² Int4 _{B,C7-endo}	-6677.063349	2.050901	-6675.215431	-6678.810591	0.375916
² TS5 _{B,C7-endo}	-6677.054162	2.046256	-6675.197569	-6678.800674	0.378810
² IntT5 _{B,C7-endo}	-6677.154592	2.052069	-6675.297970	-6678.900018	0.372764
⁴ TS4 _{B,C7-endo}	-6677.062340	2.049648	-6675.215989	-6678.808421	0.378830
⁴ Int4 _{B,C7-endo}	-6677.063344	2.050931	-6675.215805	-6678.807858	0.378635
⁴ TS5 _{B,C7-endo}	-6677.046995	2.045581	-6675.195629	-6678.796661	0.377391
⁴ Int5 _{B,C7-endo}	-6677.100191	2.049187	-6675.247700	-6678.849771	0.374099
Pathway C7-exo:					
² TS4 _{B,C7-exo}	-6677.056131	2.049153	-6675.205757	-6678.807375	0.391421
² Int4 _{B,C7-exo}	-6677.060800	2.050269	-6675.212555	-6678.807174	0.375421
² TS5 _{B,C7-exo}	-6677.055390	2.046149	-6675.210541	-6678.798992	0.384971
² Int5 _{B,C7-exo}	-6677.158151	2.051257	-6675.307672	-6678.905440	0.371572
⁴ TS4 _{B,C7-exo}	-6677.056228	2.049165	-6675.206540	-6678.806294	0.392233
⁴ Int4 _{B,C7-exo}	-6677.060800	2.050276	-6675.213204	-6678.807165	0.375439
⁴ TS5 _{B,C7-exo}	-6677.049122	2.044940	-6675.203878	-6678.795031	0.384971
⁴ Int5 _{B,C7-exo}	-6677.144509	2.049105	-6675.295677	-6678.895719	0.374360

Table S17: Relative (free) energies (in kcal mol⁻¹) of local minima and transition states for Pathway2-C7 as calculated with B3LYP with model B in Gaussian-09.

Model B-C7	ΔE	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$	ΔG	ΔE_d+ZPE
	BS1	BS1	BS1	BS2	BS2	BS2	BS2
Pathway C7-endo:							
² TS4 _{B,C7-endo}	-0.89	-0.78	-1.88	-1.10	-0.99	-2.09	1.00
² Int4 _{B,C7-endo}	-1.52	-0.63	-1.94	-2.46	-1.56	-2.88	-2.19
² TS5 _{B,C7-endo}	4.24	2.23	9.27	3.76	1.75	8.79	5.85
² Int5 _{B,C7-endo}	-58.78	-57.15	-53.73	-58.58	-56.95	-53.53	-60.29
⁴ TS4 _{B,C7-endo}	-0.89	-0.78	-2.29	-1.10	-0.99	-2.50	1.00
⁴ Int4 _{B,C7-endo}	-1.52	-0.60	-2.17	-0.75	0.17	-1.40	1.23
⁴ TS5 _{B,C7-endo}	8.74	6.30	10.49	6.28	3.84	8.03	7.47
⁴ Int5 _{B,C7-endo}	-24.64	-24.82	-22.19	-27.05	-27.22	-24.59	-27.92
Pathway C7-exo:							
² TS4 _{B,C7-exo}	3.01	2.81	4.13	-0.44	-0.64	0.68	9.56
² Int4 _{B,C7-exo}	0.08	0.58	-0.13	-0.32	0.19	-0.53	-0.36
² TS5 _{B,C7-exo}	3.47	1.39	1.13	4.82	2.73	2.48	10.77
⁴ Int5 _{B,C7-exo}	-61.01	-59.89	-59.82	-61.98	-60.86	-60.79	-64.44
⁴ TS4 _{B,C7-exo}	2.94	2.75	3.64	0.24	0.04	0.93	10.74
⁴ Int4 _{B,C7-exo}	0.08	0.58	-0.54	-0.31	0.20	-0.93	-0.34
⁴ TS5 _{B,C7-exo}	7.40	4.56	5.31	7.30	4.46	5.21	10.41
⁴ Int5 _{B,C7-exo}	-52.45	-52.68	-52.29	-55.88	-56.11	-55.72	-56.82

Table S18: Group spin densities and charges of local minima and transition states for Pathway2-C7 as calculated with B3LYP/BS1 with model B in Gaussian-09.

Spin density:

Species	ρ_{Fe}	ρ_{Porp}	ρ_{SH}	ρ_{O}	ρ_{OH}	ρ_{NO_2}	ρ_{Subs}	$\rho_{\text{Subs}(\text{NO}_2)}$	ρ_{Lig1}	ρ_{Arg}	ρ_{PheGlu}	ρ_{Tyr}	ρ_{Total}
Pathway C7-endo:													
² TS4 _{B,C7-endo}	1.27	-0.07	-0.02	0.82				-1.00	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C7-endo}	1.28	-0.07	-0.03	0.81				-0.99	0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C7-endo}	1.24	-0.07	-0.02		0.63	0.00		-0.78	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C7-endo}	0.90	-0.05	-0.01		0.17	0.00		-0.01	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C7-endo}	1.27	-0.07	-0.02	0.82				0.00	1.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C7-endo}	1.28	-0.07	-0.02	0.81				1.00	0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C7-endo}	1.51	-0.09	-0.03		0.59	0.00		1.02	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C7-endo}	0.93	1.56	0.10		0.11			0.30	0.00	0.00	0.00	0.00	3.00
Pathway C7-exo:													
² TS4 _{B,C7-exo}	1.27	-0.07	-0.02	0.82		0.00	-1.00		0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C7-exo}	1.27	-0.07	-0.02	0.82		0.00	-1.00		0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C7-exo}	1.11	-0.05	-0.01		0.49			-0.54	0.00	0.00	0.00	0.00	1.00
⁴ Int5 _{B,C7-exo}	1.17	-0.07	-0.11		0.00			0.00	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C7-exo}	1.27	-0.07	-0.02	0.82		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C7-exo}	1.23	-0.06	-0.02	0.84		0.00	1.01		0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C7-exo}	1.62	-0.10	-0.01		0.48			1.01	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C7-exo}	2.60	-0.03	0.18		0.24			0.02	0.00	0.00	0.00	0.00	3.00

Charge :

Species	Fe	Porp	SH	O	OH	NO2	Subs	Subs(NO ₂)	Lig1	Arg	PheGlu	Tyr	Total
² TS4 _{B,C7-endo}	0.42	-1.05	-0.44	-0.50				0.07	0.50	0.70	-0.62	-0.08	-1.00
² Int5 _{B,C7-endo}	0.43	-1.06	-0.44	-0.51				0.07	0.49	0.69	-0.61	-0.06	-1.00
² TS5 _{B,C7-endo}	0.41	-1.08	-0.38		-0.42			-0.04	0.50	0.71	-0.62	-0.07	-1.00
² Int5 _{B,C7-endo}	0.38	-1.18	-0.49		-0.51			0.29	0.50	0.70	-0.62	-0.07	-1.00
⁴ TS4 _{B,C7-endo}	0.42	-1.05	-0.44	-0.50				0.07	0.50	0.70	-0.62	-0.08	-1.00
⁴ Int5 _{B,C7-endo}	0.43	-1.05	-0.46	-0.50				0.08	0.50	0.69	-0.62	-0.07	-1.00
⁴ TS5 _{B,C7-endo}	0.44	-1.00	-0.35		-0.43			-0.17	0.50	0.71	-0.62	-0.07	-1.00
⁴ Int5 _{B,C7-endo}	0.32	-1.00	-0.30		-0.56			0.04	0.48	0.70	-0.62	-0.06	-1.00
² TS4 _{B,C7-exo}	0.42	-1.05	-0.44	-0.50		0.00	0.07		0.50	0.70	-0.62	-0.08	-1.00
² Int5 _{B,C7-exo}	0.41	-1.04	-0.47	-0.49				0.10	0.50	0.69	-0.64	-0.07	-1.00
² TS5 _{B,C7-exo}	0.40	-1.11	-0.39		-0.48			0.09	0.49	0.71	-0.64	-0.06	-1.00
² Int5 _{B,C7-exo}	0.43	-1.13	-0.48		-0.58			0.26	0.50	0.71	-0.63	-0.07	-1.00
⁴ TS4 _{B,C7-exo}	0.42	-1.05	-0.44	-0.50				0.07	0.50	0.70	-0.62	-0.08	-1.00
⁴ Int5 _{B,C7-exo}	0.42	-1.07	-0.49	-0.46				0.10	0.50	0.69	-0.63	-0.07	-1.00
⁴ TS5 _{B,C7-exo}	0.45	-0.96	-0.31		-0.49			-0.17	0.48	0.71	-0.64	-0.06	-1.00
⁴ Int5 _{B,C7-exo}	0.45	-1.15	-0.43		-0.63			0.24	0.50	0.71	-0.62	-0.07	-1.00

Table S19: Group spin densities and charges of local minima and transition states for Pathway2-C7 as calculated with B3LYP/BS2 with model B in Gaussian-09.

Spin density:

Species	ρ_{Fe}	ρ_{Porp}	ρ_{SH}	ρ_{O}	ρ_{OH}	ρ_{NO_2}	ρ_{Subs}	$\rho_{\text{Subs}(\text{NO}_2)}$	ρ_{Lig1}	ρ_{Arg}	ρ_{PheGlu}	ρ_{Tyr}	ρ_{Total}
Pathway C7-endo:													
² TS4 _{B,C7-endo}	1.43	-0.23	-0.03	0.83				-1.00	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C7-endo}	1.42	-0.22	-0.03	0.82				-0.99	0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C7-endo}	1.50	-0.25	-0.04		0.66	0.00		-0.87	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C7-endo}	1.11	-0.18	0.00		0.08	0.00		-0.01	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C7-endo}	1.42	-0.22	-0.03	0.83				0.00	1.01	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C7-endo}	1.41	-0.20	-0.03	0.82				1.00	0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C7-endo}	1.90	-0.28	-0.05		0.51	0.00		0.91	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C7-endo}	0.97	0.79	0.13		0.12			0.98	0.00	0.00	0.00	0.00	3.00
Pathway C7-exo:													
² TS4 _{B,C7-exo}	1.55	-0.27	-0.04	0.77		0.00	-1.01		0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C7-exo}	1.42	-0.23	-0.03	0.83		0.00	-0.99		0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C7-exo}	1.53	-0.27	-0.04		0.68			-0.89	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C7-exo}	1.19	-0.20	-0.06		0.07			0.00	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C7-exo}	1.55	-0.27	-0.04	0.78		0.00	0.99		0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C7-exo}	1.40	-0.21	-0.03	0.84		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C7-exo}	1.72	-0.30	-0.04		0.62			1.00	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C7-exo}	2.99	-0.32	0.14		0.20			0.00	0.00	0.00	0.00	0.00	3.00

Charge :

Species	Fe	Porp	SH	O	OH	NO2	Subs	Subs(NO ₂)	Lig1	Arg	PheGlu	Tyr	Total
Pathway C7-endo:													
² TS4 _{B,C7-endo}	-2.72	1.21	-0.42	-0.12				-0.10	0.96	1.02	-0.84	0.03	-1.00
² Int5 _{B,C7-endo}	-2.60	1.11	-0.47	-0.09				-0.09	0.96	1.01	-0.86	0.03	-1.00
² TS5 _{B,C7-endo}	-3.89	2.00	-0.27		0.72			-0.75	1.01	1.04	-0.88	0.03	-1.00
² Int5 _{B,C7-endo}	-2.02	0.44	-0.43		0.07			-0.22	0.99	1.01	-0.85	0.00	-1.00
⁴ TS4 _{B,C7-endo}	-2.72	1.21	-0.42	-0.12				-0.10	0.96	1.02	-0.84	0.03	-1.00
⁴ Int5 _{B,C7-endo}	-2.60	1.11	-0.47	-0.09				-0.09	0.95	1.01	-0.86	0.03	-1.00
⁴ TS5 _{B,C7-endo}	-3.61	1.88	-0.37		0.75			-0.83	1.02	1.03	-0.89	0.03	-1.00
⁴ Int5 _{B,C7-endo}	-2.08	1.15	-0.27		0.12			-1.03	0.96	1.00	-0.86	0.01	-1.00
Pathway C7-exo:													
² TS4 _{B,C7-exo}	-4.89	3.00	-0.22	0.30		0.00	-0.32		1.01	0.87	-0.91	0.17	-1.00
² Int5 _{B,C7-exo}	-2.66	1.18	-0.43	-0.13				-0.12	0.96	1.02	-0.84	0.03	-1.00
² TS5 _{B,C7-exo}	-4.06	2.28	-0.30		0.87			-0.61	0.80	0.94	-0.97	0.05	-1.00
² Int5 _{B,C7-exo}	-2.87	1.18	-0.49		0.32			-0.19	0.99	0.89	-0.89	0.05	-1.00
⁴ TS4 _{B,C7-exo}	-4.80	2.91	-0.23	0.29				-0.32	1.01	0.85	-0.90	0.19	-1.00
⁴ Int5 _{B,C7-exo}	-3.17	1.58	-0.43	0.06				-0.12	0.93	1.01	-0.88	0.03	-1.00
⁴ TS5 _{B,C7-exo}	-4.15	2.40	-0.27		0.88			-0.69	0.80	0.94	-0.97	0.05	-1.00
⁴ Int5 _{B,C7-exo}	-2.71	1.49	-0.70		0.05			-0.19	0.95	0.92	-0.87	0.05	-1.00

Table S20: Absolute (free) energies (in au) of local minima and transition states for Pathway2-C5 as calculated with B3LYP with model B in Gaussian-09.

Model B-C5	E [au]	ZPE [au]	G [au]	E [au]	E _{disp} [au]
	[BS1,au]	[BS1,au]	[BS1,au]	[BS2,au]	[BS2,au]
Pathway C5-endo:					
² TS4 _{B,C5-endo}	-6677.067924	2.050186	-6675.222340	-6678.814867	0.378108
² Int4 _{B,C5-endo}	-6677.055504	2.050010	-6675.206135	-6678.802865	0.370146
² TS5 _{B,C5-endo}	-6677.045160	2.046361	-6675.198212	-6678.790277	0.382804
² Int5 _{B,C5-endo}	-6677.155874	2.051765	-6675.306932	-6678.900861	0.374702
⁴ TS4 _{B,C5-endo}	-6677.067899	2.050205	-6675.222560	-6678.814824	0.378121
⁴ Int4 _{B,C5-endo}	-6677.067903	2.050629	-6675.222416	-6678.814570	0.378035
⁴ TS5 _{B,C5-endo}	-6677.037375	2.045225	-6675.190434	-6678.785973	0.382386
⁴ Int5 _{B,C5-endo}	-6677.098254	2.047838	-6675.254273	-6678.842613	0.375013
Pathway C5-exo:					
² TS4 _{B,C5-exo}	-6677.052930	2.049042	-6675.205705	-6678.804892	0.388247
² Int4 _{B,C5-exo}	-6677.052982	2.049708	-6675.204256	-6678.807859	0.384344
² TS5 _{B,C5-exo}	-6677.029995	2.044736	-6675.183591	-6678.774948	0.398334
² Int5 _{B,C5-exo}	-6677.143645	2.050014	-6675.292919	-6678.886361	0.390455
⁴ TS4 _{B,C5-exo}	-6677.052943	2.049062	-6675.206010	-6678.804888	0.388357
⁴ Int4 _{B,C5-exo}	-6677.052994	2.049684	-6675.205287	-6678.806894	0.385366
⁴ TS5 _{B,C5-exo}	-6677.025573	2.043977	-6675.179482	-6678.772649	0.396828
⁴ Int5 _{B,C5-exo}	-6677.086070	2.045920	-6675.241170	-6678.828365	0.390307

Table S21: Relative (free) energies (in kcal mol⁻¹) of local minima and transition states for Pathway2-C5 as calculated with B3LYP with model B in Gaussian-09.

Model B-C5	ΔE	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$	ΔG
	BS1	BS1	BS1	BS2	BS2	BS2
Pathway C5-endo:						
² TS4 _{B,C5-endo}	-4.39	-3.94	-6.28	-5.14	-4.69	-7.02
² Int4 _{B,C5-endo}	3.40	3.74	3.89	2.39	2.73	2.88
² TS5 _{B,C5-endo}	9.89	7.94	8.87	10.29	8.34	9.26
² Int5 _{B,C5-endo}	-59.58	-58.14	-59.36	-59.11	-57.67	-58.88
⁴ TS4 _{B,C5-endo}	-4.38	-3.92	-6.41	-5.12	-4.66	-7.15
⁴ Int4 _{B,C5-endo}	-4.38	-3.65	-6.32	-4.96	-4.23	-6.90
⁴ TS5 _{B,C5-endo}	14.78	12.11	13.75	12.99	10.32	11.96
⁴ Int5 _{B,C5-endo}	-23.43	-24.45	-26.31	-22.55	-23.58	-25.44
Pathway C5-exo:						
² TS4 _{B,C5-exo}	5.01	4.75	4.16	1.12	0.85	0.26
² Int4 _{B,C5-exo}	4.98	5.13	5.07	-0.75	-0.60	-0.66
² TS5 _{B,C5-exo}	19.41	16.44	18.04	19.91	16.94	18.54
² Int5 _{B,C5-exo}	-51.91	-51.57	-50.56	-50.01	-49.66	-48.66
⁴ TS4 _{B,C5-exo}	5.01	4.75	3.97	1.12	0.86	0.08
⁴ Int4 _{B,C5-exo}	4.97	5.11	4.43	-0.14	-0.01	-0.69
⁴ TS5 _{B,C5-exo}	22.18	18.73	20.62	21.35	17.90	19.79
⁴ Int5 _{B,C5-exo}	-15.78	-18.01	-18.09	-13.61	-15.84	-15.92

Table S22: Group spin densities and charges of local minima and transition states for Pathway2-C5 as calculated with B3LYP/BS1 with model B in Gaussian-09.

Spin density:

Species	ρ_{Fe}	ρ_{Porp}	ρ_{SH}	ρ_{O}	ρ_{OH}	ρ_{NO_2}	ρ_{Subs}	$\rho_{\text{Subs}(\text{NO}_2)}$	ρ_{Lig1}	ρ_{Arg}	ρ_{PheGlu}	ρ_{Tyr}	ρ_{Total}
Pathway C5-endo:													
² TS4 _{B,C5-endo}	1.35	-0.08	-0.02	0.75		0.00	-1.00		0.00	0.00	0.00	0.00	1.00
² Int4 _{B,C5-endo}	1.06	-0.07	-0.01	1.02				-1.00	0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C5-endo}	1.00	-0.05	-0.02		0.53			-0.46	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C5-endo}	0.90	-0.05	0.00		0.16	0.00		-0.01	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C5-endo}	1.36	-0.08	-0.02	0.75		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C5-endo}	1.06	-0.07	-0.01	1.02				1.00	0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C5-endo}	1.55	-0.09	-0.04		0.58			0.99	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C5-endo}	0.94	1.87	0.09		0.10			0.01	0.00	0.00	0.00	0.00	3.00
Pathway C5-exo:													
² TS4 _{B,C5-exo}	1.38	-0.08	-0.03	0.72		0.00	-1.00		0.00	0.00	0.00	0.00	1.00
² Int4 _{B,C5-exo}	1.38	-0.08	-0.03	0.72				-1.00	0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C5-exo}	1.21	-0.06	-0.02		0.68			-0.81	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C5-exo}	0.96	-0.06	-0.01		0.11			0.00	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C5-exo}	1.38	-0.08	-0.03	0.72		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C5-exo}	1.38	-0.08	-0.03	0.72				1.00	0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C5-exo}	1.78	-0.10	-0.02		0.49			0.84	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C5-exo}	0.92	1.87	0.09		0.12			0.00	0.00	0.00	0.00	0.00	3.00

Charge:

Species	Fe	Porp	SH	O	OH	NO2	Subs	Subs(NO ₂)	Lig1	Arg	PheGlu	Tyr	Total
Pathway C5-endo:													
² TS4 _{B,C5-endo}	0.44	-1.02	-0.40	-0.55		0.00	0.05		0.47	0.70	-0.64	-0.05	-1.00
² Int4 _{B,C5-endo}	0.34	-1.15	-0.35	-0.46				0.09	0.51	0.69	-0.61	-0.06	-1.00
² TS5 _{B,C5-endo}	0.37	-1.16	-0.46		-0.41			0.16	0.51	0.71	-0.63	-0.09	-1.00
² Int5 _{B,C5-endo}	0.39	-1.19	-0.49		-0.54			0.34	0.49	0.70	-0.61	-0.08	-1.00
⁴ TS4 _{B,C5-endo}	0.44	-1.02	-0.40	-0.55		0.00	0.05		0.47	0.70	-0.64	-0.05	-1.00
⁴ Int4 _{B,C5-endo}	0.34	-1.15	-0.35	-0.46				0.09	0.51	0.69	-0.61	-0.06	-1.00
⁴ TS5 _{B,C5-endo}	0.44	-0.99	-0.36		-0.41			-0.17	0.51	0.71	-0.64	-0.09	-1.00
⁴ Int5 _{B,C5-endo}	0.32	-1.24	-0.31		-0.51			0.24	0.49	0.69	-0.62	-0.06	-1.00
Pathway C5-exo:													
² TS4 _{B,C5-exo}	0.44	-1.01	-0.39	-0.56		0.00	0.02		0.50	0.69	-0.66	-0.04	-1.00
² Int4 _{B,C5-exo}	0.44	-1.01	-0.39	-0.56				0.02	0.50	0.69	-0.65	-0.04	-1.00
² TS5 _{B,C5-exo}	0.41	-1.08	-0.40		-0.38			-0.04	0.52	0.69	-0.64	-0.07	-1.00
² Int5 _{B,C5-exo}	0.31	-1.18	-0.42		-0.56			0.34	0.53	0.69	-0.64	-0.07	-1.00
⁴ TS4 _{B,C5-exo}	0.44	-1.01	-0.39	-0.56		0.00	0.02		0.50	0.69	-0.66	-0.04	-1.00
⁴ Int4 _{B,C5-exo}	0.44	-1.01	-0.39	-0.56				0.02	0.50	0.69	-0.65	-0.04	-1.00
⁴ TS5 _{B,C5-exo}	0.49	-1.03	-0.42		-0.44			-0.09	0.52	0.69	-0.65	-0.07	-1.00
⁴ Int5 _{B,C5-exo}	0.28	-1.25	-0.30		-0.54			0.30	0.52	0.68	-0.62	-0.07	-1.00

Table S23: Group spin densities and charges of local minima and transition states for Pathway2-C5 as calculated with B3LYP/BS2 with model B in Gaussian-09.

Spin density:

Species	ρ_{Fe}	ρ_{Porp}	ρ_{SH}	ρ_{O}	ρ_{OH}	ρ_{NO_2}	ρ_{Subs}	$\rho_{\text{Subs}(\text{NO}_2)}$	ρ_{Lig1}	ρ_{Arg}	ρ_{PheGlu}	ρ_{Tyr}	ρ_{Total}
Pathway C5-endo:													
² TS4 _{B,C5-endo}	1.46	-0.21	-0.03	0.79		0.00	-1.00		0.00	0.00	-0.01	0.00	1.00
² Int4 _{B,C5-endo}	1.38	-0.17	-0.03	0.82				-0.99	0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C5-endo}	1.00	-0.05	-0.02		0.53			-0.46	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C5-endo}	1.10	-0.18	0.00		0.08	0.00		0.00	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C5-endo}	1.47	-0.22	-0.03	0.79		0.00	0.99		0.00	0.00	0.01	0.00	3.00
⁴ Int4 _{B,C5-endo}	1.38	-0.17	-0.03	0.82				1.00	0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C5-endo}	1.87	-0.29	-0.05		0.55	0.00		0.91	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C5-endo}	0.99	1.83	0.09		0.10			-0.01	0.00	0.00	0.00	0.00	3.00
Pathway C5-exo:													
² TS4 _{B,C5-exo}	1.56	-0.27	-0.04	0.77		0.00	-1.01		0.00	0.00	-0.01	0.00	1.00
² Int4 _{B,C5-exo}	1.55	-0.26	-0.04	0.77				-1.01	0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C5-exo}	1.41	-0.20	-0.03		0.70			-0.89	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C5-exo}	1.09	-0.18	0.01		0.09			-0.01	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C5-exo}	1.57	-0.28	-0.04	0.77		0.00	0.99		0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C5-exo}	1.55	-0.27	-0.04	0.77				0.99	0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C5-exo}	1.86	-0.23	-0.04		0.54			0.87	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C5-exo}	0.92	1.87	0.09		0.12			0.00	0.00	0.00	0.00	0.00	3.00

Charge:

Species	Fe	Porp	SH	O	OH	NO2	Subs	Subs(NO ₂)	Lig1	Arg	PheGlu	Tyr	Total
Pathway C5-endo:													
² TS4 _{B,C5-endo}	-2.73	1.29	-0.50	0.12		0.00	-0.13		0.94	0.93	-0.94	0.03	-1.00
² Int4 _{B,C5-endo}	-1.76	0.47	-0.59	-0.10				-0.28	1.05	1.06	-0.87	0.03	-1.00
² TS5 _{B,C5-endo}	0.37	-1.16	-0.46		-0.41			0.16	0.51	0.71	-0.63	-0.09	-1.00
² Int5 _{B,C5-endo}	-1.83	0.27	-0.48		0.28			-0.54	1.05	1.07	-0.86	0.02	-1.00
⁴ TS4 _{B,C5-endo}	-2.73	1.29	-0.50	0.11		0.00	-0.14		0.94	0.93	-0.94	0.03	-1.00
⁴ Int4 _{B,C5-endo}	-1.75	0.47	-0.60	-0.10				-0.29	1.05	1.06	-0.86	0.03	-1.00
⁴ TS5 _{B,C5-endo}	0.44	-0.99	-0.36		-0.41			-0.17	0.51	0.71	-0.64	-0.09	-1.00
⁴ Int5 _{B,C5-endo}	-1.80	0.17	-0.41		0.29			-0.55	1.06	1.07	-0.86	0.03	-1.00
Pathway C5-exo:													
² TS4 _{B,C5-exo}	-4.79	2.97	-0.20	0.27		0.00	-0.31		1.01	0.92	-0.99	0.12	-1.00
² Int4 _{B,C5-exo}	-4.50	2.74	-0.23	0.26				-0.31	1.01	0.90	-0.99	0.12	-1.00
² TS5 _{B,C5-exo}	-2.34	1.15	-0.59		0.38			-0.30	0.93	0.57	-0.85	0.05	-1.00
² Int5 _{B,C5-exo}	-1.61	0.35	-0.48		0.22			-0.52	0.91	0.91	-0.83	0.04	-1.00
⁴ TS4 _{B,C5-exo}	-4.80	2.98	-0.19	0.27		0.00	-0.31		1.01	0.92	-0.99	0.13	-1.00
⁴ Int4 _{B,C5-exo}	-4.50	2.74	-0.23	0.25				-0.31	1.01	0.90	-0.99	0.12	-1.00
⁴ TS5 _{B,C5-exo}	-3.45	1.99	-0.36		0.54			-0.63	0.93	0.95	-1.00	0.02	-1.00
⁴ Int5 _{B,C5-exo}	0.28	-1.25	-0.30		-0.54			0.30	0.52	0.68	-0.62	-0.07	-1.00

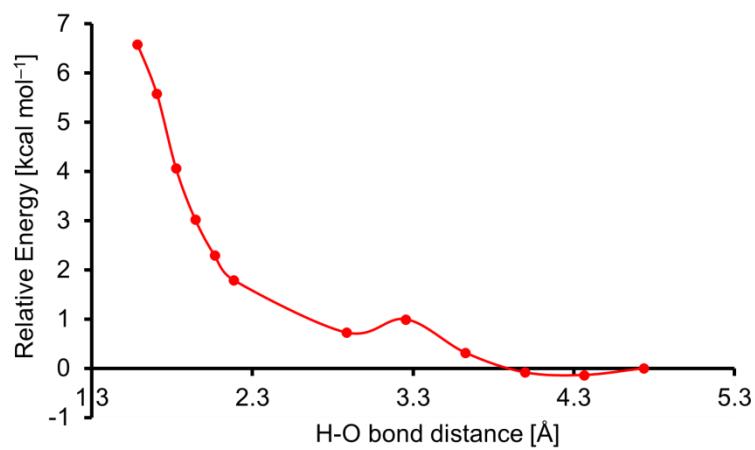


Figure S26: UB3LYP/BS1 geometry scan for proton transfer for Pathway C4-exo between the substrate to apical oxo of P450, as obtained in Gaussian-09. All points refer to a full geometry optimization. Energies are relative to ${}^2\text{Int}4_{\text{C4-oxo}}$.

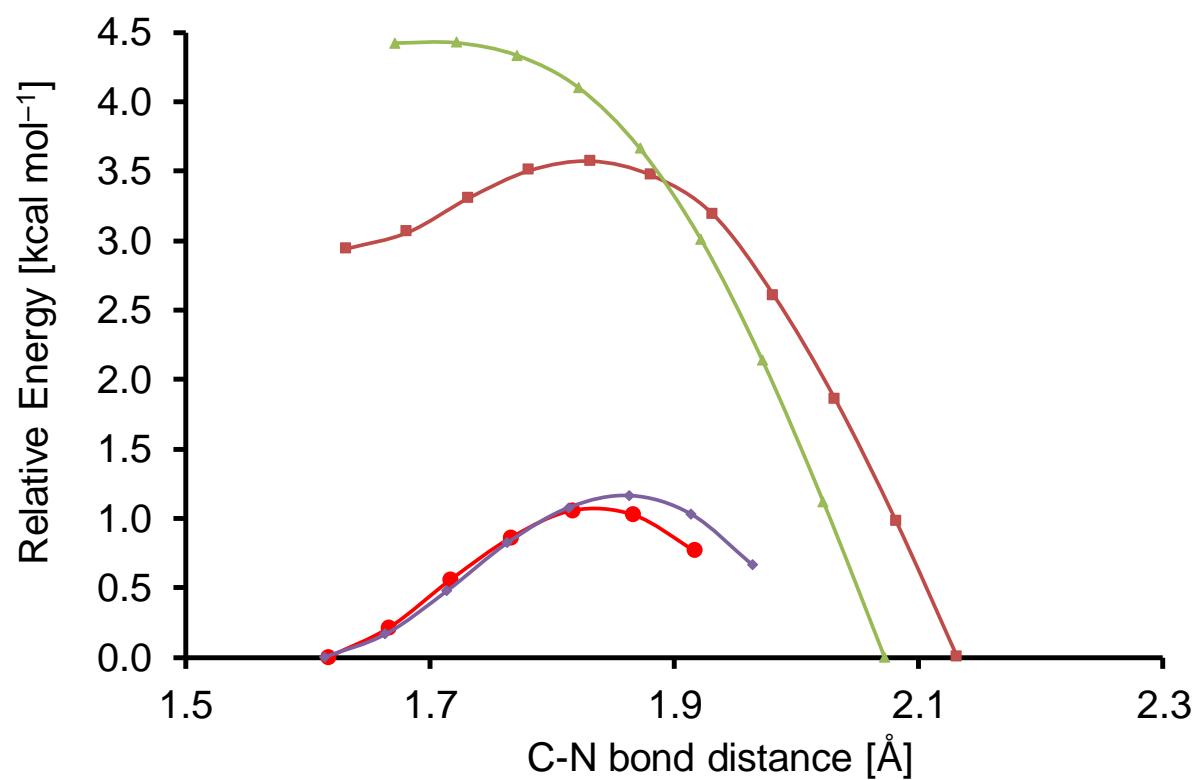


Figure S27: UB3LYP/BS1 geometry scan for NO₂ attack on a carbon position, -C⁴ (in purple), -C⁵ (in green), -C⁶ (in red), -C⁷ (in wine-red), of L-Trp substrate starting from ^{4,2}Int1_B as obtained in Gaussian-09. All points refer to a full geometry optimization. Energies are relative to ²Re..

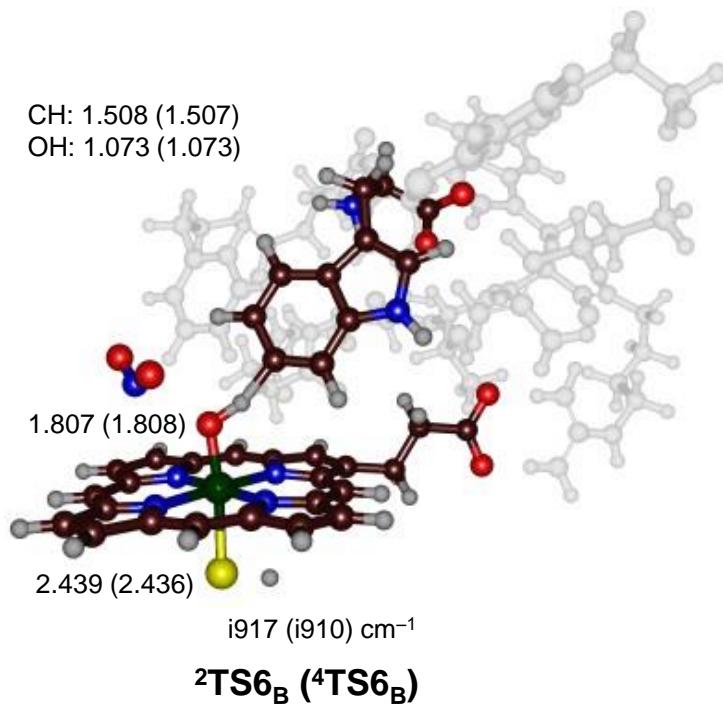


Figure S28: UB3LYP/BS1 optimized geometries of transition states ${}^4,2\text{TS6}_\text{B}$ for direct hydrogen atom abstraction from L-Trp from ${}^4,2\text{Int1}_\text{B}$ as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wavenumbers.

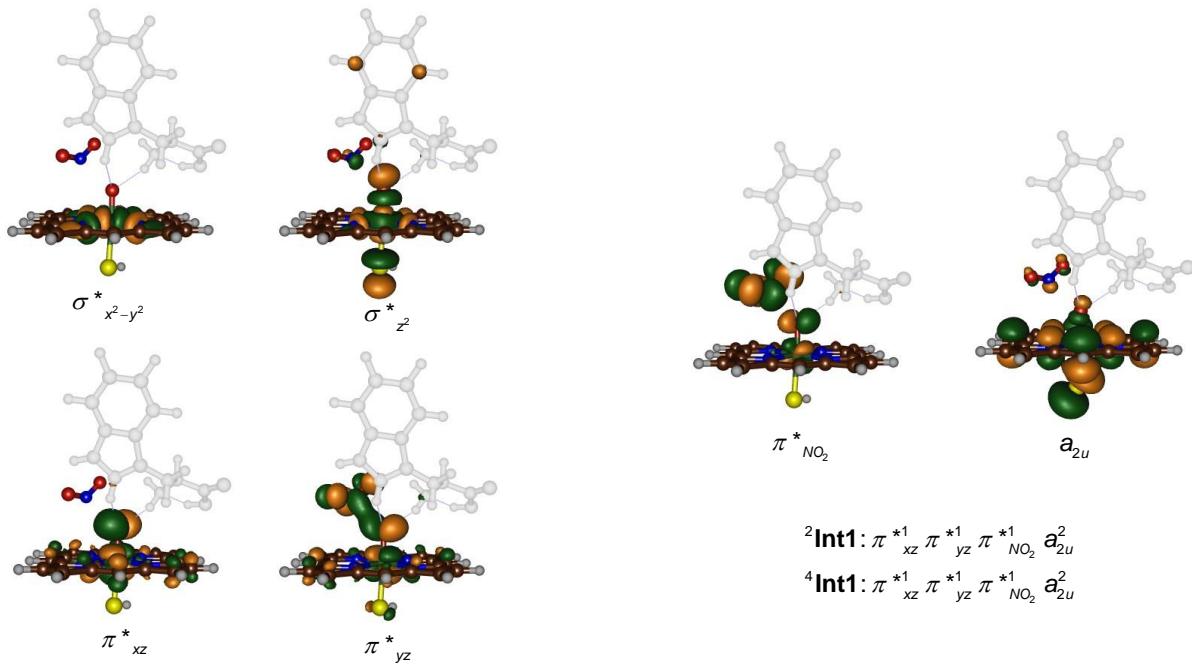


Figure S29: High-lying occupied and low-lying virtual orbitals of ^{4,2}Int1_B as obtained in Gaussian-09.

Table S24: Group spin densities and charges of local minima and transition states for Pathway2-C4 as calculated with B3LYP/BS1 with model B in Gaussian-09.

Spin density:

Species	ρ_{Fe}	ρ_{Porp}	ρ_{SH}	ρ_{O}	ρ_{OH}	ρ_{NO_2}	ρ_{Subs}	$\rho_{\text{Subs}(\text{NO}_2)}$	ρ_{Lig1}	ρ_{Arg}	ρ_{PheGlu}	ρ_{Tyr}	ρ_{Total}
Pathway C4-endo:													
² TS4 _{B,C4-endo}	-0.01	0.00	-0.01	0.01		0.00	1.00		0.00	0.00	0.00	0.00	1.00
² Int4 _{B,C4-endo}	0.00	0.00	-0.01	0.00				0.99	0.00	0.00	0.01	0.00	1.00
² Int4 _{B,C4-rot}	-0.01	0.01	0.00	0.01				0.99	0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C4-endo}	1.00	-0.06	-0.01		0.39	0.00		-0.32	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C4-endo}	0.95	-0.05	-0.01		0.12	0.00		-0.01	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C4-endo}	1.27	-0.07	-0.02	0.82		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C4-endo}	1.27	-0.07	-0.02	0.82				1.00	0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C4-rot}	1.26	-0.06	-0.02	0.83				0.99	0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C4-endo}	2.22	-0.09	0.06		0.26	0.00		0.55	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C4-endo}	0.96	1.85	0.07		0.09			0.02	0.00	0.00	0.00	0.00	3.00
Pathway C4-exo:													
² TS4 _{B,C4-exo}	-0.01	0.00	-0.01	0.01		0.00	1.00		0.00	0.00	0.00	0.00	1.00
² Int4 _{B,C4-exo}	1.27	-0.07	-0.02	0.82				-1.00	0.00	0.00	0.00	0.00	1.00
² Int4 _{B,C4-rot}	-0.06	0.02	-0.03	0.07				1.00	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C4-exo}	0.94	-0.05	-0.01		0.12			0.00	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C4-exo}	1.27	-0.07	-0.02	0.82		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C4-exo}	1.27	-0.07	-0.02	0.82				1.00	0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C4-rot}	1.26	-0.07	-0.02	0.82				1.00	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C4-exo}	0.89	1.68	0.14		0.13			0.16	0.00	0.00	0.00	0.00	3.00

Charge:

Species	Fe	Porp	SH	O	OH	NO2	Subs	Subs(NO ₂)	Lig1	Arg	PheGlu	Tyr	Total
Pathway C4-endo:													
² TS4 _{B,C4-endo}	0.40	-1.03	-0.44	-0.49		0.00	0.06		0.50	0.70	-0.62	-0.08	-1.00
² Int4 _{B,C4-endo}	0.42	-1.04	-0.46	-0.49				0.08	0.50	0.69	-0.63	-0.07	-1.00
² Int4 _{B,C4-rot}	0.38	-1.06	-0.47	-0.48				0.13	0.52	0.71	-0.62	-0.10	-1.00
² TS5 _{B,C4-endo}	0.35	-1.16	-0.38		-0.51			0.21	0.52	0.73	-0.69	-0.08	-1.00
² Int5 _{B,C4-endo}	0.34	-1.16	-0.39		-0.63			0.36	0.52	0.73	-0.69	-0.07	-1.00
⁴ TS4 _{B,C4-endo}	0.41	-1.03	-0.44	-0.50		0.00	0.06		0.50	0.70	-0.62	-0.08	-1.00
⁴ Int4 _{B,C4-endo}	0.42	-1.04	-0.46	-0.49				0.07	0.50	0.70	-0.63	-0.07	-1.00
⁴ Int4 _{B,C4-rot}	0.39	-1.06	-0.47	-0.49				0.13	0.52	0.71	-0.62	-0.10	-1.00
⁴ TS5 _{B,C4-endo}	0.47	-1.05	-0.39		-0.58			0.06	0.52	0.73	-0.68	-0.08	-1.00
⁴ Int5 _{B,C4-endo}	0.27	-1.19	-0.25		-0.62			0.35	0.51	0.74	-0.71	-0.09	-1.00
Pathway C4-exo:													
² TS4 _{B,C4-exo}	0.40	-1.03	-0.44	-0.49		0.00	0.06		0.50	0.70	-0.62	-0.08	-1.00
² Int4 _{B,C4-exo}	0.43	-1.06	-0.46	-0.50				0.11	0.50	0.69	-0.64	-0.07	-1.00
² Int4 _{B,C4-rot}	0.40	-1.06	-0.46	-0.49				0.10	0.54	0.67	-0.60	-0.10	-1.00
² Int5 _{B,C4-exo}	0.36	-1.13	-0.44		-0.62			0.28	0.48	0.73	-0.58	-0.09	-1.00
⁴ TS4 _{B,C4-exo}	0.41	-1.03	-0.44	-0.50		0.00	0.06		0.50	0.70	-0.62	-0.08	-1.00
⁴ Int4 _{B,C4-exo}	0.42	-1.03	-0.46	-0.49				0.10	0.49	0.69	-0.65	-0.07	-1.00
⁴ Int4 _{B,C4-rot}	0.41	-1.06	-0.46	-0.49				0.10	0.54	0.67	-0.60	-0.10	-1.00
⁴ Int5 _{B,C4-exo}	0.36	-1.12	-0.35		-0.62			0.18	0.49	0.73	-0.58	-0.09	-1.00

Table S25: Group spin densities and charges of local minima and transition states for Pathway2-C4 as calculated with B3LYP/BS2 with model B in Gaussian-09.

Spin density:

Species	ρ_{Fe}	ρ_{Porp}	ρ_{SH}	ρ_{O}	ρ_{OH}	ρ_{NO_2}	ρ_{Subs}	$\rho_{\text{Subs}(\text{NO}_2)}$	ρ_{Lig1}	ρ_{Arg}	ρ_{PheGlu}	ρ_{Tyr}	ρ_{Total}
Pathway C4-endo:													
² TS4 _{B,C4-endo}	0.00	0.00	-0.01	0.02		0.00	1.00		0.00	0.00	0.00	0.00	1.00
² Int4 _{B,C4-endo}	0.00	0.00	-0.01	0.01				0.99	0.00	0.00	0.00	0.00	1.00
² Int4 _{B,C4-rotate}	0.00	0.00	0.00	-0.01				1.00	0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C4-endo}	1.56	-0.30	-0.06		0.63	0.00		-0.83	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C4-endo}	1.20	-0.25	-0.02		0.06	0.00		-0.01	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C4-endo}	1.42	-0.22	-0.03	0.83		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C4-endo}	1.42	-0.21	-0.03	0.83				1.00	0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C4-rotate}	1.39	-0.20	-0.03	0.83				1.00	0.00	0.00	0.00	0.00	3.00
⁴ TS5 _{B,C4-endo}	2.25	-0.38	-0.07		0.42	0.00		0.78	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C4-endo}	1.04	1.76	0.07		0.09			0.03	0.00	0.00	0.00	0.00	3.00
Pathway C4-exo:													
² TS4 _{B,C4-exo}	1.39	-0.20	-0.03	0.83		0.00	-0.99		0.00	0.00	0.00	0.00	1.00
² Int4 _{B,C4-exo}	1.41	-0.22	-0.03	0.83				-0.99	0.00	0.00	0.00	0.00	1.00
⁴ Int4 _{B,C4-rotate}	0.00	0.00	0.00	0.01				1.00	0.00	0.00	0.00	0.00	1.00
² Int5 _{B,C4-endo}	1.20	-0.25	-0.02		0.06	0.00		-0.01	0.00	0.00	0.00	0.00	1.00
⁴ TS4 _{B,C4-endo}	1.42	-0.22	-0.03	0.83		0.00	1.00		0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C4-exo}	1.42	-0.22	-0.03	0.83				1.00	0.00	0.00	0.00	0.00	3.00
⁴ Int4 _{B,C4-rotate}	1.39	-0.19	-0.03	0.82				1.00	0.00	0.00	0.00	0.00	3.00
⁴ Int5 _{B,C4-exo}	1.07	1.81	0.06		0.07			-0.01	0.00	0.00	0.00	0.00	3.00

Charge:

Species	Fe	Porp	SH	O	OH	NO2	Subs	Subs(NO ₂)	Lig1	Arg	PheGlu	Tyr	Total
Pathway C4-endo:													
² TS4 _{B,C4-endo}	-2.95	1.46	-0.45	-0.04		0.00	-0.25		1.01	1.03	-0.84	0.02	-1.00
² Int4 _{B,C4-endo}	-2.59	1.22	-0.50	-0.10				-0.23	0.94	1.02	-0.81	0.04	-1.00
² Int4 _{B,C4-rotate}	0.00	0.00	0.00	-0.01				1.00	0.00	0.00	0.00	0.00	1.00
² TS5 _{B,C4-endo}	-4.93	3.42	-0.17		0.67			-0.71	1.00	0.96	-1.32	0.08	-1.00
² Int5 _{B,C4-endo}	-4.15	2.46	-0.17		0.35			-0.15	0.98	0.98	-1.33	0.02	-1.00
⁴ TS4 _{B,C4-endo}	-2.96	1.48	-0.45	-0.05		0.00	-0.25		1.01	1.03	-0.84	0.02	-1.00
⁴ Int4 _{B,C4-endo}	-2.60	1.24	-0.50	-0.10				-0.23	0.94	1.02	-0.81	0.04	-1.00
⁴ Int4 _{B,C4-rotate}	-2.17	1.05	-0.52	-0.25				-0.32	0.96	1.06	-0.84	0.03	-1.00
⁴ TS5 _{B,C4-endo}	-4.55	3.19	-0.29		0.65			-0.72	1.00	0.97	-1.34	0.08	-1.00
⁴ Int5 _{B,C4-endo}	-4.27	2.51	-0.11		0.41			-0.19	0.98	0.98	-1.34	0.02	-1.00
Pathway C4-exo:													
² TS4 _{B,C4-exo}	-1.80	0.68	-0.55	-0.28		0.00	-0.22		0.95	1.06	-0.88	0.05	-1.00
² Int4 _{B,C4-exo}	-2.50	1.14	-0.49	-0.14				-0.12	0.97	1.02	-0.92	0.05	-1.00
⁴ Int4 _{B,C4-rotate}	-1.59	0.57	-0.58	-0.32				-0.31	0.97	1.05	-0.80	0.01	-1.00
² Int5 _{B,C4-exo}	-3.42	1.76	-0.23		0.21			0.03	0.90	1.01	-1.32	0.06	-1.00
⁴ TS4 _{B,C4-exo}	-1.80	0.68	-0.55	-0.28		0.00	-0.22		0.95	1.06	-0.88	0.05	-1.00
⁴ Int4 _{B,C4-exo}	-2.50	1.15	-0.49	-0.14				-0.12	0.97	1.02	-0.92	0.05	-1.00
⁴ Int4 _{B,C4-rotate}	-1.60	0.59	-0.58	-0.33				-0.31	0.97	1.05	-0.80	0.01	-1.00
⁴ Int5 _{B,C4-exo}	-3.53	1.77	-0.17		0.24			0.03	0.91	1.01	-1.33	0.07	-1.00

Part III: Cartesian coordinates.

Cartesian coordinates of optimized geometries

Small model A results:

²ReA:

26	0.394425000	0.130821000	0.203226000	8	2.570138000	1.886164000	-0.222224000
7	0.362866000	-1.135833000	-1.373441000	7	3.111083000	2.392800000	-1.385990000
7	-0.296076000	1.643572000	-0.941584000	8	3.227863000	1.627738000	-2.297525000
7	1.127074000	-1.379214000	1.340969000	7	⁴ ReA:		
7	0.464854000	1.402287000	1.775644000	26	0.303950000	0.085358000	0.223202000
6	0.746683000	-2.449377000	-1.408179000	7	0.268609000	-1.141056000	-1.376542000
6	-0.562825000	2.930696000	-0.560388000	7	-0.365221000	1.613272000	-0.929388000
6	-0.046222000	-0.820522000	-2.640222000	7	1.137687000	-1.400067000	1.331623000
6	-0.626741000	1.555919000	-2.265887000	7	0.383552000	1.324955000	1.816337000
6	1.404843000	-2.664241000	0.957310000	6	0.675523000	-2.450583000	-1.419854000
6	0.103959000	2.721302000	1.803125000	6	-0.654702000	2.885715000	-0.513914000
6	1.440019000	-1.296846000	2.671187000	6	-0.124749000	-0.815187000	-2.649399000
6	0.870093000	1.084741000	3.043013000	6	-0.690289000	1.554665000	-2.257672000
6	0.576722000	-2.985334000	-2.741160000	6	1.410547000	-2.677680000	0.922913000
6	-1.075953000	3.685595000	-1.681605000	6	1.410547000	-2.677680000	0.922913000
6	0.081785000	-1.973572000	-3.504961000	6	-0.005516000	2.637676000	1.853996000
6	-1.115689000	2.831806000	-2.740819000	6	1.483165000	-1.332860000	2.654890000
6	1.910477000	-3.421531000	2.081088000	6	0.832033000	1.012974000	3.072793000
6	0.289158000	3.260658000	3.131566000	6	0.517109000	-2.973060000	-2.755402000
6	1.931262000	-2.571911000	3.145165000	6	-1.169778000	3.660672000	-1.618969000
6	0.765800000	2.244196000	3.901928000	6	0.019033000	-1.958549000	-3.516989000
1	0.826813000	-3.997562000	-3.032699000	6	-1.190536000	2.835187000	-2.701525000
1	-1.360491000	4.730212000	-1.643914000	6	1.958418000	-3.442695000	2.020376000
1	-0.170583000	-1.984248000	-4.558412000	6	0.190383000	3.170202000	3.180237000
1	-1.438074000	3.028788000	-3.756130000	6	2.003389000	-2.607115000	3.094903000
1	2.208822000	-4.461876000	2.039414000	6	0.711570000	2.162292000	3.936279000
1	0.076184000	4.283679000	3.417716000	1	0.782775000	-3.978818000	-3.054998000
1	2.251670000	-2.770377000	4.160768000	1	-1.470278000	4.699418000	-1.556210000
1	1.026631000	2.257940000	4.953452000	1	-0.219568000	-1.963011000	-4.573492000
6	1.233265000	-3.173792000	-0.325703000	1	-1.510936000	3.054784000	-3.712613000
6	-0.378533000	3.443817000	0.717880000	1	2.265116000	-4.479200000	1.955860000
6	1.324663000	-0.160233000	3.464266000	1	-0.039854000	4.186273000	3.476812000
6	-0.510582000	0.420467000	-3.059312000	1	2.353114000	-2.816983000	4.098252000
1	1.514399000	-4.207597000	-0.500529000	1	0.996556000	2.180604000	4.981197000
1	-0.632657000	4.487254000	0.881697000	6	1.198250000	-3.176952000	-0.356059000
1	1.615481000	-0.253834000	4.506986000	6	-0.494779000	3.369602000	0.777375000
1	-0.804254000	0.512610000	-4.101234000	6	1.344666000	-0.217284000	3.470647000
8	2.230433000	0.502193000	-0.269175000	6	-0.579823000	0.430365000	-3.065474000
6	1.233265000	-3.173792000	-0.325703000	1	1.492690000	-4.202753000	-0.551396000
6	-0.378533000	3.443817000	0.717880000	1	-0.766385000	4.405059000	0.960642000
6	1.324663000	-0.160233000	3.464266000	1	1.661637000	-0.313269000	4.504993000
6	-0.510582000	0.420467000	-3.059312000	1	-0.864089000	0.533701000	-4.108454000
1	1.514399000	-4.207597000	-0.500529000	8	2.394387000	0.553925000	-0.253784000
1	-0.632657000	4.487254000	0.881697000	16	-2.049095000	-0.557017000	0.931086000
1	1.615481000	-0.253834000	4.506986000	1	-2.338023000	-1.283919000	-0.173460000
1	-0.804254000	0.512610000	-4.101234000	6	5.268891000	-2.168460000	-1.241682000
8	2.230433000	0.502193000	-0.269175000	6	4.967947000	-3.648108000	-1.598493000
16	-1.782623000	-0.435035000	0.757867000	7	4.216847000	-1.328226000	-1.829695000
1	-1.668187000	-1.775856000	0.619375000	8	3.892757000	-3.782955000	-2.380747000
6	5.245934000	-2.198420000	-1.323948000	8	5.645195000	-4.581743000	-1.215556000
6	4.975873000	-3.660735000	-1.762234000	1	6.231175000	-1.939356000	-1.717870000
7	4.188085000	-1.342138000	-1.877138000	1	4.584544000	-0.598032000	-2.430663000
8	3.926723000	-3.775591000	-2.582611000	1	3.619373000	-0.839398000	-1.152483000
8	5.656814000	-4.601969000	-1.406543000	6	5.448305000	-2.027695000	0.289651000
1	6.204198000	-1.924869000	-1.784153000	6	5.997914000	-0.698268000	0.718469000
1	4.552251000	-0.527293000	-2.359982000	1	6.104282000	-2.843148000	0.613361000
1	3.541781000	-0.970316000	-1.176966000	1	4.475238000	-2.202875000	0.765431000
6	5.414251000	-2.135237000	0.214194000	6	5.259621000	0.422429000	1.011410000
6	5.900948000	-0.806749000	0.713895000	7	6.104158000	1.469736000	1.331723000
1	6.103011000	-2.938420000	0.498244000	6	7.414259000	1.051441000	1.236953000
1	4.447514000	-2.376251000	0.673870000	6	7.384783000	-0.322588000	0.852952000
6	5.111609000	0.245939000	1.107889000	1	4.183687000	0.551396000	0.981212000
7	5.903870000	1.321129000	1.465631000	6	8.611920000	1.738730000	1.457787000
6	7.231169000	0.990864000	1.294518000	6	8.604952000	-1.003079000	0.694808000
6	7.267404000	-0.355074000	0.822592000	6	9.798322000	-0.321794000	0.912324000
1	4.032200000	0.316348000	1.135380000	6	9.802507000	1.036852000	1.288992000
6	8.394623000	1.734633000	1.515881000	1	5.795483000	2.410178000	1.521157000
6	8.517713000	-0.949209000	0.576567000	1	8.614314000	2.786651000	1.749651000
6	9.676895000	-0.211688000	0.794716000	1	10.749933000	1.545311000	1.451280000
6	9.616211000	1.118357000	1.258640000	1	8.614447000	-2.050861000	0.403404000
1	5.546397000	2.228151000	1.721395000	1	10.744916000	-0.842880000	0.789719000
1	8.347625000	2.760320000	1.874833000	1	3.584621000	-2.823420000	-2.481997000
1	10.537923000	1.672465000	1.419305000	8	2.652927000	1.935573000	-0.415277000
1	8.576529000	-1.974601000	0.218796000	7	3.040110000	2.333910000	-1.676191000
1	10.646717000	-0.665403000	0.604798000	8	3.117405000	1.467960000	-2.503724000
1	3.599129000	-2.824784000	-2.655395000				

^TS1A:			
26	0.467863000	0.125661000	0.208803000
7	0.369533000	-1.175500000	-1.351445000
7	-0.257148000	1.607253000	-0.939389000
7	1.116929000	-1.405090000	1.387330000
7	0.483024000	1.384251000	1.784598000
6	0.742649000	-2.492105000	-1.365203000
6	-0.523548000	2.897275000	-0.567538000
6	-0.023726000	-0.870224000	-2.623518000
6	-0.581225000	1.511361000	-2.266040000
6	1.387434000	-2.692201000	1.008804000
6	0.125681000	2.703775000	1.799926000
6	1.429602000	-1.314870000	2.714945000
6	0.876781000	1.072649000	3.057924000
6	0.577741000	-3.041822000	-2.693767000
6	-1.028633000	3.645256000	-1.696336000
6	0.099301000	-2.034836000	-3.473796000
6	-1.063915000	2.785415000	-2.750410000
6	1.883845000	-3.446650000	2.139492000
6	0.300561000	3.250577000	3.126320000
6	1.908809000	-2.591326000	3.198412000
6	0.767878000	2.238269000	3.907206000
1	0.822302000	-4.059053000	-2.971603000
1	-1.312819000	4.690127000	-1.665699000
1	-0.144957000	-2.055693000	-4.528896000
1	-1.381931000	2.975687000	-3.768272000
1	2.173251000	-4.489720000	2.104774000
1	0.086473000	4.275714000	3.403617000
1	2.223973000	-2.786152000	4.216262000
1	1.018421000	2.257430000	4.961031000
6	1.215950000	-3.208501000	-0.271666000
6	-0.346435000	3.420023000	0.706935000
6	1.319614000	-0.169771000	3.495595000
6	-0.471642000	0.372448000	-3.053867000
1	1.485131000	-4.247600000	-0.434484000
1	-0.599262000	4.465046000	0.861202000
1	1.603466000	-0.253772000	4.540903000
1	-0.759330000	0.462520000	-4.097476000
8	2.116058000	0.384570000	-0.181351000
16	-1.773654000	-0.463665000	0.770882000
1	-1.643557000	-1.807557000	0.695731000
6	5.177580000	-2.147829000	-1.387559000
6	4.912333000	-3.597754000	-1.864685000
7	4.108731000	-1.286084000	-1.907984000
8	3.929907000	-3.678420000	-2.769522000
8	5.546279000	-4.559666000	-1.479740000
1	6.117838000	-1.851376000	-1.871736000
1	4.447007000	-0.380805000	-2.220289000
1	3.392548000	-1.066196000	-1.211521000
6	5.393570000	-2.114668000	0.144930000
6	5.878546000	-0.787764000	0.652521000
1	6.100832000	-2.913024000	0.394231000
1	4.444690000	-2.378066000	0.629114000
6	5.086649000	0.277247000	1.007696000
7	5.877847000	1.348400000	1.379894000
6	7.206597000	1.002759000	1.260528000
6	7.245018000	-0.348712000	0.803853000
1	4.006971000	0.360137000	0.998453000
6	8.369191000	1.737114000	1.515280000
6	8.497328000	-0.957040000	0.607459000
6	9.655705000	-0.229028000	0.859041000
6	9.592717000	1.106245000	1.307555000
1	5.520093000	2.258509000	1.624186000
1	8.320023000	2.766932000	1.862013000
1	10.513922000	1.652690000	1.495267000
1	8.558289000	-1.986363000	0.261587000
1	10.626854000	-0.694342000	0.707646000
1	3.611944000	-2.726065000	-2.839060000
8	2.708660000	2.217490000	-0.262816000
7	3.312815000	2.551641000	-1.306527000
8	3.530397000	1.800775000	-2.235030000
26	0.471301000	0.054822000	0.207516000
7	0.309609000	-1.167564000	-1.375048000
7	-0.294321000	1.598056000	-0.912639000
7	1.185549000	-1.450756000	1.317136000
7	0.485250000	1.275091000	1.844896000
6	0.657642000	-2.491572000	-1.426276000
6	-0.546881000	2.869734000	-0.483519000
6	-0.086010000	-0.818666000	-2.644139000
6	-0.605036000	1.563235000	-2.239246000
6	1.404681000	-2.741869000	0.907596000
6	0.117367000	2.592768000	1.883959000
6	1.541283000	-1.396118000	2.643173000
6	0.941090000	0.957692000	3.090903000
6	0.462883000	-3.003226000	-2.761895000
6	-1.039992000	3.673008000	-1.582427000
6	0.002605000	-1.965869000	-3.515460000
6	-1.074798000	2.861417000	-2.674393000
6	1.932442000	-3.523111000	2.002046000
6	0.332343000	3.122652000	3.211597000
6	2.018586000	-2.688841000	3.074977000
6	0.845565000	2.107513000	3.961422000
1	0.676605000	-4.020036000	-3.066006000
1	-1.315250000	4.718072000	-1.508287000
1	-0.249129000	-1.957583000	-4.568939000
1	-1.384541000	3.099827000	-3.684656000
1	2.196980000	-4.571123000	1.937062000
1	0.118131000	4.141501000	3.510910000
1	2.366517000	-2.912027000	4.076089000
1	1.139151000	2.119135000	5.004117000
1	1.159397000	-3.237470000	-0.365659000
6	-0.364079000	3.336897000	0.812536000
6	1.437231000	-0.286934000	3.470443000
6	-0.510388000	0.438783000	-3.052850000
1	1.409175000	-4.275441000	-0.558716000
1	-0.610726000	4.377402000	1.004268000
1	1.763150000	-0.402574000	4.500023000
1	-0.790442000	0.551530000	-4.096221000
8	2.161075000	0.568249000	-0.247273000
16	-1.930528000	-0.399501000	0.881246000
1	-2.350655000	-0.808152000	-0.338691000
6	5.185878000	-2.224846000	-1.208497000
6	4.930266000	-3.711514000	-1.568721000
7	4.081797000	-1.421256000	-1.749457000
8	3.866188000	-3.877915000	-2.361289000
8	5.632134000	-4.626168000	-1.185092000
1	6.111901000	-1.950735000	-1.730693000
1	4.393174000	-0.609974000	-2.274213000
1	3.445975000	-1.043771000	-1.041656000
6	5.435484000	-2.085937000	0.313760000
6	5.914541000	-0.723333000	0.722918000
1	6.158883000	-2.858336000	0.595847000
1	4.501828000	-2.329839000	0.836542000
6	5.115632000	0.363445000	0.982793000
7	5.898449000	1.463990000	1.276589000
6	7.229700000	1.116952000	1.193310000
6	7.278125000	-0.267901000	0.850853000
1	4.036229000	0.446110000	0.948414000
6	8.386512000	1.876125000	1.395756000
6	8.535041000	-0.883807000	0.718445000
6	9.687801000	-0.131073000	0.918594000
6	9.614950000	1.236919000	1.252155000
1	5.533193000	2.395557000	1.399123000
1	8.329073000	2.930932000	1.655154000
1	10.531948000	1.802108000	1.401062000
1	8.604387000	-1.938040000	0.460350000
1	10.662336000	-0.602595000	0.815580000
1	3.522809000	-2.932677000	-2.460100000
8	2.959145000	2.141562000	-0.553330000
7	3.423157000	2.345798000	-1.720860000
8	3.392006000	1.487198000	-2.578195000

² Int1A:			
26	0.507756000	0.038586000	0.187520000
7	0.308960000	-1.215840000	-1.389825000
7	-0.145879000	1.577406000	-0.948768000
7	1.053883000	-1.535464000	1.352344000
7	0.521009000	1.247282000	1.806729000
6	0.632719000	-2.546113000	-1.424267000
6	-0.339265000	2.870112000	-0.546004000
6	-0.051967000	-0.870545000	-2.663266000
6	-0.464306000	1.531969000	-2.277782000
6	1.270635000	-2.821822000	0.943593000
6	0.245376000	2.586060000	1.832591000
6	1.347339000	-1.495172000	2.685879000
6	0.880991000	0.897330000	3.079943000
6	0.456111000	-3.064037000	-2.762095000
6	-0.787903000	3.674473000	-1.661300000
6	0.027063000	-2.024508000	-3.529800000
6	-0.866543000	2.843863000	-2.735888000
6	1.721553000	-3.627390000	2.058970000
6	0.429770000	3.102881000	3.169347000
6	1.766189000	-2.803654000	3.140949000
6	0.823762000	2.054734000	3.943680000
1	0.655819000	-4.087083000	-3.054678000
1	-1.011779000	4.732950000	-1.606190000
1	-0.207691000	-2.017355000	-4.587272000
1	-1.167553000	3.075896000	-3.750316000
1	1.966978000	-4.680389000	1.997884000
1	0.273620000	4.135469000	3.457189000
1	2.055355000	-3.038708000	4.157996000
1	1.059540000	2.045625000	5.000924000
6	1.081215000	-3.301677000	-0.346696000
6	-0.155044000	3.350790000	0.743217000
6	1.265657000	-0.370886000	3.497577000
6	-0.422742000	0.401521000	-3.082830000
1	1.315112000	-4.344780000	-0.534005000
1	-0.343591000	4.406372000	0.915793000
1	1.529185000	-0.491303000	4.544412000
1	-0.695322000	0.521997000	-4.127374000
8	2.107225000	0.323662000	-0.168140000
16	-1.809157000	-0.417872000	0.814419000
1	-2.017740000	-1.485498000	0.010317000
6	5.142204000	-2.216263000	-1.174318000
6	4.839035000	-3.693057000	-1.525207000
7	4.094859000	-1.371797000	-1.765884000
8	3.862192000	-3.826128000	-2.431197000
8	5.443271000	-4.634738000	-1.053473000
1	6.086787000	-1.986774000	-1.685890000
1	4.468279000	-0.498584000	-2.126805000
1	3.375619000	-1.091486000	-1.091279000
6	5.370551000	-2.050482000	0.348692000
6	5.857397000	-0.679613000	0.719677000
1	6.079530000	-2.824290000	0.662186000
1	4.425827000	-2.267331000	0.862934000
6	5.061151000	0.409390000	0.977965000
7	5.843535000	1.524803000	1.211499000
6	7.172884000	1.185038000	1.080471000
6	7.220837000	-0.209981000	0.780773000
1	3.979935000	0.475913000	0.988259000
6	8.330188000	1.959853000	1.207899000
6	8.476954000	-0.820190000	0.617434000
6	9.629743000	-0.051706000	0.743479000
6	9.557467000	1.326339000	1.033229000
1	5.470397000	2.459850000	1.277648000
1	8.273430000	3.022035000	1.434969000
1	10.474464000	1.903705000	1.124104000
1	8.545761000	-1.882329000	0.393678000
1	10.603694000	-0.518505000	0.616224000
1	3.567470000	-2.877879000	-2.584876000
8	3.346046000	3.051326000	-0.150256000
7	3.084702000	2.295434000	-1.060270000
8	3.751480000	1.974647000	-2.016799000

⁴Int1A:

26	0.507528000	-0.046551000	0.142960000
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²TS2_A:

26	1.271543000	0.291322000	0.165237000
7	2.360446000	-0.171933000	-1.492273000
7	1.118181000	2.211507000	-0.440064000
7	1.346099000	-1.662538000	0.717855000
7	0.117004000	0.734565000	1.754740000
6	2.881673000	-1.389599000	-1.826857000
6	0.433533000	3.232119000	0.169030000
6	2.759069000	0.703478000	-2.460284000
6	1.678821000	2.748873000	-1.571446000
6	1.995609000	-2.683969000	0.082990000
6	-0.431797000	1.945897000	2.084735000
6	0.786977000	-2.196296000	1.841251000
6	-0.276799000	-0.143052000	2.731046000
6	3.642016000	-1.284883000	-3.052750000
6	0.575562000	4.453095000	-0.591858000
6	3.566111000	0.019267000	-3.449278000
6	1.350245000	4.154368000	-1.670449000
6	1.837098000	-3.914563000	0.829827000
6	-1.190497000	1.838283000	3.311914000
6	1.086749000	-3.611379000	1.923389000
6	-1.091523000	0.541878000	3.712791000
1	4.145414000	-2.110358000	-3.542002000
1	0.132102000	5.402369000	-0.318181000
1	3.991675000	0.483966000	-4.331037000
1	1.677908000	4.807757000	-2.469699000
1	2.251133000	-4.872262000	0.537874000
1	-1.711647000	2.666768000	3.773709000
1	0.754986000	-4.267885000	2.718808000
1	-1.527273000	0.070762000	4.585798000
6	2.710270000	-2.566395000	-1.102953000
6	-0.291663000	3.120155000	1.352138000
6	0.037014000	-1.495569000	2.781549000
6	2.447908000	2.060946000	-2.503290000
1	3.177384000	-3.465521000	-1.495744000
1	-0.786030000	4.005775000	1.738867000
1	-0.351692000	-2.060471000	3.624629000
1	2.833326000	2.632742000	-3.343154000
8	2.784165000	0.461765000	1.038322000
16	-0.718313000	-0.296552000	-1.080976000
1	-1.384049000	0.871166000	-0.923987000
6	6.233467000	2.310859000	-1.809975000
6	6.570803000	3.012275000	-3.139183000
7	6.632266000	0.895776000	-1.907557000
8	7.376905000	2.284834000	-3.930462000
8	6.180646000	4.122881000	-3.426198000
1	5.157508000	2.425009000	-1.643997000
1	5.830417000	0.331621000	-2.193737000
1	6.916797000	0.556336000	-0.989359000
6	6.993862000	3.042522000	-0.670432000
6	6.836228000	2.387587000	0.670457000
1	6.630763000	4.076923000	-0.662990000
1	8.060704000	3.083621000	-0.928904000
6	7.844311000	1.825656000	1.414958000
7	7.322097000	1.280835000	2.579133000
6	5.956533000	1.453671000	2.592561000
6	5.606891000	2.160870000	1.407535000
1	8.906533000	1.780708000	2.124209000
6	5.000803000	1.055864000	3.551145000
6	4.266958000	2.478442000	1.178651000
6	3.268188000	1.941985000	2.043300000
6	3.680241000	1.327204000	3.284081000
1	7.850479000	0.775085000	3.272210000
1	5.302742000	0.551855000	4.466424000
1	2.907134000	1.022426000	3.982290000
1	3.955015000	3.044543000	0.307971000
1	2.284457000	2.391328000	2.020145000
1	7.488535000	1.434355000	-3.417528000
8	-2.057763000	5.256861000	3.595967000
7	-1.061578000	5.699812000	4.173471000
8	-1.053822000	6.678810000	4.910022000

²Int2_A:

26	1.198154000	0.278450000	0.131124000
7	2.332324000	-0.169361000	-1.495155000
7	1.103253000	2.224417000	-0.431390000
7	1.290476000	-1.666863000	0.685204000
7	0.098001000	0.739067000	1.755502000
6	2.867534000	-1.382066000	-1.826957000
6	0.438948000	3.249307000	0.193541000
6	2.736588000	0.713353000	-2.456121000
6	1.651310000	2.759200000	-1.568918000
6	1.946252000	-2.687071000	0.055420000
6	-0.417634000	1.959483000	2.109249000
6	0.715207000	-2.204135000	1.800162000
6	-0.308329000	-0.143173000	2.721129000
6	3.647751000	-1.266352000	-3.039245000
6	0.580608000	4.471250000	-0.565552000
6	3.565610000	0.038565000	-3.433513000
6	1.333139000	4.167986000	-1.658979000
6	1.771479000	-3.921408000	0.792273000
6	-1.161680000	1.852782000	3.345501000
6	1.006033000	-3.621492000	1.876452000
6	-1.093388000	0.547287000	3.723686000
1	4.164985000	-2.086009000	-3.524113000
1	0.151699000	5.424133000	-0.281198000
1	3.994750000	0.508837000	-4.308408000
1	1.653868000	4.821535000	-2.461137000
1	2.187912000	-4.878748000	0.502224000
1	-1.651633000	2.688739000	3.827835000
1	0.662594000	-4.280906000	2.664615000
1	-1.529242000	0.074350000	4.595793000
6	2.686398000	-2.564277000	-1.114547000
6	-0.269834000	3.138723000	1.386484000
6	-0.025143000	-1.504301000	2.748394000
6	2.418853000	2.069643000	-2.502823000
1	3.161546000	-3.460789000	-1.503639000
1	-0.738552000	4.029343000	1.794469000
1	-0.422018000	-2.073704000	3.584686000
1	2.801071000	2.639676000	-3.345439000
8	2.822844000	0.474100000	1.095326000
16	-0.732746000	-0.220074000	-1.091052000
1	-1.431358000	0.909489000	-0.831419000
6	6.310426000	2.250303000	-1.860222000
6	6.728433000	2.874215000	-3.206730000
7	6.690301000	0.826616000	-1.858820000
8	7.544499000	2.085821000	-3.924294000
8	6.386132000	3.980723000	-3.561570000
1	5.228263000	2.383113000	-1.765960000
1	5.888211000	0.258628000	-2.137488000
1	6.944438000	0.533507000	-0.916745000
6	7.015711000	3.049291000	-0.731243000
6	6.838073000	2.469719000	0.642113000
1	6.629681000	4.073922000	-0.788977000
1	8.089463000	3.105792000	-0.954866000
6	7.849283000	2.097063000	1.487371000
7	7.309991000	1.592315000	2.670372000
6	5.946785000	1.602532000	2.599562000
6	5.591142000	2.164493000	1.334126000
1	8.920974000	2.162174000	1.357541000
6	4.990954000	1.119968000	3.542687000
6	4.255167000	2.278118000	1.001464000
6	3.192667000	1.616843000	1.836413000
6	3.679996000	1.153724000	3.190687000
1	7.846933000	1.219639000	3.438432000
1	5.321124000	0.710574000	4.495403000
1	2.917987000	0.751337000	3.851989000
1	3.925937000	2.698815000	0.058095000
1	2.342061000	2.301233000	1.981988000
1	7.611990000	1.260351000	-3.365319000
8	-1.928046000	5.271811000	3.709784000
7	-1.086888000	5.745018000	4.483579000
8	-1.307181000	6.674507000	5.255592000

⁴TS2_A:

26	1.287058000	0.281799000	0.175332000
7	2.348323000	-0.188748000	-1.494383000
7	1.144931000	2.210261000	-0.434380000
7	1.319064000	-1.670331000	0.717800000
7	0.136680000	0.737274000	1.771710000
6	2.845180000	-1.413454000	-1.836633000
6	0.473705000	3.234982000	0.179407000
6	2.768616000	0.686776000	-2.453379000
6	1.718875000	2.745817000	-1.557640000
6	1.940235000	-2.701653000	0.069293000
6	-0.399947000	1.955620000	2.099640000
6	0.772782000	-2.197238000	1.852587000
6	-0.249126000	-0.130863000	2.758236000
6	3.613337000	-1.314687000	-3.058309000
6	0.635168000	4.459366000	-0.572864000
6	3.566586000	-0.006004000	-3.444095000
6	1.411128000	4.156827000	-1.650018000
6	1.772177000	-3.930992000	0.815678000
6	-1.145267000	1.859023000	3.336109000
6	1.049257000	-3.617244000	1.924851000
6	-1.047726000	0.565048000	3.745590000
1	4.103390000	-2.145982000	-3.551202000
1	0.203954000	5.413362000	-0.295648000
1	4.006693000	0.456968000	-4.319639000
1	1.752318000	4.811040000	-2.442968000
1	2.163864000	-4.895166000	0.514308000
1	-1.661965000	2.689737000	3.799058000
1	0.722107000	-4.270112000	2.725191000
1	-1.475513000	0.102717000	4.627192000
6	2.648803000	-2.592127000	-1.121196000
6	-0.254164000	3.125678000	1.362377000
6	0.052840000	-1.486815000	2.808539000
6	2.480049000	2.049692000	-2.491499000
1	3.096312000	-3.498127000	-1.520880000
1	-0.738203000	4.017382000	1.749368000
1	-0.325872000	-2.045936000	3.659911000
1	2.879663000	2.619342000	-3.326188000
8	2.806463000	0.468343000	1.032291000
16	-0.796010000	-0.284436000	-1.017847000
1	-1.349870000	0.949881000	-1.047871000
6	6.280163000	2.300492000	-1.835562000
6	6.616677000	2.987400000	-3.171777000
7	6.668702000	0.881401000	-1.922669000
8	7.415260000	2.247298000	-3.959397000
8	6.232197000	4.097592000	-3.469046000
1	5.205834000	2.422396000	-1.665318000
1	5.859841000	0.319228000	-2.191798000
1	6.960256000	0.552452000	-1.002572000
6	7.048825000	3.034577000	-0.702401000
6	6.889871000	2.385234000	0.641072000
1	6.691347000	4.071093000	-0.700319000
1	8.115085000	3.068430000	-0.964983000
6	7.897182000	1.819681000	1.386714000
7	7.373509000	1.278641000	2.549609000
6	6.004388000	1.453119000	2.557485000
6	5.658659000	2.161126000	1.374327000
1	8.959354000	1.771797000	1.185450000
6	5.043165000	1.061171000	3.514268000
6	4.318375000	2.486016000	1.141566000
6	3.308691000	1.929285000	1.988988000
6	3.723640000	1.330233000	3.242988000
1	7.897020000	0.759946000	3.236439000
1	5.341724000	0.565471000	4.435649000
1	2.950062000	1.029284000	3.942742000
1	4.013735000	3.058692000	0.272441000
1	2.336106000	2.404358000	1.980377000
1	7.521287000	1.400639000	-3.438278000
8	-2.206293000	5.286175000	3.581225000
7	-1.559131000	5.852546000	4.457846000
8	-1.964567000	6.733359000	5.201532000

⁴Int2_A:

26	1.224314000	0.279355000	0.169906000
7	2.318221000	-0.193169000	-1.478058000
7	1.131203000	2.219125000	-0.413550000
7	1.258828000	-1.672757000	0.711606000
7	0.101223000	0.747825000	1.778071000
6	2.830105000	-1.413814000	-1.810776000
6	0.476883000	3.250527000	0.205203000
6	2.745649000	0.682770000	-2.433552000
6	1.695345000	2.746848000	-1.545013000
6	1.889926000	-2.704927000	0.075035000
6	-0.412588000	1.972562000	2.119371000
6	0.692010000	-2.199938000	1.835817000
6	-0.307535000	-0.124806000	2.751443000
6	3.617545000	-1.312149000	-3.019921000
6	0.640216000	4.472197000	-0.550501000
6	3.564591000	-0.005313000	-3.410351000
6	1.398473000	4.160054000	-1.637452000
6	1.703674000	-3.935676000	0.814923000
6	-1.165017000	1.875322000	3.350864000
6	0.960144000	-3.621729000	1.910105000
6	-1.096949000	0.574107000	3.743579000
1	4.122729000	-2.140516000	-3.502343000
1	0.222109000	5.430925000	-0.269553000
1	4.014102000	0.459472000	-4.280064000
1	1.736809000	4.809718000	-2.435315000
1	2.099965000	-4.900033000	0.520297000
1	-1.667465000	2.709358000	3.823501000
1	0.617562000	-4.274342000	2.704169000
1	-1.537577000	0.109575000	4.617646000
6	2.624561000	-2.593533000	-1.099293000
6	-0.247533000	3.145488000	1.390821000
6	-0.028828000	-1.486610000	2.789074000
6	2.451650000	2.044618000	-2.478456000
1	3.082754000	-3.498109000	-1.490009000
1	-0.717833000	4.042370000	1.782702000
1	-0.422332000	-2.047057000	3.632898000
1	2.851400000	2.610657000	-3.315546000
8	2.821508000	0.458652000	1.081020000
16	-0.791185000	-0.220456000	-1.025894000
1	-1.449393000	0.942439000	-0.811651000
6	6.344372000	2.303557000	-1.868045000
6	6.706935000	2.958501000	-3.213145000
7	6.763443000	0.890149000	-1.900998000
8	7.534725000	2.208161000	-3.959818000
8	6.315761000	4.054926000	-3.550804000
1	5.262972000	2.404023000	-1.735894000
1	5.966461000	0.301899000	-2.147615000
1	7.060011000	0.603768000	-0.968245000
6	7.055846000	3.090995000	-0.732408000
6	6.905230000	2.459502000	0.620595000
1	6.648001000	4.108728000	-0.757652000
1	8.124161000	3.173969000	-0.975449000
6	7.933901000	2.023860000	1.422843000
7	7.416808000	1.466904000	2.582063000
6	6.039322000	1.499508000	2.531368000
6	5.668483000	2.132420000	1.313523000
1	9.003148000	2.082335000	1.267302000
6	5.083018000	1.007789000	3.467901000
6	4.321524000	2.303587000	1.008180000
6	3.256892000	1.598412000	1.814795000
6	3.764084000	1.093631000	3.151285000
1	7.960813000	1.030652000	3.309214000
1	5.413317000	0.567976000	4.408151000
1	3.009232000	0.698815000	3.826037000
1	3.998199000	2.808352000	0.104511000
1	2.410783000	2.279832000	1.990639000
1	7.636813000	1.377278000	-3.412673000
8	-2.197795000	5.344744000	3.628100000
7	-1.579952000	5.904242000	4.525221000
8	-1.988914000	6.783607000	5.264695000

²TS3A:

26	1.141346000	0.172826000	0.115410000
7	2.141054000	0.164116000	-1.647118000
7	1.124325000	2.241432000	0.032302000
7	1.244111000	-1.822240000	0.243790000
7	0.195325000	0.237243000	1.894148000
6	2.610182000	-0.956588000	-2.283040000
6	0.402056000	3.072170000	0.888550000
6	2.479870000	1.229907000	-2.433629000
6	1.480111000	3.033899000	-1.060707000
6	1.821419000	-2.663529000	-0.665543000
6	-0.274015000	1.345563000	2.538481000
6	0.788680000	-2.610710000	1.260975000
6	-0.114086000	-0.831856000	2.695961000
6	3.286490000	-0.583223000	-3.501550000
6	0.387465000	4.408026000	0.361504000
6	3.205592000	0.777037000	-3.597090000
6	1.049716000	4.385214000	-0.835192000
6	1.713877000	-4.036914000	-0.210945000
6	-0.890357000	0.968053000	3.794824000
6	1.074316000	-4.004752000	0.988804000
6	-0.786553000	-0.385689000	3.896178000
1	3.747493000	-1.279584000	-4.191566000
1	-0.091576000	5.252747000	0.842076000
1	3.587103000	1.421473000	-4.380039000
1	1.218426000	5.207225000	-1.520576000
1	2.093300000	-4.895074000	-0.752744000
1	-1.336646000	1.666120000	4.493408000
1	0.810490000	-4.809189000	1.663188000
1	-1.110440000	-1.063825000	4.676098000
6	2.457938000	-2.266141000	-1.836092000
6	-0.192624000	2.659793000	2.069890000
6	0.147564000	-2.165235000	2.414244000
6	2.162635000	2.568347000	-2.172161000
1	2.882471000	-3.049858000	-2.457982000
1	-0.669168000	3.426546000	2.675184000
1	-0.149020000	-2.913772000	3.150838000
1	2.444905000	3.299028000	-2.925460000
8	2.818386000	0.206289000	1.063585000
16	-0.871924000	-0.031019000	-1.002551000
1	-0.859014000	1.156332000	-1.653614000
6	7.324692000	1.596518000	-1.757289000
6	8.114633000	1.526886000	-3.083183000
7	7.966495000	0.702596000	-0.775767000
8	8.933173000	0.466756000	-3.158414000
8	7.995985000	2.339539000	-3.972630000
1	6.341431000	1.167610000	-1.984276000
1	7.269323000	0.288943000	-0.160513000
1	8.600141000	1.230980000	-0.177024000
6	7.142920000	3.074288000	-1.324664000
6	6.666631000	3.264717000	0.087074000
1	6.456009000	3.538662000	-2.041931000
1	8.098733000	3.599267000	-1.449754000
6	7.263374000	4.067576000	1.023552000
7	6.541261000	4.034299000	2.210901000
6	5.470864000	3.191491000	2.072413000
6	5.504175000	2.681668000	0.736983000
1	8.145773000	4.687485000	0.937289000
6	4.488690000	2.815171000	3.015278000
6	4.541140000	1.761895000	0.343098000
6	3.442223000	1.400446000	1.237386000
6	3.529484000	1.920438000	2.617418000
1	6.774638000	4.544769000	3.048382000
1	4.515746000	3.201951000	4.031504000
1	2.760473000	1.575641000	3.300739000
1	4.522292000	1.321812000	-0.647215000
1	2.595514000	2.168087000	0.779620000
1	8.843218000	0.031085000	-2.269057000
8	-0.106487000	-4.893021000	4.163021000
7	-0.720697000	-4.578799000	5.208678000
8	-1.109799000	-3.398637000	5.358594000

²Int3A:

26	0.880300000	0.086401000	-0.192269000
7	1.494799000	-0.439776000	-2.047231000
7	1.718764000	2.034826000	-0.484443000
7	0.181728000	-1.746838000	0.105820000
7	0.307049000	0.703412000	1.629797000
6	1.440747000	-1.693450000	-2.595873000
6	1.387258000	3.186409000	0.320446000
6	2.083422000	0.363493000	-2.977207000
6	1.987028000	2.550764000	-1.800819000
6	0.251383000	-2.813524000	-0.741332000
6	0.503652000	1.915012000	2.231698000
6	-0.459836000	-2.175904000	1.229312000
6	-0.304490000	-0.090786000	2.566781000
6	2.035475000	-1.686463000	-3.914637000
6	1.568732000	4.345475000	-0.467105000
6	2.431253000	-0.407201000	-4.154058000
6	1.921423000	3.963927000	-1.745811000
6	-0.384024000	-3.964674000	-0.139238000
6	0.030773000	1.887291000	3.600912000
6	-0.829489000	-3.567271000	1.084977000
6	-0.482744000	0.645356000	3.803252000
1	2.121404000	-2.551979000	-4.559875000
1	1.402629000	5.351992000	-0.105227000
1	2.915661000	-0.002858000	-5.034124000
1	2.081655000	4.612284000	-2.598309000
1	-0.467117000	-4.938999000	-0.604750000
1	0.135593000	2.728739000	4.274404000
1	-1.351657000	-4.148543000	1.834857000
1	-0.932168000	0.238247000	4.700765000
6	0.856957000	-2.800562000	-1.996059000
6	0.971694000	3.091657000	1.629654000
6	-0.680794000	-1.412406000	2.376122000
6	2.270022000	1.751327000	-2.886127000
1	0.860079000	-3.731235000	-2.556469000
1	0.967304000	3.983709000	2.253958000
1	-1.178044000	-1.906687000	3.206181000
1	2.617248000	2.253865000	-3.784636000
8	2.591244000	-0.570710000	0.447662000
16	-1.161682000	0.737205000	-1.098721000
1	-1.376096000	1.844617000	-0.351146000
6	7.761514000	2.254022000	-0.680161000
6	8.421905000	2.650492000	-2.010759000
7	8.791204000	2.221287000	0.375467000
8	9.652175000	3.173305000	-1.857514000
8	7.876466000	2.544715000	-3.087195000
1	7.272794000	1.283522000	-0.825765000
1	9.138403000	1.273686000	0.508212000
1	8.361595000	2.502883000	1.258976000
6	6.664640000	3.299978000	-0.327341000
6	6.000810000	3.033818000	0.989009000
1	5.945171000	3.297069000	-1.155042000
1	7.131592000	4.294459000	-0.314190000
6	6.142659000	3.777083000	2.148958000
7	5.439200000	3.220629000	3.189279000
6	4.775994000	2.115345000	2.688145000
6	5.086388000	1.964167000	1.313534000
1	6.689295000	4.702027000	2.291234000
6	3.896269000	1.245234000	3.345317000
6	4.398002000	0.986659000	0.557137000
6	3.407099000	0.196266000	1.178682000
6	3.236012000	0.290113000	2.594583000
1	4.962695000	3.782126000	3.945537000
1	3.693804000	1.369498000	4.404877000
1	2.509683000	-0.370215000	3.056758000
1	4.586477000	0.844954000	-0.506162000
1	2.626695000	1.683666000	-0.097411000
1	9.813787000	3.092841000	-0.877084000
8	1.614179000	4.749636000	4.338952000
7	2.751489000	4.358208000	3.975843000
8	3.683184000	4.503406000	4.839562000

⁴TS3A:

26	0.931855000	0.292635000	0.135417000
7	2.020159000	0.177564000	-1.577467000
7	1.085065000	2.367922000	0.022535000
7	0.862208000	-1.704673000	0.289071000
7	-0.144805000	0.464187000	1.848457000
6	2.477216000	-0.977213000	-2.151246000
6	0.361698000	3.265793000	0.815000000
6	2.445114000	1.203878000	-2.387218000
6	1.507780000	3.106836000	-1.092814000
6	1.477501000	-2.598355000	-0.552259000
6	-0.565334000	1.622654000	2.443473000
6	0.270831000	-2.439191000	1.275387000
6	-0.615687000	-0.559899000	2.626677000
6	3.225497000	-0.680901000	-3.336795000
6	0.448981000	4.586704000	0.249654000
6	3.198606000	0.686620000	-3.488247000
6	1.148719000	4.491437000	-0.917564000
6	1.242191000	-3.952883000	-0.086645000
6	-1.314235000	1.329591000	3.632388000
6	0.493420000	-3.855021000	1.041919000
6	-1.344131000	-0.035682000	3.748706000
1	3.691235000	-1.418865000	-3.978734000
1	0.003706000	5.470023000	0.691354000
1	3.648780000	1.285587000	-4.270825000
1	1.388817000	5.280834000	-1.619655000
1	1.614655000	-4.845177000	-0.575656000
1	-1.737995000	2.077000000	4.291411000
1	0.121047000	-4.649719000	1.677445000
1	-1.816762000	-0.6366631000	4.516322000
6	2.227880000	-2.274266000	-1.666193000
6	-0.334918000	2.924950000	1.960513000
6	-0.424807000	-1.920122000	2.359842000
6	2.184246000	2.567844000	-2.165914000
1	2.656549000	-3.097291000	-2.232084000
1	-0.818762000	3.732133000	2.498692000
1	-0.850485000	-2.628612000	3.065248000
1	2.523661000	3.259261000	-2.933405000
8	2.520699000	0.249347000	1.178951000
16	-1.037366000	0.217227000	-1.119698000
1	-0.875384000	1.372718000	-1.806691000
6	7.278089000	1.135419000	-1.391402000
6	8.240393000	0.869446000	-2.568609000
7	7.682815000	0.288987000	-0.251449000
8	8.967218000	-0.249317000	-2.416070000
8	8.325045000	1.587047000	-3.540684000
1	6.299461000	0.772717000	-1.727800000
1	6.859487000	-0.003283000	0.272249000
1	8.245424000	0.835779000	0.400122000
6	7.177595000	2.659014000	-1.108115000
6	6.615223000	3.007989000	0.240821000
1	6.581346000	3.099026000	-1.916599000
1	8.176406000	3.104185000	-1.203873000
6	7.188943000	3.875269000	1.138166000
7	6.392799000	3.985387000	2.266982000
6	5.289519000	3.174029000	2.129284000
6	5.385621000	2.538801000	0.855926000
1	8.103493000	4.447372000	1.052421000
6	4.235319000	2.920224000	3.033169000
6	4.402284000	1.626197000	0.475313000
6	3.229562000	1.413130000	1.316140000
6	3.265205000	2.027867000	2.654075000
1	6.583568000	4.574218000	3.062036000
1	4.190696000	3.403632000	4.005278000
1	2.442257000	1.793626000	3.319805000
1	4.429126000	1.102338000	-0.473266000
1	2.403712000	2.192767000	0.759914000
1	8.706647000	-0.574933000	-1.511402000
8	-0.239785000	4.666021000	4.849351000
7	0.763468000	4.055982000	4.505844000
8	1.768479000	3.873978000	5.177454000

⁴Int3A:

26	0.929515000	0.969512000	0.094773000
7	1.758238000	1.516350000	-1.672810000
7	-0.067696000	2.910294000	0.220459000
7	1.982613000	-0.704995000	0.076234000
7	0.093333000	0.544828000	1.890305000
6	2.645660000	0.793121000	-2.426360000
6	-1.197546000	3.173181000	1.058689000
6	1.515960000	2.676548000	-2.375782000
6	-0.216402000	3.754789000	-0.929050000
6	2.835468000	-1.153553000	-0.907220000
6	-0.818959000	1.266654000	2.618648000
6	1.982803000	-1.651027000	1.069533000
6	0.382927000	-0.569213000	2.637597000
6	2.988038000	1.505961000	-3.615544000
6	-1.958643000	4.224739000	0.462160000
6	2.276537000	2.685357000	-3.582919000
6	-1.367949000	4.577521000	-0.722680000
6	3.392579000	-2.436533000	-0.518323000
6	-1.106248000	0.605248000	3.850938000
6	2.870822000	-2.738457000	0.699949000
6	-0.349845000	-0.544061000	3.866589000
1	3.673385000	1.151708000	-4.375666000
1	-2.881143000	4.614144000	0.875467000
1	2.270819000	3.486466000	-4.312538000
1	-1.730438000	5.300638000	-1.443502000
1	4.096560000	-2.998121000	-1.119962000
1	-1.783926000	0.978450000	4.608992000
1	3.050860000	-3.615010000	1.311491000
1	-0.297813000	-1.304985000	4.636028000
6	3.146396000	-0.480174000	-2.071969000
6	-1.458356000	2.464951000	2.202949000
6	1.258450000	-1.596448000	2.247564000
6	0.575799000	3.680097000	-2.041225000
1	3.868048000	-0.942590000	-2.738642000
1	-2.292380000	2.800087000	2.812335000
1	1.375968000	-2.427200000	2.938265000
1	0.412580000	4.442623000	-2.799669000
8	2.190553000	2.111686000	1.111049000
16	-0.856247000	0.004049000	-0.969242000
1	-0.196556000	-0.502018000	-2.035673000
6	6.845944000	-0.885957000	-0.409647000
6	7.128212000	-1.935625000	-1.496541000
7	7.648350000	-1.216242000	0.785947000
8	8.228626000	-2.669163000	-1.253685000
8	6.453097000	-2.072194000	-2.495062000
1	5.770707000	-0.897759000	-0.207868000
1	7.083342000	-1.743899000	1.448869000
1	7.908972000	-0.347098000	1.254312000
6	7.230134000	0.519261000	-0.952890000
6	7.072638000	1.607556000	0.067359000
1	6.601586000	0.702150000	-1.831964000
1	8.271586000	0.485554000	-1.302146000
6	8.089711000	2.337122000	0.645186000
7	7.565207000	3.233067000	1.555381000
6	6.180728000	3.101779000	1.573382000
6	5.836130000	2.080814000	0.654243000
1	9.155389000	2.299037000	0.457382000
6	5.199637000	3.776066000	2.310790000
6	4.488786000	1.722838000	0.468148000
6	3.487421000	2.382324000	1.196753000
6	3.876801000	3.410649000	2.116003000
1	8.091149000	3.931276000	2.054858000
1	5.460141000	4.562373000	3.017117000
1	3.082484000	3.902672000	2.670306000
1	4.210744000	0.954991000	-0.239725000
1	0.835479000	3.074148000	0.724116000
1	8.519885000	-2.348851000	-0.354764000
8	-1.016272000	4.326067000	4.943157000
7	-0.238462000	4.191107000	4.019044000
8	0.676398000	4.908342000	3.673268000

²TS4_A:

26	1.509262000	0.119696000	-0.357359000
7	2.220934000	-0.374382000	-2.191790000
7	1.286383000	2.039897000	-0.963277000
7	1.565910000	-1.828193000	0.187575000
7	0.684704000	0.598303000	1.435566000
6	2.592366000	-1.619015000	-2.614911000
6	0.813510000	3.084837000	-0.217521000
6	2.479683000	0.481779000	-3.223973000
6	1.686072000	2.566501000	-2.162073000
6	2.022618000	-2.873769000	-0.564867000
6	0.275960000	1.834669000	1.845254000
6	1.220641000	-2.343337000	1.405418000
6	0.461597000	-0.252560000	2.480533000
6	3.106379000	-1.549947000	-3.966871000
6	0.905033000	4.314579000	-0.973829000
6	3.040121000	-0.244829000	-4.344511000
6	1.450427000	3.993435000	-2.179290000
6	1.957701000	-4.099050000	0.200692000
6	-0.223900000	1.768927000	3.203774000
6	1.461298000	-3.769319000	1.424906000
6	-0.104698000	0.472122000	3.598641000
1	3.466774000	-2.400221000	-4.533427000
1	0.595406000	5.286863000	-0.610040000
1	3.340743000	0.207120000	-5.281394000
1	1.684468000	4.645821000	-3.011482000
1	2.256826000	-5.072983000	-0.167931000
1	-0.611586000	2.613524000	3.760723000
1	1.266465000	-4.415789000	2.272270000
1	-0.376638000	0.027042000	4.548270000
6	2.499992000	-2.786914000	-1.868283000
6	0.328998000	2.997622000	1.083728000
6	0.713067000	-1.618902000	2.478510000
6	2.242680000	1.851387000	-3.217391000
1	2.831088000	-3.708022000	-2.339876000
1	-0.031899000	3.913611000	1.543549000
1	0.480612000	-2.170129000	3.385517000
1	2.517936000	2.408854000	-4.107489000
8	3.045226000	0.408916000	0.198816000
16	-0.748289000	-0.404108000	-1.170920000
1	-1.092598000	0.829252000	-1.609296000
6	5.660579000	2.182499000	-1.223964000
6	5.926007000	2.707614000	-2.655075000
7	5.521817000	0.720231000	-1.269259000
8	5.838811000	1.750177000	-3.583531000
8	6.191036000	3.866320000	-2.906425000
1	4.697422000	2.604943000	-0.916291000
1	4.637674000	0.444784000	-0.815732000
1	6.276014000	0.268815000	-0.755237000
6	6.770665000	2.713622000	-0.281769000
6	6.680791000	2.204839000	1.126281000
1	6.731952000	3.808125000	-0.318036000
1	7.747883000	2.430237000	-0.697443000
6	7.600656000	1.399417000	1.746551000
7	7.189665000	1.115912000	3.043940000
6	5.977023000	1.714292000	3.273800000
6	5.621246000	2.428932000	2.093628000
1	8.540683000	1.014834000	1.373957000
6	5.127880000	1.638021000	4.406142000
6	4.415489000	3.118091000	2.048296000
6	3.568272000	3.168435000	3.234574000
6	3.940495000	2.310763000	4.374519000
1	7.658001000	0.487533000	3.677480000
1	5.399405000	1.024601000	5.262340000
1	3.250121000	2.259950000	5.208747000
1	4.083220000	3.628526000	1.152509000
1	2.496582000	3.179095000	3.024692000
1	5.628331000	0.931584000	-3.035027000
8	4.261573000	5.658669000	3.270754000
7	3.612891000	4.821317000	3.874487000
8	2.957732000	5.009760000	4.890964000

⁴TS4_A:

26	1.511381000	0.096929000	-0.361728000
7	2.216287000	-0.390710000	-2.200092000
7	1.299994000	2.022574000	-0.956307000
7	1.556143000	-1.853776000	0.172303000
7	0.694083000	0.571012000	1.436159000
6	2.578684000	-1.635308000	-2.631036000
6	0.835267000	3.066022000	-0.203587000
6	2.479305000	0.469764000	-3.227687000
6	1.701213000	2.553617000	-2.152628000
6	2.003882000	-2.898111000	-0.587338000
6	0.294104000	1.807617000	1.853401000
6	1.210032000	-2.373633000	1.387936000
6	0.467603000	-0.284047000	2.476843000
6	3.091307000	-1.561772000	-3.983270000
6	0.933802000	4.299685000	-0.952653000
6	3.033408000	-0.254014000	-4.353149000
6	1.475241000	3.982191000	-2.160939000
6	1.932069000	-4.127334000	0.171182000
6	-0.203720000	1.737629000	3.212478000
6	1.440739000	-3.801328000	1.398454000
6	-0.092119000	0.438045000	3.600035000
1	3.445135000	-2.411127000	-4.555322000
1	0.630939000	5.271815000	-0.582762000
1	3.335620000	0.201388000	-5.287863000
1	1.712427000	4.638013000	-2.989525000
1	2.223525000	-5.101160000	-0.203809000
1	-0.585401000	2.581593000	3.774556000
1	1.243277000	-4.451413000	2.242442000
1	-0.365160000	-0.010575000	4.547688000
6	2.479443000	-2.806912000	-1.891077000
6	0.352438000	2.974292000	1.098086000
6	0.709854000	-1.651997000	2.466445000
6	2.251206000	1.840844000	-3.213027000
1	2.803322000	-3.727514000	-2.368638000
1	-0.003200000	3.889675000	1.563288000
1	0.475522000	-2.206963000	3.370691000
1	2.528887000	2.401573000	-4.100309000
8	3.049901000	0.374890000	0.193197000
16	-0.751535000	-0.405633000	-1.172551000
1	-1.082210000	0.828310000	-1.619649000
6	5.654581000	2.187474000	-1.219591000
6	5.916066000	2.718411000	-2.649437000
7	5.521180000	0.724925000	-1.270003000
8	5.833974000	1.763145000	-3.580502000
8	6.174196000	3.879408000	-2.897403000
1	4.690992000	2.606440000	-0.908368000
1	4.637069000	0.443168000	-0.819894000
1	6.275785000	0.274382000	-0.755851000
6	6.765157000	2.718082000	-0.277736000
6	6.670041000	2.215280000	1.131968000
1	6.730741000	3.812536000	-0.318298000
1	7.741750000	2.428825000	-0.690925000
6	7.575802000	1.394824000	1.753084000
7	7.161327000	1.121733000	3.051678000
6	5.960117000	1.742382000	3.281582000
6	5.615991000	2.461007000	2.100114000
1	8.508254000	0.992275000	1.380445000
6	5.111270000	1.684645000	4.415028000
6	4.423807000	3.172927000	2.054942000
6	3.577594000	3.239895000	3.241046000
6	3.936080000	2.378508000	4.382878000
1	7.617897000	0.484755000	3.685244000
1	5.372531000	1.068772000	5.272628000
1	3.245857000	2.342394000	5.218059000
1	4.100294000	3.687124000	1.157850000
1	2.506109000	3.267255000	3.031819000
1	5.628189000	0.941965000	-3.033803000
8	4.341675000	5.708899000	3.296563000
7	3.650413000	4.891467000	3.879844000
8	2.973754000	5.098176000	4.878613000

²Int4A:

26	1.515887000	0.120406000	-0.337914000
7	2.213121000	-0.363069000	-2.180654000
7	1.300962000	2.046640000	-0.927240000
7	1.563742000	-1.832183000	0.191247000
7	0.705779000	0.589091000	1.464095000
6	2.574142000	-1.606543000	-2.615970000
6	0.839080000	3.088194000	-0.170188000
6	2.471257000	0.499692000	-3.207442000
6	1.696772000	2.580579000	-2.124101000
6	2.008416000	-2.874514000	-0.572872000
6	0.308907000	1.824905000	1.886845000
6	1.221894000	-2.355339000	1.406577000
6	0.484337000	-0.268504000	2.503903000
6	3.080626000	-1.529837000	-3.970351000
6	0.933568000	4.323602000	-0.916906000
6	3.020462000	-0.221330000	-4.337121000
6	1.469854000	4.009031000	-2.128231000
6	1.939285000	-4.105832000	0.182562000
6	-0.180265000	1.752124000	3.249003000
6	1.452409000	-3.783118000	1.412463000
6	-0.067955000	0.451351000	3.632232000
1	3.432274000	-2.377763000	-4.545848000
1	0.631584000	5.294670000	-0.543523000
1	3.318575000	0.236252000	-5.272065000
1	1.702535000	4.666747000	-2.956621000
1	2.229200000	-5.078672000	-0.196156000
1	-0.554647000	2.595787000	3.816243000
1	1.257781000	-4.435451000	2.255373000
1	-0.335266000	0.000682000	4.580544000
6	2.478559000	-2.779888000	-1.878355000
6	0.363198000	2.993536000	1.133875000
6	0.726089000	-1.636423000	2.488969000
6	2.242767000	1.870670000	-3.188450000
1	2.800659000	-3.699222000	-2.359549000
1	0.010871000	3.907785000	1.603737000
1	0.495446000	-2.193618000	3.392792000
1	2.515956000	2.433557000	-4.075793000
8	3.056647000	0.396507000	0.211617000
16	-0.749766000	-0.383235000	-1.141646000
1	-1.085153000	0.852854000	-1.579282000
6	5.684234000	2.170845000	-1.230231000
6	5.954923000	2.693825000	-2.661002000
7	5.520535000	0.711316000	-1.277876000
8	5.847765000	1.739831000	-3.590941000
8	6.239085000	3.848302000	-2.911257000
1	4.729451000	2.609524000	-0.918949000
1	4.635682000	0.447016000	-0.818866000
1	6.270666000	0.246580000	-0.769730000
6	6.804996000	2.679360000	-0.288101000
6	6.690507000	2.184469000	1.122693000
1	6.797541000	3.774159000	-0.334266000
1	7.775343000	2.364178000	-0.697250000
6	7.566128000	1.335069000	1.749824000
7	7.134841000	1.075620000	3.044441000
6	5.950474000	1.734110000	3.264475000
6	5.636629000	2.462943000	2.082438000
1	8.487065000	0.902198000	1.382492000
6	5.092300000	1.705828000	4.395425000
6	4.474232000	3.219204000	2.024128000
6	3.579780000	3.295355000	3.201275000
6	3.939513000	2.427772000	4.364119000
1	7.562063000	0.418796000	3.678083000
1	5.334149000	1.087237000	5.257110000
1	3.244608000	2.412025000	5.195917000
1	4.181203000	3.750875000	1.126901000
1	2.521902000	3.184708000	2.933025000
1	5.624990000	0.923999000	-3.042881000
8	4.269734000	5.659726000	3.269168000
7	3.530140000	4.824682000	3.768252000
8	2.730329000	5.031133000	4.675555000

⁴Int4A:

26	1.541711000	0.067227000	-0.319744000
7	2.210830000	-0.360519000	-2.186378000
7	1.312763000	2.008571000	-0.852313000
7	1.603575000	-1.898423000	0.155268000
7	0.758765000	0.481759000	1.507813000
6	2.563123000	-1.591193000	-2.663290000
6	0.848764000	3.024007000	-0.062798000
6	2.457476000	0.531942000	-3.190287000
6	1.694642000	2.579119000	-2.037015000
6	2.034046000	-2.917859000	-0.647329000
6	0.355870000	1.702026000	1.967033000
6	1.288539000	-2.456269000	1.362210000
6	0.561186000	-0.403749000	2.528658000
6	3.050398000	-1.475327000	-4.021767000
6	0.927262000	4.280910000	-0.774875000
6	2.989006000	-0.156123000	-4.348455000
6	1.457635000	4.005360000	-1.998402000
6	1.982867000	-4.169995000	0.074416000
6	-0.113270000	1.590097000	3.333423000
6	1.521917000	-3.883026000	1.323124000
6	0.017956000	0.281953000	3.682755000
1	3.391474000	-2.306453000	-4.627338000
1	0.618879000	5.238414000	-0.372631000
1	3.274314000	0.328037000	-5.274047000
1	1.677026000	4.688221000	-2.809994000
1	2.266137000	-5.131189000	-0.337593000
1	-0.490808000	2.415035000	3.925710000
1	1.345972000	-4.559424000	2.151076000
1	-0.231370000	-0.195247000	4.623002000
6	2.479282000	-2.785250000	-1.958182000
6	0.387001000	2.889463000	1.243437000
6	0.811198000	-1.769002000	2.473554000
6	2.230537000	1.902114000	-3.127542000
1	2.792519000	-3.690246000	-2.471385000
1	0.024597000	3.786433000	1.738688000
1	0.599595000	-2.351688000	3.365926000
1	2.492088000	2.491031000	-4.001494000
8	3.089427000	0.331833000	0.214701000
16	-0.734117000	-0.419403000	-1.104758000
1	-1.033040000	0.795749000	-1.620592000
6	5.734276000	2.130722000	-1.236396000
6	6.054039000	2.678416000	-2.647935000
7	5.509892000	0.682288000	-1.326804000
8	5.880156000	1.765561000	-3.608617000
8	6.420608000	3.817111000	-2.860555000
1	4.789316000	2.597658000	-0.934927000
1	4.634159000	0.428536000	-0.844398000
1	6.262755000	0.169874000	-0.871197000
6	6.846303000	2.568101000	-0.250413000
6	6.621188000	2.098980000	1.154947000
1	6.921588000	3.659891000	-0.303476000
1	7.807718000	2.177252000	-0.613312000
6	7.335623000	1.132214000	1.814126000
7	6.813921000	0.938123000	3.087321000
6	5.727143000	1.758606000	3.257874000
6	5.576626000	2.526330000	2.068423000
1	8.198268000	0.568188000	1.485326000
6	4.824711000	1.857653000	4.349269000
6	4.544226000	3.446936000	1.963413000
6	3.610512000	3.646379000	3.095654000
6	3.791757000	2.739362000	4.270779000
1	7.099495000	0.212409000	3.725624000
1	4.934626000	1.211767000	5.217638000
1	3.064438000	2.823298000	5.070116000
1	4.379071000	4.020401000	1.058622000
1	2.561179000	3.671961000	2.774823000
1	5.604786000	0.948451000	-3.087243000
8	4.614198000	5.889527000	3.224546000
7	3.733377000	5.166326000	3.665651000
8	2.909861000	5.483375000	4.518524000

²TS5_A:

26	1.619871000	-0.116949000	-0.181853000
7	2.426952000	-0.698197000	-1.957520000
7	1.863151000	1.816551000	-0.690464000
7	1.235940000	-2.065102000	0.255976000
7	0.705564000	0.458203000	1.528919000
6	2.616277000	-1.979559000	-2.393850000
6	1.505963000	2.914276000	0.043789000
6	2.933360000	0.124750000	-2.921185000
6	2.433854000	2.290700000	-1.842263000
6	1.591830000	-3.160730000	-0.481258000
6	0.524107000	1.735478000	1.974690000
6	0.647649000	-2.535764000	1.394586000
6	0.186643000	-0.367000000	2.487067000
6	3.265724000	-1.970824000	-3.685979000
6	1.862872000	4.123631000	-0.664409000
6	3.462049000	-0.660299000	-4.016358000
6	2.437894000	3.737210000	-1.833891000
6	1.202616000	-4.370605000	0.209961000
6	-0.131480000	1.723829000	3.265188000
6	0.615736000	-3.982241000	1.375436000
6	-0.342014000	0.418588000	3.582934000
1	3.512144000	-2.855846000	-4.260963000
1	1.698476000	5.126050000	-0.289781000
1	3.901765000	-0.249062000	-4.917705000
1	2.841628000	4.355237000	-2.626344000
1	1.366474000	-5.374578000	-0.163325000
1	-0.385660000	2.609705000	3.834220000
1	0.196936000	-4.600366000	2.160637000
1	-0.808834000	0.004283000	4.468551000
6	2.232082000	-3.131278000	-1.714891000
6	0.891523000	2.887247000	1.289913000
6	0.155903000	-1.754155000	2.435356000
6	2.943280000	1.516329000	-2.876375000
1	2.446706000	-4.085205000	-2.189041000
1	0.685360000	3.841008000	1.765753000
1	-0.291596000	-2.273513000	3.278369000
1	3.372673000	2.040296000	-3.725654000
8	3.112775000	-0.256742000	0.580507000
16	-0.537720000	0.009715000	-1.303841000
1	-0.670323000	-1.304149000	-1.598808000
6	7.015370000	0.448702000	-3.043741000
6	7.306641000	1.010942000	-4.448585000
7	6.812848000	-1.006362000	-3.148813000
8	7.558564000	0.054096000	-5.357466000
8	7.345291000	2.195528000	-4.699641000
1	6.127066000	0.962709000	-2.660087000
1	5.815555000	-1.213154000	-3.227074000
1	7.142329000	-1.459761000	-2.297242000
6	8.224049000	0.789641000	-2.129318000
6	8.118011000	0.202872000	-0.753214000
1	8.301482000	1.882702000	-2.101083000
1	9.139931000	0.419526000	-2.609875000
6	8.936724000	-0.769378000	-0.226819000
7	8.521774000	-1.091352000	1.053671000
6	7.402212000	-0.351152000	1.367774000
6	7.115150000	0.489798000	0.257429000
1	9.800447000	-1.251908000	-0.664943000
6	6.623744000	-0.335329000	2.553932000
6	6.037703000	1.371067000	0.308623000
6	5.100774000	1.289924000	1.442670000
6	5.535712000	0.482693000	2.610481000
1	8.925439000	-1.810143000	1.632752000
1	6.890381000	-0.962145000	3.402229000
1	4.908565000	0.523436000	3.492103000
1	5.800723000	2.049559000	-0.500662000
1	4.095241000	0.748119000	1.040946000
1	7.438512000	-0.789520000	-4.834213000
8	4.651461000	3.580809000	1.075805000
7	4.551720000	2.645933000	1.867364000
8	3.988298000	2.716299000	2.959602000

⁴TS5_A:

26	1.609030000	-0.106066000	-0.175240000
7	2.388667000	-0.666733000	-1.960769000
7	1.739733000	1.835567000	-0.746535000
7	1.351633000	-2.051295000	0.329309000
7	0.666931000	0.447090000	1.527758000
6	2.606724000	-1.949201000	-2.384234000
6	1.329399000	2.921013000	-0.025566000
6	2.871130000	0.159290000	-2.939231000
6	2.310560000	2.321269000	-1.890291000
6	1.712764000	-3.139953000	-0.415299000
6	0.412873000	1.728024000	1.931208000
6	0.827220000	-2.532230000	1.495633000
6	0.239131000	-0.373245000	2.533403000
6	3.238857000	-1.937610000	-3.682683000
6	1.642618000	4.138666000	-0.741836000
6	3.405242000	-0.626208000	-4.027981000
6	2.252504000	3.767420000	-1.897652000
6	1.407601000	-4.355403000	0.306539000
6	-0.207627000	1.719258000	3.237547000
6	0.860290000	-3.977978000	1.494033000
6	-0.314769000	0.415955000	3.611856000
1	3.503096000	-2.822836000	-4.249022000
1	1.430838000	5.136189000	-0.378247000
1	3.835150000	-0.215484000	-4.934011000
1	2.643811000	4.394438000	-2.689171000
1	1.594848000	-5.355766000	-0.064854000
1	-0.505039000	2.607023000	3.781777000
1	0.501815000	-4.603089000	2.303016000
1	-0.723991000	0.006201000	4.527391000
6	2.292092000	-3.104141000	-1.676271000
6	0.710060000	2.880909000	1.216338000
6	0.311904000	-1.760616000	2.530515000
6	2.846101000	1.551172000	-2.914030000
1	2.523632000	-4.055497000	-2.146927000
1	0.455481000	3.830806000	1.676053000
1	-0.074647000	-2.283827000	3.400398000
1	3.267341000	2.074314000	-3.767506000
8	3.126878000	-0.036826000	0.566203000
16	-0.614373000	-0.153607000	-1.186324000
1	-0.242129000	0.227234000	-2.429930000
6	7.012006000	0.391583000	-3.020862000
6	7.298403000	0.952504000	-4.426232000
7	6.773109000	-1.058138000	-3.130358000
8	7.523180000	-0.006884000	-5.340754000
8	7.355474000	2.136558000	-4.676831000
1	6.143431000	0.925753000	-2.620004000
1	5.771063000	-1.241434000	-3.196999000
1	7.102577000	-1.519648000	-2.282690000
6	8.239015000	0.692597000	-2.115799000
6	8.124250000	0.098201000	-0.743993000
1	8.347123000	1.782934000	-2.080888000
1	9.139231000	0.299849000	-2.608206000
6	8.908696000	-0.914358000	-0.235899000
7	8.492402000	-1.230121000	1.043476000
6	7.407062000	-0.443903000	1.376005000
6	7.143313000	0.417228000	0.277189000
1	9.748069000	-1.426937000	-0.687319000
6	6.651462000	-0.395211000	2.578866000
6	6.102976000	1.346550000	0.347925000
6	5.184472000	1.283204000	1.493496000
6	5.603251000	0.472555000	2.654469000
1	8.873988000	-1.966620000	1.614914000
1	6.910163000	-1.029287000	3.424470000
1	5.001914000	0.553039000	3.551306000
1	5.882147000	2.044330000	-0.448958000
1	4.117513000	0.683554000	1.040464000
1	7.391049000	-0.848968000	-4.817713000
8	4.529597000	3.473564000	1.011368000
7	4.552218000	2.576865000	1.863776000
8	3.997387000	2.661490000	2.969111000

² Int5A:				⁴ Int5A:			
26	1.374842000	-0.553541000	-1.042298000	26	1.436713000	-0.617310000	-1.053266000
7	1.326712000	-1.097535000	-2.982561000	7	1.208319000	-1.156235000	-2.949351000
7	0.385737000	1.171773000	-1.453939000	7	0.436015000	1.267443000	-1.477111000
7	2.383215000	-2.252957000	-0.616524000	7	2.484442000	-2.434033000	-0.639721000
7	1.435682000	0.011772000	0.916264000	7	1.533439000	-0.112190000	0.878759000
6	1.880632000	-2.209073000	-3.551191000	6	1.703532000	-2.302789000	-3.520223000
6	0.025809000	2.168255000	-0.584978000	6	0.095533000	2.211810000	-0.563552000
6	0.742557000	-0.391469000	-3.995667000	6	0.619147000	-0.412437000	-3.943150000
6	-0.082018000	1.544065000	-2.684796000	6	-0.091918000	1.630599000	-2.672033000
6	2.793253000	-3.218679000	-1.492149000	6	2.769694000	-3.405652000	-1.537812000
6	0.967960000	1.172531000	1.469840000	6	1.083891000	1.061257000	1.435598000
6	2.786144000	-2.660947000	0.625148000	6	2.924665000	-2.844216000	0.574915000
6	1.983424000	-0.716447000	1.936657000	6	2.126468000	-0.852900000	1.871868000
6	1.635444000	-2.213320000	-4.978708000	6	1.394962000	-2.293648000	-4.933643000
6	-0.691073000	3.208165000	-1.290375000	6	-0.669109000	3.263489000	-1.217229000
6	0.925834000	-1.086297000	-5.254159000	6	0.727212000	-1.133527000	-5.193124000
6	-0.760979000	2.818831000	-2.593095000	6	-0.786497000	2.901576000	-2.528601000
6	3.482746000	-4.276890000	-0.783411000	6	3.456606000	-4.502088000	-0.867284000
6	1.241901000	1.191139000	2.889113000	6	1.405319000	1.061249000	2.845186000
6	3.475005000	-3.932265000	0.532446000	6	3.552394000	-4.152837000	0.447425000
6	1.868869000	0.012877000	3.181470000	6	2.044153000	-0.119589000	3.114574000
1	1.972972000	-2.983875000	-5.661114000	1	1.669642000	-3.078303000	-5.628259000
1	-1.085062000	4.107323000	-0.831985000	1	-1.070670000	4.145251000	-0.731284000
1	0.558236000	-0.736353000	-6.211263000	1	0.345825000	-0.778532000	-6.143073000
1	-1.222614000	3.333609000	-3.427144000	1	-1.302074000	3.430624000	-3.321800000
1	3.909619000	-5.156733000	-1.249330000	1	3.807342000	-5.410129000	-1.343588000
1	0.963917000	1.992827000	3.563117000	1	1.149956000	1.856486000	3.535947000
1	3.896562000	-4.468743000	1.373838000	1	3.997062000	-4.718982000	1.257460000
1	2.207911000	-0.350367000	4.144747000	1	2.418818000	-0.476185000	4.066951000
6	2.568933000	-3.203660000	-2.865431000	6	2.409345000	-3.334790000	-2.887427000
6	0.307790000	2.184790000	0.777092000	6	0.423891000	2.120295000	0.791946000
6	2.599671000	-1.958967000	1.811053000	6	2.758379000	-2.099834000	1.745163000
6	0.080710000	0.824815000	-3.865007000	6	0.014206000	0.846822000	-3.826568000
1	2.955018000	-4.037141000	-3.445408000	1	2.701465000	-4.167518000	-3.522257000
1	-0.025231000	3.047503000	1.347430000	1	0.122984000	2.946961000	1.431041000
1	2.986753000	-2.412227000	2.719513000	1	3.160293000	-2.522160000	2.662648000
1	-0.339126000	1.257930000	-4.768835000	1	-0.422176000	1.247461000	-4.738274000
8	3.024029000	0.319814000	-1.349148000	8	3.087027000	0.266777000	-1.443878000
16	-0.689450000	-1.602403000	-0.683501000	16	-0.696909000	-1.633979000	-0.483327000
1	-0.372261000	-2.829954000	-1.156457000	1	-1.019919000	-2.069367000	-1.722109000
6	6.905546000	0.776038000	-2.039385000	6	6.999624000	0.793502000	-2.015519000
6	7.607109000	0.141529000	-3.267891000	6	7.730568000	0.125767000	-3.207126000
7	5.581032000	1.262467000	-2.457887000	7	5.677747000	1.251049000	-2.473777000
8	6.945775000	0.351390000	-4.410802000	8	7.106589000	0.317336000	-4.375245000
8	8.660178000	-0.457800000	-3.200508000	8	8.775826000	-0.479909000	-3.096686000
1	7.522268000	1.645305000	-1.773909000	1	7.599390000	1.681231000	-1.772666000
1	5.396627000	2.187613000	-2.082060000	1	5.455925000	2.161109000	-2.080818000
1	4.792775000	0.670269000	-2.150266000	1	4.903811000	0.630739000	-2.189252000
6	6.924127000	-0.209248000	-0.847644000	6	7.003617000	-0.142873000	-0.785752000
6	6.447657000	0.379266000	0.450592000	6	6.476454000	0.491053000	0.471216000
1	7.947235000	-0.587798000	-0.754629000	1	8.030156000	-0.496410000	-0.645538000
1	6.296930000	-1.070928000	-1.109474000	1	6.401860000	-1.027634000	-1.030587000
6	5.134501000	0.495368000	0.834405000	6	5.149258000	0.645688000	0.790144000
7	5.056983000	1.090707000	2.082855000	7	5.029079000	1.273475000	2.019255000
6	6.316264000	1.362750000	2.542351000	6	6.271569000	1.527588000	2.530955000
6	7.234320000	0.932728000	1.527417000	6	7.225066000	1.054877000	1.569557000
1	4.238469000	0.231005000	0.275396000	1	4.270073000	0.384104000	0.203000000
6	6.746079000	1.939830000	3.745411000	6	6.658416000	2.124692000	3.738894000
6	8.604939000	1.100383000	1.746117000	6	8.587573000	1.201394000	1.846196000
6	9.013200000	1.679689000	2.946950000	6	8.953220000	1.802084000	3.050242000
6	8.107777000	2.098892000	3.944274000	6	8.012640000	2.262403000	3.995637000
1	4.188894000	1.212165000	2.589798000	1	4.143619000	1.396800000	2.495026000
1	6.034219000	2.256939000	4.502725000	1	5.919704000	2.474093000	4.455161000
1	8.498682000	2.539883000	4.851873000	1	8.371333000	2.717923000	4.909328000
1	9.348601000	0.794939000	1.019484000	1	9.356986000	0.863725000	1.161887000
1	2.801711000	1.253716000	-1.195792000	1	2.771172000	1.168143000	-1.629026000
1	6.126813000	0.846160000	-4.102546000	1	6.281862000	0.821574000	-4.106330000
8	11.233831000	1.499082000	2.314455000	8	11.195882000	1.563754000	2.523423000
7	10.439619000	1.862336000	3.187807000	7	10.370728000	1.964104000	3.350716000
8	10.789731000	2.374291000	4.258375000	8	10.682748000	2.496888000	4.422889000

Large model structures:

⁴FeOO+NO:

26	-2.580902000	-4.949569000	-4.292668000	8	-1.219270000	5.639384000	4.943266000
7	-2.915750000	-4.448410000	-2.360324000	6	-0.699704000	2.523152000	3.279068000
7	-2.236514000	-6.866019000	-3.785016000	8	-1.434271000	2.620447000	2.038590000
7	-2.169814000	-5.421045000	-6.217587000	6	-1.558485000	1.956354000	4.405121000
7	-2.831274000	-3.003484000	-4.793787000	7	-2.078118000	5.244568000	2.871885000
6	-3.284906000	-3.229964000	-1.852818000	6	-2.936242000	6.406141000	2.865427000
6	-3.550501000	-3.332031000	-0.423323000	6	-4.384006000	6.022466000	3.158446000
6	-3.306752000	-4.633836000	-0.098643000	6	-4.889484000	4.958904000	2.758035000
6	-2.918617000	-5.318947000	-1.307932000	6	-2.858071000	7.155845000	1.493483000
6	-2.304358000	-7.383645000	-2.521249000	6	-1.496590000	7.680479000	1.182158000
6	-1.998963000	-8.797765000	-2.544941000	6	-0.558815000	7.058979000	0.379816000
6	-1.744057000	-9.121579000	-3.841308000	6	1.341489000	9.941941000	1.390509000
6	-1.893151000	-7.904429000	-4.608035000	6	-0.389251000	10.979767000	2.764679000
6	-1.843510000	-6.648153000	-6.726567000	6	0.910430000	10.977886000	2.214489000
6	-1.643782000	-6.560981000	-8.155755000	7	-5.123959000	6.943465000	3.817460000
6	-1.847714000	-5.259920000	-8.498142000	6	-6.543032000	6.764239000	4.094107000
6	-2.172819000	-4.554873000	-7.277658000	6	-6.826537000	6.289337000	5.533819000
6	-2.742054000	-2.480899000	-6.056314000	6	-6.258141000	4.905961000	5.897131000
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6	-2.435594000	-3.192611000	-7.211680000	1	4.124006000	-0.715770000	1.365911000
1	-3.683546000	-1.152650000	-2.081218000	1	4.773460000	2.536149000	1.307911000
1	-2.655313000	-7.232595000	-0.437764000	1	3.244615000	3.115760000	0.742282000
1	-1.446750000	-8.723966000	-6.514767000	1	6.059341000	1.086612000	1.853626000
1	-2.399256000	-2.634279000	-8.142994000	1	6.103220000	-0.508196000	2.575841000
1	-3.403286000	-5.103887000	0.873553000	1	6.651998000	2.650746000	3.372189000
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16	-4.857891000	-5.341889000	-4.595605000	1	-1.895518000	0.941592000	4.172304000
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6	5.535536000	0.430375000	2.556962000	1	-2.156787000	1.944030000	2.017291000
6	5.607967000	0.961923000	3.991018000	1	-2.045905000	4.621778000	2.070619000
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6	3.243187000	1.186764000	1.461257000	1	-3.177413000	6.454073000	0.715031000
8	2.033387000	0.959690000	1.276952000	1	-0.669743000	6.159472000	-0.212175000
7	3.832994000	2.308374000	1.019988000	1	-2.280001000	9.963987000	2.932338000
7	6.274190000	2.142512000	4.169897000	1	-0.696510000	11.806044000	3.401492000
6	6.517979000	2.650239000	5.508113000	1	2.338668000	9.930732000	0.959403000
6	5.294770000	3.208242000	6.254171000	1	1.584092000	11.802056000	2.435788000
8	5.316173000	3.378412000	7.472411000	1	1.512262000	7.420302000	-0.025201000
7	4.263293000	3.524426000	5.447632000	1	-4.662145000	7.776822000	4.157507000
6	2.930389000	3.855538000	5.886744000	1	-6.926149000	6.057459000	3.356504000
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7	8.195714000	4.445020000	-0.025147000	6	-2.152660000	-0.600428000	-5.913094000
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1	5.361516000	7.283710000	1.104633000	1	0.390534000	-7.989375000	-6.398370000
1	6.033019000	6.580375000	-0.355948000	1	-0.975595000	-1.952294000	-7.950894000
1	4.525319000	4.920546000	1.729236000	1	-3.081787000	-5.008994000	0.714492000
1	5.007981000	4.415730000	0.114692000	1	-0.853586000	-9.060238000	-1.763014000
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6	5.268242000	7.751634000	5.075485000	1	-8.137267000	3.775154000	5.525875000
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6	-0.363851000	10.868711000	2.483113000	1	-3.303332000	2.613739000	-1.269354000
6	0.937887000	10.823080000	1.938565000	1	-5.865447000	2.416042000	1.045826000
7	-5.121109000	6.925218000	3.809325000	1	-6.118743000	4.061152000	1.208764000
6	-6.543032000	6.764239000	4.094107000	1	-7.378797000	8.156153000	-1.305626000
6	-6.826119000	6.272327000	5.528124000	6	-8.555019000	2.165242000	-3.902891000
6	-6.293552000	4.868141000	5.865794000	6	-7.771446000	2.392703000	-5.212856000
6	-7.094001000	3.743661000	5.189169000	6	-6.485598000	3.147084000	-4.956345000
7	-6.592138000	2.396486000	5.454968000	6	-5.325290000	2.471733000	-4.554076000
6	-5.734222000	1.711276000	4.655000000	6	-6.445642000	4.547645000	-4.983657000
7	-5.181106000	2.288014000	3.595370000	6	-4.196886000	3.155508000	-4.102820000
7	-5.451984000	0.431701000	4.931300000	6	-5.325350000	5.250151000	-4.540952000
1	3.926951000	-0.643563000	2.746162000	6	-4.215430000	4.555959000	-4.035639000
1	4.585931000	-0.725586000	1.118138000	8	-3.253065000	5.280334000	-3.400564000
1	4.848265000	2.476469000	1.410694000	1	-8.402137000	2.946557000	-5.920955000
1	3.265139000	2.987001000	0.933266000	1	-7.556233000	1.421403000	-5.675867000
1	6.296913000	1.114528000	1.833878000	1	-5.312567000	1.383591000	-4.562531000
1	6.454251000	-0.476550000	2.546200000	1	-7.316272000	5.100447000	-5.333818000
1	6.736196000	2.676573000	3.385594000	1	-3.324229000	2.618575000	-3.742146000
1	6.912096000	1.850272000	6.142989000	1	-5.302471000	6.336888000	-4.543855000
1	7.266340000	3.449076000	5.472205000	1	-2.424606000	4.740184000	-3.169006000
1	4.296921000	3.209636000	4.460195000	1	-7.955587000	1.589685000	-3.188900000
1	2.581802000	3.091701000	6.628751000	1	-9.487074000	1.615929000	-4.085761000
1	3.413939000	5.119918000	7.502789000	1	-8.808519000	3.121976000	-3.430824000
1	1.800161000	5.414611000	6.862386000	6	6.994001000	5.915234000	1.497102000
1	5.392546000	6.132957000	6.497050000	6	7.563722000	4.551479000	1.136990000
1	1.494562000	6.896001000	4.859003000	8	7.471713000	3.558316000	1.872561000
1	6.325276000	7.997539000	5.149080000	6	5.730698000	6.292944000	0.690290000
1	2.417540000	8.749046000	3.508341000	6	4.681711000	5.190080000	0.762098000
1	4.835673000	9.309991000	3.643710000	6	3.272205000	5.524929000	0.237246000
1	0.365711000	4.464476000	5.549019000	8	3.083051000	6.681814000	-0.223066000
1	0.462390000	4.266984000	2.738696000	8	2.424373000	4.587483000	0.335867000
1	0.209592000	1.890004000	3.118125000	7	8.197473000	4.464562000	-0.059968000

6	8.662921000	3.181251000	-0.572884000	8	-1.050669000	4.181080000	-2.523908000
6	9.285380000	3.333502000	-1.970439000	6	1.592643000	2.482904000	-2.331316000
6	8.318477000	3.891196000	-2.997585000	6	1.783419000	1.020526000	-2.644805000
6	7.230033000	3.125967000	-3.445214000	6	0.856810000	0.084189000	-3.073011000
6	8.463995000	5.195794000	-3.488457000	6	3.033876000	0.311992000	-2.533974000
6	6.309059000	3.654620000	-4.348524000	7	1.450288000	-1.144040000	-3.239557000
6	7.543396000	5.728551000	-4.396083000	6	2.781267000	-1.038525000	-2.915531000
6	6.462093000	4.959739000	-4.825678000	6	4.337925000	0.676084000	-2.146074000
1	5.320005000	7.222996000	1.095259000	6	3.789565000	-2.013618000	-2.920764000
1	5.984416000	6.503624000	-0.356854000	6	5.336359000	-0.292060000	-2.142346000
1	4.556942000	4.863992000	1.803476000	6	5.064116000	-1.623988000	-2.529471000
1	5.036350000	4.314526000	0.204035000	8	-1.764444000	2.152136000	-1.818245000
1	6.748456000	5.881393000	2.562915000	1	1.382546000	3.081084000	-3.227312000
1	9.638438000	2.342007000	-2.280446000	1	2.527151000	2.876351000	-1.918739000
1	10.171172000	3.978139000	-1.903770000	1	-0.197673000	0.210630000	-3.282186000
1	7.093336000	2.108404000	-3.086200000	1	4.559489000	1.694906000	-1.838089000
1	9.311998000	5.797396000	-3.164815000	1	6.344603000	-0.025261000	-1.829394000
1	5.469917000	3.045861000	-4.673129000	1	3.572073000	-3.034002000	-3.219193000
1	7.672663000	6.743459000	-4.763353000	1	5.866019000	-2.358243000	-2.519443000
1	5.740115000	5.372776000	-5.524610000	1	0.797792000	3.741876000	-0.781968000
1	7.826717000	2.470795000	-0.609267000	1	-0.338700000	2.061740000	0.456949000
1	8.076992000	5.220491000	-0.723032000	1	-0.037154000	0.925807000	-0.728742000
1	9.397226000	2.769116000	0.127683000	1	1.219330000	1.490346000	0.233563000
1	7.772493000	6.678610000	1.359902000	1	0.964482000	-2.040404000	-3.449168000
8	0.327980000	-3.685648000	-3.577779000	8	1.486524000	-4.463192000	-3.839367000
7	0.334297000	1.764356000	-0.270592000	7	1.776371000	-5.263801000	-2.739019000
6	0.479546000	2.839137000	-1.309478000	8	2.771774000	-5.900927000	-2.951356000
6	-0.902942000	3.074444000	-1.945864000				

Cartesian coordinates of optimized geometries:

Model B system – C6

² Re _B								
26	0.044462000	-5.961780000	-2.255076000	7	4.443612000	3.889952000	5.111186000	
7	-0.082372000	-4.584191000	-0.768116000	1	4.577217000	3.658667000	4.133690000	
7	1.962518000	-5.428300000	-2.547481000	6	3.125958000	4.391248000	5.466122000	
7	0.139835000	-7.307814000	-3.763423000	1	2.724548000	3.756486000	6.265654000	
7	-1.890786000	-6.478050000	-1.974403000	6	3.126671000	5.845290000	6.027037000	
6	-1.218615000	-4.222542000	-0.086977000	1	3.701416000	5.801687000	6.957016000	
6	-0.938548000	-3.116879000	0.827035000	6	3.691703000	6.908017000	5.113461000	
6	0.394220000	-2.851910000	0.683514000	6	5.055962000	7.231025000	5.155196000	
6	0.911039000	-3.753946000	-0.317139000	6	2.863042000	7.604706000	4.221126000	
6	2.700251000	-4.520269000	-1.832729000	6	5.582089000	8.222399000	4.323631000	
6	4.049119000	-4.460727000	-2.348212000	6	3.385179000	8.596245000	3.387807000	
6	4.110712000	-5.339953000	-3.387252000	6	4.747134000	8.907683000	3.436850000	
6	2.802365000	-5.944336000	-3.501779000	1	5.705676000	6.709636000	5.853982000	
6	1.234911000	-7.548770000	-4.550574000	1	1.800187000	7.373760000	4.188559000	
6	0.937130000	-8.590974000	-5.508288000	1	6.640494000	8.465330000	4.375215000	
6	-0.347362000	-8.981835000	-5.276898000	1	2.729194000	9.128811000	2.705057000	
6	-0.836601000	-8.172641000	-4.183420000	1	5.152179000	9.683280000	2.792323000	
6	-2.603597000	-7.456080000	-2.620243000	6	2.247254000	4.232343000	4.223728000	
6	-3.954957000	-7.504978000	-2.110750000	8	2.729350000	4.235239000	3.085134000	
6	-4.050224000	-6.531399000	-1.162400000	7	0.932133000	4.063724000	4.482928000	
6	-2.753624000	-5.894918000	-1.084887000	1	0.616559000	4.252571000	5.426285000	
6	-2.457148000	-4.838512000	-0.226177000	6	-0.080918000	4.122616000	3.449378000	
6	2.221338000	-3.742985000	-0.783086000	1	0.438573000	4.316406000	2.505571000	
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6	-2.116236000	-8.260556000	-3.644301000	1	-0.000293000	2.014431000	3.159378000	
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1	3.245734000	-7.218265000	-5.136247000	6	-1.654910000	2.368644000	4.499178000	
1	-2.792064000	-8.995335000	-4.071430000	1	-1.046235000	2.303820000	5.407991000	
1	0.978914000	-2.094171000	1.194400000	1	-2.111674000	1.386864000	4.336918000	
1	4.830196000	-3.819671000	-1.958548000	1	-2.459494000	3.094798000	4.661754000	
1	4.953811000	-5.571369000	-4.026425000	6	-0.983241000	5.341854000	3.735177000	
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1	-4.908302000	-6.255289000	-0.562012000	6	-2.945767000	6.590812000	2.965880000	
6	-1.926035000	-2.392924000	1.705262000	1	-2.596144000	7.236184000	3.774845000	
6	-2.392948000	-1.046022000	1.112269000	6	-2.932400000	7.372549000	1.615431000	
6	-3.434772000	-0.309231000	1.963464000	1	-3.642785000	8.204121000	1.703808000	
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8	-4.130353000	-0.955434000	2.777215000	6	-1.595697000	7.871588000	1.161641000	
1	-1.465137000	-2.201389000	2.682117000	6	-0.715390000	7.165647000	0.369620000	
1	-2.807332000	-3.009969000	1.902278000	7	0.392698000	7.921393000	0.079284000	
1	-1.539778000	-0.378416000	0.950063000	1	-0.811564000	6.155964000	-0.007879000	
1	-2.840183000	-1.210465000	0.121409000	1	1.169922000	7.607186000	-0.523005000	
16	0.760054000	-7.743023000	-0.826271000	6	-0.987331000	9.160018000	1.382366000	
1	1.538549000	-7.035955000	0.024855000	6	0.258131000	9.150015000	0.683107000	
8	-0.577687000	-4.726537000	-3.554875000	6	-1.359594000	10.326484000	2.078387000	
7	3.762214000	1.806918000	1.801397000	6	1.121808000	10.253824000	0.670742000	
1	4.733268000	2.073131000	1.666154000	6	-0.507421000	11.425852000	2.064119000	
1	3.101197000	2.573772000	1.876808000	6	0.722803000	11.389285000	1.369478000	
6	3.384493000	0.610497000	2.318563000	1	-2.301014000	10.370429000	2.621999000	
8	2.209132000	0.355823000	2.603275000	1	-0.788072000	12.329515000	2.599481000	
6	4.474810000	-0.447250000	2.497642000	1	1.368363000	12.263726000	1.382362000	
1	4.108961000	-1.133129000	3.265298000	1	2.068266000	10.198831000	0.139950000	
1	4.548666000	-1.019264000	1.563489000	6	-4.378339000	6.118021000	3.224125000	
6	5.872490000	0.069280000	2.882389000	8	-4.791966000	5.043249000	2.759503000	
1	6.307290000	0.687694000	2.092993000	7	-5.167649000	6.978046000	3.896040000	
1	6.532462000	-0.799257000	2.999536000	1	-4.749982000	7.816082000	4.279094000	
6	5.877304000	0.797422000	4.225737000	6	-6.604577000	6.787316000	4.074927000	
8	5.428367000	0.279836000	5.249878000	1	-7.069927000	7.777053000	4.037637000	
7	6.436385000	2.041668000	4.225998000	1	-6.970442000	6.220602000	3.215190000	
1	6.713346000	2.459152000	3.339435000	6	-6.973058000	6.108236000	5.400130000	
6	6.601234000	2.779770000	5.464661000	1	-6.492372000	6.666764000	6.213092000	
1	6.963664000	2.111416000	6.248846000	1	-8.055363000	6.233452000	5.548144000	
1	7.354847000	3.557921000	5.304178000	6	-6.618282000	4.622817000	5.540288000	
6	5.335541000	3.449747000	6.029792000	1	-6.744939000	4.326726000	6.588875000	
8	5.195633000	3.609800000	7.243203000	1	-5.564031000	4.456702000	5.294033000	

6	-7.511437000	3.723830000	4.673800000	6	5.341917000	0.795231000	-2.508132000
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1	-7.421193000	3.977445000	3.613656000	6	4.493991000	1.640639000	-3.230593000
7	-7.225169000	2.297790000	4.819948000	1	7.272039000	0.555189000	-1.590218000
1	-7.668790000	1.805343000	5.583371000	1	6.542902000	4.348441000	-3.476563000
6	-6.271000000	1.641253000	4.136087000	1	5.012642000	-0.205446000	-2.240756000
7	-5.512311000	2.276050000	3.229022000	1	4.286182000	3.581607000	-4.148887000
1	-5.385084000	3.287509000	3.258303000	1	3.506914000	1.298827000	-3.530051000
1	-4.757680000	1.737647000	2.752021000	7	1.078421000	4.525241000	-2.130013000
7	-6.083843000	0.330597000	4.326141000	1	0.621228000	4.048862000	-1.331553000
1	-6.774802000	-0.213401000	4.823037000	1	1.601875000	3.816968000	-2.653373000
1	-5.363967000	-0.170039000	3.765754000	1	1.746176000	5.299655000	-1.777183000
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1	-7.063424000	8.564716000	0.520994000	1	0.021372000	6.172764000	-2.882691000
1	-8.095856000	7.291921000	-0.152529000	6	-1.396858000	4.678493000	-2.275778000
1	-7.204690000	8.376052000	-1.233266000	8	-2.440516000	5.137987000	-2.795680000
6	-5.951202000	6.869759000	-0.260731000	8	-1.299486000	3.942012000	-1.249437000
1	-5.904438000	6.360914000	0.709340000	6	0.038115000	4.680703000	-4.431640000
1	-5.024096000	7.444359000	-0.354480000	1	-0.895010000	5.025718000	-4.892891000
6	-5.960592000	5.805236000	-1.373604000	1	0.841445000	5.262284000	-4.899758000
1	-6.921627000	5.277194000	-1.409863000	6	0.294871000	3.217100000	-4.699986000
1	-5.842698000	6.280667000	-2.351782000	6	-0.040169000	2.113086000	-3.933082000
7	-4.868115000	4.832148000	-1.248657000	1	-0.565405000	2.062958000	-2.988571000
1	-4.000626000	4.991778000	-1.788262000	7	0.438389000	0.964592000	-4.524523000
6	-4.893923000	3.734573000	-0.478569000	1	0.364846000	0.026669000	-4.146724000
7	-3.809182000	2.967976000	-0.371899000	6	1.097124000	1.292120000	-5.690657000
1	-5.958715000	2.709289000	0.919738000	6	1.026186000	2.705308000	-5.837126000
1	-6.780842000	4.024036000	0.241732000	6	1.628338000	3.305871000	-6.959690000
7	-6.042954000	3.344292000	0.133092000	6	2.275564000	2.498686000	-7.887020000
1	-3.797025000	2.166256000	0.263785000	6	1.748937000	0.474149000	-6.623880000
1	-2.895867000	3.316731000	-0.708033000	6	2.334555000	1.097012000	-7.719542000
6	-8.555047000	2.165240000	-3.902878000	1	1.585224000	4.382583000	-7.102686000
1	-8.458948000	1.077569000	-3.999474000	1	2.744184000	2.949853000	-8.757502000
1	-9.613703000	2.400476000	-3.740088000	1	1.794515000	-0.601030000	-6.483678000
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6	-8.018258000	2.878527000	-5.157641000	7	0.758786000	-3.109400000	-4.416729000
6	-6.552885000	2.599576000	-5.427453000	8	1.117893000	-1.956884000	-4.355688000
6	-5.548428000	3.276352000	-4.721877000	8	-0.105945000	-3.387690000	-3.402263000
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1	-4.495998000	0.621519000	-7.326708000				
8	2.418466000	6.667340000	-1.391148000				
8	3.816251000	8.190579000	-0.536279000				
6	3.492931000	7.012486000	-0.758252000				
6	4.356828000	5.860464000	-0.207212000				
1	3.728893000	5.326573000	0.521031000				
1	4.558181000	5.142621000	-1.013159000				
6	5.645034000	6.337736000	0.472849000				
1	5.411219000	7.255557000	1.018629000				
1	6.384780000	6.630619000	-0.284315000				
6	6.246983000	5.342157000	1.482738000				
1	5.470192000	5.020953000	2.182253000				
1	7.013928000	5.860223000	2.075968000				
6	6.900422000	4.077256000	0.939818000				
8	6.634223000	2.951603000	1.407088000				
7	7.833985000	4.248268000	-0.021195000				
1	8.014065000	5.191427000	-0.340706000				
6	8.662980000	3.181227000	-0.572899000				
1	8.414224000	2.275041000	-0.018457000				
1	9.716446000	3.418040000	-0.380611000				
6	8.459069000	2.971767000	-2.086030000				
1	9.202192000	2.229650000	-2.407311000				
1	8.704070000	3.902638000	-2.612572000				
6	7.068745000	2.512841000	-2.478233000				
6	6.616639000	1.227508000	-2.140003000				
6	6.207333000	3.352243000	-3.197161000				

²TS1_B

26	-0.169613000	-5.175592000	-2.207672000
7	-0.225556000	-3.920687000	-0.629976000
7	1.736007000	-4.681932000	-2.524770000
7	-0.082047000	-6.551258000	-3.704167000
7	-2.068588000	-5.789847000	-1.802012000
6	-1.314709000	-3.655171000	0.164892000
6	-0.975164000	-2.652188000	1.166424000
6	0.338723000	-2.345994000	0.958415000
6	0.790384000	-3.128443000	-0.164613000
6	2.493781000	-3.786603000	-1.812037000
6	3.818539000	-3.696535000	-2.378109000
6	3.850633000	-4.545119000	-3.442493000
6	2.549033000	-5.163614000	-3.524243000
6	0.976620000	-6.765828000	-4.543896000
6	0.641510000	-7.778938000	-5.517759000
6	-0.635251000	-8.171295000	-5.250589000
6	-1.081725000	-7.393913000	-4.117393000
6	-2.800463000	-6.733661000	-2.476691000
6	2.067897000	-3.066150000	-0.704246000
6	2.204347000	-6.118108000	-4.470464000
6	-2.344686000	-7.494565000	-3.545881000
1	-3.326994000	-3.962136000	0.760268000
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1	2.959249000	-6.390952000	-5.201148000
1	-3.034908000	-8.210684000	-3.980966000
1	0.947664000	-1.638055000	1.510524000
1	4.608905000	-3.064381000	-1.993295000
1	4.671302000	-4.752446000	-4.117566000
1	1.309021000	-8.130768000	-6.294272000
1	-1.236398000	-8.911760000	-5.763209000
1	-4.903690000	-7.488456000	-2.268908000

1	-5.024324000	-5.666331000	-0.260717000	6	-0.968625000	6.996722000	0.351513000
6	-1.912115000	-2.012317000	2.152485000	7	0.177052000	7.684008000	0.026038000
6	-2.502376000	-0.708035000	1.587110000	1	-1.120506000	5.987561000	-0.011134000
6	-3.450230000	0.041960000	2.522417000	1	0.942307000	7.337607000	-0.571414000
8	-3.719721000	1.262533000	2.176868000	6	-1.094742000	9.020375000	1.339227000
8	-3.907762000	-0.519387000	3.537156000	6	0.133216000	8.924980000	0.620026000
1	-1.368390000	-1.783499000	3.076059000	6	-1.379855000	10.211788000	2.034574000
1	-2.726104000	-2.687620000	2.433851000	6	1.071677000	9.965998000	0.592086000
1	-1.691090000	-0.025135000	1.308619000	6	-0.457027000	11.251776000	2.001641000
1	-3.051421000	-0.912290000	0.657195000	6	0.759050000	11.127824000	1.291881000
16	0.601255000	-6.926782000	-0.706146000	1	-2.308259000	10.320822000	2.591210000
1	-0.311478000	-7.871975000	-1.020518000	1	-0.668815000	12.174977000	2.535318000
8	-0.916095000	-4.098631000	-3.253868000	1	1.462954000	11.956207000	1.293166000
7	3.526138000	1.555665000	2.055140000	1	2.009125000	9.842319000	0.056267000
1	4.500572000	1.780051000	1.874548000	6	-4.411814000	6.522627000	3.714794000
1	2.901805000	2.350390000	2.149457000	8	-5.037410000	5.541696000	3.280628000
6	3.131751000	0.400908000	2.646722000	7	-4.936426000	7.398468000	4.596169000
8	1.964178000	0.213507000	3.008891000	1	-4.351614000	8.155500000	4.925494000
6	4.182446000	-0.698933000	2.806014000	6	-6.311131000	7.335178000	5.090371000
1	3.831956000	-1.340847000	3.617629000	1	-6.688910000	8.360964000	5.141025000
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6	5.621402000	-0.235242000	3.094290000	6	-6.445083000	6.676484000	6.473749000
1	6.031292000	0.353687000	2.269582000	1	-5.828124000	7.235269000	7.188369000
1	6.251204000	-1.128500000	3.186311000	1	-7.486284000	6.801528000	6.802064000
6	5.734548000	0.510249000	4.422693000	6	-6.057034000	5.190778000	6.539146000
8	5.361784000	0.006695000	5.483946000	1	-6.039395000	4.876793000	7.590333000
7	6.293675000	1.752608000	4.364459000	1	-5.039067000	5.049837000	6.156525000
1	6.509978000	2.159305000	3.455545000	6	-7.024875000	4.274963000	5.773422000
6	6.543548000	2.505803000	5.578748000	1	-8.040645000	4.388490000	6.166546000
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1	7.298231000	3.269298000	5.362008000	7	-6.684787000	2.855421000	5.875092000
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8	5.272744000	3.398584000	7.423866000	6	-5.873345000	2.180058000	5.034228000
7	4.386127000	3.646508000	5.338821000	7	-5.332493000	2.763653000	3.964915000
1	4.440148000	3.386369000	4.360557000	1	-5.298118000	3.776251000	3.848112000
6	3.127122000	4.229985000	5.764466000	1	-4.741575000	2.195502000	3.335864000
1	2.709891000	3.612089000	6.569783000	7	-5.622021000	0.884080000	5.265989000
6	3.269438000	5.670832000	6.344566000	1	-6.180011000	0.373184000	5.934526000
1	3.958335000	5.580394000	7.189010000	1	-5.004999000	0.350805000	4.624846000
1	2.296123000	5.961989000	6.757610000	6	-7.329113000	6.610608000	-1.371977000
6	3.753353000	6.726833000	5.376280000	1	-7.480310000	7.496559000	-0.746361000
6	5.123011000	6.995527000	5.237195000	1	-8.196863000	5.953315000	-1.237469000
6	2.842114000	7.469241000	4.608687000	1	-7.317281000	6.937924000	-2.418502000
6	5.573371000	7.975667000	4.349538000	6	-6.025835000	5.895644000	-1.002035000
6	3.288930000	8.448506000	3.718357000	1	-6.044440000	5.603969000	0.056968000
6	4.656735000	8.704469000	3.586489000	1	-5.174841000	6.578074000	-1.119136000
1	5.838768000	6.441510000	5.839592000	6	-5.781523000	4.656231000	-1.877851000
1	1.775287000	7.282842000	4.714233000	1	-6.622867000	3.955980000	-1.804502000
1	6.638151000	8.175843000	4.260815000	1	-5.721357000	4.953329000	-2.929446000
1	2.571220000	9.014519000	3.130367000	7	-4.538126000	3.952325000	-1.572410000
1	5.004085000	9.469937000	2.897844000	1	-3.690254000	4.213728000	-2.107645000
6	2.176420000	4.167171000	4.558314000	6	-4.398957000	3.014414000	-0.631072000
8	2.600569000	3.964739000	3.414385000	7	-3.222852000	2.407083000	-0.451774000
7	0.864868000	4.325133000	4.840278000	1	-5.217739000	2.013610000	0.917389000
1	0.594176000	4.668405000	5.753803000	1	-6.258999000	3.188433000	0.213372000
6	-0.154350000	4.377221000	3.808422000	7	-5.451396000	2.592262000	0.113336000
1	0.350016000	4.588629000	2.859479000	1	-3.130957000	1.859873000	0.404867000
6	-0.851734000	2.998913000	3.644791000	1	-2.373005000	2.800377000	-0.887781000
1	-0.045267000	2.267019000	3.492092000	6	-7.557082000	0.102408000	-5.467632000
8	-1.640027000	3.089346000	2.454355000	1	-7.250126000	-0.569387000	-6.277548000
1	-2.329872000	2.386575000	2.453986000	1	-8.597839000	-0.128629000	-5.210375000
6	-1.675946000	2.588272000	4.864695000	1	-6.933000000	-0.121811000	-4.594862000
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6	-1.089383000	5.569582000	4.105756000	6	-5.502645000	1.795332000	-7.561218000
8	-0.832372000	6.375462000	5.005510000	6	-3.752848000	2.700577000	-5.590672000
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6	-1.785651000	7.768552000	1.151974000	1	-6.177742000	1.447256000	-8.340595000

1	-3.086525000	3.084353000	-4.821643000	6	0.677668000	-4.673073000	1.797103000
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8	3.794829000	8.094903000	-0.550553000	6	4.758082000	-7.038695000	1.910556000
6	3.403054000	6.943917000	-0.796362000	6	4.244368000	-6.779543000	0.583311000
6	4.157878000	5.733472000	-0.214710000	6	4.397717000	-6.917298000	-1.876531000
1	3.430996000	5.167968000	0.385950000	6	5.067287000	-7.324498000	-3.092241000
1	4.447218000	5.064233000	-1.036360000	6	4.277553000	-6.924537000	-4.126950000
6	5.359731000	6.113207000	0.655380000	6	3.125896000	-6.272122000	-3.543777000
1	5.071395000	6.959986000	1.284443000	6	0.966997000	-5.086330000	-3.740020000
1	6.178951000	6.494559000	0.030271000	6	-0.094309000	-4.501502000	-4.526129000
6	5.838980000	4.991329000	1.589831000	6	-0.978956000	-3.953484000	-3.645389000
1	5.002026000	4.647721000	2.206132000	6	-0.456683000	-4.203727000	-2.320339000
1	6.585513000	5.396317000	2.288722000	6	-1.062142000	-3.763236000	-1.145410000
6	6.471680000	3.746242000	0.982454000	6	1.698214000	-5.265552000	2.532031000
8	6.370430000	2.636366000	1.545730000	6	4.880049000	-7.156709000	-0.593718000
7	7.192951000	3.905305000	-0.145289000	6	2.079938000	-5.723621000	-4.277215000
1	7.271125000	4.838197000	-0.528947000	1	-1.986480000	-3.203755000	-1.248809000
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1	7.712839000	1.918733000	-0.270746000	1	5.827438000	-7.679728000	-0.505116000
1	9.058220000	3.032189000	-0.529280000	1	2.141414000	-5.790433000	-5.359243000
6	7.820506000	2.768301000	-2.279858000	1	-0.562554000	-3.786789000	3.442585000
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6	6.441206000	2.342459000	-2.743257000	1	6.014926000	-7.847374000	-3.127879000
6	5.912301000	1.095747000	-2.372042000	1	4.441354000	-7.049205000	-5.190099000
6	5.681429000	3.162855000	-3.586664000	1	-0.139499000	-4.516466000	-5.607969000
6	4.662420200	0.681264000	-2.831528000	1	-1.905589000	-3.432626000	-3.854387000
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1	6.489167000	0.436530000	-1.727178000	6	-3.461096000	-0.337818000	1.954416000
1	6.078798000	4.128131000	-3.892700000	8	-3.469575000	0.937439000	1.746837000
1	4.272079000	-0.289819000	-2.538365000	8	-4.338077000	-0.939990000	2.610720000
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1	2.955844000	1.170944000	-4.059804000	1	-3.193990000	-2.971762000	0.717195000
7	1.329878000	4.457676000	-2.461559000	1	-1.393317000	-0.843468000	1.998405000
1	0.934538000	3.851838000	-1.719140000	1	-2.057210000	-0.803244000	0.380013000
1	1.934163000	3.882077000	-3.055416000	16	0.760041000	-7.742993000	-0.826246000
1	1.889103000	5.274650000	-2.014350000	1	1.878065000	-8.464865000	-0.589618000
6	0.132722000	4.983687000	-3.201829000	8	2.745764000	-3.998846000	-0.909881000
1	0.094042000	6.057815000	-3.000149000	7	3.944385000	1.947788000	1.861709000
6	-1.141556000	4.361403000	-2.564240000	1	4.905152000	2.199518000	1.652051000
8	-2.238454000	4.695206000	-3.070569000	1	3.296724000	2.725275000	1.950327000
8	-0.940837000	3.598136000	-1.573380000	6	3.601901000	0.800093000	2.504906000
6	0.233293000	4.786929000	-4.720925000	8	2.459460000	0.600728000	2.927696000
1	-0.705759000	5.178415000	-5.131085000	6	4.685458000	-0.271095000	2.641781000
1	1.026404000	5.441216000	-5.103074000	1	4.341282000	-0.957108000	3.418919000
6	0.498616000	3.377122000	-5.191671000	1	4.728891000	-0.837679000	1.702539000
6	0.136689000	2.175286000	-4.603353000	6	6.098986000	0.237051000	2.984598000
1	-0.385638000	1.992590000	-3.674040000	1	6.512951000	0.853616000	2.181952000
7	0.580909000	1.120214000	-5.364026000	1	6.756339000	-0.634596000	3.086115000
1	0.473393000	0.124005000	-5.156962000	6	6.132164000	0.973312000	4.321433000
6	1.241154000	1.606790000	-6.471056000	8	5.765427000	0.440607000	5.370420000
6	1.216156000	3.028053000	-6.397826000	7	6.599414000	2.253620000	4.281469000
6	1.832457000	3.773951000	-7.421933000	1	6.817731000	2.674808000	3.380169000
6	2.448547000	3.097459000	-8.467832000	6	6.711289000	3.036325000	5.496807000
6	1.857279000	0.921430000	-7.527219000	1	7.135021000	2.424651000	6.296227000
6	2.458556000	1.685273000	-8.520331000	1	7.392056000	3.873230000	5.308624000
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1	2.945315000	1.187237000	-9.354556000	1	4.623661000	3.727029000	4.144919000
7	0.215419000	-2.725389000	-5.061469000	6	3.125957000	4.391230000	5.466108000
8	0.636627000	-1.724903000	-5.658331000	1	2.719037000	3.721768000	6.234177000
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				6	3.764539000	6.904943000	5.267479000
26	1.938070000	-5.428029000	-0.873036000	6	5.125319000	7.180623000	5.470564000
7	0.561553000	-4.688131000	0.433522000	6	3.060655000	7.658120000	4.316890000
7	3.049100000	-6.114337000	0.665070000	6	5.770150000	8.179610000	4.738244000
7	3.222136000	-6.283768000	-2.177462000	6	3.701515000	8.659247000	3.583599000
7	0.718647000	-4.902657000	-2.403191000	6	5.058686000	8.921604000	3.791414000
6	-0.572482000	-3.973869000	0.1366679000	1	5.675329000	6.615782000	6.219341000
6	-1.205171000	-3.484443000	1.358237000	1	2.001376000	7.465100000	4.160480000

1	6.823274000	8.384262000	4.913902000	1	-5.612113000	6.259584000	-2.266807000
1	3.138544000	9.237446000	2.857022000	7	-4.647005000	4.860926000	-1.081062000
1	5.555003000	9.705493000	3.225277000	1	-3.722584000	5.085035000	-1.453677000
6	2.269668000	4.264920000	4.208761000	6	-4.722221000	3.684898000	-0.443155000
8	2.759591000	4.327756000	3.075771000	7	-3.669704000	2.865983000	-0.435814000
7	0.955693000	4.064979000	4.446470000	1	-5.842407000	2.469689000	0.727423000
1	0.628970000	4.196198000	5.395479000	1	-6.521254000	3.994115000	0.454206000
6	-0.046333000	4.154820000	3.405799000	7	-5.888030000	3.280522000	0.121195000
1	0.484834000	4.378739000	2.475124000	1	-3.624691000	2.081408000	0.221909000
6	-0.752886000	2.790127000	3.209622000	1	-2.798441000	3.218206000	-0.839780000
1	0.056237000	2.058600000	3.070735000	6	-8.455566000	1.954831000	-4.226740000
8	-1.521243000	2.895162000	2.009019000	1	-8.014996000	0.956885000	-4.118805000
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6	-1.611697000	2.370153000	4.404013000	1	-8.126992000	2.557293000	-3.371774000
1	-1.008502000	2.294637000	5.315488000	6	-8.025501000	2.603331000	-5.554772000
1	-2.056571000	1.387180000	4.220560000	6	-6.523970000	2.767520000	-5.654038000
1	-2.424679000	3.084919000	4.573903000	6	-5.870166000	3.798882000	-4.964845000
6	-0.951473000	5.365171000	3.719146000	6	-5.730507000	1.866966000	-6.378299000
8	-0.650518000	6.171111000	4.604619000	6	-4.482300000	3.923342000	-4.974981000
7	-2.041103000	5.481377000	2.929739000	6	-4.339901000	1.975769000	-6.404168000
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7	0.407897000	8.042865000	0.179460000	1	-3.734335000	1.269575000	-6.965321000
1	-0.919333000	6.396051000	-0.136129000	8	2.412559000	6.353378000	-0.796075000
1	1.219862000	7.660214000	-0.327717000	8	3.767973000	8.068505000	-0.327333000
6	-0.882427000	9.183443000	1.655193000	6	3.509596000	6.852345000	-0.332061000
6	0.358735000	9.184939000	0.946694000	6	4.500497000	5.853698000	0.292903000
6	-1.184433000	10.274841000	2.492064000	1	4.018960000	5.462184000	1.199928000
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6	-0.268163000	11.315140000	2.607359000	6	5.852349000	6.479099000	0.647350000
6	0.956143000	11.291373000	1.902672000	1	5.665197000	7.447248000	1.119785000
1	-2.122033000	10.306808000	3.043188000	1	6.417319000	6.692135000	-0.269555000
1	-0.493913000	12.161252000	3.251628000	6	6.711514000	5.639108000	1.616410000
1	1.652514000	12.118272000	2.016129000	1	6.148308000	5.438960000	2.532413000
1	2.224072000	10.190153000	0.520124000	1	7.600107000	6.219068000	1.898974000
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6	-6.973020000	6.108254000	5.400110000	6	9.046856000	3.467213000	-2.035264000
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6	-6.617673000	4.624557000	5.537406000	6	7.872359000	3.814119000	-2.927698000
1	-6.760134000	4.320815000	6.581679000	6	7.014233000	2.808324000	-3.397085000
1	-5.560143000	4.459640000	5.304736000	6	7.606418000	5.141103000	-3.293053000
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1	-8.554188000	3.888551000	4.900140000	6	6.510098000	5.458922000	-4.099744000
1	-7.385228000	3.993787000	3.593145000	6	5.663168000	4.448211000	-4.559397000
7	-7.231199000	2.309540000	4.798273000	1	7.207205000	1.770890000	-3.132109000
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6	-6.271002000	1.641194000	4.136097000	1	5.271914000	2.324645000	-4.564237000
7	-5.467263000	2.264200000	3.264346000	1	6.322236000	6.494291000	-4.371351000
1	-5.355341000	3.277310000	3.261580000	1	4.814513000	4.691217000	-5.193148000
1	-4.730268000	1.722484000	2.772648000	7	0.968145000	4.202204000	-1.204221000
7	-6.120429000	0.323045000	4.326396000	1	0.116649000	4.224899000	-0.618807000
1	-6.870541000	-0.202203000	4.754075000	1	1.355199000	3.254312000	-1.155883000
1	-5.464567000	-0.187951000	3.702683000	1	1.684758000	4.931988000	-0.868794000
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6	-0.074817000	1.397200000	-3.829637000	6	5.084901000	-0.359025000	2.374789000
1	-0.961379000	1.684382000	-4.379681000	1	5.461196000	0.223640000	1.529646000
7	0.128178000	0.096841000	-3.440873000	1	5.656543000	-1.295039000	2.392985000
1	-0.489389000	-0.676554000	-3.643431000	6	5.364566000	0.349319000	3.698893000
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6	-6.044766000	1.654991000	4.962159000	1	5.302909000	3.627349000	-6.716616000
7	-5.389410000	2.217930000	3.944606000	1	8.366364000	6.162832000	-5.072338000
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6	-6.249757000	4.767345000	-0.918641000	8	-1.129513000	3.429051000	-1.131976000
1	-6.256254000	4.478854000	0.140887000	6	0.268135000	3.423445000	-4.382323000
1	-5.452248000	5.512626000	-1.030904000	1	-0.479795000	3.811774000	-5.079837000
6	-5.898790000	3.549151000	-1.787072000	1	1.245034000	3.699809000	-4.797589000
1	-6.680198000	2.782091000	-1.722676000	6	0.134979000	1.928060000	-4.269019000
1	-5.849967000	3.848169000	-2.838574000	6	-1.062446000	1.226523000	-4.371545000
7	-4.602313000	2.955771000	-1.464751000	1	-2.051251000	1.599829000	-4.596969000
1	-3.779481000	3.315259000	-1.971264000	7	-0.843660000	-0.105032000	-4.143333000
6	-4.375000000	2.069657000	-0.490753000	1	-1.551784000	-0.824690000	-4.158342000
7	-3.126407000	1.643444000	-0.252519000	6	0.500441000	-0.314840000	-3.888123000
1	-5.109883000	1.016382000	1.067419000	6	1.142633000	0.963949000	-3.976210000
1	-6.303501000	1.919745000	0.201305000	6	2.551343000	1.026453000	-3.742336000
7	-5.380425000	1.514909000	0.221742000	6	3.240743000	-0.108068000	-3.419215000
1	-2.998545000	1.132488000	0.623189000	6	1.158814000	-1.478236000	-3.548728000
1	-2.351613000	2.243176000	-0.5666597000	6	2.594517000	-1.426876000	-3.369457000
6	-8.716201000	6.935027000	-6.256532000	1	3.083554000	1.973101000	-3.818122000
1	-8.918643000	5.981263000	-6.757773000	1	4.308901000	-0.069190000	-3.231714000
1	-9.536500000	7.623636000	-6.491851000	1	0.635040000	-2.420290000	-3.433457000
1	-8.726082000	6.752041000	-5.175539000	1	2.994485000	-2.128290000	-2.633962000
6	-7.361931000	7.515591000	-6.703336000	7	3.349718000	-2.321258000	-4.788978000
6	-6.191741000	6.603236000	-6.396917000	8	4.557099000	-2.502751000	-4.713290000
6	-5.542908000	6.646189000	-5.154974000	8	2.630461000	-2.671005000	-5.710896000
6	-5.736516000	5.661202000	-7.332054000				
6	-4.486494000	5.786373000	-4.847733000				
6	-4.684373000	4.793194000	-7.044411000				
6	-4.050807000	4.846127000	-5.794901000				
8	-3.024073000	3.985253000	-5.555776000				
1	-2.721623000	4.066155000	-4.614745000				
1	-7.210441000	8.485252000	-6.211367000				
1	-7.397888000	7.716487000	-7.781729000				
1	-5.860388000	7.374973000	-4.411329000				
1	-6.213215000	5.606669000	-8.308956000				
1	-3.986595000	5.847232000	-3.884849000				
1	-4.339121000	4.070116000	-7.778009000				
8	1.980316000	6.319067000	-1.412043000				
8	3.432340000	7.883956000	-0.726324000				
6	3.090179000	6.700684000	-0.859381000				
6	3.972753000	5.577389000	-0.285980000				
1	3.540701000	5.308394000	0.690170000				
1	3.878182000	4.683293000	-0.914552000				
6	5.444218000	5.959692000	-0.111091000				
1	5.497913000	6.919907000	0.409582000				
1	5.902686000	6.127435000	-1.095513000				
6	6.256261000	4.926482000	0.695341000				
1	5.876426000	4.872530000	1.719722000				
1	7.304436000	5.249591000	0.752932000				
6	6.223767000	3.504859000	0.146605000				
8	5.888560000	2.533517000	0.851844000				
7	6.596415000	3.344813000	-1.139476000				
1	6.787382000	4.169112000	-1.696073000				
6	6.604180000	2.055163000	-1.822942000				
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²Int4_{B,C6-endo}

26	2.275104000	-4.881032000	-0.406903000
7	1.165626000	-4.224668000	1.158949000
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6	0.545258000	-3.479845000	3.249401000
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6	3.924143000	-4.836164000	2.150736000
6	5.254235000	-5.091175000	2.659082000
6	5.993973000	-5.546618000	1.610147000
6	5.115544000	-5.574336000	0.461735000
6	4.659196000	-6.043620000	-1.917890000
6	5.064215000	-6.507961000	-3.226300000
6	3.965582000	-6.429754000	-4.027023000
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6	-0.786399000	-4.953498000	-3.397019000
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6	-0.609683000	-4.352013000	-1.231081000
6	-0.972012000	-3.865255000	0.022903000
6	2.876121000	-4.335248000	2.916137000
6	5.496336000	-5.991090000	-0.808189000
6	1.594696000	-5.695691000	-3.662516000
1	-1.994682000	-3.520974000	0.138973000
1	3.074680000	-4.140158000	3.965618000
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1	1.385285000	-5.926631000	-4.702416000	1	-2.657262000	4.543906000	2.722879000
1	0.637180000	-3.235622000	4.301091000	6	-3.371131000	6.517494000	3.171842000
1	5.561401000	-4.933235000	3.685412000	1	-2.960877000	7.300996000	3.812919000
1	7.035711000	-5.842168000	1.595378000	6	-3.485613000	7.040581000	1.704438000
1	6.061678000	-6.846397000	-3.477872000	1	-4.203948000	7.871224000	1.702756000
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1	-1.112202000	-5.164384000	-4.408071000	6	-2.180311000	7.466906000	1.104512000
1	-2.543133000	-4.122353000	-2.349077000	6	-1.340966000	6.682407000	0.339437000
6	-1.875128000	-2.726518000	2.819184000	7	-0.217811000	7.387416000	-0.021905000
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1	-1.167225000	-0.683702000	2.592848000	6	-0.955374000	11.026945000	1.777600000
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8	2.735182000	-3.348164000	-0.804163000	1	0.938971000	11.754746000	1.024888000
7	2.987432000	1.569921000	1.489429000	1	1.544180000	9.601289000	-0.111536000
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1	5.665132000	-1.285426000	2.371558000	1	-8.034760000	6.232487000	6.523654000
6	5.367274000	0.350747000	3.686564000	6	-6.505816000	4.704224000	6.364344000
8	5.058189000	-0.155514000	4.767236000	1	-6.580941000	4.387888000	7.412430000
7	5.994900000	1.559236000	3.603626000	1	-5.447293000	4.621762000	6.089989000
1	6.153516000	1.979536000	2.688881000	6	-7.333819000	3.739322000	5.501586000
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6	5.263912000	3.041325000	5.525763000	1	-7.291544000	1.883967000	6.523074000
8	5.286876000	3.189075000	6.748888000	6	-6.044766000	1.654991000	4.962159000
7	4.309203000	3.580806000	4.729730000	7	-5.389362000	2.216759000	3.944277000
1	4.286532000	3.363548000	3.739438000	1	-5.383376000	3.223428000	3.782557000
6	3.109716000	4.198289000	5.265748000	1	-4.729459000	1.636985000	3.404831000
1	2.759715000	3.591429000	6.109827000	7	-5.804084000	0.373132000	5.265527000
6	3.339068000	5.635730000	5.822800000	1	-6.417118000	-0.117455000	5.900293000
1	4.090296000	5.531077000	6.611051000	1	-5.111507000	-0.178309000	4.721088000
1	2.409676000	5.956952000	6.308776000	6	-7.598912000	5.379367000	-1.308401000
6	3.773920000	6.668126000	4.808023000	1	-7.822719000	6.253215000	-0.687471000
6	5.135075000	6.912957000	4.575455000	1	-8.418536000	4.661133000	-1.183711000
6	2.824998000	7.406989000	4.083895000	1	-7.595502000	5.704673000	-2.355844000
6	5.540815000	7.868868000	3.640634000	6	-6.251956000	4.762019000	-0.918937000
6	3.226978000	8.360557000	3.146273000	1	-6.258796000	4.475670000	0.141191000
6	4.586869000	8.595089000	2.923097000	1	-5.451349000	5.503655000	-1.033231000
1	5.880494000	6.359432000	5.141272000	6	-5.907149000	3.540570000	-1.785459000
1	1.764545000	7.235288000	4.257986000	1	-6.692596000	2.777725000	-1.719702000
1	6.600305000	8.050967000	3.479397000	1	-5.856815000	3.837787000	-2.837374000
1	2.479788000	8.922708000	2.592567000	7	-4.613943000	2.940329000	-1.462378000
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6	2.050137000	4.153893000	4.154862000	6	-4.392118000	2.054046000	-0.487214000
8	2.369407000	3.993900000	2.970729000	7	-3.147366000	1.616578000	-0.251281000
7	0.770057000	4.279158000	4.564197000	1	-5.132970000	1.011838000	1.075224000
1	0.580993000	4.539844000	5.523059000	1	-6.319072000	1.927553000	0.213633000
6	-0.354493000	4.237036000	3.649056000	7	-5.401365000	1.510398000	0.229141000
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6	-1.011677000	2.830366000	3.666224000	1	-2.367291000	2.206832000	-0.571088000
1	-0.197315000	2.116647000	3.482381000	6	-8.716201000	6.935027000	-6.256532000
8	-1.925459000	2.799406000	2.566220000	1	-8.914569000	5.990552000	-6.776654000
1	-2.430248000	1.954000000	2.585382000	1	-9.532793000	7.629040000	-6.488814000
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1	-0.978331000	2.520979000	5.820549000	6	-7.356192000	7.521393000	-6.678077000
1	-2.111461000	1.478469000	4.956781000	6	-6.189205000	6.603123000	-6.376234000
1	-2.512621000	3.188155000	5.206379000	6	-5.540153000	6.636099000	-5.134111000
6	-1.291626000	5.430166000	3.935298000	6	-5.735505000	5.666718000	-7.317897000
8	-0.953188000	6.346089000	4.689008000	6	-4.484725000	5.772575000	-4.833049000
7	-2.462334000	5.392177000	3.255492000	6	-4.684605000	4.795281000	-7.036517000

6	-4.050167000	4.838668000	-5.786916000	7	1.828378000	-3.620196000	0.480091000
8	-3.023838000	3.975452000	-5.555441000	7	4.481625000	-4.129458000	-0.471549000
1	-2.720691000	4.046011000	-4.613745000	7	3.391994000	-5.335131000	-2.830254000
1	-7.208869000	8.481876000	-6.167274000	7	0.755800000	-4.756693000	-1.928581000
1	-7.380731000	7.741860000	-7.753010000	6	0.499259000	-3.446823000	0.764983000
1	-5.856181000	7.360344000	-4.385433000	6	0.335782000	-2.845650000	2.085165000
1	-6.212159000	5.619880000	-8.295231000	6	1.599494000	-2.658353000	2.563614000
1	-3.984391000	5.826288000	-3.869931000	6	2.519664000	-3.140417000	1.559166000
1	-4.340425000	4.076992000	-7.775306000	6	4.809638000	-3.552481000	0.724062000
8	1.970778000	6.268731000	-1.412484000	6	6.248563000	-3.483460000	0.864444000
8	3.408720000	7.856468000	-0.749368000	6	6.778296000	-4.028573000	-0.266618000
6	3.077795000	6.668227000	-0.867604000	6	5.662193000	-4.435765000	-1.092946000
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1	3.549649000	5.301328000	0.698293000	6	4.879041000	-6.244381000	-4.344923000
1	3.882808000	4.657847000	-0.900060000	6	3.625266000	-6.494895000	-4.813723000
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6	6.236628000	3.513830000	0.141866000	6	3.904295000	-3.106317000	1.680957000
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6	6.604180000	2.055163000	-1.822942000	1	4.313475000	-2.701259000	2.600925000
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1	8.624594000	2.174881000	-2.575089000	1	7.820616000	-4.161626000	-0.528767000
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1	5.251225000	3.605407000	-6.709036000	8	-3.340433000	-1.388910000	3.838289000
1	8.334818000	6.146066000	-5.111053000	1	-0.817269000	-2.472113000	3.836768000
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7	1.191453000	3.882962000	-2.066302000	1	-0.715991000	-0.339433000	2.474216000
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1	1.900192000	3.243361000	-2.428409000	16	2.511315000	-6.574968000	-0.009812000
1	1.646655000	4.832767000	-1.744657000	1	2.645512000	-7.419100000	-1.058875000
6	0.078992000	4.137413000	-3.043713000	8	2.676293000	-2.838516000	-1.915521000
1	0.077608000	5.213233000	-3.243009000	7	3.475250000	1.558187000	2.970050000
6	-1.243893000	3.772504000	-2.320132000	1	4.384246000	1.814123000	2.596282000
8	-2.325003000	3.907258000	-2.959578000	1	2.728892000	2.222082000	2.791653000
8	-1.133063000	3.373207000	-1.132463000	6	3.324240000	0.737351000	4.039722000
6	0.275327000	3.386829000	-4.381161000	8	2.229866000	0.560695000	4.585047000
1	-0.466398000	3.788372000	-5.078039000	6	4.565022000	-0.020321000	4.517916000
1	1.255706000	3.665298000	-4.786998000	1	4.393870000	-0.256600000	5.570857000
6	0.134569000	1.889620000	-4.297062000	1	4.598573000	-0.973639000	3.976762000
6	-1.065696000	1.198805000	-4.439129000	6	5.920756000	0.689853000	4.359902000
1	-2.050193000	1.583289000	-4.663837000	1	6.147698000	0.909122000	3.313091000
7	-0.850740000	-0.143498000	-4.260895000	1	6.702128000	0.006575000	4.714498000
1	-1.560415000	-0.859737000	-4.310188000	6	6.018532000	1.942909000	5.225486000
6	0.491573000	-0.369419000	-4.002256000	8	5.813673000	1.908211000	6.440860000
6	1.134356000	0.912413000	-4.029675000	7	6.367411000	3.093301000	4.583797000
6	2.546893000	0.959702000	-3.782844000	1	6.425128000	3.107844000	3.566665000
6	3.241109000	-0.175000000	-3.506542000	6	6.543595000	4.319239000	5.339119000
6	1.137704000	-1.553656000	-3.734785000	1	7.148561000	4.127412000	6.227994000
6	2.599500000	-1.532017000	-3.487401000	1	7.077352000	5.037773000	4.708343000
1	3.079713000	1.908808000	-3.817347000	6	5.249509000	4.985692000	5.838447000
1	4.307839000	-0.142501000	-3.312255000	8	5.231396000	5.610704000	6.900622000
1	0.611170000	-2.499624000	-3.685168000	7	4.186507000	4.888634000	5.007239000
1	2.871246000	-2.110626000	-2.590079000	1	4.242303000	4.327516000	4.164306000
7	3.361879000	-2.402719000	-4.598399000	6	2.867057000	5.396954000	5.329084000
8	4.558720000	-2.593185000	-4.405569000	1	2.580548000	5.040987000	6.327102000
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				1	3.510497000	7.264503000	6.138882000
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6	3.650842000	8.876425000	1.589113000	1	-6.149499000	5.187262000	-1.686603000
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1	1.519834000	8.816259000	1.261924000	7	-5.365360000	2.592427000	-1.303397000
1	3.864567000	9.337004000	0.629299000	1	-4.523158000	2.753311000	-1.876352000
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6	-1.005388000	10.418945000	-0.556832000	1	5.048702000	6.440085000	-0.663580000
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6	-6.377219000	4.089820000	6.371879000	6	7.207332000	0.591808000	-2.468209000
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1	-7.333752000	3.231189000	4.607340000	6	7.691431000	1.070329000	-5.204391000
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6	-0.531930000	1.342439000	-4.633471000	1	4.273551000	-0.750683000	1.375754000
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6	0.847482000	-2.017879000	-4.722176000	1	7.011254000	2.126868000	6.061854000
6	2.269469000	-1.876339000	-4.381604000	1	7.341227000	3.609464000	5.148405000
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1	3.864178000	-0.373658000	-4.172622000	8	5.217197000	3.511539000	7.152883000
1	0.437051000	-3.008049000	-4.878182000	7	4.438281000	3.922650000	5.052883000
1	2.466223000	-2.414663000	-3.310797000	1	4.563280000	3.773956000	4.058146000
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²INT5_{B,C6-endo}							
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8	3.532799000	-2.024140000	-0.525897000	1	2.139178000	10.589911000	0.827447000
7	3.691245000	2.095914000	1.662224000	1			

6	-4.392118000	6.215012000	3.268524000	6	7.173806000	4.334563000	1.035764000
8	-4.744107000	5.111788000	2.820313000	8	6.634782000	3.261263000	1.373272000
7	-5.240797000	7.065518000	3.876263000	7	8.148343000	4.369109000	0.105209000
1	-4.866145000	7.918403000	4.270961000	1	8.512114000	5.269446000	-0.182140000
6	-6.661933000	6.795035000	4.064285000	6	8.662955000	3.181227000	-0.572900000
1	-7.182738000	7.756454000	4.024312000	1	7.963415000	2.853402000	-1.351881000
1	-7.002727000	6.202709000	3.211673000	1	8.726107000	2.374569000	0.163185000
6	-6.973028000	6.108255000	5.400128000	6	10.047160000	3.447408000	-1.186618000
1	-6.475364000	6.676903000	6.195673000	1	10.377190000	2.510162000	-1.650367000
1	-8.051631000	6.216292000	5.585939000	1	10.758521000	3.675878000	-0.384107000
6	-6.597802000	4.628284000	5.535000000	6	10.053483000	4.564966000	-2.212858000
1	-6.706227000	4.331990000	6.585562000	6	9.446910000	4.389273000	-3.468137000
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6	-7.500989000	3.726147000	4.683434000	6	9.429881000	5.425141000	-4.402736000
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6	5.069130000	7.221737000	5.163997000	1	-8.086936000	7.276427000	-0.152401000
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1	3.751259000	5.393203000	0.516994000	6	0.735875000	-7.465784000	-5.612885000	
1	4.561155000	5.226310000	-1.028980000	6	-0.579845000	-7.780611000	-5.446594000	
6	5.677552000	6.384843000	0.464997000	6	-1.044676000	-7.034673000	-4.302943000	
1	5.461534000	7.305139000	1.014062000	6	-2.819533000	-6.292000000	-2.767145000	
1	6.418593000	6.667026000	-0.295029000	6	-4.178727000	-6.312520000	-2.287095000	
6	6.267646000	5.377964000	1.470903000	6	-4.236070000	-5.466416000	-1.220300000	
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8	6.629030000	2.984145000	1.403605000	6	2.333934000	-5.955370000	-4.421698000	
7	7.838340000	4.259500000	-0.035148000	6	-2.354040000	-7.045497000	-3.833610000	
1	8.028132000	5.198692000	-0.360754000	1	-3.346589000	-3.749523000	0.660374000	
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1	8.411073000	2.283756000	-0.005919000	1	3.099487000	-6.243665000	-5.135351000	
1	9.717135000	3.417393000	-0.383785000	1	-3.067162000	-7.681988000	-4.347805000	
6	8.458700000	2.950260000	-2.082848000	1	1.037488000	-1.739634000	1.722894000	
1	9.202396000	2.204191000	-2.393311000	1	4.767643000	-3.129204000	-1.699175000	
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6	6.199795000	3.317141000	-3.184334000	1	-4.972960000	-6.907681000	-2.719783000	
6	5.350310000	0.757693000	-2.484401000	1	-5.087017000	-5.224912000	-0.595961000	
6	4.924177000	2.878784000	-3.554811000	6	-1.870399000	-1.981069000	2.231897000	
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1	6.529206000	4.314014000	-3.468597000	8	-3.714613000	1.270175000	2.182020000	
1	5.027097000	-0.243981000	-2.213218000	8	-3.907596000	-0.504970000	3.551244000	
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6	-0.039782000	5.243797000	-2.987140000	8	-0.589350000	-3.607235000	-3.293715000	
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1	6.606071000	8.056653000	3.503279000	1	-5.849645000	3.848669000	-2.838554000
1	2.488073000	8.938337000	2.614755000	7	-4.601679000	2.956627000	-1.464788000
1	4.908073000	9.354236000	2.223811000	1	-3.778957000	3.316824000	-1.970983000
6	2.050498000	4.156412000	4.154631000	6	-4.374031000	2.070498000	-0.490886000
8	2.368667000	3.990466000	2.970990000	7	-3.125215000	1.644956000	-0.252538000
7	0.771240000	4.288906000	4.563948000	1	-5.108534000	1.016506000	1.066985000
1	0.583156000	4.556128000	5.521220000	1	-6.302576000	1.919267000	0.200753000

7	-5.379231000	1.515055000	0.221359000	6	3.245495000	-0.098504000	-3.423194000
1	-2.997214000	1.133896000	0.623080000	6	1.164598000	-1.471446000	-3.548348000
1	-2.350733000	2.245223000	-0.566332000	6	2.600990000	-1.418470000	-3.372342000
6	-8.716201000	6.935027000	-6.256532000	1	3.085040000	1.982137000	-3.822993000
1	-8.918383000	5.980837000	-6.757066000	1	4.313841000	-0.058374000	-3.237220000
1	-9.536932000	7.623084000	-6.491968000	1	0.642011000	-2.413863000	-3.430942000
1	-8.725562000	6.752746000	-5.175416000	1	3.003030000	-2.118253000	-2.636859000
6	-7.362388000	7.515922000	-6.704250000	7	3.353286000	-2.311278000	-4.791899000
6	-6.191817000	6.604173000	-6.397575000	8	4.561715000	-2.487852000	-4.720936000
6	-5.543213000	6.647616000	-5.155532000	8	2.631632000	-2.665899000	-5.710096000
6	-5.736200000	5.662054000	-7.332424000				
6	-4.486669000	5.788123000	-4.847892000				
6	-4.683910000	4.794357000	-7.044380000				
6	-4.050642000	4.847721000	-5.794748000	26	2.282966000	-4.882215000	-0.398275000
8	-3.023849000	3.987053000	-5.555134000	7	1.169197000	-4.225285000	1.164003000
1	-2.721674000	4.068342000	-4.614048000	7	3.866471000	-5.149365000	0.832023000
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1	-5.861026000	7.376488000	-4.412115000	6	-0.134129000	-3.801482000	1.132402000
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6	3.091582000	6.702494000	-0.857840000	6	5.992103000	-5.561339000	1.632124000
6	3.973061000	5.577999000	-0.285068000	6	5.117941000	-5.585313000	0.480368000
1	3.540199000	5.308264000	0.690519000	6	4.669946000	-6.049254000	-1.901963000
1	3.878271000	4.684631000	-0.914648000	6	5.079453000	-6.510553000	-3.210112000
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6	6.222651000	3.503417000	0.147518000	6	-0.963772000	-3.860349000	0.020735000
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7	6.596308000	3.344239000	-1.138383000	6	5.502426000	-6.001868000	-0.788512000
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6	6.604180000	2.055163000	-1.822942000	1	-1.986255000	-3.514485000	0.133677000
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1	6.844141000	1.288119000	-1.083229000	1	6.531242000	-6.323598000	-0.918938000
6	7.631485000	2.030765000	-2.968633000	1	1.409213000	-5.911936000	-4.700914000
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8	5.201241000	3.439281000	7.129748000	6	-6.271004000	1.641188000	4.136076000
7	4.431927000	3.915397000	5.040265000	7	-5.500212000	2.284289000	3.243646000
1	4.554064000	3.788715000	4.042101000	1	-5.360560000	3.292268000	3.301349000
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6	3.740844000	6.920625000	5.369311000	1	-7.117536000	8.468754000	0.552228000
6	5.113237000	7.203937000	5.432536000	1	-8.042058000	7.203743000	-0.275462000
6	2.923484000	7.730710000	4.566918000	1	-7.092433000	8.367236000	-1.214989000
6	5.657923000	8.269523000	4.712051000	6	-5.881467000	6.850113000	-0.202441000
6	3.464400000	8.797357000	3.845928000	1	-5.907335000	6.296242000	0.743228000
6	4.833453000	9.070300000	3.917476000	1	-4.972563000	7.458832000	-0.178716000
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6	-4.707971000	3.780750000	-0.407151000	1	10.362140000	2.491651000	-1.661154000
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7	-5.884969000	3.372755000	0.123855000	6	10.615813000	5.776254000	-2.020815000
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6	4.054995000	0.943718000	-3.146270000	6	-2.240767000	-2.168003000	2.340716000
6	3.740619000	-0.163010000	-2.354135000	6	-2.353288000	-0.654467000	2.085848000
1	6.617561000	-0.346551000	-0.545076000	6	-3.435526000	0.075671000	2.879538000
1	5.519717000	2.453564000	-3.616960000	8	-3.674031000	1.292016000	2.493001000
1	4.441311000	-1.483945000	-0.800381000	8	-4.002750000	-0.477363000	3.840667000
1	3.358312000	1.283864000	-3.908845000	1	-2.023581000	-2.341236000	3.399438000
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7	1.271058000	3.826131000	-2.566416000	1	-1.394395000	-0.171251000	2.321148000
1	0.878175000	3.360422000	-1.728154000	1	-2.524248000	-0.462554000	1.020345000
1	1.920136000	3.180323000	-3.022930000	16	-0.188622000	-6.259727000	-2.006717000
1	1.790724000	4.738713000	-2.250987000	1	-0.894576000	-6.128409000	-0.860863000
6	0.076870000	4.150932000	-3.417995000	8	0.867483000	-2.283444000	-2.607338000
1	0.049796000	5.239547000	-3.516922000	7	3.185333000	1.360352000	2.302763000
6	-1.200203000	3.734360000	-2.633561000	1	4.157900000	1.519995000	2.056682000
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8	-0.998627000	3.221381000	-1.492525000	6	2.789969000	0.301365000	3.055411000
6	0.150192000	3.545090000	-4.828574000	8	1.655084000	0.220293000	3.537033000
1	-0.805992000	3.795073000	-5.303816000	6	3.802127000	-0.830775000	3.240522000
1	0.922696000	4.075160000	-5.398181000	1	3.469248000	-1.403303000	4.109354000
6	0.428221000	2.062836000	-4.899365000	1	3.731870000	-1.491985000	2.367055000
6	0.140846000	1.074492000	-3.950788000	6	5.269212000	-0.403984000	3.430240000
1	-0.318338000	1.171898000	-2.976445000	1	5.658910000	0.112947000	2.549087000
7	0.568072000	-0.145583000	-4.391235000	1	5.872063000	-1.312315000	3.552411000
1	0.577766000	-1.006773000	-3.814786000	6	5.475964000	0.422848000	4.698222000
6	1.161403000	0.004692000	-5.630490000	8	5.121002000	0.014344000	5.805500000
6	1.076286000	1.391712000	-5.976742000	7	6.101656000	1.623257000	4.530794000
6	1.569109000	1.816319000	-7.249614000	1	6.292278000	1.956198000	3.587006000
6	2.161985000	0.916174000	-8.083340000	6	6.440865000	2.448147000	5.675028000
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6	2.373670000	-0.484853000	-7.688322000	1	7.256381000	3.120733000	5.388033000
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1	-5.122338000	-4.283054000	-1.488535000	6	-1.610319000	7.073020000	0.455966000
6	-2.127747000	-2.619210000	2.660250000	7	-0.532076000	7.795543000	0.002195000
6	-2.488935000	-1.194571000	2.202087000	1	-1.877999000	6.151285000	-0.040933000
6	-3.399407000	-0.441330000	3.177805000	1	0.075207000	7.518559000	-0.777596000
8	-3.764880000	0.749358000	2.818579000	6	-1.430637000	8.902237000	1.762051000
8	-3.729321000	-0.970183000	4.257524000	6	-0.390513000	8.921725000	0.784110000
1	-1.726242000	-2.559792000	3.676944000	6	-1.512517000	9.964615000	2.683034000
1	-3.050124000	-3.208140000	2.736289000	6	0.556566000	9.952434000	0.717310000
1	-1.578169000	-0.594696000	2.070158000	6	-0.578690000	10.993441000	2.616382000
1	-2.974923000	-1.204363000	1.218271000	6	0.447954000	10.984713000	1.645656000
16	-0.591071000	-7.722598000	-0.346712000	1	-2.295992000	9.985116000	3.437703000
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8	0.264762000	-4.313309000	-2.623024000	1	1.164656000	11.801818000	1.621192000
7	3.543469000	1.782164000	1.094965000	1	1.345652000	9.922963000	-0.029174000
1	4.454232000	2.185830000	0.889476000	6	-4.375494000	6.177584000	4.355719000
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6	3.340964000	0.487554000	1.413396000	7	-4.871026000	7.053431000	5.254359000
8	2.211217000	0.056509000	1.708940000	1	-4.315911000	7.866241000	5.488130000
6	4.528467000	-0.466205000	1.347281000	6	-6.192749000	6.929667000	5.869022000
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1	4.476502000	-0.981464000	0.379473000	1	-6.818691000	6.363501000	5.175151000
6	5.925917000	0.144532000	1.535760000	6	-6.173705000	6.282335000	7.263623000
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1	6.662580000	-0.659025000	1.415115000	1	-7.184151000	6.372221000	7.686455000
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8	5.925833000	0.027940000	3.949226000	1	-5.596729000	4.512579000	8.351591000
7	6.569390000	1.995936000	3.009433000	1	-4.746364000	4.703669000	6.824589000
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1	3.144122000	3.246472000	5.844450000	7	-5.343191000	0.472035000	6.049652000
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6	4.529073000	6.693240000	0.016937000	6	0.731319000	-4.812382000	-6.527947000
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8	-0.794182000	6.612310000	4.836859000	6	-3.944896000	1.181932000	-4.925951000
7	-2.117548000	5.742401000	3.184001000	6	-4.366949000	-0.291927000	-6.799044000
1	-2.263364000	4.903708000	2.621108000	6	-3.486498000	0.516244000	-6.069044000
6	-2.967852000	6.903204000	2.998296000	8	-2.202614000	0.626345000	-6.527593000
1	-2.483283000	7.730783000	3.521805000	1	-1.666688000	1.133783000	-5.892429000
6	-3.103075000	7.239964000	1.484310000	1	-7.951563000	0.940927000	-4.279635000
1	-3.792623000	8.090249000	1.394116000	1	-8.247937000	-0.158900000	-5.619523000
1	-3.593032000	6.388452000	0.997519000	1	-5.610642000	1.542384000	-3.627286000
6	-1.795803000	7.543948000	0.815259000	1	-6.362031000	-1.062476000	-6.959071000
6	-1.050253000	6.685957000	0.032546000	1	-3.278687000	1.836789000	-4.368097000
7	0.109641000	7.297897000	-0.382897000	1	-4.004034000	-0.796540000	-7.689766000
1	-1.259430000	5.663911000	-0.258499000	8	2.237046000	6.149582000	-1.915206000
1	0.832540000	6.882531000	-0.986078000	8	3.770464000	7.602211000	-1.164514000
6	-1.042229000	8.771045000	0.893242000	6	3.309195000	6.454931000	-1.252459000
6	0.147909000	8.574144000	0.132391000	6	3.989021000	5.293808000	-0.500242000
6	-1.243640000	10.014595000	1.523490000	1	3.217209000	4.822117000	0.124445000
6	1.129356000	9.566349000	0.000589000	1	4.293464000	4.525133000	-1.224625000
6	-0.276951000	11.005471000	1.389618000	6	5.163355000	5.737284000	0.377863000
6	0.900106000	10.781445000	0.639905000	1	4.869362000	6.650112000	0.903424000
1	-2.141728000	10.201387000	2.108379000	1	6.013803000	6.039194000	-0.248993000
1	-0.423797000	11.968172000	1.872942000	6	5.581088000	4.713168000	1.444917000
1	1.639455000	11.574373000	0.560394000	1	4.710530000	4.431903000	2.045906000
1	2.035854000	9.369515000	-0.566053000	1	6.285966000	5.190594000	2.141396000

6	6.250419000	3.415277000	1.013235000	6	2.282684000	-3.887918000	0.596763000
8	6.126529000	2.377030000	1.694984000	6	3.256135000	-5.038749000	-4.005336000
7	7.035251000	3.456831000	-0.082706000	6	-1.332787000	-4.042443000	-5.216454000
1	7.106569000	4.334759000	-0.579839000	1	-3.180072000	-2.541635000	-0.086400000
6	7.899483000	2.362829000	-0.515486000	1	2.853683000	-3.863875000	1.519940000
1	7.804439000	1.576589000	0.234401000	1	4.134998000	-5.378516000	-4.544574000
1	8.938191000	2.715319000	-0.501914000	1	-1.904525000	-4.069558000	-6.138923000
6	7.570808000	1.828446000	-1.920078000	1	0.777564000	-2.939686000	2.827408000
1	8.368588000	1.118782000	-2.180646000	1	5.000900000	-4.703515000	0.254539000
1	7.644217000	2.648740000	-2.644936000	1	5.548998000	-5.338987000	-2.327360000
6	6.221288000	1.150114000	-2.051535000	1	2.773011000	-5.450336000	-6.789940000
6	5.896556000	0.032413000	-1.266701000	1	0.201712000	-4.901137000	-7.465242000
6	5.281726000	1.596658000	-2.989927000	1	-4.050692000	-3.225664000	-4.870096000
6	4.668270000	-0.613732000	-1.410377000	1	-4.592890000	-2.592840000	-2.289376000
6	4.054958000	0.942993000	-3.147126000	6	-2.058368000	-2.137210000	2.411142000
6	3.739485000	-0.162366000	-2.353516000	6	-2.189144000	-0.628862000	2.135459000
1	6.614843000	-0.344213000	-0.541766000	6	-3.276199000	0.096321000	2.925452000
1	5.520685000	2.451457000	-3.619027000	8	-3.541333000	1.300753000	2.520075000
1	4.438361000	-1.481100000	-0.797091000	8	-3.824495000	-0.450178000	3.901311000
1	3.359095000	1.282185000	-3.910885000	1	-1.809956000	-2.292497000	3.465751000
1	2.791703000	-0.680515000	-2.472470000	1	-3.029758000	-2.620193000	2.247464000
7	1.270439000	3.823013000	-2.569187000	1	-1.234662000	-0.131371000	2.358360000
1	0.878119000	3.356125000	-1.731328000	1	-2.369384000	-0.453887000	1.068617000
1	1.919755000	3.178165000	-3.026714000	16	-0.145878000	-6.266209000	-1.940848000
1	1.789740000	4.735441000	-2.252867000	1	-0.820855000	-6.111752000	-0.779439000
6	0.075798000	4.148372000	-3.419927000	8	0.914511000	-2.304481000	-2.620371000
1	0.049162000	5.236986000	-3.518885000	7	3.227289000	1.430240000	2.362149000
6	-1.200901000	3.732270000	-2.634632000	1	4.198630000	1.603701000	2.120011000
8	-2.298532000	3.959003000	-3.194695000	1	2.647799000	2.261519000	2.416943000
8	-0.998779000	3.218041000	-1.494269000	6	2.843312000	0.375628000	3.125757000
6	0.147633000	3.542421000	-4.830578000	8	1.706831000	0.283966000	3.602380000
1	-0.809208000	3.792231000	-5.304597000	6	3.869317000	-0.740562000	3.330743000
1	0.919295000	4.072623000	-5.401194000	1	3.543728000	-1.300814000	4.210252000
6	0.425910000	2.060224000	-4.901628000	1	3.804893000	-1.418722000	2.469824000
6	0.139254000	1.071787000	-3.952929000	6	5.331960000	-0.295218000	3.510992000
1	-0.319492000	1.169087000	-2.978373000	1	5.713846000	0.214423000	2.622185000
7	0.566446000	-0.148183000	-4.393657000	1	5.945054000	-1.195284000	3.643169000
1	0.577126000	-1.009200000	-3.816886000	6	5.533846000	0.549888000	4.767918000
6	1.159156000	0.002273000	-5.633193000	8	5.180965000	0.154151000	5.880384000
6	1.073518000	1.389288000	-5.979399000	7	6.155910000	1.750006000	4.584571000
6	1.565225000	1.813943000	-7.252706000	1	6.340612000	2.072847000	3.636426000
6	2.157603000	0.913898000	-8.086879000	6	6.491315000	2.593142000	5.716608000
6	1.717300000	-0.948360000	-6.467387000	1	6.834490000	1.971338000	6.545782000
6	2.370274000	-0.486945000	-7.691745000	1	7.312428000	3.256617000	5.424209000
1	1.441510000	2.847618000	-7.565279000	6	5.353935000	3.465365000	6.278037000
1	2.523715000	1.224393000	-9.060742000	8	5.330153000	3.778235000	7.469576000
1	1.741931000	-2.002423000	-6.213174000	7	4.446610000	3.901857000	5.372518000
1	2.368036000	-1.211526000	-8.506203000	1	4.456442000	3.530985000	4.428364000
7	4.108630000	-0.665659000	-7.354201000	6	3.231734000	4.600520000	5.751730000
8	4.716967000	0.291214000	-6.900588000	1	2.812061000	4.112432000	6.640526000
8	4.560432000	-1.792232000	-7.517134000	6	3.459804000	6.093836000	6.135713000
				1	4.180730000	6.080262000	6.958325000
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26	0.496306000	-3.879921000	-2.325698000	6	2.519069000	6.480477000	6.546293000
7	0.064603000	-3.500310000	-0.384773000	6	3.943218000	6.995477000	5.021936000
7	2.394625000	-4.374228000	-1.806033000	6	5.315411000	7.181317000	4.797940000
7	0.878286000	-4.459031000	-4.226280000	6	3.031194000	7.677361000	4.200641000
7	-1.434167000	-3.531616000	-2.818316000	6	5.767143000	8.021895000	3.777833000
6	-1.126881000	-3.044814000	0.118946000	6	3.479114000	8.516333000	3.177399000
6	-0.998643000	-2.752923000	1.542065000	1	4.849289000	8.691373000	2.963527000
6	0.292406000	-3.050400000	1.865034000	1	6.033396000	6.673173000	5.436885000
6	0.947367000	-3.509704000	0.662809000	1	1.962751000	7.555682000	4.366954000
6	2.947561000	-4.288453000	-0.557650000	1	6.834414000	8.160776000	3.625257000
6	4.339957000	-4.680368000	-0.602936000	1	2.759994000	9.036185000	2.549682000
6	4.614518000	-5.000129000	-1.897819000	6	5.198137000	9.349397000	2.172258000
6	3.390494000	-4.805537000	-2.642839000	8	2.245219000	4.427525000	4.587328000
6	2.082899000	-4.872543000	-4.734151000	7	4.038202000	3.477405000	
6	1.964064000	-5.114971000	-6.153185000	1	0.701996000	5.190125000	5.706284000
6	0.672673000	-4.839004000	-6.492193000	6	-0.069881000	4.623451000	3.828041000
6	0.002510000	-4.426374000	-5.281145000	1	0.429055000	4.730655000	2.858674000
6	-1.992349000	-3.628396000	-4.066648000	6	-0.750332000	3.227967000	3.819020000
6	-3.386642000	-3.248494000	-4.015627000	1	0.061818000	2.489475000	3.763174000
6	-3.657537000	-2.927017000	-2.720633000	8	-1.520378000	3.174514000	2.614880000
6	-2.428019000	-3.107469000	-1.980540000	1	-2.181832000	2.446267000	2.669369000
6	-2.294697000	-2.879796000	-0.614371000	6	-1.584779000	2.950572000	5.069061000

1	-0.964142000	3.027779000	5.968237000	6	-7.706430000	-0.147143000	-4.500855000
1	-1.995566000	1.935896000	5.037490000	6	-6.287366000	0.054297000	-4.993909000
1	-2.420123000	3.654207000	5.154491000	6	-5.386584000	0.873887000	-4.299994000
6	-1.018531000	5.827724000	3.986613000	6	-5.817842000	-0.592294000	-6.147487000
8	-0.775774000	6.736950000	4.786581000	6	-4.067985000	1.045118000	-4.725963000
7	-2.075799000	5.811849000	3.144308000	6	-4.503495000	-0.439277000	-6.587161000
1	-2.204288000	4.958916000	2.598631000	6	-3.619366000	0.378605000	-5.872404000
6	-2.947956000	6.951435000	2.932417000	8	-2.342608000	0.497241000	-6.348561000
1	-2.479355000	7.800245000	3.436169000	1	-1.799633000	1.004106000	-5.718710000
6	-3.091139000	7.249796000	1.411537000	1	-8.061901000	0.774822000	-4.022456000
1	-3.790333000	8.090081000	1.303224000	1	-8.369141000	-0.328213000	-5.356914000
1	-3.573173000	6.381481000	0.947247000	1	-5.718814000	1.396591000	-3.405563000
6	-1.789385000	7.550190000	0.730020000	1	-6.493939000	-1.227375000	-6.716493000
6	-1.045888000	6.682966000	-0.044306000	1	-3.399793000	1.710991000	-4.183863000
7	0.108474000	7.292879000	-0.477804000	1	-4.149185000	-0.943897000	-7.481347000
1	-1.252595000	5.655377000	-0.316912000	8	2.228664000	6.143546000	-2.025040000
1	0.826615000	6.872558000	-1.082900000	8	3.765619000	7.608798000	-1.307147000
6	-1.040383000	8.781476000	0.783156000	6	3.299993000	6.461280000	-1.366957000
6	0.144982000	8.577424000	0.016642000	6	3.973854000	5.317890000	-0.582204000
6	-1.242077000	10.034049000	1.395185000	1	3.195866000	4.856366000	0.042358000
6	1.121198000	9.571345000	-0.138450000	1	4.290161000	4.535695000	-1.286881000
6	-0.280357000	11.026455000	1.238624000	6	5.135841000	5.785040000	0.300316000
6	0.891876000	10.795420000	0.483503000	1	4.835355000	6.713808000	0.793354000
1	-2.136590000	10.226619000	1.983652000	1	5.995752000	6.066875000	-0.322762000
1	-0.427536000	11.996045000	1.707865000	6	5.535439000	4.794035000	1.405227000
1	1.627218000	11.590028000	0.385698000	1	4.655190000	4.528608000	1.998754000
1	2.023994000	9.369620000	-0.709352000	1	6.226574000	5.294608000	2.099276000
6	-4.335867000	6.675857000	3.527175000	6	6.216444000	3.486331000	1.026061000
8	-4.979955000	5.666215000	3.198301000	8	6.066106000	2.462646000	1.724600000
7	-4.813762000	7.609796000	4.374373000	7	7.041385000	3.504229000	-0.040601000
1	-4.213918000	8.387239000	4.617652000	1	7.138830000	4.374166000	-0.547558000
6	-6.154371000	7.574148000	4.956569000	6	7.922642000	2.402955000	-0.415439000
1	-6.530972000	8.601722000	4.975637000	1	7.770170000	1.616754000	0.325017000
1	-6.786884000	7.005472000	4.271039000	1	8.961867000	2.744802000	-0.332027000
6	-6.201451000	6.991520000	6.379413000	6	7.683501000	1.874378000	-1.840599000
1	-5.533605000	7.580042000	7.020657000	1	8.500747000	1.171999000	-2.055932000
1	-7.217511000	7.147736000	6.767833000	1	7.794964000	2.699607000	-2.555064000
6	-5.826250000	5.506459000	6.503254000	6	6.350644000	1.185534000	-2.058820000
1	-5.758255000	5.248554000	7.567549000	6	6.007210000	0.036600000	-1.328830000
1	-4.830861000	5.331567000	6.077630000	6	5.448602000	1.652077000	-3.023953000
6	-6.843671000	4.565534000	5.838695000	6	4.797156000	-0.621304000	-1.552158000
1	-7.839002000	4.725252000	6.265998000	6	4.240795000	0.987271000	-3.261518000
1	-6.922811000	4.763049000	4.767254000	6	3.906658000	-0.149675000	-2.522036000
7	-6.530205000	3.147138000	6.018194000	1	6.697598000	-0.355557000	-0.584997000
1	-6.756798000	2.741985000	6.916403000	1	5.702853000	2.532605000	-3.610100000
6	-5.723807000	2.416234000	5.219503000	1	4.551947000	-1.512000000	-0.979472000
7	-5.195904000	2.926069000	4.107216000	1	3.574887000	1.344338000	-4.043655000
1	-5.185128000	3.926669000	3.910230000	1	2.971140000	-0.673367000	-2.698668000
1	-4.581705000	2.321249000	3.536521000	7	1.251230000	3.806988000	-2.634687000
7	-5.467622000	1.139999000	5.540540000	1	0.879128000	3.348810000	-1.782752000
1	-6.012189000	0.684535000	6.258685000	1	1.891319000	3.157945000	-3.099033000
1	-4.884993000	0.546909000	4.919239000	1	1.774087000	4.723713000	-2.340666000
6	-7.304228000	6.217714000	-1.624516000	6	0.036563000	4.113619000	-3.463776000
1	-7.412096000	7.186764000	-1.126000000	1	-0.000520000	5.200586000	-3.576371000
1	-8.186996000	5.614698000	-1.378904000	6	-1.219503000	3.697950000	-2.646432000
1	-7.311914000	6.395592000	-2.706575000	8	-2.330493000	3.905404000	-3.187428000
6	-6.012808000	5.518846000	-1.188054000	8	-0.989553000	3.203055000	-1.502784000
1	-6.008774000	5.381697000	-0.098190000	6	0.080320300	3.486859000	-4.866926000
1	-5.145394000	6.147528000	-1.424379000	1	-0.889851000	3.711487000	-5.320299000
6	-5.831066000	4.158837000	-1.880398000	1	0.830433000	4.020907000	-5.465227000
1	-6.684169000	3.500440000	-1.675161000	6	0.387260000	2.008954000	-4.918142000
1	-5.806989000	4.296222000	-2.965875000	6	0.115001000	1.030306000	-3.954067000
7	-4.589822000	3.478321000	-1.519203000	1	-0.343129000	1.133926000	-2.979943000
1	-3.755865000	3.650405000	-2.109367000	7	0.565697000	-0.189150000	-4.377893000
6	-4.418659000	2.699103000	-0.446632000	1	0.597667000	-1.040781000	-3.788830000
7	-3.227259000	2.149319000	-0.197953000	6	1.160161000	-0.045564000	-5.618020000
1	-5.205062000	1.917390000	1.242991000	6	1.048574000	1.335064000	-5.982913000
1	-6.286185000	2.940646000	0.377433000	6	1.544174000	1.753390000	-7.261066000
7	-5.450815000	2.376019000	0.370332000	6	2.164768000	0.865411000	-8.078806000
1	-3.109190000	1.734370000	0.729356000	6	1.741234000	-1.000241000	-6.426924000
1	-2.392432000	2.501548000	-0.693768000	6	2.391960000	-0.555819000	-7.687923000
6	-7.847385000	-1.312672000	-3.503992000	1	1.403552000	2.781337000	-7.585698000
1	-7.534274000	-2.258926000	-3.960179000	1	2.533931000	1.174854000	-9.051885000
1	-8.886879000	-1.422584000	-3.172535000	1	1.788065000	-2.048878000	-6.155172000
1	-7.223792000	-1.146952000	-2.617646000	1	2.230574000	-1.260881000	-8.509351000

7	3.987444000	-0.793632000	-7.469674000	6	3.397137000	3.977767000	5.065882000
8	4.670265000	0.140491000	-7.069558000	1	3.142720000	3.242225000	5.839935000
8	4.391098000	-1.936584000	-7.661392000	6	3.513537000	5.351686000	5.797996000
⁴TS5_{B,C6-exo}							
26	0.164887000	-5.649720000	-1.597340000	6	3.884470000	6.536068000	4.934163000
7	-0.171690000	-4.617134000	0.124771000	6	5.228747000	6.904058000	4.775095000
7	2.006215000	-6.158597000	-0.922938000	6	2.897052000	7.305034000	4.298404000
7	0.433199000	-6.829942000	-3.223651000	6	5.581117000	8.011304000	3.999781000
7	-1.752178000	-5.342735000	-2.146093000	6	3.245937000	8.413593000	3.522589000
6	-1.338216000	-4.007613000	0.510800000	6	4.589299000	8.770107000	3.371774000
6	-1.178639000	-3.383437000	1.820267000	1	6.001423000	6.326973000	5.277368000
6	0.113727000	-3.626704000	2.184598000	1	1.848578000	7.042517000	4.424555000
6	0.728571000	-4.401984000	1.132865000	1	6.627388000	8.287984000	3.896782000
6	2.606983000	-5.725262000	0.228118000	1	2.469483000	9.002700000	3.041284000
6	3.945075000	-6.263845000	0.320153000	1	4.859957000	9.637257000	2.775198000
6	4.140980000	-7.022452000	-0.793513000	6	2.280579000	3.963189000	4.010807000
6	2.923954000	-6.946453000	-1.569344000	8	2.523813000	3.914748000	2.800685000
6	1.573757000	-7.510960000	-3.557747000	7	1.026880000	3.980955000	4.518801000
6	1.402100000	-8.163343000	-4.836251000	1	0.913883000	4.184323000	5.503410000
6	0.145497000	-7.860615000	-5.266453000	6	-0.172599000	4.047772000	3.706020000
6	-0.452710000	-7.025875000	-4.249079000	1	0.148446000	4.207069000	2.671560000
6	-2.344365000	-5.744659000	-3.317857000	6	-0.916632000	2.685948000	3.757918000
6	-3.702199000	-5.257926000	-3.375006000	1	-0.181802000	1.932736000	3.439407000
6	-3.919618000	-4.561733000	-2.223524000	8	-1.983973000	2.741402000	2.806884000
6	-2.692601000	-4.615216000	-1.464109000	1	-2.568587000	1.945828000	2.914922000
6	-2.514481000	-4.003998000	-0.226130000	6	-1.435902000	2.327832000	5.151045000
6	2.024065000	-4.902252000	1.186167000	1	-0.614427000	2.273571000	5.872820000
6	2.732538000	-7.577644000	-2.792100000	1	-1.924148000	1.347777000	5.135005000
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1	-3.370564000	-3.482978000	0.190239000	6	-0.994309000	5.290276000	4.132503000
1	2.622785000	-4.646064000	2.054665000	8	-0.529843000	6.114130000	4.925067000
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1	-2.342159000	-6.761581000	-5.179283000	1	-2.547363000	4.609326000	3.012260000
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1	4.629532000	-6.072815000	1.137130000	1	-2.496524000	7.287557000	4.305328000
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1	-0.347945000	-8.166519000	-6.180577000	1	-3.924435000	6.481261000	1.713272000
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6	-2.236090000	-2.673296000	2.621580000	7	-0.521427000	7.829801000	0.022887000
6	-2.494036000	-1.211863000	2.210172000	1	-1.864807000	6.183994000	-0.034838000
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8	-3.777836000	-0.989583000	4.238277000	6	-0.382108000	8.949587000	0.814104000
1	-1.940172000	-2.680969000	3.675089000	6	-1.507769000	9.976249000	2.719698000
1	-3.182802000	-3.225630000	2.572022000	6	0.563909000	9.981865000	0.756668000
1	-1.546133000	-0.657785000	2.167477000	6	-0.575253000	11.006845000	2.662067000
1	-2.914860000	-1.148233000	1.199079000	6	0.452770000	11.006876000	1.692741000
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1	-1.753867000	-7.924177000	-1.007811000	1	-0.633690000	11.825217000	3.375445000
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7	3.576731000	1.794092000	1.109883000	1	1.354125000	9.958604000	0.011144000
1	4.488018000	2.195032000	0.902258000	6	-4.366788000	6.176031000	4.361045000
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1	4.503888000	-0.982649000	0.427940000	1	-6.812380000	6.364536000	5.173226000
6	5.954883000	0.153283000	1.572569000	6	-6.173705000	6.282335000	7.263623000
1	6.182772000	0.892397000	0.799019000	1	-5.517100000	6.871675000	7.915669000
1	6.688405000	-0.654091000	1.458808000	1	-7.185487000	6.372673000	7.683141000
6	6.159086000	0.727657000	2.973273000	6	-5.727267000	4.812926000	7.305298000
8	5.959778000	0.056310000	3.986971000	1	-5.602730000	4.511797000	8.353165000
7	6.597394000	2.017847000	3.030231000	1	-4.745418000	4.703082000	6.830030000
1	6.655715000	2.562780000	2.172801000	6	-6.729074000	3.857407000	6.639340000
6	6.904637000	2.639793000	4.302741000	1	-7.711377000	3.951835000	7.114863000
1	7.433603000	1.929776000	4.941895000	1	-6.861757000	4.098156000	5.582516000
1	7.566791000	3.492948000	4.120736000	7	-6.338395000	2.451524000	6.737898000
6	5.707236000	3.142427000	5.125817000	1	-6.457666000	2.007499000	7.638550000
8	5.782249000	3.211143000	6.354057000	6	-5.627757000	1.761925000	5.821507000
7	4.626667000	3.556614000	4.421514000	7	-5.217554000	2.321971000	4.683674000
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1	-4.725624000	1.732007000	3.992088000	7	1.225028000	4.424090000	-2.791185000
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1	-5.839294000	-0.028290000	6.779015000	1	2.041586000	4.289643000	-3.398954000
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1	-6.807619000	3.620589000	-2.547010000	1	-0.935749000	2.227861000	-4.283766000
6	-5.363604000	2.022437000	-2.548993000	1	0.757049000	2.371133000	-4.686938000
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1	-5.081758000	2.162368000	-3.597268000	6	0.302703000	1.718445000	-1.368545000
7	-4.336586000	2.708526000	-1.764198000	1	-0.150265000	2.526705000	-0.814170000
1	-3.735499000	3.383260000	-2.254447000	7	0.826770000	0.631228000	-0.709277000
6	-4.001510000	2.434567000	-0.495932000	1	1.030430000	0.572338000	0.289914000
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1	-5.321750000	0.900243000	-0.236824000	6	1.539061000	-0.437707000	-4.076089000
7	-4.647964000	1.498154000	0.216537000	6	2.175667000	-1.632829000	-3.920735000
1	-2.634694000	2.871632000	0.979650000	6	2.036529000	-1.430761000	-1.416390000
1	-2.426907000	3.759245000	-0.488128000	6	2.366654000	-2.246028000	-2.587825000
6	-5.907048000	7.610529000	-9.451466000	1	1.374265000	-0.043283000	-5.076013000
1	-6.623886000	6.788748000	-9.564323000	1	2.523340000	-2.197315000	-4.777635000
1	-6.109431000	8.348481000	-10.236897000	1	2.220431000	-1.814275000	-0.421528000
1	-6.095130000	8.085815000	-8.481669000	1	1.569135000	-3.249900000	-2.508371000
6	-4.459027000	7.093558000	-9.539251000	7	3.637806000	-3.019028000	-2.469471000
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6	4.548404000	6.711039000	0.028825000				
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6	5.242825000	5.617224000	0.858976000				
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1	5.917797000	6.093323000	1.584373000				
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1	6.842711000	5.990350000	-1.101542000				
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7	3.784298000	1.650693000	1.899363000	1	1.396495000	9.635135000	-0.630805000
1	4.705983000	1.970651000	1.617179000	6	-4.443559000	6.084358000	3.780366000
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6	6.164561000	0.177657000	2.829756000	6	-6.205813000	5.905210000	6.708234000
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1	6.908821000	-0.625639000	2.890934000	1	-7.214421000	5.946554000	7.142557000
6	6.262608000	0.960202000	4.137162000	6	-5.750010000	4.441637000	6.602329000
8	6.026312000	0.436381000	5.227367000	1	-5.644994000	4.031986000	7.614815000
7	6.649425000	2.263473000	4.023462000	1	-4.756744000	4.390447000	6.141054000
1	6.753313000	2.673032000	3.096105000	6	-6.728254000	3.555108000	5.815643000
6	6.865072000	3.075077000	5.205673000	1	-7.726210000	3.605144000	6.263609000
1	7.335624000	2.469767000	5.983006000	1	-6.824376000	3.897105000	4.783020000
1	7.548628000	3.891370000	4.948208000	7	-6.345322000	2.142793000	5.795460000
6	5.612124000	3.696573000	5.846997000	1	-6.547525000	1.605915000	6.628250000
8	5.587784000	3.954402000	7.051977000	6	-5.525253000	1.560831000	4.895593000
7	4.599056000	3.991411000	4.999143000	7	-5.037705000	2.235316000	3.852579000
1	4.640657000	3.686507000	4.033269000	1	-5.082798000	3.252048000	3.785886000
6	3.315229000	4.496969000	5.448766000	1	-4.413496000	1.741364000	3.194747000
1	2.986450000	3.901592000	6.309978000	7	-5.212185000	0.266210000	5.037759000
6	3.363013000	5.980536000	5.930254000	1	-5.702487000	-0.300706000	5.714049000
1	4.095362000	6.002899000	6.742102000	1	-4.599422000	-0.206723000	4.345959000
1	2.389170000	6.219761000	6.374000000	6	-7.818462000	5.992639000	-1.253582000
6	3.712257000	7.003960000	4.872994000	1	-8.091590000	6.832643000	-0.606269000
6	5.049192000	7.354470000	4.632889000	1	-8.588568000	5.219540000	-1.142230000
6	2.708056000	7.634884000	4.121900000	1	-7.848853000	6.346814000	-2.291227000
6	5.377077000	8.305604000	3.663966000	6	-6.430772000	5.452391000	-0.894194000
6	3.031914000	8.585398000	3.150627000	1	-6.412624000	5.130150000	0.155837000
6	4.368379000	8.923117000	2.918784000	1	-5.680136000	6.247160000	-0.985736000
1	5.836219000	6.888881000	5.220900000	6	-6.016010000	4.282905000	-1.800218000
1	1.664926000	7.385107000	4.305122000	1	-6.754438000	3.473168000	-1.754095000
1	6.418091000	8.571297000	3.498436000	1	-5.989308000	4.612137000	-2.843972000
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7	1.014436000	4.361250000	4.630591000	1	-5.130194000	1.577297000	0.851641000
1	0.752471000	4.744937000	5.531170000	1	-6.307101000	2.649355000	0.210931000
6	-0.039358000	4.313060000	3.633857000	7	-5.428133000	2.170899000	0.082718000
1	0.406487000	4.567677000	2.666041000	1	-3.021416000	1.709510000	0.347506000
6	-0.612381000	2.877741000	3.489895000	1	-2.402932000	2.858343000	-0.850597000
1	0.253359000	2.220670000	3.320143000	6	-8.698008000	5.859391000	-6.274444000
8	-1.431878000	2.899772000	2.319522000	1	-9.171688000	4.930191000	-6.611816000
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6	-1.364523000	2.392632000	4.728536000	1	-8.414396000	5.726668000	-5.223652000
1	-0.710569000	2.412618000	5.606884000	6	-7.467569000	6.194597000	-7.137201000
1	-1.702402000	1.359910000	4.590285000	6	-6.407252000	5.113082000	-7.100444000
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6	-1.068175000	5.413208000	3.969849000	6	-6.421759000	4.048166000	-8.014176000
8	-0.857741000	6.228729000	4.873882000	6	-4.438685000	4.103195000	-6.056068000
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1	-4.414458000	1.741943000	3.194111000	7	1.005081000	3.910363000	-2.951925000
7	-5.212157000	0.266144000	5.037410000	1	0.723491000	3.305761000	-2.167910000
1	-5.703743000	-0.301173000	5.712448000	1	1.725975000	3.454878000	-3.514688000
1	-4.601459000	-0.206930000	4.343900000	1	1.403786000	4.836291000	-2.516265000
6	-7.818462000	5.992639000	-1.253582000	6	-0.240395000	4.220142000	-3.728544000
1	-8.093155000	6.831781000	-0.605811000	1	-0.093341000	5.203186000	-4.181767000
1	-8.587351000	5.218223000	-1.142971000	6	-1.406522000	4.269860000	-2.710685000
1	-7.849120000	6.347444000	-2.291005000	8	-2.519341000	4.662801000	-3.138617000
6	-6.430039000	5.454393000	-0.894135000	8	-1.131491000	3.846845000	-1.551225000
1	-6.411696000	5.131482000	0.155686000	6	-0.536852000	3.181685000	-4.838686000
1	-5.680637000	6.250411000	-0.984925000	1	-1.272928000	3.656321000	-5.494926000
6	-6.013242000	4.286165000	-1.800813000	1	0.362897000	3.047597000	-5.452285000
1	-6.750685000	3.475466000	-1.755777000	6	-1.048407000	1.846513000	-4.354995000
1	-5.986301000	4.616152000	-2.844312000	6	-2.336535000	1.572507000	-3.936183000
7	-4.686573000	3.752522000	-1.497954000	1	-3.187232000	2.232458000	-3.846936000
1	-3.883541000	4.139410000	-2.024891000	7	-2.424675000	0.268811000	-3.502080000
6	-4.429499000	2.781217000	-0.615203000	1	-3.255667000	-0.158181000	-3.120862000
7	-3.186107000	2.325192000	-0.457235000	6	-1.193099000	-0.335494000	-3.613995000
1	-5.126033000	1.580376000	0.850338000	6	-0.295128000	0.628114000	-4.159426000

6	1.045503000	0.255068000	-4.382861000	1	6.708779000	2.640316000	3.012226000
6	1.459919000	-1.031961000	-4.041871000	6	6.873616000	3.076206000	5.112846000
6	-0.793001000	-1.638456000	-3.269881000	1	7.368544000	2.482848000	5.884235000
6	0.535249000	-1.927636000	-3.488274000	1	7.547504000	3.889215000	4.821895000
1	1.756074000	0.954712000	-4.818227000	6	5.638568000	3.704218000	5.783104000
1	2.490354000	-1.335596000	-4.201744000	8	5.640374000	3.960194000	6.988646000
1	-1.487575000	-2.356380000	-2.843373000	7	4.610671000	4.006324000	4.955990000
1	1.125054000	-3.275363000	-3.160210000	1	4.632792000	3.702494000	3.989139000
7	2.658992000	-4.262398000	-5.572746000	6	3.334648000	4.511934000	5.427748000
8	3.694875000	-3.648810000	-5.503626000	1	3.017790000	3.914277000	6.291825000
8	1.663030000	-4.091583000	-6.228898000	6	3.390554000	5.994355000	5.911117000
1				1	4.139054000	6.016274000	6.708141000
1	⁴ Int6 _{B,HAT}			1	2.425488000	6.231632000	6.374778000
26	1.685610000	-5.338835000	-1.647222000	6	3.717035000	7.019406000	4.848080000
7	1.074207000	-4.153709000	-0.123252000	6	5.048333000	7.372259000	4.581597000
7	3.552970000	-5.448039000	-0.873984000	6	2.697059000	7.648176000	4.116667000
7	2.276997000	-6.569662000	-3.145388000	6	5.355240000	8.323621000	3.606085000
7	-0.179479000	-5.223228000	-2.422664000	6	3.000009000	8.598689000	3.138698000
6	-0.190304000	-3.688459000	0.136412000	6	4.330979000	8.938879000	2.880536000
6	-0.206856000	-2.918000000	1.374902000	1	5.847639000	6.908039000	5.153901000
6	1.083892000	-2.907702000	1.818376000	1	1.658221000	7.395747000	4.319543000
6	1.869520000	-3.688810000	0.890181000	1	6.392300000	8.590912000	3.419669000
6	3.997705000	-4.780857000	0.233519000	1	2.199062000	9.076858000	2.580934000
6	5.399649000	-5.068890000	0.459950000	1	4.566821000	9.683343000	2.124865000
6	5.786568000	-5.925708000	-0.525504000	6	2.325654000	4.304423000	4.288951000
6	4.623398000	-6.153045000	-1.357009000	8	2.699350000	4.072271000	3.132717000
6	3.507635000	-7.140031000	-3.325205000	7	1.022807000	4.378393000	4.634748000
6	3.515145000	-7.938932000	-4.531812000	1	0.767453000	4.758422000	5.538655000
6	2.273388000	-7.827759000	-5.080723000	6	-0.037472000	4.323373000	3.645443000
6	1.507473000	-6.966201000	-4.205072000	1	0.400706000	4.581655000	2.675109000
6	-0.598133000	-5.807410000	-3.592105000	6	-0.600471000	2.884036000	3.502770000
6	-1.997504000	-5.520058000	-3.814832000	1	0.269084000	2.231745000	3.335858000
6	-2.420562000	-4.776155000	-2.752267000	8	-1.418230000	2.900512000	2.330767000
6	-1.275354000	-4.599366000	-1.887225000	1	-2.007411000	2.110852000	2.312329000
6	-1.294799000	-3.902235000	-0.679720000	6	-1.351017000	2.396546000	4.741505000
6	3.225270000	-3.959076000	1.051094000	1	-0.698692000	2.424810000	5.620937000
6	4.606582000	-6.961530000	-2.488764000	1	-1.679024000	1.360351000	4.606263000
6	0.180030000	-6.606840000	-4.424779000	1	-2.236300000	3.011189000	4.937763000
1	-2.245874000	-3.481779000	-0.367986000	6	-1.072786000	5.414785000	3.986318000
1	3.717875000	-3.513520000	1.910166000	8	-0.864452000	6.235574000	4.885892000
1	5.527552000	-7.471815000	-2.755138000	7	-2.166666000	5.419524000	3.191712000
1	-0.298454000	-7.003330000	-5.315752000	1	-2.253590000	4.642855000	2.536241000
1	1.479318000	-2.408415000	2.695301000	6	-3.128501000	6.507834000	3.175373000
1	5.988943000	-4.664722000	1.273927000	1	-2.680258000	7.327776000	3.744514000
1	6.761005000	-6.368308000	-0.691957000	6	-3.413685000	6.970158000	1.717450000
1	4.368047000	-8.497346000	-4.897669000	1	-4.162537000	7.772076000	1.768908000
1	1.894884000	-8.276145000	-5.991151000	1	-3.890874000	6.133403000	1.193829000
1	-2.569223000	-5.861494000	-4.6669096000	6	-2.196552000	7.425075000	0.969674000
1	-3.410177000	-4.381720000	-2.556134000	6	-1.462777000	6.672676000	0.076248000
6	-1.412636000	-2.314503000	2.039514000	7	-0.397623000	7.397936000	-0.403314000
6	-1.823243000	-0.928109000	1.512648000	1	-1.618433000	5.656410000	-0.262898000
6	-3.007036000	-0.323048000	2.272242000	1	0.298410000	7.055199000	-1.078527000
8	-3.304061000	0.908326000	1.995753000	6	-1.537075000	8.704728000	1.053517000
8	-3.615512000	-1.012695000	3.113774000	6	-0.410904000	8.646129000	0.178587000
1	-1.212430000	-2.225509000	3.112624000	6	-1.775851000	9.894458000	1.768716000
1	-2.271364000	-2.989781000	1.951264000	6	0.470087000	9.723693000	0.014985000
1	-0.982261000	-0.226217000	1.578368000	6	-0.907803000	10.968945000	1.604941000
1	-2.088491000	-0.972235000	0.447511000	6	0.206049000	10.882951000	0.739354000
16	1.031873000	-7.304887000	-0.370004000	1	-2.626582000	9.975382000	2.442114000
1	-0.195443000	-6.890864000	0.019143000	1	-1.084385000	11.890825000	2.153612000
8	2.234694000	-3.869317000	-2.635020000	1	0.868485000	11.738865000	0.637425000
7	3.695212000	1.641138000	1.871932000	1	1.330687000	9.630797000	-0.641741000
1	4.617808000	1.932889000	1.563638000	6	-4.449650000	6.067465000	3.821398000
1	3.025945000	2.392099000	2.009564000	8	-5.071906000	5.083385000	3.388344000
6	3.502638000	0.516358000	2.609503000	7	-4.903094000	6.838342000	4.830664000
8	2.427864000	0.271786000	3.167210000	1	-4.320062000	7.601699000	5.148075000
6	4.667453000	-0.472269000	2.671989000	6	-6.201253000	6.656070000	5.479891000
1	4.471761000	-1.126661000	3.524421000	1	-6.603303000	7.652318000	5.689335000
1	4.634595000	-1.091427000	1.766395000	1	-6.861609000	6.183201000	4.749268000
6	6.070482000	0.148673000	2.805620000	6	-6.144491000	5.848689000	6.788353000
1	6.335433000	0.744891000	1.928320000	1	-5.468163000	6.358021000	7.485990000
1	6.798578000	-0.669590000	2.861661000	1	-7.144033000	5.887538000	7.243308000
6	6.220224000	0.952687000	4.095170000	6	-5.699796000	4.385039000	6.646115000
8	6.006482000	0.451281000	5.200674000	1	-5.588103000	3.952456000	7.648272000
7	6.621680000	2.247987000	3.949007000	1	-4.711289000	4.337174000	6.174280000

6	-6.691434000	3.523547000	5.848890000	6	5.767855000	-0.719453000	-1.631901000
1	-7.686113000	3.574316000	6.304078000	6	4.085357000	0.753137000	-2.537858000
1	-6.790112000	3.887221000	4.824072000	6	4.439720000	-0.487951000	-2.004886000
7	-6.322962000	2.108419000	5.799465000	1	7.763280000	0.080431000	-1.527470000
1	-6.531436000	1.557207000	6.621244000	1	4.769441000	2.707505000	-3.139492000
6	-5.511192000	1.533224000	4.887466000	1	6.055243000	-1.685011000	-1.223562000
7	-5.022332000	2.219023000	3.852936000	1	3.058534000	0.936737000	-2.842512000
1	-5.073044000	3.236081000	3.795175000	1	3.698484000	-1.276091000	-1.904709000
1	-4.398789000	1.733481000	3.188261000	7	1.003706000	3.985002000	-3.035534000
7	-5.207147000	0.234608000	5.015223000	1	0.742270000	3.328613000	-2.287352000
1	-5.717393000	-0.335550000	5.674195000	1	1.722343000	3.576194000	-3.635727000
1	-4.646492000	-0.244325000	4.283786000	1	1.397037000	4.892021000	-2.553951000
6	-7.838747000	6.010664000	-1.312969000	6	-0.255213000	4.333190000	-3.772784000
1	-8.109050000	6.869242000	-0.689362000	1	-0.136460000	5.360785000	-4.125025000
1	-8.613955000	5.245426000	-1.184456000	6	-1.416451000	4.263871000	-2.749473000
1	-7.861972000	6.337039000	-2.359868000	8	-2.547359000	4.633936000	-3.152073000
6	-6.454828000	5.472012000	-0.932091000	8	-1.118306000	3.789303000	-1.617013000
1	-6.443765000	5.178974000	0.126548000	6	-0.527896000	3.413332000	-4.984913000
1	-5.699775000	6.260287000	-1.042016000	1	-1.306860000	3.919677000	-5.563870000
6	-6.040234000	4.275150000	-1.802416000	1	0.358735000	3.403667000	-5.630259000
1	-6.773699000	3.463508000	-1.724107000	6	-0.944113000	1.997774000	-4.660372000
1	-6.022883000	4.571281000	-2.856408000	6	-2.149369000	1.599431000	-4.113004000
7	-4.708213000	3.755477000	-1.494040000	1	-2.988797000	2.195912000	-3.786766000
1	-3.910445000	4.130722000	-2.037130000	7	-2.159448000	0.232456000	-3.938989000
6	-4.439478000	2.785966000	-0.613114000	1	-2.925340000	-0.295108000	-3.546762000
7	-3.194765000	2.322242000	-0.479963000	6	-0.963646000	-0.293246000	-4.367384000
1	-5.111359000	1.593199000	0.870000000	6	-0.162903000	0.792750000	-4.832665000
1	-6.293474000	2.675674000	0.256635000	6	1.128157000	0.529391000	-5.335318000
7	-5.422481000	2.188534000	0.107330000	6	1.598649000	-0.785358000	-5.357536000
1	-3.011482000	1.721241000	0.328041000	6	-0.518060000	-1.629539000	-4.391263000
1	-2.410140000	2.852419000	-0.891624000	6	0.751116000	-1.784449000	-4.885029000
6	-8.655675000	6.001185000	-6.315308000	1	1.758249000	1.333750000	-5.708031000
1	-9.139535000	5.080241000	-6.660808000	1	2.593024000	-1.016557000	-5.727998000
1	-9.391679000	6.812369000	-6.366431000	1	-1.136779000	-2.455184000	-4.048798000
1	-8.379825000	5.858464000	-5.263724000	1	1.437873000	-3.338048000	-2.803589000
6	-7.416083000	6.324844000	-7.168953000	7	3.663850000	-3.836458000	-4.835068000
6	-6.371044000	5.228842000	-7.130192000	8	4.454435000	-2.959404000	-4.592311000
6	-5.387878000	5.197992000	-6.132600000	8	2.884203000	-3.986333000	-5.742072000
6	-6.375600000	4.184156000	-8.066827000				
6	-4.445136000	4.169483000	-6.056078000				
6	-5.444483000	3.148880000	-8.009752000				
6	-4.473560000	3.134210000	-6.999992000				
8	-3.585131000	2.093962000	-7.005011000				
1	-2.999904000	2.137861000	-6.225660000				
1	-6.975896000	7.266617000	-6.816822000				
1	-7.730783000	6.496314000	-8.206324000				
1	-5.346004000	6.000212000	-5.398188000				
1	-7.121249000	4.180815000	-8.859375000				
1	-3.696515000	4.192431000	-5.267109000				
1	-5.453629000	2.346110000	-8.741391000				
8	1.673981000	6.306816000	-2.071943000				
8	3.061330000	7.925851000	-1.380841000				
6	2.745902000	6.730829000	-1.479122000				
6	3.625479000	5.650672000	-0.819942000				
1	2.971312000	5.065658000	-0.158179000				
1	3.969214000	4.947509000	-1.591632000				
6	4.795948000	6.225497000	-0.015441000				
1	4.420382000	7.068203000	0.571841000				
1	5.540807000	6.669385000	-0.690079000				
6	5.440980000	5.238971000	0.970078000				
1	4.669927000	4.811632000	1.619128000				
1	6.118536000	5.792852000	1.636512000				
6	6.265325000	4.073598000	0.438886000				
8	6.399504000	3.031006000	1.110869000				
7	6.901663000	4.246461000	-0.738167000				
1	6.760512000	5.120195000	-1.227418000				
6	7.898557000	3.328129000	-1.280300000				
1	8.137080000	2.615317000	-0.488814000				
1	8.802687000	3.906621000	-1.502919000				
6	7.448981000	2.587699000	-2.557124000				
1	8.347995000	2.122895000	-2.982667000				
1	7.103035000	3.325253000	-3.291895000				
6	6.387150000	1.527398000	-2.345932000				
6	6.729205000	0.278309000	-1.802990000				
6	5.051383000	1.750347000	-2.705431000				

Model B system – C7

2	TS4 _{B,C7-endo}	6	3.039150000	4.385981000	5.286708000
26	2.512545000	-4.553530000	-0.180364000	1	2.671129000
7	1.233969000	-4.178861000	1.347504000	6	3.262675000
7	3.951042000	-5.089877000	1.137515000	6	5.874807000
7	3.728659000	-5.101823000	-1.706361000	1	5.856455000
7	1.017779000	-4.187098000	-1.496741000	1	6.484195000
6	-0.046680000	-3.696320000	1.259781000	6	2.331648000
6	-0.589734000	-3.448528000	2.591971000	6	6.241243000
6	0.396565000	-3.807972000	3.461934000	1	6.138083000
6	1.527034000	-4.253808000	2.681702000	6	3.694030000
6	3.859934000	-5.048171000	2.502308000	1	4.574571000
6	5.119341000	-5.442837000	3.096643000	1	3.274109000
6	5.968518000	-5.716602000	2.068520000	6	4.311499000
6	5.227457000	-5.492652000	0.845788000	8	3.793916000
6	5.037738000	-5.493549000	-1.615065000	6	3.294116000
6	5.586149000	-5.706134000	-2.936616000	7	2.773314000
6	4.588554000	-5.436209000	-3.823416000	1	2.521939000
6	3.431084000	-5.057047000	-3.043137000	6	4.918206000
6	1.090671000	-4.285391000	-2.860830000	1	3.989869000
6	-0.164429000	-3.879076000	-3.454607000	1	3.110166000
6	-0.988960000	-3.529470000	-2.422755000	1	2.177199000
6	-0.237575000	-3.729100000	-1.203938000	8	2.000000000
6	-0.740199000	-3.493872000	0.073786000	6	1.730583000
6	2.735378000	-4.671180000	3.227811000	1	4.218267000
6	5.744239000	-5.678683000	-0.430981000	1	3.023589000
6	2.204756000	-4.692621000	-3.588396000	1	4.532037000
1	-1.761318000	-3.132977000	0.139101000	6	1.998123000
1	2.813848000	-4.683502000	4.310673000	8	3.823419000
1	6.777842000	-6.001752000	-0.510218000	6	4.337997000
1	2.110710000	-4.719575000	-4.669419000	1	2.592773000
1	0.374168000	-3.764445000	4.544395000	8	3.730405000
1	5.307627000	-5.494745000	4.161739000	6	2.110446000
1	7.000507000	-6.042007000	2.112013000	1	2.592773000
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1	4.614318000	-5.473985000	-4.905192000	1	3.632176000
1	-0.371141000	-3.879470000	-4.517749000	8	3.782205000
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6	-1.929715000	-2.853801000	2.922311000	1	2.211045000
6	-1.999691000	-1.342015000	2.630120000	6	5.115487000
6	-3.236082000	-0.644982000	3.202160000	1	5.184339000
8	-3.555287000	0.489328000	2.659135000	6	3.204053000
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1	-2.729977000	-3.364150000	2.369754000	6	1.002179000
1	-1.118520000	-0.845079000	3.061061000	6	7.267235000
1	-1.950294000	-1.148912000	1.553261000	6	1.414668000
16	1.685032000	-6.951784000	-0.086508000	1	0.989075000
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8	3.037727000	-2.995037000	-0.226237000	1	-0.326712000
7	2.877603000	1.252014000	1.929615000	1	7.243197000
1	3.821969000	1.361453000	1.573691000	6	-0.767256000
1	2.358513000	2.118225000	2.039478000	8	-0.001686000
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8	1.487497000	0.231015000	3.409021000	1	5.415238000
6	3.544846000	-0.913273000	2.886048000	1	-0.286446000
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6	8.988290000	4.318885000	-2.779151000	1	-4.027291000	-5.647360000	-3.309483000
6	8.573346000	3.955929000	-5.511424000	1	-4.237420000	-4.502076000	-0.856965000
6	9.296953000	5.346290000	-3.675136000	6	-1.089935000	-2.458835000	2.971589000
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1	7.872689000	1.989178000	-4.986058000	6	-2.765109000	-0.501286000	3.351067000
1	9.165558000	4.461063000	-1.715544000	8	-3.289468000	0.578371000	2.855113000
1	8.416056000	3.804550000	-6.576140000	8	-3.097430000	-1.005907000	4.439725000
1	9.704518000	6.282310000	-3.302322000	1	-0.619500000	-2.331016000	3.951949000
1	9.331807000	5.964564000	-5.742935000	1	-1.910683000	-3.172557000	3.110898000
7	1.010116000	3.757280000	-2.370066000	1	-0.849050000	-0.373441000	2.435219000
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6	-0.174241000	3.821701000	-3.290480000	8	0.823313000	-3.136941000	-2.531255000
1	-0.325350000	4.873501000	-3.551767000	7	3.577782000	1.512577000	2.590478000
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6	-0.327886000	0.531980000	-3.922056000	6	5.982816000	0.335734000	3.810543000
1	-1.382594000	0.504084000	-3.688793000	1	6.245106000	0.795433000	2.853908000
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				1	6.176130000	8.742719000	2.967453000
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				7	0.792464000	4.755191000	4.695703000
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6	-4.779134000	5.821017000	3.390124000	6	6.100468000	3.686786000	0.710621000
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1	-5.351950000	-0.008166000	6.817014000	1	1.992172000	2.796680000	-2.597549000
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6	-7.674161000	4.218524000	-1.751210000	6	0.105482000	3.598210000	-3.140000000
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8	3.196173000	-2.795494000	-0.181644000	1	0.892965000	11.821792000	1.080949000
7	2.997664000	1.444625000	1.644522000	1	1.530128000	9.684690000	-0.066795000
1	3.941747000	1.563922000	1.292661000	8	-4.761208000	6.103246000	3.640833000
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6	2.665940000	0.385921000	2.436552000	1	-4.890525000	7.784276000	4.774313000
8	1.601929000	0.352519000	3.065301000	6	-6.789643000	6.824422000	4.881320000
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8	1.789095000	6.140529000	-1.904787000	6	5.020193000	-5.632417000	3.270041000
8	3.289833000	7.620215000	-1.139321000	6	5.846381000	-6.042148000	2.268611000
6	2.882932000	6.459406000	-1.281432000	6	5.115998000	-5.872886000	1.031075000
6	3.647944000	5.285858000	-0.639201000	6	4.923085000	-6.044641000	-1.423924000
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6	5.076055000	5.620999000	-0.200428000	6	3.364273000	-5.568886000	-2.892396000
1	5.061708000	6.596256000	0.294128000	6	1.080382000	-4.634347000	-2.780132000
1	5.721488000	5.751473000	-1.080649000	6	-0.139590000	-4.175048000	-3.407179000
6	5.678958000	4.604592000	0.784278000	6	-0.963275000	-3.759115000	-2.400511000
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1	6.675741000	4.945454000	1.098992000	6	-0.748116000	-3.652258000	0.096646000
6	5.841216000	3.161075000	0.320645000	6	2.680949000	-4.726757000	3.337594000
8	5.713938000	2.214059000	1.121470000	6	5.614498000	-6.193529000	-0.225834000
7	6.161451000	2.958268000	-0.974480000	6	2.176180000	-5.138229000	-3.472840000
1	6.279294000	3.767646000	-1.569581000	1	-1.754432000	-3.248549000	0.135073000
6	6.448747000	1.648769000	-1.551009000	1	2.760874000	-4.659225000	4.418274000
1	5.817290000	1.504862000	-2.434687000	1	6.624106000	-6.589862000	-0.277343000
1	6.163651000	0.905874000	-0.804914000	1	2.103255000	-5.188204000	-4.554674000
6	7.935471000	1.472497000	1.929139000	1	0.345458000	-3.659476000	4.578620000
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6	8.956427000	3.672732000	-2.686227000	1	-0.325287000	-4.186679000	-4.473632000
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7	0.940357000	3.725990000	-2.331702000	1	-1.144122000	-0.811679000	2.896881000
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1	1.639846000	3.059178000	-2.668980000	16	1.538379000	-7.233557000	0.195502000
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6	2.249019000	-6.039173000	-4.229494000		7	0.792464000	4.755191000	4.695703000
6	1.937898000	-6.737073000	-5.455100000		1	0.509205000	5.329276000	5.481036000
6	0.579827000	-6.783525000	-5.546406000		6	-0.241233000	4.447552000	3.726192000
6	0.059632000	-6.118266000	-4.374331000		1	0.205963000	4.508573000	2.727749000
6	-1.823982000	-5.390860000	-2.950953000		6	-0.745013000	2.989467000	3.896213000
6	-3.237141000	-5.301869000	-2.654320000		1	0.150520000	2.351343000	3.879887000
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6	3.538623000	-5.766553000	-3.787123000		1	-1.783377000	1.698241000	5.295138000
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1	-2.505160000	-3.645102000	0.911095000		6	-1.325912000	5.541651000	3.811616000
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1	4.362514000	-6.100087000	-4.410491000		7	-2.413851000	5.309929000	3.044420000
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6	-2.765109000	-0.501286000	3.351067000		1	0.402503000	6.621051000	-1.056922000
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8	-3.097430000	-1.005907000	4.439725000		6	-0.645856000	8.290020000	-0.210971000
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16	0.948840000	-6.852174000	-0.634430000		1	-3.282710000	9.694263000	1.483051000
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6	6.502976000	2.473440000	4.847986000	1	-8.402655000	3.834133000	5.712455000
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6	3.214046000	8.384572000	3.152318000	1	-6.224304000	4.530579000	0.143077000
6	4.576166000	8.631584000	2.958626000	1	-5.439690000	5.467034000	-1.120094000
1	5.842311000	6.389802000	5.186899000	6	-5.961519000	3.471684000	-1.734693000
1	1.738538000	7.240761000	4.226595000	1	-6.751796000	2.726501000	-1.581410000
1	6.582382000	8.098993000	3.551210000	1	-5.958758000	3.702437000	-2.804423000
1	2.473509000	8.945297000	2.588286000	7	-4.660558000	2.870492000	-1.439515000
1	4.896899000	9.385224000	2.244581000	1	-3.863417000	3.140940000	-2.037450000
6	2.061210000	4.116083000	4.147232000	6	-4.406265000	2.014537000	-0.446204000
8	2.376011000	3.829141000	2.986192000	7	-3.171266000	1.521483000	-0.284252000
7	0.787800000	4.345606000	4.531098000	1	-5.077774000	1.065919000	1.206017000
1	0.603349000	4.739547000	5.444923000	1	-6.259817000	2.054638000	0.432702000
6	-0.329282000	4.277019000	3.609826000	7	-5.385020000	1.556880000	0.369070000
1	0.066466000	4.424427000	2.598995000	1	-2.992997000	1.051038000	0.603351000
6	-0.968242000	2.863444000	3.638105000	1	-2.383614000	2.004313000	-0.742922000
1	-0.144212000	2.153470000	3.481082000	6	-8.716227000	6.935047000	-6.256543000
8	-1.863435000	2.808855000	2.525232000	1	-8.969669000	5.990341000	-6.751511000
1	-2.365996000	1.961688000	2.557119000	1	-9.522339000	7.651135000	-6.457783000
6	-1.662424000	2.538264000	4.962595000	1	-8.690049000	6.748503000	-5.176468000
1	-0.956298000	2.608067000	5.797178000	6	-7.361085000	7.467452000	-6.753477000
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6	-1.286529000	5.451251000	3.899848000	6	-5.874430000	5.518607000	-7.425641000
8	-0.963869000	6.366786000	4.661972000	6	-4.565178000	5.556863000	-4.968137000
7	-2.457016000	5.396279000	3.222409000	6	-4.889274000	4.570830000	-7.154962000
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6	-3.378073000	6.511919000	3.132903000	8	-3.279839000	3.633898000	-5.688525000
1	-2.966978000	7.308734000	3.756795000	1	-2.952259000	3.701443000	-4.754457000

1	-7.150276000	8.426965000	-6.263625000	7	-1.345780000	-3.565541000	-2.842678000
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1	-5.802180000	7.249449000	-4.512336000	6	-0.823684000	-2.703938000	1.493588000
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1	-4.039545000	5.580128000	-4.017734000	6	1.113773000	-3.444095000	0.580668000
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8	1.909056000	6.326886000	-1.583435000	6	4.477878000	-4.648063000	-0.729950000
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6	2.997951000	6.640340000	-0.954786000	6	3.480981000	-4.837606000	-2.741923000
6	3.803667000	5.453105000	-0.397091000	6	2.120433000	-4.985471000	-4.794880000
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1	3.798479000	4.638247000	-1.131601000	6	0.668245000	-5.008778000	-6.518185000
6	5.232128000	5.797900000	0.030429000	6	0.032075000	-4.538606000	-5.309004000
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7	6.347824000	3.279927000	-1.074459000	6	-1.298005000	-4.140111000	-5.227797000
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6	1.528031000	0.791612000	-5.604543000	8	5.360948000	0.156246000	5.919567000
6	1.699854000	2.147155000	-5.220697000	7	6.325842000	1.766138000	4.633328000
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6	-5.869537000	5.512379000	-1.179260000	8	-0.845981000	3.085875000	-1.554412000

6	0.205447000	3.442449000	-4.921849000	8	1.519509000	0.181331000	3.246369000
1	-0.757531000	3.700664000	-5.378852000	6	3.574550000	-0.953389000	2.697900000
1	0.968373000	3.978583000	-5.500758000	1	3.323183000	-1.508747000	3.604600000
6	0.473177000	1.960563000	-5.020341000	1	3.409194000	-1.628381000	1.846956000
6	0.377994000	0.980385000	-4.043674000	6	5.061485000	-0.550286000	2.733417000
1	0.073307000	1.056066000	-3.009061000	1	5.370927000	-0.057132000	1.807400000
7	0.750114000	-0.237496000	-4.563830000	1	5.655163000	-1.469283000	2.810564000
1	0.809111000	-1.104770000	-3.998210000	6	5.408384000	0.295810000	3.956024000
6	1.079462000	-0.079629000	-5.878708000	8	5.194029000	-0.098600000	5.104352000
6	0.919067000	1.281644000	-6.212519000	7	5.986838000	1.505209000	3.702284000
6	1.130757000	1.706637000	-7.546010000	1	6.070594000	1.829452000	2.738998000
6	1.457252000	0.741748000	-8.518934000	6	6.429927000	2.350655000	4.794148000
6	1.564525000	-1.069004000	-6.815673000	1	6.915403000	1.741920000	5.559835000
6	1.608988000	-0.596793000	-8.199583000	1	7.165345000	3.062770000	4.404552000
1	1.008581000	2.748170000	-7.827451000	6	5.329735000	3.147527000	5.518140000
1	1.565105000	1.052353000	-9.554570000	8	5.427320000	3.415343000	6.716935000
1	1.271791000	-2.107208000	-6.664921000	7	4.308612000	3.573897000	4.736514000
1	1.846524000	-1.322735000	-8.970379000	1	4.234762000	3.242164000	3.780880000
7	3.330630000	-1.362956000	-6.453703000	6	3.109728000	4.198279000	5.265727000
8	3.961648000	-0.476524000	-5.901763000	1	2.764309000	3.618075000	6.131240000
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6	5.148934000	-6.137102000	-0.931608000	7	0.768884000	4.308188000	4.559872000
6	5.824588000	-6.407697000	-2.181038000	1	0.586459000	4.684348000	5.481478000
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1	4.780407000	-6.079645000	4.839908000	1	-2.964648000	7.284645000	3.734806000
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6	-2.032466000	-2.867655000	2.788520000	7	-0.331335000	7.343294000	-0.208814000
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16	1.538379000	-7.233557000	0.195502000	1	-2.753443000	9.956831000	2.439068000
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7	-6.979767000	2.340635000	5.653069000	1	8.796326000	1.967892000	-4.393361000
1	-7.345212000	1.883862000	6.477716000	1	9.411259000	3.790777000	-0.551150000
6	-6.044763000	1.654992000	4.962165000	1	10.192562000	3.716438000	-5.450108000
7	-5.352781000	2.212187000	3.967245000	1	10.805408000	5.545318000	-1.603306000
1	-5.358286000	3.215651000	3.785983000	1	11.203567000	5.518110000	-4.060500000
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1	-6.463250000	-0.107824000	5.892513000	1	1.738947000	3.290704000	-2.635844000
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7	-3.245781000	1.498839000	-0.196277000	6	2.159358000	0.015829000	-4.094632000
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1	-2.474180000	2.069742000	-0.568724000	6	4.435315000	-0.098852000	-5.003927000
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6	-6.231975000	6.374796000	-6.383787000	8	4.998180000	-1.647927000	-2.542823000
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8	5.355435000	0.154694000	5.927555000	1	-5.623370000	5.242330000	7.601593000
7	6.327622000	1.763526000	4.645335000	1	-4.696584000	5.320495000	6.111122000
1	6.515528000	2.092624000	3.699867000	6	-6.709179000	4.552722000	5.875572000
6	6.641520000	2.608181000	5.782112000	1	-7.703262000	4.709154000	6.306932000
1	6.977113000	1.988193000	6.615685000	1	-6.793483000	4.750481000	4.804533000
1	7.462283000	3.277314000	5.501837000	7	-6.390532000	3.134844000	6.052709000
6	5.490946000	3.472594000	6.327688000	1	-6.612002000	2.727660000	6.951276000
8	5.452938000	3.790541000	7.517594000	6	-5.588497000	2.406650000	5.247353000
7	4.588083000	3.897195000	5.412076000	7	-5.067715000	2.919544000	4.133419000
1	4.610578000	3.525085000	4.468693000	1	-5.060279000	3.920375000	3.937198000
6	3.367044000	4.590936000	5.779580000	1	-4.456670000	2.317288000	3.556411000
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6	3.585401000	6.086491000	6.161976000	1	-5.867397000	0.669056000	6.280907000
1	4.300181000	6.077911000	6.989950000	1	-4.747617000	0.541276000	4.935013000
1	2.639797000	6.469552000	6.564641000	6	-7.168918000	6.208130000	-1.596666000
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6	5.445571000	7.180401000	4.835641000	1	-8.038840000	5.590385000	-1.342079000
6	3.163406000	7.664988000	4.221406000	1	-7.195138000	6.392464000	-2.677359000
6	5.900641000	8.021574000	3.817500000	6	-5.861141000	5.525770000	-1.182968000
6	3.614676000	8.504640000	3.200193000	1	-5.842226000	5.381795000	-0.094157000
6	4.985525000	8.685654000	2.995728000	1	-5.005960000	6.169049000	-1.424247000
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1	2.094415000	7.538897000	4.380763000	1	-6.521008000	3.510202000	-1.691820000
1	6.968321000	8.165286000	3.672415000	1	-5.638577000	4.320225000	-2.971103000
1	2.897621000	9.020402000	2.566752000	7	-4.428519000	3.491536000	-1.523689000
1	5.337011000	9.344441000	2.206248000	1	-3.597416000	3.635782000	-2.124627000
6	2.388140000	4.412431000	4.610089000	6	-4.266149000	2.713599000	-0.448608000
8	2.779029000	4.028175000	3.501211000	7	-3.086622000	2.139262000	-0.203194000
7	1.091014000	4.675442000	4.874627000	1	-5.057594000	1.955850000	1.248440000
1	0.837140000	5.161431000	5.726365000	1	-6.114781000	3.012986000	0.396439000
6	0.073060000	4.599943000	3.843913000	7	-5.300940000	2.417795000	0.376532000
1	0.573653000	4.714764000	2.876191000	1	-2.971113000	1.732962000	0.727871000
6	-0.600747000	3.201166000	3.825477000	1	-2.246619000	2.449749000	-0.719044000
1	0.215385000	2.467103000	3.769032000	6	-7.847385000	-1.312672000	-3.503992000
8	-1.365619000	3.149321000	2.617786000	1	-7.546953000	-2.241137000	-4.003227000
1	-2.042830000	2.435821000	2.675939000	1	-8.883773000	-1.429067000	-3.164956000
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1	-1.843727000	1.896800000	5.033395000	6	-6.292622000	0.098691000	-4.951975000
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6	-5.838780000	-0.520618000	-6.126470000	
6	-4.062633000	1.062350000	-4.675175000	
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8	-2.359333000	0.549022000	-6.330629000	
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7	7.198321000	3.508092000	-0.002801000	
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6	-0.376625000	8.588621000	0.370708000	6	3.649930000	5.435944000	-0.569613000
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6	0.227729000	10.814744000	0.983112000	1	4.977008000	6.668728000	0.577009000
1	-2.754577000	9.955139000	2.437332000	1	5.717751000	6.024111000	-0.862097000
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8	-5.308100000	5.027942000	3.220287000	8	5.748289000	2.232207000	0.855127000
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1	-4.869641000	7.759567000	4.752887000	1	6.403185000	4.158385000	-1.556631000
6	-6.779854000	6.8222631000	4.881079000	6	6.604168000	2.055179000	-1.822908000
1	-7.198465000	7.833606000	4.904754000	1	6.286546000	2.184766000	-2.862309000
1	-7.309019000	6.268491000	4.102142000	1	6.021618000	1.239022000	-1.391189000
6	-6.970213000	6.165371000	6.259162000	6	8.108397000	1.712015000	-1.762237000
1	-6.429979000	6.756262000	7.009167000	1	8.244077000	0.748239000	-2.268535000
1	-8.036336000	6.241076000	6.514249000	1	8.385141000	1.566166000	-0.711912000
6	-6.518043000	4.700086000	6.361478000	6	8.993526000	2.762758000	-2.398260000
1	-6.614316000	4.375532000	7.405277000	6	9.223332000	2.762616000	-3.782924000
1	-5.455118000	4.613616000	6.105583000	6	9.575047000	3.780560000	-1.628147000
6	-7.334998000	3.748159000	5.474039000	6	10.008620000	3.749920000	-4.381061000
1	-8.401593000	3.837012000	5.706871000	6	10.361255000	4.771481000	-2.222215000
1	-7.214251000	3.999210000	4.418862000	6	10.580108000	4.759685000	-3.601559000
7	-6.979660000	2.340664000	5.653148000	1	8.786753000	1.976957000	-4.396130000
1	-7.345454000	1.883712000	6.477538000	1	9.415467000	3.792061000	-0.552500000
6	-6.044763000	1.654992000	4.962165000	1	10.178323000	3.728197000	-5.454498000
7	-5.352856000	2.212133000	3.967139000	1	10.805249000	5.549240000	-1.606234000
1	-5.358368000	3.215581000	3.785800000	1	11.194101000	5.527258000	-4.064993000
1	-4.673839000	1.628492000	3.457092000	7	1.003273000	3.925487000	-2.313197000
7	-5.821119000	0.372622000	5.278749000	1	0.624185000	3.545125000	-1.427058000
1	-6.463027000	-0.107761000	5.892771000	1	1.738079000	3.291011000	-2.638189000

1	1.417578000	4.927825000	-2.106120000
6	-0.165038000	3.942793000	-3.253261000
1	-0.350223000	4.985875000	-3.527035000
6	-1.401974000	3.445983000	-2.459146000
8	-2.498443000	3.362436000	-3.082155000
8	-1.217853000	3.178493000	-1.244068000
6	0.113979000	3.126739000	-4.537272000
1	-0.823603000	3.079497000	-5.098978000
1	0.813251000	3.696458000	-5.158739000
6	0.684912000	1.757729000	-4.275578000
6	0.056699000	0.674537000	-3.689704000
1	-0.961509000	0.558171000	-3.347041000
7	0.951415000	-0.365711000	-3.584009000
1	0.729881000	-1.282609000	-3.205030000
6	2.159429000	0.015286000	-4.094042000
6	2.037775000	1.338211000	-4.547159000
6	3.131931000	1.961547000	-5.209297000
6	4.299433000	1.201573000	-5.440155000
6	3.407067000	-0.757677000	-4.141684000
6	4.436034000	-0.098270000	-5.001716000
1	3.061524000	2.980898000	-5.575331000
1	5.110814000	1.647353000	-6.009496000
1	3.291375000	-1.827633000	-4.336409000
1	5.341229000	-0.661748000	-5.199672000
7	4.097562000	-0.825486000	-2.660340000
8	4.998996000	-1.644862000	-2.539499000
8	3.738690000	-0.022881000	-1.809916000

Model B system – C5

²TS4_{B,C5-endo}

26	-1.665559000	-4.876806000	-2.082238000	6	4.383991000	5.291081000	5.607091000
7	-1.338956000	-4.251825000	-0.185911000	1	5.265325000	5.153478000	6.240597000
7	0.260736000	-5.494919000	-2.213421000	1	3.567804000	5.616275000	6.263716000
7	-2.041673000	-5.697501000	-3.893630000	6	4.647259000	6.343496000	4.553830000
7	-3.624881000	-4.393610000	-1.896918000	6	5.950235000	6.583308000	4.093934000
6	-2.242587000	-3.650361000	0.652575000	6	3.596611000	7.110428000	4.025193000
6	-1.597522000	-3.266701000	1.903487000	6	6.199505000	7.560501000	3.126888000
6	-0.296052000	-3.655321000	1.781062000	1	3.841714000	8.084094000	3.054366000
6	-0.142079000	-4.263186000	0.480898000	1	5.144778000	8.312509000	2.603006000
6	1.233538000	-5.340573000	-1.263433000	1	6.775909000	6.008624000	4.506625000
6	2.490602000	-5.867030000	-1.750621000	1	2.580915000	6.946417000	4.379916000
6	2.257006000	-6.339246000	-3.006486000	1	7.217246000	7.738514000	2.788969000
6	0.857586000	-6.104255000	-3.285758000	1	3.017423000	8.666934000	2.652051000
6	-1.129538000	-6.273984000	-4.739242000	1	5.335581000	9.073333000	1.851050000
6	-1.771691000	-6.651539000	-5.977262000	6	2.787970000	3.880280000	4.160235000
6	-3.079192000	-6.284666000	-5.869301000	1	2.895346000	3.740010000	2.936552000
6	-3.236760000	-5.682203000	-4.565426000	6	1.601080000	4.032389000	4.785889000
6	-4.602814000	-4.560644000	-2.841748000	1	0.316454000	1.986101000	3.799440000
6	-5.858257000	-4.035400000	-2.352669000	8	0.341487000	4.099787000	4.069045000
6	-5.619284000	-3.553150000	-1.100723000	1	-1.489857000	2.818509000	3.221769000
6	-4.217132000	-3.782877000	-0.827066000	1	-2.130391000	2.089851000	3.393234000
6	-3.583738000	-3.435768000	0.362384000	6	-0.404101000	2.739349000	4.148590000
6	1.055781000	-4.769984000	-0.007592000	1	-0.018367000	2.333642000	6.248739000
6	0.220004000	-6.468932000	-4.465056000	1	-1.349389000	1.394928000	5.565457000
6	-4.432163000	-5.159420000	-4.083882000	1	-1.590517000	3.112652000	5.936761000
1	-4.194516000	-2.958125000	1.121001000	6	-0.444072000	5.343847000	4.539467000
1	1.923102000	-4.713437000	0.642936000	8	0.084796000	6.206129000	5.246343000
1	0.821717000	-6.945995000	-5.232571000	7	-1.707629000	5.417646000	4.061001000
1	-5.300934000	-5.223150000	-4.732045000	1	-2.042269000	4.607393000	3.538302000
1	0.503309000	-3.535411000	2.502639000	6	-2.508885000	6.626265000	4.106024000
1	3.416030000	-5.869497000	-1.188294000	1	-2.899726000	7.393728000	4.578862000
1	2.951002000	-6.809395000	-3.691973000	6	-3.556019000	7.951085000	2.753197000
1	-1.270441000	-7.130630000	-6.809024000	1	-3.505078000	6.274302000	2.223294000
1	-3.875385000	-6.399146000	-6.594259000	6	-1.715614000	7.386198000	1.798608000
1	-6.789190000	-4.050101000	-2.905761000	6	-1.073164000	6.522561000	0.933813000
1	-6.314278000	-3.093266000	-0.409182000	7	0.006991000	7.140371000	0.347649000
6	-2.248392000	-2.536617000	3.043952000	1	-1.313802000	5.496318000	0.683119000
6	-2.406012000	-1.033363000	2.752077000	1	0.688131000	6.689965000	-0.283964000
6	-3.148453000	-0.241323000	3.829625000	6	-0.977148000	8.623622000	1.748226000
8	-3.517659000	0.953664000	3.497213000	6	0.098554000	8.425267000	0.832560000
8	-3.344516000	-0.746716000	4.953748000	6	-1.109683000	9.878283000	2.374802000
1	-1.651139000	-2.666263000	3.951938000	6	1.034463000	9.428742000	0.545041000
1	-3.235000000	-2.963470000	3.262496000	6	-0.188218000	10.879422000	2.087038000
1	-1.416195000	-0.572819000	2.625573000	6	0.875958000	10.655026000	1.184274000
1	-2.921816000	-0.881596000	1.797723000	1	-1.920963000	10.065355000	3.075281000
16	-2.204411000	-7.083197000	-1.029692000	1	-0.282972000	11.850888000	2.565986000
1	-2.280129000	-7.8444834000	-2.144946000	1	1.583108000	11.456357000	0.985072000
8	-1.306596000	-3.400326000	-2.736028000	1	1.854841000	9.229597000	-0.139026000
7	3.327925000	1.529170000	1.099701000	6	-3.784159000	6.379341000	4.920362000
1	4.249797000	1.687928000	0.703618000	8	-4.513470000	5.404715000	4.678990000
1	2.890883000	2.356177000	1.498674000	7	-4.079250000	7.304555000	5.857075000
6	3.027537000	0.359646000	1.741229000	1	-3.419127000	8.054492000	6.015070000
8	2.028145000	0.244226000	2.453092000	6	-5.302103000	7.290707000	6.658485000
6	3.958249000	-0.826931000	1.494413000	1	-5.636817000	8.327264000	6.766743000
1	3.711769000	-1.573483000	2.252549000	1	-6.059931000	6.759577000	6.078035000
1	3.715972000	-1.255809000	0.513354000	6	-5.123283000	6.665798000	8.053184000
6	5.465874000	-0.5111431000	1.536471000	1	-4.356203000	7.232988000	8.595045000
1	5.761061000	0.147054000	0.715372000	1	-6.062020000	6.810780000	8.605770000
1	6.011952000	-1.452712000	1.399740000	6	-4.738845000	5.177787000	8.065269000
6	5.910079000	0.058453000	2.882419000	1	-4.489226000	4.887183000	9.093619000
8	5.727297000	-0.545470000	3.940737000	1	-3.832790000	5.019686000	7.468512000
7	6.537662000	1.268665000	2.829389000	6	-5.855531000	4.253937000	7.554310000
1	6.615322000	1.7444971000	1.931724000	1	-6.763389000	4.395902000	8.150752000
6	7.110136000	1.865426000	4.020667000	1	-6.114378000	4.485065000	6.519217000
1	7.557595000	1.086745000	4.641960000	7	-5.510098000	2.834424000	7.630974000
1	7.903803000	2.556243000	3.716145000	1	-5.520814000	2.414386000	8.550693000
6	6.141438000	2.633325000	4.936072000	6	-4.947403000	2.100261000	6.646898000
8	6.360595000	2.719920000	6.145542000	7	-4.686776000	2.616546000	5.446685000
7	5.096036000	3.240202000	4.324594000	1	-4.661410000	3.621717000	5.277275000
1	4.905797000	3.066035000	3.343979000	1	-4.286788000	1.996933000	4.720733000
6	4.023323000	3.871746000	5.071559000	7	-4.671728000	0.808870000	6.876981000
1	3.809451000	3.252967000	5.951414000				

1	-5.027641000	0.355089000	7.705452000	1	1.656875000	2.513334000	-1.299790000
1	-4.199098000	0.229607000	6.156697000	1	1.582611000	4.253007000	-1.123904000
6	-7.332534000	0.370746000	-3.744286000	6	0.000680000	3.392098000	-2.289369000
1	-8.315503000	0.801961000	-3.961385000	1	-0.051103000	4.445896000	-2.583369000
1	-7.482118000	-0.673432000	-3.443682000	6	-1.369138000	3.029099000	-1.657726000
1	-6.753080000	0.371596000	-4.675158000	8	-2.345467000	2.840382000	-2.437948000
6	-6.613786000	1.168068000	-2.651321000	8	-1.405459000	2.991171000	-0.401856000
1	-7.235553000	1.209265000	-1.746375000	6	0.379502000	2.550745000	-3.523728000
1	-6.467695000	2.205535000	-2.976288000	1	-0.430195000	2.676203000	-4.247877000
6	-5.242706000	0.562305000	-2.316005000	1	1.273046000	2.993179000	-3.979979000
1	-5.345025000	-0.475856000	-1.976467000	6	0.616784000	1.092110000	-3.245845000
1	-4.623444000	0.537572000	-3.217961000	6	-0.325909000	0.091805000	-3.152313000
7	-4.482638000	1.328082000	-1.325897000	1	-1.397575000	0.144468000	-3.282203000
1	-3.754933000	1.965017000	-1.683791000	7	0.279974000	-1.115308000	-2.871775000
6	-4.518981000	1.148059000	-0.004335000	1	-0.228113000	-2.011274000	-2.770904000
7	-3.692524000	1.826506000	0.793343000	6	1.627550000	-0.930894000	-2.783735000
1	-5.474121000	0.279950000	1.561612000	6	1.898113000	0.453789000	-3.020605000
1	-6.209549000	-0.014465000	0.048268000	6	3.208985000	0.917538000	-2.985779000
7	-5.379987000	0.258129000	0.554550000	6	4.315725000	-0.044397000	-2.833879000
1	-3.625745000	1.542396000	1.779542000	6	2.657252000	-1.861668000	-2.479080000
1	-2.878929000	2.304913000	0.378455000	6	3.951730000	-1.430000000	-2.470721000
6	-8.241224000	4.686078000	-7.313429000	1	3.461500000	1.958086000	-3.165696000
1	-8.450055000	3.628682000	-7.513621000	1	5.168217000	0.359688000	-2.282592000
1	-8.968745000	5.287821000	-7.871255000	1	2.411348000	-2.890770000	-2.233296000
1	-8.404098000	4.861406000	-6.243609000	1	4.756923000	-2.117284000	-2.232054000
6	-6.799818000	5.048110000	-7.716335000	7	5.078893000	-0.087083000	-4.368124000
6	-5.753427000	4.243169000	-6.972588000	8	4.934028000	-1.070879000	-5.075197000
6	-5.232633000	4.682391000	-5.747440000	8	5.675567000	0.938099000	-4.693179000
6	-5.295327000	3.012258000	-7.466578000				
6	-4.294963000	3.931738000	-5.035919000				
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6	-3.850858000	2.703273000	-5.547672000				
8	-2.934290000	1.925742000	-4.904176000				
1	-2.665498000	2.346313000	-4.049582000				
1	-6.637279000	6.118457000	-7.535361000				
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1	-5.561015000	5.636145000	-5.338436000				
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8	3.460266000	7.415008000	-0.923162000				
6	3.161886000	6.211878000	-0.880249000				
6	4.219337000	5.171482000	-0.465033000				
1	3.941578000	4.829951000	0.543268000				
1	4.129435000	4.291579000	-1.114938000				
6	5.650164000	5.711881000	-0.455077000				
1	5.647557000	6.683945000	0.045707000				
1	5.986422000	5.897299000	-1.483685000				
6	6.665320000	4.804724000	0.274226000				
1	6.353748000	4.667036000	1.314217000				
1	7.644383000	5.299791000	0.284098000				
6	6.809013000	3.422650000	-0.343427000				
8	6.240940000	2.416271000	0.130260000				
7	7.587184000	3.345763000	-1.440779000				
1	7.970402000	4.202970000	-1.820952000				
6	7.818481000	2.114251000	-2.190353000				
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6	9.169886000	2.148949000	-2.924905000				
1	9.291604000	1.177442000	-3.419024000				
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6	9.273974000	3.264790000	-3.946712000				
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6	10.054359000	4.402289000	-3.695359000				
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6	10.128571000	5.443249000	-4.626685000				
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1	10.618585000	4.469204000	-2.767496000				
1	8.088458000	4.154029000	-7.022992000				
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1	9.478845000	6.164133000	-6.553779000				
7	1.028620000	3.316259000	-1.196439000				
1	0.483578000	3.180301000	-0.326392000				
				1	-1.317149000	-0.768935000	1.933574000
				1	-2.474879000	-1.668412000	1.254363000

16	-0.104348000	-8.167299000	0.380060000	1	-2.101531000	9.858499000	2.664213000
1	-1.082805000	-8.933124000	-0.154142000	1	-0.492550000	11.714639000	2.352795000
8	-0.232611000	-5.040175000	-2.420414000	1	1.470404000	11.464864000	0.863105000
7	3.553184000	0.960449000	1.477695000	1	1.873930000	9.315839000	-0.367048000
1	4.466962000	1.191978000	1.100380000	6	-4.134454000	5.987738000	4.006403000
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6	3.337700000	-0.167111000	2.206046000	7	-4.655423000	6.859999000	4.893304000
8	2.292040000	-0.351370000	2.837192000	1	-4.086211000	7.644129000	5.184348000
6	4.431289000	-1.235408000	2.168480000	6	-6.030850000	6.792449000	5.390736000
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1	4.281567000	-1.842415000	1.266081000	1	-6.620951000	6.274936000	4.630714000
6	5.881678000	-0.719039000	2.193794000	6	-6.177549000	6.116508000	6.764818000
1	6.117330000	-0.125821000	1.306303000	1	-5.579584000	6.673217000	7.496944000
1	6.550572000	-1.588103000	2.180423000	1	-7.226136000	6.224917000	7.074819000
6	6.194718000	0.050990000	3.475392000	6	-5.772229000	4.634780000	6.817379000
8	6.029479000	-0.449583000	4.589417000	1	-5.803333000	4.298989000	7.861666000
7	6.685045000	1.312139000	3.307544000	1	-4.734347000	4.515910000	6.483764000
1	6.732148000	1.709241000	2.369712000	6	-6.683164000	3.721293000	5.982249000
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7	4.920281000	3.222599000	4.494604000	7	-4.907030000	2.180151000	4.246595000
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1	5.270402000	8.903283000	1.773280000	1	-3.749019000	3.176918000	-1.808497000
6	2.609276000	3.718156000	4.056430000	6	-4.302899000	2.012825000	-0.253012000
8	2.840748000	3.422983000	2.878069000	7	-3.068172000	1.508434000	-0.109000000
7	1.363015000	3.944957000	4.526436000	1	-4.986364000	1.021430000	1.373995000
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6	0.193858000	3.941504000	3.666005000	7	-5.278657000	1.539878000	0.549830000
1	0.537594000	4.106285000	2.638756000	1	-2.910622000	0.996632000	0.762523000
6	-0.501781000	2.553725000	3.682868000	1	-2.285776000	2.073053000	-0.466482000
1	0.282991000	1.818906000	3.449974000	6	-8.663142000	7.295225000	-5.593022000
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6	-1.745298000	7.267039000	1.245367000	1	-6.474428000	5.853277000	-7.821746000
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6	0.091580000	8.407755000	0.454710000	6	4.091265000	5.185555000	-0.633034000
6	-1.247074000	9.735045000	2.002112000	1	3.657435000	4.895108000	0.336304000
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1	6.019144000	5.781032000	-1.418727000	6	-3.103598000	-4.964768000	-2.751524000
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6	6.407886000	3.137619000	-0.209710000	6	3.148498000	-3.863641000	0.902648000
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6	7.841662000	3.528858000	-6.298282000	1	-4.164660000	-4.165895000	-0.988962000
6	9.236335000	4.777747000	-4.773427000	6	-1.151957000	-2.590004000	3.169875000
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6	0.088205000	3.666674000	-3.156227000	8	1.079921000	-3.046807000	-2.226201000
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²TSS_{B,C5-endo}							
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1	-6.741814000	7.667887000	5.960077000	1	5.234105000	0.268263000	-2.156849000
1	-6.939603000	6.029764000	5.337040000	1	5.864262000	0.098125000	-0.512375000
6	-5.985276000	6.149840000	7.300948000	6	7.352692000	-0.198270000	-2.065905000
1	-5.303253000	6.841373000	7.811176000	1	7.157892000	-1.277954000	-2.064079000
1	-6.932323000	6.184310000	7.857301000	1	8.186229000	-0.017206000	-1.377241000
6	-5.395921000	4.731881000	7.374575000	6	7.724214000	0.257522000	-3.463071000
1	-5.126930000	4.519472000	8.417050000	6	7.036724000	-0.236206000	-4.584444000
1	-4.465328000	4.680253000	6.797060000	6	8.744165000	1.198902000	-3.664667000
6	-6.362119000	3.640166000	6.887976000	6	7.365396000	0.200646000	-5.868987000
1	-7.299546000	3.687470000	7.452233000	6	9.073863000	1.637985000	-4.950349000
1	-6.614418000	3.781253000	5.835274000	6	8.385217000	1.138652000	-6.057352000
7	-5.836301000	2.284383000	7.055425000	1	6.235692000	-0.959319000	-4.449421000
1	-5.865377000	1.900663000	7.990462000	1	9.291179000	1.584664000	-2.807129000
6	-5.097002000	1.602836000	6.154602000	1	6.825853000	-0.195303000	-6.725603000
7	-4.831186000	2.100148000	4.945450000	1	9.870591000	2.365167000	-5.084746000
1	-4.976706000	3.082587000	4.714050000	1	8.641318000	1.474826000	-7.058628000
1	-4.251465000	1.536351000	4.303352000	7	0.862898000	2.321190000	-2.271723000
7	-4.644013000	0.382985000	6.472532000	1	0.554118000	1.542267000	-1.662293000
1	-4.967184000	-0.072927000	7.313268000	1	1.642918000	2.013854000	-2.853833000
1	-4.069023000	-0.165805000	5.803857000	1	1.185906000	3.172946000	-1.679776000
6	-8.262103000	3.204518000	-2.067469000	6	-0.347257000	2.721998000	-3.069838000
1	-8.646899000	4.222434000	-1.945692000	1	-0.479621000	3.789119000	-2.874286000
1	-8.953877000	2.521369000	-1.559613000	6	-1.558176000	1.972160000	-2.464241000
1	-8.281631000	2.965403000	-3.137557000	8	-2.708064000	2.304265000	-2.874312000
6	-6.843670000	3.085120000	-1.500841000	8	-1.298847000	1.113878000	-1.585028000
1	-6.841126000	3.361346000	-0.437530000	6	-0.172682000	2.543827000	-4.596757000
1	-6.174375000	3.793237000	-2.005171000	1	-0.844575000	3.272045000	-5.059661000
6	-6.275242000	1.666657000	-1.6666847000	1	0.843608000	2.875530000	-4.854738000
1	-6.913277000	0.929190000	-1.166020000	6	-0.471812000	1.205026000	-5.218186000
1	-6.262057000	1.397006000	-2.728044000	6	-1.510815000	1.013822000	-6.099017000
7	-4.906401000	1.518705000	-1.177577000	1	-2.278878000	1.711398000	-6.403572000
1	-4.134714000	1.753998000	-1.819900000	7	-1.475620000	-0.267957000	-6.606121000
6	-4.561533000	1.158145000	0.062724000	1	-2.125966000	-0.644360000	-7.280385000
7	-3.283665000	0.966362000	0.376971000	6	-0.411081000	-0.940374000	-6.067312000
1	-5.145808000	0.737535000	1.949907000	6	0.248988000	-0.056831000	-5.159021000
1	-6.379325000	1.421470000	0.974417000	6	1.366716000	-0.514342000	-4.467136000
7	-5.500464000	0.926429000	1.017395000	6	1.791111000	-1.925819000	-4.605955000
1	-3.050346000	0.797484000	1.360197000	6	0.082759000	-2.236003000	-6.372304000
1	-2.553116000	0.958121000	-0.349855000	6	1.193051000	-2.688305000	-5.726910000

1	1.928286000	0.096388000	-3.772046000	6	5.215102000	3.177720000	5.547863000
1	1.527838000	-2.502894000	-3.594752000	8	5.262660000	3.375252000	6.763210000
1	-0.404812000	-2.845333000	-7.128455000	7	4.236468000	3.669922000	4.750381000
1	1.599443000	-3.667748000	-5.944574000	1	4.190428000	3.397993000	3.773991000
7	3.317734000	-2.023088000	-4.559936000	6	3.031615000	4.281867000	5.280974000
8	3.902532000	-2.693209000	-5.404936000	1	2.685359000	3.683004000	6.132939000
8	3.880923000	-1.434888000	-3.634947000	6	3.245570000	5.727629000	5.820465000
				1	3.996002000	5.639167000	6.611187000
2	INT5_{B,C5-endo}			1	2.313206000	6.046039000	6.302511000
26	0.966956000	-6.197925000	-0.537000000	6	3.673253000	6.754470000	4.796939000
7	0.469404000	-4.906348000	0.948958000	6	5.033224000	7.006464000	4.564595000
7	2.737444000	-6.519804000	0.394422000	6	2.720692000	7.484681000	4.068741000
7	1.449734000	-7.512883000	-2.001031000	6	5.434217000	7.961418000	3.626957000
7	-0.806758000	-5.881260000	-1.458810000	6	3.118049000	8.436942000	3.127693000
6	-0.727083000	-4.246411000	1.074199000	6	4.476681000	8.679237000	2.905708000
6	-0.750221000	-3.462221000	2.305728000	1	5.781107000	6.460144000	5.134115000
6	0.470074000	-3.653415000	2.885792000	1	1.661004000	7.309474000	4.243497000
6	1.217495000	-4.555827000	2.041184000	1	6.492747000	8.149740000	3.466563000
6	3.199507000	-5.944048000	1.548115000	1	2.368196000	8.992659000	2.571055000
6	4.521724000	-6.442332000	1.859247000	1	4.784887000	9.423286000	2.176289000
6	4.845978000	-7.328990000	0.877239000	6	1.970324000	4.202092000	4.172171000
6	3.723684000	-7.370027000	-0.035917000	8	2.283546000	3.946802000	3.002930000
6	2.618171000	-8.220101000	-2.087620000	7	0.693746000	4.395623000	4.564994000
6	2.615534000	-9.040629000	-3.280331000	1	0.503324000	4.754656000	5.491788000
6	1.430974000	-8.808957000	-3.912419000	6	-0.421054000	4.327778000	3.639328000
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6	-1.248103000	-6.419533000	-2.639188000	6	-1.065515000	2.915536000	3.664123000
6	-2.562536000	-5.906897000	-2.959199000	1	-0.243489000	2.203076000	3.508150000
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6	-1.799951000	-5.052704000	-1.014924000	1	-2.464128000	2.024196000	2.568963000
6	-1.776615000	-4.308488000	0.164380000	6	-1.772815000	2.586503000	4.980094000
6	2.497176000	-5.024357000	2.323101000	1	-1.073358000	2.638718000	5.821653000
6	3.673023000	-8.161519000	-1.179185000	1	-2.176481000	1.568594000	4.950049000
6	-0.548234000	-7.341430000	-3.411798000	1	-2.602909000	3.277063000	5.166217000
1	-2.664682000	-3.724374000	0.385650000	6	-1.374998000	5.509404000	3.911405000
1	2.979672000	-4.654324000	3.222740000	8	-1.061864000	6.421857000	4.681010000
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1	-0.214870000	-7.693746000	-4.323738000	1	-2.705073000	4.616701000	2.667427000
1	0.830678000	-3.239885000	3.820285000	6	-3.451954000	6.579266000	3.115525000
1	5.107025000	-6.143508000	2.720147000	1	-3.051281000	7.371171000	3.752324000
1	5.754097000	-7.908417000	0.764203000	6	-3.576523000	7.093299000	1.646109000
1	3.423805000	-9.696429000	-3.580139000	1	-4.304852000	7.915185000	1.643200000
1	1.064398000	-9.236032000	-4.837868000	1	-4.017057000	6.282072000	1.054127000
1	-3.132895000	-6.175064000	-3.840172000	6	-2.278427000	7.530277000	1.040704000
1	-3.819480000	-4.487872000	-1.828115000	6	-1.441621000	6.753623000	0.265699000
6	-1.911656000	-2.677886000	2.849249000	7	-0.322676000	7.464108000	-0.096141000
6	-2.097093000	-1.266422000	2.259544000	1	-1.561457000	5.726479000	-0.055781000
6	-3.254099000	-0.486357000	2.898378000	1	0.454633000	7.103788000	-0.668544000
8	-3.567704000	0.644686000	2.346704000	6	-1.628096000	8.810472000	1.172984000
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1	-1.791279000	-2.577011000	3.932581000	6	-1.946348000	10.020202000	1.820428000
1	-2.841591000	-3.241559000	2.704108000	6	0.501388000	9.794372000	0.369431000
1	-1.178700000	-0.678228000	2.395336000	6	-1.057481000	11.086949000	1.738062000
1	-2.267179000	-1.306533000	1.176480000	6	0.156816000	10.973564000	1.023819000
16	-0.012820000	-8.005488000	0.747399000	1	-2.873887000	10.122590000	2.379770000
1	-0.729439000	-8.596858000	-0.235758000	1	-1.295456000	12.023941000	2.235471000
8	1.723560000	-4.838306000	-1.535181000	1	0.833271000	11.823603000	0.984892000
7	2.857202000	1.446113000	1.611580000	1	1.437217000	9.681050000	-0.171496000
1	3.788642000	1.596269000	1.238243000	6	-4.844204000	6.148792000	3.586857000
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6	2.566618000	0.363740000	2.383398000	7	-5.492431000	7.021528000	4.384165000
8	1.514180000	0.279134000	3.025356000	1	-4.995929000	7.847691000	4.691002000
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1	3.469405000	-1.344131000	1.450951000	1	-7.395061000	6.295766000	4.021014000
6	5.059747000	-0.345110000	2.512232000	6	-7.062063000	6.223510000	6.180614000
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1	5.673264000	-1.253995000	2.539943000	1	-8.127303000	6.288022000	6.443073000
6	5.342944000	0.408141000	3.810136000	6	-6.592420000	4.764380000	6.297952000
8	5.080862000	-0.072679000	4.914440000	1	-6.668305000	4.456926000	7.348636000
7	5.928652000	1.632037000	3.669152000	1	-5.533115000	4.683667000	6.026421000
1	6.041439000	2.025907000	2.735873000	6	-7.414537000	3.787446000	5.442471000
6	6.331701000	2.398196000	4.832308000	1	-8.477132000	3.865397000	5.696431000
1	6.762491000	1.730539000	5.581255000	1	-7.320274000	4.021703000	4.380588000
1	7.103291000	3.113168000	4.526587000	7	-7.033857000	2.387740000	5.636414000

1	-7.361685000	1.942247000	6.482791000	1	9.728355000	3.382195000	-0.689038000
6	-6.112002000	1.706331000	4.925749000	1	10.184281000	3.020490000	-5.616669000
7	-5.461728000	2.261414000	3.898603000	1	11.330818000	4.838681000	-1.888702000
1	-5.455609000	3.267332000	3.732199000	1	11.567796000	4.665963000	-4.360458000
1	-4.789066000	1.685865000	3.372048000	7	1.298939000	3.949656000	-2.309805000
7	-5.857250000	0.429430000	5.234946000	1	0.985414000	3.343752000	-1.536887000
1	-6.432581000	-0.058790000	5.905375000	1	2.112571000	3.544198000	-2.774562000
1	-5.116772000	-0.095826000	4.730360000	1	1.597190000	4.936688000	-1.875103000
6	-7.629056000	5.377174000	-1.385331000	6	0.129817000	4.112793000	-3.233421000
1	-7.923208000	6.224376000	-0.756830000	1	0.163152000	5.142014000	-3.599704000
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6	-6.264306000	4.827151000	-0.959080000	8	-0.975187000	3.461415000	-1.221694000
1	-6.291419000	4.522659000	0.095694000	6	0.177292000	3.151501000	-4.451034000
1	-5.502053000	5.612860000	-1.033729000	1	-0.444843000	3.607203000	-5.226594000
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1	-6.568942000	2.836854000	-1.805606000	6	-0.314130000	1.746613000	-4.222280000
1	-5.754167000	3.960887000	-2.876599000	6	-1.531819000	1.279251000	-4.653750000
7	-4.513371000	3.103846000	-1.473146000	1	-2.304915000	1.804659000	-5.197709000
1	-3.691082000	3.498780000	-1.954564000	7	-1.696032000	-0.041436000	-4.286780000
6	-4.286390000	2.187708000	-0.527276000	1	-2.509303000	-0.604110000	-4.491030000
7	-3.037268000	1.772603000	-0.280302000	6	-0.589463000	-0.466631000	-3.602244000
1	-5.026387000	1.071920000	0.981518000	6	0.318816000	0.638384000	-3.539147000
1	-6.213014000	2.012821000	0.152641000	6	1.538565000	0.456225000	-2.882229000
7	-5.296666000	1.591677000	0.147281000	6	1.797937000	-0.787032000	-2.306326000
1	-2.912170000	1.237894000	0.580268000	6	-0.302559000	-1.716909000	-3.037621000
1	-2.255009000	2.360588000	-0.598707000	6	0.904570000	-1.877187000	-2.377749000
6	-8.712634000	6.890995000	-6.353892000	1	2.285612000	1.234639000	-2.799811000
1	-8.819700000	5.966236000	-6.932717000	1	2.308954000	-4.357121000	-0.926528000
1	-9.567949000	7.537291000	-6.584656000	1	-1.005799000	-2.541702000	-3.106538000
1	-8.763264000	6.626847000	-5.290971000	1	1.165309000	-2.841906000	-1.947606000
6	-7.383009000	7.594754000	-6.682139000	7	3.046661000	-0.950309000	-1.578256000
6	-6.170603000	6.739137000	-6.377886000	8	3.257351000	-2.018625000	-0.991876000
6	-5.542760000	6.785454000	-5.125766000	8	3.847816000	-0.005915000	-1.561712000
6	-5.658241000	5.840260000	-7.326280000				
6	-4.453227000	5.967225000	-4.819277000				
6	-4.573567000	5.013693000	-7.039490000				
6	-3.963860000	5.066663000	-5.778015000				
8	-2.906617000	4.243840000	-5.538193000				
1	-2.631004000	4.303373000	-4.584671000				
1	-7.324603000	8.531479000	-6.113104000				
1	-7.380047000	7.874381000	-7.743629000				
1	-5.904962000	7.482435000	-4.372219000				
1	-6.117047000	5.785709000	-8.311745000				
1	-3.970465000	6.029947000	-3.847866000				
1	-4.185220000	4.322180000	-7.781985000				
8	1.851447000	6.320430000	-1.469174000				
8	3.287529000	7.883219000	-0.750839000				
6	2.949853000	6.700327000	-0.887318000				
6	3.813362000	5.578980000	-0.284342000				
1	3.350585000	5.311515000	0.677960000				
1	3.741960000	4.681761000	-0.911474000				
6	5.277752000	5.964812000	-0.064165000				
1	5.313062000	6.924287000	0.459189000				
1	5.764919000	6.133558000	-1.034201000				
6	6.066608000	4.932052000	0.764892000				
1	5.649392000	4.867350000	1.773928000				
1	7.109071000	5.263862000	0.865270000				
6	6.070709000	3.514545000	0.203913000				
8	5.719051000	2.535068000	0.888452000				
7	6.476344000	3.378803000	-1.076981000				
1	6.805508000	4.203519000	-1.561187000				
6	6.588242000	2.095656000	-1.763496000				
1	6.257160000	2.235819000	-2.797911000				
1	5.899847000	1.402297000	-1.279211100				
6	8.019036000	1.515461000	-1.741087000				
1	7.975126000	0.520848000	-2.202016000				
1	8.317578000	1.373779000	-0.696065000				
6	9.031554000	2.377847000	-2.464779000				
6	9.177953000	2.290782000	-3.858159000				
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6	10.082804000	3.107891000	-4.538018000				
6	10.726732000	4.127821000	-2.446580000				
6	10.860541000	4.031272000	-3.833348000				
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26	-1.664842000	-4.877436000	-2.083642000
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6	1.234014000	-5.341006000	-1.263939000
6	2.491070000	-5.868094000	-1.750473000
6	2.257586000	-6.341373000	-3.005948000
6	0.858250000	-6.106378000	-3.285654000
6	-1.128621000	-6.276918000	-4.739394000
6	-1.770577000	-6.655239000	-5.977285000
6	-3.078005000	-6.287934000	-5.869916000
6	-3.235727000	-5.684462000	-4.566524000
6	-4.601908000	-4.561295000	-2.843984000
6	-5.857388000	-4.035559000	-2.355528000
6	-5.618648000	-3.552608000	-1.103810000
6	-4.216593000	-3.782377000	-0.829682000
6	-3.583459000	-3.434795000	0.359773000
6	1.056105000	-4.769403000	-0.008579000
6	0.220824000	-6.471926000	-4.464763000
6	-4.431099000	-5.160995000	-4.085653000
1	-4.194376000	-2.956776000	1.118042000
1	1.923295000	-4.712510000	0.642094000
1	0.822599000	-6.949728000	-5.231768000
1	-5.299736000	-5.224984000	-4.733970000
1	0.503077000	-3.533839000	2.501015000
1	3.416409000	-5.870225000	-1.188000000
1	2.951605000	-6.812244000	-3.690916000
1	-1.269253000	-7.135077000	-6.808573000
1	-3.874051000	-6.402734000	-6.594985000
1	-6.788193000	-4.050469000	-2.908828000
6	-6.313749000	-3.092234000	-0.412702000
6	-2.248846000	-2.535579000	3.041817000
6	-2.406543000	-1.032223000	2.750555000
6	-3.148955000	-0.240651000	3.828510000

8	-3.517996000	0.954553000	3.496685000	6	-0.976316000	8.625066000	1.749668000
8	-3.345152000	-0.746561000	4.952374000	6	0.099409000	8.426970000	0.833967000
1	-1.651808000	-2.665508000	3.949906000	6	-1.108608000	9.879418000	2.376914000
1	-3.235470000	-2.962587000	3.259984000	6	1.035573000	9.430385000	0.547074000
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16	-2.204411000	-7.083197000	-1.029692000	1	-1.919898000	10.066297000	3.077434000
1	-2.279330000	-7.845710000	-2.144399000	1	-0.281411000	11.851727000	2.569242000
8	-1.305733000	-3.401795000	-2.739143000	1	1.584653000	11.457635000	0.988254000
7	3.328051000	1.529095000	1.100153000	1	1.855964000	9.231447000	-0.137040000
1	4.249877000	1.687789000	0.703939000	6	-3.783920000	6.379648000	4.920469000
1	2.891019000	2.356188000	1.498959000	8	-4.512997000	5.404877000	4.678991000
6	3.027753000	0.359716000	1.741987000	7	-4.079301000	7.304789000	5.857163000
8	2.028408000	0.244435000	2.453943000	1	-3.419330000	8.054838000	6.015257000
6	3.958467000	-0.826903000	1.495392000	6	-5.302203000	7.290657000	6.658482000
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1	3.715998000	-1.256096000	0.514524000	1	-6.059867000	6.759341000	6.077987000
6	5.466092000	-0.511371000	1.537046000	6	-5.123283000	6.665798000	8.053184000
1	5.761095000	0.146969000	0.715760000	1	-4.356242000	7.233082000	8.595003000
1	6.012154000	-1.452668000	1.400369000	1	-6.062010000	6.810692000	8.605810000
6	5.910545000	0.058764000	2.882800000	6	-4.738685000	5.177815000	8.065303000
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7	6.538046000	1.268998000	2.829451000	1	-3.832750000	5.019760000	7.468354000
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6	7.110514000	1.866050000	4.020585000	1	-6.763098000	4.395664000	8.151394000
1	7.558331000	1.087585000	4.641890000	1	-6.114609000	4.484902000	6.519665000
1	7.903891000	2.557114000	3.715870000	7	-5.509805000	2.834319000	7.631209000
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6	5.950569000	6.583214000	4.094595000	1	-7.481568000	-0.673442000	-3.443445000
6	3.597023000	7.110656000	4.025633000	1	-6.753163000	0.371682000	-4.675208000
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1	7.217896000	7.738416000	2.789933000	1	-4.623345000	0.539358000	-3.218218000
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8	2.895471000	3.740326000	2.936458000	7	-3.693607000	1.828571000	0.793364000
7	1.601128000	4.032541000	4.785775000	1	-5.474444000	0.280940000	1.561194000
1	1.591847000	4.300232000	5.761622000	1	-6.209290000	-0.014013000	0.047674000
6	0.341563000	4.100129000	4.068907000	7	-5.380044000	0.259171000	0.554156000
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8	0.085010000	6.206273000	5.246588000	6	-4.294989000	3.933179000	-5.035496000
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1	5.648432000	6.684365000	0.045913000	6	-3.093951000	-7.025574000	-1.908664000
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1	7.644760000	5.299654000	0.284213000	6	-2.445181000	-4.742768000	0.726508000
6	6.809043000	3.422740000	-0.343454000	6	2.377955000	-4.739728000	0.337572000
8	6.240956000	2.416389000	0.130276000	6	2.078633000	-7.999150000	-3.233751000
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6	9.273640000	3.264785000	-3.946984000	1	0.858416000	-9.741516000	-5.139550000
6	8.565732000	3.192339000	-5.158282000	1	-1.850704000	-9.678717000	-4.980955000
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6	8.639365000	4.228223000	-6.089816000	1	-5.157269000	-5.409692000	0.123488000
6	10.127836000	5.443301000	-4.627274000	6	-1.449753000	-2.705853000	2.870581000
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6	0.000368000	3.394161000	-2.287857000	8	-0.252606000	-5.045519000	-2.424138000
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6	-1.369832000	3.031827000	-1.656672000	1	4.476555000	1.172160000	1.120167000
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6	-0.326703000	0.093726000	-3.146634000	6	5.880253000	-0.737030000	2.227027000
1	-1.398473000	0.146792000	-3.275469000	1	6.120218000	-0.153612000	1.334245000
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8	4.929931000	-1.071634000	-5.074566000	1	3.456377000	3.238821000	5.974564000
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⁴Int4_{B,C5-endo}							
26	-0.192040000	-6.277075000	-1.333144000	6	4.331930000	6.291264000	4.518169000
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1	-0.369563000	2.204218000	5.818035000	6	-7.279283000	7.787402000	-6.057192000
1	-1.566742000	1.197910000	4.994231000	6	-6.185628000	6.751308000	-5.890115000
1	-1.918780000	2.910630000	5.292848000	6	-5.426468000	6.674605000	-4.714441000
6	-0.695821000	5.146481000	4.043200000	6	-5.912805000	5.811852000	-6.896896000
8	-0.294941000	6.010145000	4.829371000	6	-4.438666000	5.702574000	-4.538241000
7	-1.893843000	5.183722000	3.414779000	6	-4.933264000	4.832958000	-6.739775000
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1	-3.684252000	7.730258000	2.041000000	1	-7.343801000	8.085417000	-7.111769000
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6	-1.744429000	7.267122000	1.245144000	1	-6.477343000	5.848002000	-7.826812000
6	-1.029095000	6.472237000	0.372779000	1	-3.850745000	5.672011000	-3.624998000
7	0.068238000	7.147863000	-0.105024000	1	-4.730880000	4.112905000	-7.527735000
1	-1.225231000	5.456106000	0.052829000	8	2.061836000	5.928032000	-1.697390000
1	0.763329000	6.767408000	-0.763960000	8	3.567014000	7.476900000	-1.092238000
6	-1.037667000	8.521662000	1.315679000	6	3.197249000	6.298299000	-1.190954000
6	0.094887000	8.404720000	0.455729000	6	4.077875000	5.168938000	-0.627248000
6	-1.240647000	9.733136000	2.004818000	1	3.628993000	4.869708000	0.332471000
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6	-0.332774000	10.772174000	1.829394000	6	5.540926000	5.561343000	-0.409396000
6	0.786549000	10.628986000	0.978570000	1	5.570790000	6.505960000	0.140173000
1	-2.094797000	9.857737000	2.667096000	1	6.019008000	5.771025000	-1.376429000
1	-0.481645000	11.710607000	2.357788000	6	6.345599000	4.519000000	0.387899000
1	1.480784000	11.458111000	0.867880000	1	5.931462000	4.420795000	1.395889000
1	1.879569000	9.309531000	-0.364589000	1	7.382321000	4.864712000	0.504467000
6	-4.134049000	5.988475000	4.005850000	6	6.396428000	3.111035000	-0.193592000
8	-4.747642000	4.985938000	3.604057000	8	6.280343000	2.103560000	0.533111000
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1	-5.579744000	6.673001000	7.497240000	1	8.021062000	0.691674000	-3.565847000
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6	-5.772283000	4.634754000	6.817187000	6	8.111323000	2.764299000	-4.139658000
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1	-4.734396000	4.515899000	6.483565000	6	8.857816000	3.928203000	-3.903288000
6	-6.683239000	3.721283000	5.982041000	6	7.496786000	3.657089000	-6.319359000
1	-7.723607000	3.826330000	6.308500000	6	8.923690000	4.946357000	-4.859311000
1	-6.649319000	3.994060000	4.925995000	6	8.242691000	4.813436000	-6.070693000
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1	-5.821838000	-0.156429000	6.262519000	1	1.9556666000	2.866534000	-2.564340000
1	-4.578583000	-0.219303000	5.011960000	1	1.692264000	4.488838000	-1.975377000
6	-7.300650000	5.564083000	-0.766101000	6	0.083198000	3.667192000	-3.163967000
1	-7.396791000	6.439610000	-0.115374000	1	0.111111000	4.692487000	-3.543627000
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1	3.267028000	-2.822449000	-2.668806000	1	4.547182000	3.722515000	3.663381000
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6	-6.368742000	9.228000000	-3.092774000	1	2.133883000	0.312360000	-3.908700000
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1	-6.628294000	10.258012000	-2.819659000	1	-0.271634000	-3.022602000	-6.810828000
1	-6.593597000	8.582611000	-2.235560000	1	1.895704000	-3.608902000	-5.771073000
6	-4.885315000	9.116828000	-3.489028000	7	3.544528000	-1.858851000	-4.525753000
6	-4.481795000	7.707771000	-3.871638000	8	4.095967000	-2.882743000	-4.945454000
6	-4.034803000	6.796378000	-2.905251000	8	4.160652000	-0.933585000	-3.969823000
6	-4.578525000	7.253376000	-5.195625000				
6	-3.698579000	5.483164000	-3.236636000				
6	-4.246015000	5.945548000	-5.546966000	26	1.008455000	-6.178920000	-0.545608000
6	-3.802674000	5.046285000	-4.566944000	7	0.493488000	-4.892809000	0.948918000
8	-3.480170000	3.779584000	-4.949489000	7	2.771600000	-6.524378000	0.416142000
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1	-4.686898000	9.798586000	-4.326217000	6	-0.708557000	-4.227624000	1.069409000
1	-3.932642000	7.116585000	-1.870209000	6	-0.743897000	-3.457565000	2.313641000
1	-4.916360000	7.938431000	-5.971196000	6	0.465208000	-3.656462000	2.905494000
1	-3.344107000	4.797452000	-2.472597000	6	1.227855000	-4.551316000	2.060818000
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8	1.349509000	4.616411000	-1.149316000	6	4.528296000	-6.441275000	1.899124000
8	2.703253000	6.391140000	-1.405308000	6	4.864900000	-7.342433000	0.902019000
6	2.503450000	5.204161000	-1.107493000	6	3.766910000	-7.376269000	-0.000440000
6	3.659116000	4.343522000	-0.564951000	6	2.660267000	-8.239641000	-2.072826000
1	3.601800000	4.416641000	0.531319000	6	2.656201000	-9.067025000	-3.265124000
1	3.471596000	3.289600000	-0.803056000	6	1.483271000	-8.828932000	-3.906959000
6	5.047686000	4.772246000	-1.046062000	6	0.759034000	-7.855434000	-3.110897000
1	5.134307000	5.858182000	-0.943863000	6	-1.208984000	-6.388308000	-2.675291000
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1	7.164141000	4.402847000	-0.715888000	6	-1.737844000	-4.277541000	0.150184000
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8	5.946270000	2.003695000	0.893751000	6	3.701616000	-8.178683000	-1.166432000
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6	8.056563000	0.198138000	-3.121104000	1	3.461363000	-9.731203000	-3.554392000

1	1.121315000	-9.257103000	-4.833607000	1	-4.019108000	6.282490000	1.054449000
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6	-0.593656000	-0.473312000	-3.580862000	8	5.201616000	-0.008802000	5.879728000
6	0.315481000	0.631744000	-3.529943000	7	6.161003000	1.610843000	4.601824000
6	1.540043000	0.452883000	-2.881190000	1	6.352088000	1.941948000	3.657326000
6	1.803692000	-0.787888000	-2.302048000	6	6.478482000	2.448108000	5.743092000
6	-0.303501000	-1.721214000	-3.012360000	1	6.827098000	1.824305000	6.568529000
6	0.909341000	-1.877816000	-2.362138000	1	7.290745000	3.126625000	5.460766000
1	2.287576000	1.231744000	-2.807748000	6	5.325831000	3.298286000	6.306630000
1	2.361659000	-4.346689000	-0.922555000	8	5.295861000	3.604788000	7.499820000
1	-1.008117000	-2.546030000	-3.069516000	7	4.412977000	3.724827000	5.402255000
1	1.176342000	-2.839495000	-1.931091000	1	4.432430000	3.363827000	4.454668000
7	3.057172000	-0.948864000	-1.582250000	6	3.193906000	4.415949000	5.780567000
8	3.271775000	-2.015167000	-0.993141000	1	2.766211000	3.914466000	6.658041000
8	3.858697000	-0.004784000	-1.574774000	6	3.418053000	5.903808000	6.189292000
1				1	4.127297000	5.877182000	7.021523000
² TS4 _{B,C5-exo}				1	2.472083000	6.285916000	6.591971000
26	0.439753000	-3.917970000	-2.330901000	6	3.918721000	6.819856000	5.095100000
7	-0.045932000	-3.514358000	-0.407370000	6	5.294343000	7.005044000	4.892316000
7	2.327717000	-4.388870000	-1.756053000	6	3.019675000	7.515211000	4.270836000
7	0.875152000	-4.519504000	-4.212720000	6	5.762018000	7.857737000	3.889565000
7	-1.480638000	-3.591646000	-2.877115000	6	3.483610000	8.366267000	3.264864000
6	-1.254609000	-3.065080000	0.060672000	6	4.856991000	8.540207000	3.071739000

1	6.002317000	6.486775000	5.534309000	6	-5.815713000	4.238480000	-1.962672000
1	1.948809000	7.394781000	4.421692000	1	-6.684419000	3.592485000	-1.784571000
1	6.831623000	7.995630000	3.753256000	1	-5.766153000	4.390345000	-3.045285000
1	2.774509000	8.896480000	2.634474000	7	-4.594951000	3.530450000	-1.584754000
1	5.218133000	9.207291000	2.293669000	1	-3.746363000	3.688012000	-2.157637000
6	2.216434000	4.262577000	4.605514000	6	-4.458946000	2.750238000	-0.507675000
8	2.606503000	3.891978000	3.491789000	7	-3.283281000	2.178073000	-0.235790000
7	0.921088000	4.532796000	4.873110000	1	-5.291304000	1.987270000	1.168712000
1	0.674631000	5.012988000	5.730404000	1	-6.338553000	3.025660000	0.277111000
6	-0.097947000	4.494139000	3.841005000	7	-5.511683000	2.449007000	0.290614000
1	0.405932000	4.606743000	2.874771000	1	-3.192829000	1.761521000	0.693385000
6	-0.808122000	3.113599000	3.808357000	1	-2.431404000	2.514910000	-0.713690000
1	-0.010028000	2.360576000	3.740186000	6	-7.826005000	-1.151923000	-3.886395000
8	-1.579489000	3.095113000	2.603854000	1	-7.512463000	-2.098416000	-4.341834000
1	-2.277122000	2.401407000	2.658151000	1	-8.881226000	-1.244598000	-3.602611000
6	-1.648845000	2.832552000	5.053202000	1	-7.238881000	-1.011476000	-2.971229000
1	-1.027437000	2.880278000	5.953805000	6	-7.616470000	0.023328000	-4.858932000
1	-2.081824000	1.827827000	5.003454000	6	-6.171731000	0.197959000	-5.280987000
1	-2.468702000	3.552773000	5.150725000	6	-5.291204000	0.999804000	-4.542251000
6	-1.021450000	5.716128000	4.018771000	6	-5.657119000	-0.462364000	-6.407169000
8	-0.759467000	6.605972000	4.834341000	6	-3.949051000	1.142176000	-4.899349000
7	-2.079459000	5.738868000	3.177441000	6	-4.318973000	-0.338406000	-6.778088000
1	-2.225887000	4.900125000	2.614817000	6	-3.456105000	0.463530000	-6.020369000
6	-2.921205000	6.904664000	2.983013000	8	-2.155206000	0.555803000	-6.430871000
1	-2.431543000	7.732129000	3.501964000	1	-1.634613000	1.053172000	-5.773780000
6	-3.051053000	7.232523000	1.466700000	1	-7.973865000	0.946557000	-4.384515000
1	-3.734435000	8.087020000	1.369680000	1	-8.242503000	-0.132467000	-5.747010000
1	-3.546051000	6.381392000	0.984345000	1	-5.658277000	1.531454000	-3.666760000
6	-1.740214000	7.523131000	0.798649000	1	-6.316085000	-1.085302000	-7.008818000
6	-0.999316000	6.655382000	0.022194000	1	-3.295996000	1.793081000	-4.321815000
7	0.165735000	7.256587000	-0.394392000	1	-3.929211000	-0.852982000	-7.651630000
1	-1.215466000	5.633334000	-0.263850000	8	2.285377000	6.081334000	-1.914388000
1	0.887218000	6.832493000	-0.993570000	8	3.825743000	7.532201000	-1.174244000
6	-0.977892000	8.745127000	0.871381000	6	3.360206000	6.385914000	-1.256693000
6	0.212190000	8.535335000	0.113878000	6	4.039698000	5.225515000	-0.502326000
6	-1.171391000	9.993634000	1.494302000	1	3.266873000	4.753291000	0.120658000
6	1.201098000	9.519621000	-0.021620000	1	4.346686000	4.457153000	-1.225921000
6	-0.197249000	10.976680000	1.356744000	6	5.211470000	5.671449000	0.378349000
6	0.979495000	10.739930000	0.610431000	1	4.919476000	6.592083000	0.891267000
1	-2.069200000	10.190269000	2.076398000	1	6.067889000	5.960979000	-0.246170000
1	-0.337993000	11.943126000	1.834390000	6	5.615898000	4.658005000	1.460630000
1	1.724723000	11.527030000	0.527862000	1	4.739070000	4.386955000	2.057228000
1	2.107093000	9.312786000	-0.585517000	1	6.316280000	5.140986000	2.157864000
6	-4.318870000	6.659043000	3.567874000	6	6.284725000	3.352779000	1.051448000
8	-4.986912000	5.670089000	3.224856000	8	6.148133000	2.323017000	1.743835000
7	-4.778755000	7.597588000	4.420370000	7	7.083331000	3.378114000	-0.034988000
1	-4.160789000	8.357002000	4.674859000	1	7.166794000	4.250483000	-0.540135000
6	-6.127511000	7.596484000	4.985314000	6	7.950761000	2.276029000	-0.440471000
1	-6.476094000	8.633971000	5.003782000	1	7.825904000	1.492630000	0.307810000
1	-6.765841000	7.047965000	4.288859000	1	8.992122000	2.618294000	-0.395474000
6	-6.210451000	7.009625000	6.405084000	6	7.661399000	1.742698000	-1.853503000
1	-5.537972000	7.578937000	7.058637000	1	8.455938000	1.018715000	-2.083691000
1	-7.228031000	7.188682000	6.779189000	1	7.775058000	2.558318000	-2.578491000
6	-5.871740000	5.515186000	6.526518000	6	6.305505000	1.087997000	-2.033758000
1	-5.814322000	5.252243000	7.590174000	6	5.908521000	0.009390000	-1.227500000
1	-4.879004000	5.318595000	6.104283000	6	5.434176000	1.515988000	-3.043875000
6	-6.908387000	4.600665000	5.854579000	6	4.675317000	-0.614595000	-1.419899000
1	-7.900214000	4.778214000	6.282974000	6	4.203123000	0.884579000	-3.250198000
1	-6.983256000	4.807930000	4.784673000	6	3.815256000	-0.180713000	-2.433794000
7	-6.625444000	3.174133000	6.021591000	1	6.572140000	-0.354480000	-0.446289000
1	-6.863211000	2.763598000	6.914407000	1	5.730253000	2.337353000	-3.692755000
6	-5.845913000	2.430602000	5.208564000	1	4.387888000	-1.450905000	-0.787858000
7	-5.301427000	2.942054000	4.105517000	1	3.566388000	1.211421000	-4.068445000
1	-5.256275000	3.945112000	3.926334000	1	2.863165000	-0.681545000	-2.586222000
1	-4.710918000	2.328607000	3.518848000	7	1.280291000	3.761357000	-2.551238000
7	-5.630258000	1.140372000	5.505988000	1	0.876164000	3.311060000	-1.709827000
1	-6.199645000	0.684883000	6.204734000	1	1.913663000	3.095634000	-3.001824000
1	-5.068561000	0.5444100000	4.870019000	1	1.816745000	4.664053000	-2.245019000
6	-7.266921000	6.311813000	-1.695038000	6	0.093931000	4.098605000	-3.408971000
1	-7.368200000	7.275633000	-1.185149000	1	0.079413000	5.187240000	-3.510502000
1	-8.159157000	5.716281000	-1.465996000	6	-1.190826000	3.696519000	-2.630646000
1	-7.261726000	6.503676000	-2.774733000	8	-2.283723000	3.926680000	-3.198694000
6	-5.988628000	5.591889000	-1.254711000	8	-0.999656000	3.188673000	-1.485351000
1	-5.998768000	5.440636000	-0.166789000	6	0.173291000	3.484927000	-4.816025000
1	-5.110907000	6.212818000	-1.472627000	1	-0.774585000	3.740400000	-5.305000000

1	0.957286000	4.004706000	-5.380066000	1	3.640704000	-1.422800000	4.195068000
6	0.445562000	2.002667000	-4.870606000	1	3.905545000	-1.522643000	2.453650000
6	0.137852000	1.020555000	-3.945954000	6	5.436704000	-0.420165000	3.510834000
1	-0.357178000	1.102833000	-2.988046000	1	5.825059000	0.092078000	2.626386000
7	0.609933000	-0.203730000	-4.372776000	1	6.043834000	-1.324466000	3.641157000
1	0.595683000	-1.067840000	-3.799230000	6	5.636551000	0.418037000	4.772422000
6	1.243578000	-0.047640000	-5.570343000	8	5.286611000	0.014427000	5.883049000
6	1.171697000	1.332092000	-5.932677000	7	6.250511000	1.623061000	4.595243000
6	1.743643000	1.769501000	-7.121857000	1	6.440252000	1.948740000	3.648786000
6	2.533651000	0.834015000	-7.927043000	6	6.582993000	2.459733000	5.732774000
6	1.860028000	-1.020002000	-6.406665000	1	6.938748000	1.835468000	6.554875000
6	2.451461000	-0.603068000	-7.561172000	1	7.394102000	3.135652000	5.441101000
1	1.671799000	2.803090000	-7.444994000	6	5.438844000	3.313814000	6.308270000
1	2.495996000	1.008520000	-9.004749000	8	5.419959000	3.617716000	7.502320000
1	1.831445000	-2.073105000	-6.142298000	7	4.521050000	3.746147000	5.411879000
1	2.924009000	-1.315143000	-8.229449000	1	4.532154000	3.386873000	4.463453000
7	4.199703000	1.224562000	-7.740729000	6	3.306732000	4.441225000	5.798459000
8	4.953017000	0.744254000	-8.578760000	1	2.881598000	3.940345000	6.677515000
8	4.541201000	1.906044000	-6.785039000	6	3.538619000	5.927866000	6.206576000
				1	4.252451000	5.898400000	7.034817000
² Int4_{B,C5,exo}				1	2.596383000	6.313435000	6.614698000
26	0.549841000	-3.866473000	-2.321732000	6	4.036815000	6.841940000	5.109571000
7	0.065451000	-3.479752000	-0.394096000	6	5.412034000	7.022067000	4.899678000
7	2.437262000	-4.346050000	-1.751791000	6	3.136085000	7.539639000	4.289139000
7	0.982431000	-4.454103000	-4.208605000	6	5.877670000	7.872114000	3.893736000
7	-1.369877000	-3.530441000	-2.864135000	6	3.597961000	8.388052000	3.279986000
6	-1.141027000	-3.028897000	0.077982000	6	4.970954000	8.556939000	3.079758000
6	-1.050812000	-2.732917000	1.503472000	1	6.121381000	6.501821000	5.538552000
6	0.233642000	-3.021618000	1.859368000	1	2.065546000	7.422916000	4.445115000
6	0.921366000	-3.480539000	0.675559000	1	6.947054000	8.006062000	3.751868000
6	2.957247000	-4.251642000	-0.490102000	1	2.887573000	8.920062000	2.652557000
6	4.352250000	-4.637133000	-0.497504000	1	5.330517000	9.221874000	2.299128000
6	4.661344000	-4.962673000	-1.783178000	6	2.323640000	4.291752000	4.627265000
6	3.455849000	-4.778010000	-2.560401000	8	2.708310000	3.917855000	3.512709000
6	2.200571000	-4.867499000	-4.682864000	7	1.030203000	4.567943000	4.897579000
6	2.117397000	-5.122230000	-6.102211000	1	0.786704000	5.051131000	5.754030000
6	0.833955000	-4.852978000	-6.475621000	6	0.010020000	4.528538000	3.866538000
6	0.132719000	-4.432829000	-5.284937000	1	0.513453000	4.637899000	2.899744000
6	-1.895074000	-3.634261000	-4.126205000	6	-0.701919000	3.148903000	3.837495000
6	-3.290746000	-3.256065000	-4.113660000	1	0.094740000	2.394415000	3.770109000
6	-3.596075000	-2.928926000	-2.827794000	8	-1.474129000	3.129289000	2.633597000
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6	-2.289769000	-2.870776000	-0.686150000	6	-1.542009000	2.871460000	5.083600000
6	2.260190000	-3.850996000	0.645061000	1	-0.919806000	2.920371000	5.983619000
6	3.356254000	-5.022429000	-3.923913000	1	-1.976072000	1.867089000	5.036228000
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1	-3.189616000	-2.5333472000	-0.182616000	6	-0.911773000	5.751961000	4.041003000
1	2.806699000	-3.821450000	1.582747000	8	-0.649919000	6.643147000	4.855149000
1	4.249418000	-5.363612000	-4.438235000	7	-1.968071000	5.773986000	3.197525000
1	-1.753151000	-4.087202000	-6.192825000	1	-2.116000000	4.933144000	2.638361000
1	0.694858000	-2.903092000	2.832500000	6	-2.811398000	6.938167000	3.001541000
1	4.991012000	-4.653100000	0.376765000	1	-2.323457000	7.766927000	3.520060000
1	5.608039000	-5.300013000	-2.186430000	6	-2.941697000	7.264467000	1.485046000
1	2.941994000	-5.463031000	-6.715758000	1	-3.625934000	8.118236000	1.387367000
1	0.387378000	-4.925262000	-7.459393000	1	-3.435925000	6.412411000	1.003522000
1	-3.932264000	-3.239362000	-4.985447000	6	-1.631377000	7.555435000	0.816222000
1	-4.543012000	-2.594538000	-2.422679000	6	-0.892625000	6.688874000	0.036513000
6	-2.134456000	-2.124563000	2.349101000	7	0.272330000	7.290002000	-0.380484000
6	-2.266186000	-0.615898000	2.077965000	1	-1.110115000	5.6667646000	-0.251421000
6	-3.340382000	0.116242000	2.880932000	1	0.991726000	6.867317000	-0.982893000
8	-3.569445000	1.336784000	2.501925000	6	-0.867816000	8.7776616000	0.890603000
8	-3.909798000	-0.437597000	3.840110000	6	0.320837000	8.567477000	0.130709000
1	-1.908717000	-2.282801000	3.408427000	6	-1.058971000	10.023807000	1.516881000
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1	-1.308323000	-0.120110000	2.289165000	6	-0.083940000	11.006110000	1.380235000
1	-2.458023000	-0.438324000	1.013386000	6	1.091433000	10.769910000	0.631585000
16	-0.074052000	-6.257545000	-1.946868000	1	-1.955654000	10.220036000	2.100838000
1	-0.771713000	-6.113189000	-0.797531000	1	-0.222904000	11.971548000	1.860429000
8	0.966639000	-2.290448000	-2.616388000	1	1.837420000	11.556375000	0.549866000
7	3.344434000	1.326157000	2.367831000	1	2.215658000	9.344466000	-0.569519000
1	4.315878000	1.489617000	2.119517000	6	-4.208599000	6.689902000	3.586310000
1	2.771708000	2.161746000	2.429624000	8	-4.874074000	5.698753000	3.244686000
6	2.954344000	0.270886000	3.128304000	7	-4.670806000	7.628629000	4.437192000
8	1.819844000	0.187776000	3.610232000	1	-4.054683000	8.389849000	4.690732000
6	3.971871000	-0.854996000	3.322503000	6	-6.018661000	7.623729000	5.003927000

1	-6.369453000	8.660412000	5.024347000	1	7.908505000	1.498273000	0.299052000
1	-6.657008000	7.074781000	4.307807000	1	9.104632000	2.635828000	-0.332440000
6	-6.097625000	7.034901000	6.422976000	6	7.819645000	1.808606000	-1.859336000
1	-5.423667000	7.603670000	7.075477000	1	8.631054000	1.104671000	-2.091544000
1	-7.114275000	7.213191000	6.800023000	1	7.937490000	2.648908000	-2.554905000
6	-5.758535000	5.540380000	6.542300000	6	6.480408000	1.137115000	-2.091552000
1	-5.700448000	5.276352000	7.605657000	6	6.117898000	-0.013091000	-1.373011000
1	-4.766068000	5.344251000	6.119272000	6	5.590224000	1.623302000	-3.057924000
6	-6.795680000	4.626547000	5.870163000	6	4.899892000	-0.652087000	-1.607483000
1	-7.787513000	4.804996000	6.298160000	6	4.374068000	0.978212000	-3.306688000
1	-6.869925000	4.833659000	4.800190000	6	4.020806000	-0.159696000	-2.577428000
7	-6.514169000	3.199779000	6.037685000	1	6.798530000	-0.420596000	-0.628561000
1	-6.753411000	2.789672000	6.930305000	1	5.859663000	2.504324000	-3.636449000
6	-5.733087000	2.455878000	5.226456000	1	4.639713000	-1.543845000	-1.043114000
7	-5.186929000	2.966875000	4.123885000	1	3.719548000	1.352388000	-4.090202000
1	-5.141472000	3.969872000	3.944565000	1	3.078517000	-0.668295000	-2.761078000
1	-4.593805000	2.353100000	3.540253000	7	1.375069000	3.802130000	-2.545232000
7	-5.518188000	1.165841000	5.524702000	1	0.976866000	3.352405000	-1.700788000
1	-6.086565000	0.711397000	6.224928000	1	2.006342000	3.136631000	-2.998793000
1	-4.953479000	0.568847000	4.891933000	1	1.912823000	4.705933000	-2.242694000
6	-7.154095000	6.337089000	-1.677146000	6	0.183127000	4.133970000	-3.397325000
1	-7.252550000	7.304454000	-1.173432000	1	0.162163000	5.222663000	-3.497350000
1	-8.049375000	5.746773000	-1.446446000	6	-1.095909000	3.723806000	-2.613965000
1	-7.145722000	6.522279000	-2.757988000	8	-2.192303000	3.945425000	-3.178702000
6	-5.879857000	5.614578000	-1.229817000	8	-0.897484000	3.219658000	-1.468245000
1	-5.892155000	5.469933000	-0.141001000	6	0.260252000	3.522688000	-4.805237000
1	-4.999111000	6.230247000	-1.450512000	1	-0.687926000	3.779895000	-5.292896000
6	-5.711814000	4.256275000	-1.929184000	1	1.043761000	4.043184000	-5.369768000
1	-6.580433000	3.612536000	-1.742940000	6	0.530086000	2.040285000	-4.863596000
1	-5.666938000	4.400875000	-3.013046000	6	0.256261000	1.061413000	-3.924646000
7	-4.489886000	3.550222000	-1.552012000	1	-0.205467000	1.146758000	-2.950492000
1	-3.643377000	3.707759000	-2.128154000	7	0.710202000	-0.164388000	-4.365298000
6	-4.350325000	2.769210000	-0.476204000	1	0.709510000	-1.027194000	-3.789920000
7	-3.173130000	2.197676000	-0.208729000	6	1.295238000	-0.012709000	-5.588458000
1	-5.176949000	2.003604000	1.201833000	6	1.211135000	1.365109000	-5.952522000
1	-6.227523000	3.042712000	0.314939000	6	1.725705000	1.799264000	-7.168310000
7	-5.400234000	2.466570000	0.325148000	6	2.462130000	0.853407000	-8.026905000
1	-3.078810000	1.781197000	0.720090000	6	1.869260000	-0.990747000	-6.449553000
1	-2.323692000	2.536817000	-0.689093000	6	2.400962000	-0.586020000	-7.634935000
6	-7.826005000	-1.151923000	-3.886395000	1	1.640291000	2.831919000	-7.490613000
1	-7.520193000	-2.086401000	-4.370937000	1	2.295898000	1.000327000	-9.098274000
1	-8.884863000	-1.240687000	-3.615253000	1	1.852932000	-2.042126000	-6.177461000
1	-7.245555000	-1.050207000	-2.961834000	1	2.835730000	-1.303840000	-8.322305000
6	-7.593056000	0.052874000	-4.816678000	7	4.083094000	1.238677000	-8.007646000
6	-6.143220000	0.224022000	-5.223202000	8	4.761175000	0.737463000	-8.898058000
6	-5.267454000	1.022926000	-4.475836000	8	4.507238000	1.956671000	-7.112977000
6	-5.620309000	-0.434548000	-6.346851000				
6	-3.922201000	1.165020000	-4.822366000				
6	-4.279292000	-0.311300000	-6.706891000				
6	-3.421445000	0.488501000	-5.940928000				
8	-2.117585000	0.580202000	-6.341686000				
1	-1.602135000	1.083442000	-5.685093000				
1	-7.942068000	0.964288000	-4.314226000				
1	-8.214520000	-0.064717000	-5.713938000				
1	-5.641139000	1.552988000	-3.602234000				
1	-6.275306000	-1.054861000	-6.955528000				
1	-3.272433000	1.815372000	-4.240416000				
1	-3.883318000	-0.824052000	-7.578714000				
8	2.387191000	6.119174000	-1.911842000				
8	3.934475000	7.558464000	-1.163569000				
6	3.462205000	6.415303000	-1.250524000				
6	4.133219000	5.248292000	-0.498602000				
1	3.355915000	4.776157000	0.118814000				
1	4.440441000	4.482310000	-1.224667000				
6	5.303460000	5.685019000	0.388477000				
1	5.013572000	6.603968000	0.905547000				
1	6.162428000	5.974455000	-0.232527000				
6	5.701322000	4.664455000	1.466825000				
1	4.822061000	4.392432000	2.059201000				
1	6.400776000	5.142969000	2.168086000				
6	6.368839000	3.360298000	1.051768000				
8	6.214399000	2.321494000	1.726680000				
7	7.188579000	3.397957000	-0.018654000				
1	7.289692000	4.279469000	-0.504478000				
6	8.063587000	2.301305000	-0.422579000				

²TS5_{B,C5-e/o}

26	1.114277000	-4.982658000	-1.225948000
7	0.388933000	-4.309008000	0.553737000
7	2.933226000	-5.275840000	-0.386695000
7	1.778078000	-5.843805000	-2.938311000
7	-0.756837000	-4.881701000	-1.981857000
6	-0.899324000	-3.941078000	0.857269000
6	-0.979190000	-3.430279000	2.224532000
6	0.285812000	-3.542492000	2.726662000
6	1.123168000	-4.097875000	1.690207000
6	3.304892000	-4.942563000	0.886614000
6	4.705407000	-5.245643000	1.089661000
6	5.168436000	-5.761515000	-0.082473000
6	4.051186000	-5.774650000	-1.002081000
6	3.053663000	-6.255850000	-3.210696000
6	3.142726000	-6.719380000	-4.578712000
6	1.903754000	-6.568473000	-5.124443000
6	1.057455000	-6.016341000	-4.088405000
6	-1.129263000	-5.208602000	-3.261394000
6	-2.546808000	-4.986389000	-3.435241000
6	-3.023169000	-4.538328000	-2.239738000
6	-1.894676000	-4.474083000	-1.338808000
6	-1.973759000	-4.045090000	-0.015865000
6	2.471646000	-4.393359000	1.855800000
6	4.117028000	-6.234349000	-2.312585000
6	-0.292187000	-5.718661000	-4.247893000

1	-2.953836000	-3.750875000	0.346097000	6	-1.215004000	5.526421000	3.821264000
1	2.909199000	-4.185632000	2.827449000	8	-0.873125000	6.549509000	4.419755000
1	5.076202000	-6.601832000	-2.665105000	7	-2.362287000	5.404112000	3.114370000
1	-0.735100000	-5.922403000	-5.218328000	1	-2.592961000	4.480446000	2.752681000
1	0.635269000	-3.257676000	3.712192000	6	-3.276151000	6.505906000	2.883780000
1	5.243962000	-5.077514000	2.014033000	1	-2.855378000	7.371733000	3.399771000
1	6.166871000	-6.106488000	-0.321320000	6	-3.421645000	6.818247000	1.360977000
1	4.043046000	-7.104075000	-5.041782000	1	-4.135276000	7.648168000	1.264319000
1	1.574255000	-6.804428000	-6.128819000	1	-3.890899000	5.946275000	0.889707000
1	-3.089993000	-5.165940000	-4.354855000	6	-2.130541000	7.141298000	0.666355000
1	-4.038777000	-4.271341000	-1.974440000	6	-1.408778000	6.286810000	-0.140304000
6	-2.179225000	-2.818183000	2.902792000	7	-0.269702000	6.901146000	-0.604679000
6	-2.233028000	-1.286181000	2.720714000	1	-1.624588000	5.271865000	-0.438412000
6	-3.382632000	-0.559148000	3.426642000	1	0.428612000	6.472936000	-1.223308000
8	-3.601825000	0.654280000	3.024532000	6	-1.384817000	8.376019000	0.704726000
8	-4.020379000	-1.109362000	4.344934000	6	-0.222326000	8.182935000	-0.101474000
1	-2.145930000	-3.040583000	3.974626000	6	-1.575637000	9.626164000	1.324566000
1	-3.109503000	-3.260720000	2.527542000	6	0.738657000	9.185974000	-0.286638000
1	-1.298630000	-0.842931000	3.094765000	6	-0.629506000	10.628309000	1.136069000
1	-2.276110000	-1.022423000	1.659471000	6	0.518360000	10.408568000	0.342207000
16	0.516794000	-7.287241000	-0.437379000	1	-2.451738000	9.809955000	1.942859000
1	1.553234000	-7.953842000	-0.994408000	1	-0.770305000	11.596298000	1.610623000
8	1.621003000	-3.503101000	-1.870978000	1	1.242898000	11.209760000	0.220212000
7	2.910111000	1.173420000	2.642152000	1	1.625453000	8.990188000	-0.883490000
1	3.818756000	1.203344000	2.193161000	6	-4.652682000	6.143488000	3.457829000
1	2.355426000	2.020486000	2.585990000	8	-5.163783000	5.036764000	3.224472000
6	2.546274000	0.219762000	3.527871000	7	-5.271769000	7.106295000	4.171638000
8	1.452855000	0.235220000	4.109312000	1	-4.773411000	7.969785000	4.342490000
6	3.544349000	-0.912073000	3.770302000	6	-6.636776000	6.994410000	4.685426000
1	3.301837000	-1.333315000	4.748919000	1	-7.106067000	7.977561000	4.579275000
1	3.354372000	-1.686677000	3.018327000	1	-7.172215000	6.303481000	4.030034000
6	5.033538000	-0.523381000	3.727272000	6	-6.718008000	6.551349000	6.156702000
1	5.331666000	-0.169882000	2.736396000	1	-6.128896000	7.249679000	6.763921000
1	5.624796000	-1.425116000	3.929039000	1	-7.761718000	6.666405000	6.481045000
6	5.397391000	0.487163000	4.812108000	6	-6.244621000	5.117554000	6.447208000
8	5.158801000	0.275313000	6.003126000	1	-6.190514000	4.976855000	7.534009000
7	6.021563000	1.623089000	4.388006000	1	-5.228682000	4.970267000	6.062435000
1	6.088928000	1.811876000	3.388431000	6	-7.177483000	4.044313000	5.863949000
6	6.444264000	2.628273000	5.344677000	1	-8.192870000	4.180068000	6.250587000
1	6.908456000	2.145908000	6.207109000	1	-7.239492000	4.123946000	4.776165000
1	7.192319000	3.268913000	4.865613000	7	-6.778107000	2.675576000	6.193802000
6	5.329363000	3.529269000	5.906548000	1	-7.018675000	2.335361000	7.114928000
8	5.394466000	3.976864000	7.052645000	6	-5.947746000	1.904491000	5.462127000
7	4.332517000	3.831207000	5.040835000	7	-5.418424000	2.336232000	4.318643000
1	4.294974000	3.374117000	4.136661000	1	-5.410935000	3.320996000	4.056030000
6	3.133684000	4.550876000	5.431394000	1	-4.775231000	1.698290000	3.815675000
1	2.760406000	4.125516000	6.371690000	7	-5.658589000	0.662739000	5.887006000
6	3.368215000	6.069367000	5.698803000	1	-6.227805000	0.240743000	6.606876000
1	4.093417000	6.117558000	6.515718000	1	-5.081621000	0.027820000	5.304281000
1	2.427731000	6.487183000	6.078263000	6	-7.597284000	3.810453000	-2.254316000
6	3.851677000	6.875556000	4.515406000	1	-8.271264000	4.607399000	-1.922492000
6	5.224003000	7.054563000	4.288444000	1	-8.063459000	2.850856000	-1.999116000
6	2.940636000	7.468266000	3.627319000	1	-7.523993000	3.868222000	-3.346816000
6	5.677476000	7.802509000	3.199429000	6	-6.219369000	3.952932000	-1.602119000
6	3.389975000	8.214407000	2.535762000	1	-6.317512000	3.947397000	-0.508439000
6	4.760689000	8.383776000	2.319212000	1	-5.774116000	4.919069000	-1.869443000
1	5.939650000	6.614098000	4.978460000	6	-5.259746000	2.836506000	-2.041532000
1	1.872178000	7.347155000	3.795280000	1	-5.675762000	1.850235000	-1.798272000
1	6.744847000	7.936639000	3.042992000	1	-5.139630000	2.863659000	-3.129015000
1	2.671168000	8.6655228000	1.856988000	7	-3.919059000	2.953552000	-1.473696000
1	5.109719000	8.967806000	1.471886000	1	-3.211187000	3.421474000	-2.054841000
6	2.091236000	4.302789000	4.333430000	6	-3.537526000	2.476417000	-0.278268000
8	2.426795000	3.943689000	3.198060000	7	-2.249916000	2.540553000	0.073092000
7	0.803380000	4.475839000	4.699198000	1	-4.095879000	1.382131000	1.381815000
1	0.596266000	4.911560000	5.588578000	1	-5.402268000	1.889820000	0.346282000
6	-0.299668000	4.283440000	3.777260000	7	-4.420019000	1.918239000	0.568848000
1	0.132843000	4.239406000	2.772332000	1	-1.980083000	2.470298000	1.054505000
6	-0.979169000	2.912237000	4.037066000	1	-1.572226000	2.936086000	-0.594009000
1	-0.178675000	2.161082000	4.009030000	6	-8.963627000	6.190631000	-6.275068000
8	-1.883241000	2.683140000	2.947561000	1	-9.117767000	5.205323000	-6.730450000
1	-2.417464000	1.860719000	3.110010000	1	-9.852955000	6.800144000	-6.475612000
6	-1.701573000	2.828323000	5.381407000	1	-8.886982000	6.048268000	-5.190663000
1	-1.004799000	3.001693000	6.208513000	6	-7.695436000	6.862725000	-6.832503000
1	-2.131286000	1.830082000	5.516159000	6	-6.435320000	6.060916000	-6.578240000
1	-2.514198000	3.560636000	5.442368000	6	-5.681877000	6.239596000	-5.409760000

				⁴ TS4 _{B,C5-exo}			
6	-5.996190000	5.086769000	-7.488170000				
6	-4.539648000	5.480256000	-5.147280000				
6	-4.860069000	4.317476000	-7.244375000				
6	-4.121297000	4.505588000	-6.067053000				
8	-3.018218000	3.734566000	-5.870762000				
1	-2.607755000	3.928039000	-4.983161000				
1	-7.593621000	7.859454000	-6.383968000				
1	-7.820034000	7.018938000	-7.911881000				
1	-5.986785000	6.995691000	-4.688516000				
1	-6.553162000	4.928367000	-8.409835000				
1	-3.962411000	5.643914000	-4.241555000				
1	-4.527913000	3.568747000	-7.958174000				
8	1.917350000	5.709222000	-2.196353000				
8	3.351142000	7.201553000	-1.330747000				
6	2.948802000	6.038337000	-1.483629000				
6	3.636460000	4.885874000	-0.723210000				
1	2.956730000	4.618590000	0.100094000				
1	3.685950000	3.996702000	-1.363737000				
6	5.013652000	5.237982000	-0.151579000				
1	4.953798000	6.244117000	0.272317000				
1	5.754532000	5.310775000	-0.961123000				
6	5.496195000	4.291234000	0.959587000				
1	4.769168000	4.287971000	1.778560000				
1	6.435386000	4.672945000	1.385289000				
6	5.747255000	2.828335000	0.615405000				
8	5.642230000	1.938198000	1.484434000				
7	6.119638000	2.534118000	-0.645397000				
1	6.249599000	3.295593000	-1.296520000				
6	6.444140000	1.180223000	-1.089013000				
1	6.250876000	1.134239000	-2.164814000				
1	5.751891000	0.495705000	-0.595054000				
6	7.901041000	0.766758000	-0.790677000				
1	8.004223000	-0.288221000	-1.074315000				
1	8.059844000	0.826160000	0.291526000				
6	8.930841000	1.602169000	-1.520801000				
6	9.263306000	1.321102000	-2.855232000				
6	9.554051000	2.692338000	-0.896498000				
6	10.188496000	2.105651000	-3.546131000				
6	10.481019000	3.480824000	-1.583603000				
6	10.800943000	3.190321000	-2.911682000				
1	8.796208000	0.474842000	-3.354962000				
1	9.316285000	2.920789000	0.139864000				
1	10.435083000	1.867325000	-4.577618000				
1	10.955011000	4.319042000	-1.079337000				
1	11.523972000	3.800180000	-3.446729000				
7	1.544663000	3.374290000	-3.294520000				
1	1.455964000	2.649055000	-2.574799000				
1	2.326494000	3.141116000	-3.911426000				
1	1.754713000	4.333436000	-2.768343000				
6	0.254720000	3.472057000	-4.052347000				
1	0.356937000	4.330620000	-4.721295000				
6	-0.846827000	3.7444986000	-3.000975000				
8	-1.998926000	4.071481000	-3.411912000				
8	-0.503975000	3.577492000	-1.806670000				
6	-0.036465000	2.186055000	-4.892873000				
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6	0.979305000	10.743434000	0.614431000	1	4.923208000	6.593863000	0.893948000
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1	2.108120000	9.316996000	-0.581227000	1	6.319467000	5.141209000	2.159585000
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7	0.610989000	-0.199757000	-4.373362000	1	6.044581000	-1.324989000	3.638844000
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1	1.833643000	-2.068065000	-6.143336000	7	4.520933000	3.745768000	5.412050000
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26	0.553348000	-3.866901000	-2.320804000	6	4.037167000	6.313905000	6.614107000
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6	3.359997000	-5.025875000	-3.920316000	1	-1.979096000	1.869794000	5.037410000
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1	0.595414000	4.949340000	5.575898000	1	-5.398249000	1.883340000	0.351355000
6	-0.300060000	4.297707000	3.773038000	7	-4.415346000	1.912822000	0.570853000
1	0.131663000	4.257480000	2.767579000	1	-1.973521000	2.465776000	1.042891000
6	-0.974600000	2.923450000	4.029815000	1	-1.572834000	2.928209000	-0.606593000
1	-0.172131000	2.174444000	4.001153000	6	-8.963627000	6.190631000	-6.275068000

1	-9.130595000	5.190499000	-6.691930000	1	1.392901000	-2.067665000	-1.723585000
1	-9.853232000	6.797656000	-6.482090000	1	-2.127758000	-1.158590000	-0.539911000
1	-8.868858000	6.086936000	-5.187731000	1	0.148475000	-1.512870000	0.403632000
6	-7.701529000	6.833876000	-6.877948000	7	2.470507000	-0.658240000	-0.651797000
6	-6.445355000	6.029925000	-6.613578000	8	2.573184000	-1.169166000	0.466099000
6	-5.681939000	6.233543000	-5.455733000	8	3.401409000	-0.074027000	-1.225590000
6	-6.024562000	5.025027000	-7.498157000				
6	-4.548212000	5.467300000	-5.178270000				
6	-4.896837000	4.248443000	-7.239132000				
6	-4.149340000	4.460315000	-6.071532000				
8	-3.056963000	3.679241000	-5.857317000				
1	-2.641956000	3.891296000	-4.975765000				
1	-7.585279000	7.845343000	-6.467557000				
1	-7.842772000	6.951373000	-7.960151000				
1	-5.973152000	7.013647000	-4.754688000				
1	-6.590146000	4.846995000	-8.410953000				
1	-3.963416000	5.648443000	-4.280801000				
1	-4.578891000	3.474773000	-7.932500000				
8	1.899945000	5.721309000	-2.219909000				
8	3.339876000	7.203646000	-1.347250000				
6	2.932402000	6.042786000	-1.505660000				
6	3.614846000	4.883218000	-0.750751000				
1	2.926315000	4.604929000	0.061490000				
1	3.673106000	4.001571000	-1.401002000				
6	4.984994000	5.231566000	-0.160178000				
1	4.920805000	6.236424000	0.266004000				
1	5.736437000	5.306323000	-0.959753000				
6	5.452300000	4.281424000	0.954597000				
1	4.713066000	4.274082000	1.762573000				
1	6.384129000	4.663650000	1.395800000				
6	5.712726000	2.820223000	0.609949000				
8	5.600403000	1.928024000	1.476293000				
7	6.102786000	2.530622000	-0.646148000				
1	6.238404000	3.294899000	-1.292809000				
6	6.444140000	1.180223000	-1.089013000				
1	6.274239000	1.139542000	-2.168924000				
1	5.744915000	0.488193000	-0.617248000				
6	7.897792000	0.775941000	-0.762536000				
1	8.015887000	-0.275531000	-1.053250000				
1	8.032520000	0.826746000	0.323416000				
6	8.936585000	1.626010000	-1.462291000				
6	9.312994000	1.349715000	-2.785990000				
6	9.523936000	2.726258000	-0.820958000				
6	10.245700000	2.148583000	-3.449966000				
6	10.458091000	3.529162000	-1.481053000				
6	10.821780000	3.243211000	-2.798855000				
1	8.874301000	0.495985000	-3.298585000				
1	9.251973000	2.951423000	0.207695000				
1	10.526402000	1.913685000	-4.473508000				
1	10.903460000	4.375101000	-0.963744000				
1	11.550566000	3.864216000	-3.312874000				
7	1.521119000	3.391286000	-3.332109000				
1	1.448478000	2.655707000	-2.620700000				
1	2.297237000	3.171392000	-3.961008000				
1	1.730658000	4.345510000	-2.799770000				
6	0.221917000	3.485172000	-4.074631000				
1	0.313425000	4.343639000	-4.745410000				
6	-0.868941000	3.753286000	-3.012196000				
8	-2.028114000	4.067955000	-3.414073000				
8	-0.514291000	3.593897000	-1.820582000				
6	-0.076716000	2.197624000	-4.908540000				
1	-0.724415000	2.501196000	-5.736283000				
1	0.862621000	1.852292000	-5.361250000				
6	-0.767582000	1.123421000	-4.113728000				
6	-2.131924000	0.944087000	-4.094747000				
1	-2.884198000	1.393731000	-4.727204000				
7	-2.483670000	0.110680000	-3.054839000				
1	-3.427822000	-0.149399000	-2.811751000				
6	-1.356053000	-0.250455000	-2.360806000				
6	-0.232362000	0.313100000	-3.035368000				
6	1.053539000	0.037260000	-2.569246000				
6	1.199986000	-0.853865000	-1.409089000				
6	-1.239244000	-0.877490000	-1.095342000				
6	0.003552000	-1.064402000	-0.568647000				
1	1.947816000	0.364976000	-3.083769000				

Model B system – C4

²TS4_{B,C4-endo}

26	2.601809000	-4.490955000	-0.150338000	1	2.661798000	3.933482000	6.145006000
7	1.315748000	-4.122207000	1.372215000	6	3.203178000	5.946942000	5.642137000
7	4.032847000	-5.034071000	1.172847000	1	3.971070000	5.939305000	6.421154000
7	3.824987000	-5.033903000	-1.673803000	1	2.276475000	6.298511000	6.111996000
7	1.117006000	-4.110160000	-1.474972000	6	3.595710000	6.878038000	4.517992000
6	0.030800000	-3.652341000	1.280150000	6	4.946352000	7.107100000	4.217903000
6	-0.523626000	-3.420932000	2.610861000	6	2.617555000	7.539395000	3.758610000
6	0.462427000	-3.772668000	3.484055000	6	5.312899000	7.971214000	3.183034000
6	1.602028000	-4.201545000	2.707554000	6	2.980501000	8.400449000	2.720934000
6	3.937419000	-4.990894000	2.537087000	6	4.330113000	8.619293000	2.430442000
6	5.192775000	-5.391401000	3.136388000	1	5.714724000	6.614023000	4.808303000
6	6.043564000	-5.671705000	2.111589000	6	1.564880000	7.379021000	3.983030000
6	5.307788000	-5.444379000	0.886019000	8	6.364994000	8.142629000	2.969848000
6	5.128059000	-5.443322000	-1.575955000	7	0.650330000	4.437587000	4.544028000
6	5.679126000	-5.667669000	-2.894217000	1	0.455414000	4.817418000	5.461319000
6	4.688823000	-5.386559000	-3.785855000	6	-0.469069000	4.279069000	3.635529000
6	3.534017000	-4.986822000	-3.011819000	1	-0.071496000	4.361360000	2.618459000
6	1.197917000	-4.197894000	-2.839302000	6	-1.073677000	2.854923000	3.762450000
6	-0.055256000	-3.791031000	-3.436551000	1	-0.233195000	2.156434000	3.650892000
6	-0.887000000	-3.452195000	-2.406686000	8	-1.968147000	2.700617000	2.656554000
6	-0.141869000	-3.660039000	-1.185610000	1	-2.454275000	1.849033000	2.748097000
6	-0.655412000	-3.442910000	0.091177000	6	-1.764289000	2.602829000	5.103988000
6	2.810287000	-4.613251000	3.258297000	1	-1.063890000	2.741401000	5.934952000
6	5.827756000	-5.635026000	-0.388667000	1	-2.133279000	1.572901000	5.154078000
6	2.314001000	-4.608377000	-3.562428000	1	-2.616435000	3.277293000	5.242848000
1	-1.679601000	-3.090314000	0.152918000	6	-1.452169000	5.451807000	3.831444000
1	2.884054000	-4.627185000	4.341463000	8	-1.154467000	6.431790000	4.519375000
1	6.858568000	-5.967868000	-0.463743000	7	-2.615386000	5.318437000	3.151898000
1	2.226011000	-4.632173000	-4.644664000	1	-2.774211000	4.425475000	2.683950000
1	0.433060000	-3.737114000	4.566627000	6	-3.574763000	6.392654000	2.994028000
1	5.377130000	-5.442894000	4.202171000	1	-3.192343000	7.241557000	3.565293000
1	7.073467000	-6.003107000	2.158889000	6	-3.727023000	6.791617000	1.492214000
1	6.691198000	-5.999278000	-3.090471000	1	-4.493786000	7.755566000	1.432708000
1	4.717867000	-5.437906000	-4.867220000	1	-4.128543000	5.919618000	0.962002000
1	-0.262260000	-3.792144000	-4.499985000	6	-2.451713000	7.249789000	0.851015000
1	-1.913872000	-3.111025000	-2.452740000	6	-1.575253000	6.470346000	0.123168000
6	-1.875818000	-2.853220000	2.939228000	7	-0.495570000	7.215131000	-0.289487000
6	-1.981729000	-1.344006000	2.645247000	1	-1.641931000	5.419624000	-0.131297000
6	-3.224270000	-0.672336000	3.234965000	1	0.296134000	6.875016000	-0.854633000
8	-3.576656000	0.452288000	2.692675000	6	-1.871314000	8.569671000	0.893805000
8	-3.809858000	-1.188951000	4.206524000	6	-0.643961000	8.503455000	0.169529000
1	-2.083124000	-3.011100000	4.001663000	6	-2.255739000	9.801692000	1.457872000
1	-2.664706000	-3.382628000	2.388104000	6	0.197224000	9.613609000	0.010725000
1	-1.105168000	-0.826951000	3.061519000	6	-1.428067000	10.907973000	1.297185000
1	-1.952912000	-1.151595000	1.567569000	6	-0.211106000	10.813846000	0.584851000
16	1.771335000	-6.878845000	-0.075548000	1	-3.186707000	9.891028000	2.013664000
1	2.945685000	-7.500421000	-0.329090000	1	-1.717260000	11.862360000	1.730105000
8	3.133499000	-2.933717000	-0.182462000	1	0.416161000	11.695660000	0.482768000
7	2.826373000	1.388930000	1.804174000	1	1.134962000	9.519258000	-0.530926000
1	3.760649000	1.528730000	1.432522000	6	-4.943165000	5.949526000	3.524133000
1	2.294380000	2.241762000	1.951874000	8	-5.423449000	4.849459000	3.204941000
6	2.543998000	0.353756000	2.641737000	7	-5.600000000	6.846807000	4.287124000
8	1.494383000	0.306154000	3.293130000	1	-5.126600000	7.708608000	4.524503000
6	3.563479000	-0.780949000	2.699527000	6	-6.973511000	6.672487000	4.758356000
1	3.301010000	-1.390191000	3.566692000	1	-7.461964000	7.650690000	4.707897000
1	3.436586000	-1.408269000	1.806726000	1	-7.477972000	6.016620000	4.044961000
6	5.038397000	-0.343119000	2.795379000	6	-7.079953000	6.126475000	6.192301000
1	5.364421000	0.180583000	1.892597000	1	-6.544106000	6.805490000	6.867050000
1	5.651518000	-1.249531000	2.871621000	1	-8.138116000	6.171726000	6.485510000
6	5.328554000	0.485603000	4.044784000	6	-6.549585000	4.699110000	6.399901000
8	5.076507000	0.070002000	5.177563000	1	-6.567768000	4.470492000	7.472998000
7	5.907086000	1.702826000	3.828873000	1	-5.500890000	4.635461000	6.086094000
1	6.008046000	2.046476000	2.875330000	6	-7.371666000	3.632969000	5.659076000
6	6.297670000	2.545322000	4.942399000	1	-8.422752000	3.690673000	5.961495000
1	6.720213000	1.928189000	5.737717000	1	-7.341154000	3.793304000	4.579566000
1	7.072585000	3.239214000	4.598665000	7	-6.927878000	2.265349000	5.929519000
6	5.173852000	3.369524000	5.594061000	1	-7.203771000	1.865278000	6.816143000
8	5.209075000	3.646297000	6.794367000	6	-6.009065000	1.573662000	5.224173000
7	4.201376000	3.806790000	4.757949000	7	-5.425504000	2.085258000	4.139254000
1	4.168769000	3.481635000	3.797523000	1	-5.470118000	3.076756000	3.905733000
6	2.995380000	4.455682000	5.239815000	1	-4.747771000	1.500236000	3.626833000

7	-5.689484000	0.331612000	5.613696000	1	0.572493000	3.403831000	-1.280960000
1	-6.262528000	-0.140877000	6.297861000	1	1.663289000	3.120196000	-2.503450000
1	-5.012429000	-0.236391000	5.067988000	1	1.395353000	4.772310000	-1.968116000
6	-7.730410000	4.747220000	-1.396171000	6	-0.217783000	3.846372000	-3.097891000
1	-7.939404000	5.667513000	-0.840495000	1	-0.444750000	4.906806000	-3.248471000
1	-8.546576000	4.042443000	-1.195049000	6	-1.426470000	3.217760000	-2.355039000
1	-7.752346000	4.989980000	-2.465363000	8	-2.496238000	3.053311000	-3.008857000
6	-6.374071000	4.161487000	-0.991525000	8	-1.249717000	2.937201000	-1.142208000
1	-6.350959000	3.973449000	0.089909000	6	0.087954000	3.200974000	-4.464891000
1	-5.576203000	4.885750000	-1.197859000	1	-0.828320000	3.262749000	-5.059815000
6	-6.056308000	2.862960000	-1.749625000	1	0.829349000	3.810282000	-4.989940000
1	-6.841209000	2.113126000	-1.589453000	6	0.581263000	1.780338000	-4.364554000
1	-6.037482000	3.058758000	-2.825884000	6	-0.150476000	0.678349000	-3.925355000
7	-4.753209000	2.293292000	-1.411865000	1	-1.183881000	0.619673000	-3.615112000
1	-3.944666000	2.570455000	-1.988829000	7	0.644335000	-0.432162000	-3.929307000
6	-4.481891000	1.565365000	-0.324632000	1	0.354181000	-1.357490000	-3.625448000
7	-3.214841000	1.211756000	-0.059131000	6	1.908022000	-0.092777000	-4.363208000
1	-5.161043000	0.714418000	1.382243000	6	1.892026000	1.295336000	-4.645774000
1	-6.407279000	1.410204000	0.391484000	6	3.085611000	1.921321000	-5.203700000
7	-5.452904000	1.102221000	0.488188000	6	4.288528000	1.105400000	-5.183179000
1	-3.060944000	0.824765000	0.874185000	6	3.058286000	-0.886352000	-4.475010000
1	-2.462913000	1.793454000	-0.455170000	6	4.248881000	-0.242662000	-4.878198000
6	-8.369037000	7.578511000	-5.559941000	1	3.213819000	2.988849000	-5.034893000
1	-8.759418000	6.777941000	-6.199106000	1	5.225142000	1.568547000	-5.477741000
1	-9.033674000	8.445355000	-5.657157000	1	3.045486000	-1.943159000	-4.228785000
1	-8.416350000	7.229182000	-4.521704000	1	5.163969000	-0.826137000	-4.927755000
6	-6.925193000	7.941765000	-5.952721000	7	2.679631000	2.171548000	-7.001021000
6	-5.964100000	6.776292000	-5.835734000	8	3.035839000	1.328494000	-7.805990000
6	-5.278641000	6.515128000	-4.641455000	8	2.015718000	3.169572000	-7.251991000
6	-5.750028000	5.897859000	-6.909231000				
6	-4.417758000	5.423386000	-4.511470000				
6	-4.895821000	4.802315000	-6.799435000				
6	-4.222618000	4.551912000	-5.594660000				
8	-3.401295000	3.469373000	-5.533352000				
1	-3.035512000	3.367963000	-4.619046000				
1	-6.579944000	8.767653000	-5.317438000				
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1	-5.410289000	7.184130000	-3.792988000				
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1	-3.886526000	5.247293000	-3.580301000				
1	-4.735709000	4.131332000	-7.638720000				
8	1.732768000	6.210817000	-1.713154000				
8	3.213627000	7.769738000	-1.077588000				
6	2.840197000	6.591279000	-1.152964000				
6	3.676170000	5.478192000	-0.492642000				
1	3.249220000	5.320989000	0.509909000				
1	3.529239000	4.536505000	-1.034608000				
6	5.167881000	5.798931000	-0.368441000				
1	5.274116000	6.806588000	0.043037000				
1	5.623876000	5.835375000	-1.367760000				
6	5.935906000	4.824496000	0.545316000				
1	5.556290000	4.896584000	1.568723000				
1	6.996228000	5.112056000	0.575818000				
6	5.869248000	3.348950000	0.166068000				
8	5.612046000	2.469588000	1.010257000				
7	6.117347000	3.044481000	-1.126090000				
1	6.361857000	3.799801000	-1.752697000				
6	6.174786000	1.682808000	-1.647983000				
1	5.653688000	1.659267000	-2.610659000				
1	5.627003000	1.047858000	-0.949807000				
6	7.617016000	1.153976000	-1.810948000				
1	7.546723000	0.103318000	-2.118112000				
1	8.104515000	1.172104000	-0.829308000				
6	8.434865000	1.934157000	-2.818683000				
6	8.398715000	1.601024000	-4.181782000				
6	9.219144000	3.027928000	-2.422508000				
6	9.118577000	2.340765000	-5.122088000				
6	9.940276000	3.772148000	-3.360207000				
6	9.891112000	3.431723000	-4.713789000				
1	7.807426000	0.747506000	-4.506657000				
1	9.271394000	3.293329000	-1.369160000				
1	9.080654000	2.061995000	-6.171936000				
1	10.543836000	4.614138000	-3.031308000				
1	10.454025000	4.007170000	-5.443700000				
7	0.956530000	3.779567000	-2.166703000				
				2	Int4B,C4-endo		
				26	2.508328000	-4.872221000	0.028943000
				7	1.200346000	-4.353985000	1.485804000
				7	3.855424000	-5.443662000	1.424648000
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				6	0.306194000	-3.837452000	3.545919000
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				6	3.724962000	-5.316412000	2.780517000
				6	4.926680000	-5.779649000	3.441216000
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				6	5.581115000	-6.380746000	-2.549638000
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				6	3.511040000	-5.519618000	-2.776850000
				6	1.239061000	-4.548740000	-2.725411000
				6	0.045942000	-4.065841000	-3.384549000
				6	-0.812717000	-3.670486000	-2.398543000
				6	-0.139575000	-3.911480000	-1.141212000
				6	-0.687816000	-3.627298000	0.106983000
				6	2.607467000	-4.820981000	3.443590000
				6	5.638327000	-6.272045000	-0.042959000
				6	2.354390000	-5.049430000	-3.389709000
				1	-1.691174000	-3.214652000	0.119264000
				1	2.649598000	-4.777208000	4.527611000
				1	6.639904000	-6.690772000	-0.066831000
				1	2.317675000	-5.078516000	-4.474613000
				1	0.245843000	-3.740803000	4.623488000
				1	5.076412000	-5.784267000	4.513648000
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				1	6.568189000	-6.802139000	-2.694128000
				1	4.729265000	-6.113867000	-4.567760000
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16	1.538381000	-7.233576000	0.195498000	1	-2.746498000	9.949906000	2.429552000
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8	3.138324000	-3.355145000	-0.056870000	1	0.917756000	11.640903000	0.914732000
7	2.931259000	1.253292000	1.734757000	1	1.442563000	9.521063000	-0.320030000
1	3.874159000	1.383812000	1.382707000	6	-4.769466000	6.070340000	3.625636000
1	2.408010000	2.110141000	1.888660000	8	-5.308248000	5.026165000	3.221719000
6	2.609387000	0.203507000	2.539917000	7	-5.380957000	6.940135000	4.455385000
8	1.542405000	0.161117000	3.162070000	1	-4.864484000	7.757123000	4.753962000
6	3.606444000	-0.951414000	2.600182000	6	-6.776645000	6.823990000	4.882215000
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1	3.460282000	-1.587501000	1.716464000	1	-7.306995000	6.272516000	4.102176000
6	5.090691000	-0.545014000	2.685489000	6	-6.970227000	6.165372000	6.259183000
1	5.422145000	-0.027105000	1.781045000	1	-6.429989000	6.754154000	7.010826000
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8	5.160803000	-0.148686000	5.069086000	1	-6.620318000	4.372934000	7.403123000
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6	6.411517000	2.307555000	4.843161000	1	-8.403552000	3.839463000	5.698059000
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8	2.356453000	3.823974000	2.994427000	7	-3.293470000	1.455330000	-0.182766000
7	0.771296000	4.303339000	4.553482000	1	-5.226318000	0.967647000	1.284560000
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6	8.544555000	4.017745000	-5.488958000	1	-0.481350000	-3.966116000	-4.906395000
6	9.269766000	5.392111000	-3.641228000	6	0.496998000	-5.681852000	0.091811000
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6	0.516123000	1.708625000	-4.292860000	1	5.025597000	-3.043675000	1.413705000
6	-0.269209000	0.670215000	-3.791326000	6	6.018438000	-1.705717000	2.796511000
1	-1.309798000	0.670319000	-3.500659000	1	6.159454000	-0.883231000	2.089811000
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²Int4_{B,C4-endo-rot}							
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1	-8.433756000	-1.385247000	5.969672000	1	8.299657000	3.046571000	-0.436059000
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1	-6.292007000	-2.622978000	6.432723000	6	7.035953000	3.983755000	-3.463149000
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1	-7.087863000	2.390879000	-0.095880000		6	3.060735000	0.363762000	-4.037590000
7	-6.401875000	1.728445000	0.235969000		6	4.212359000	-0.239094000	-4.751205000
1	-4.085964000	1.046238000	1.094055000		6	2.913454000	-0.618038000	-6.769746000
1	-3.430473000	0.662799000	-0.506994000		6	4.107532000	-0.731007000	-6.029595000
6	-5.326513000	8.846825000	-4.899657000		1	2.709355000	-0.387564000	-3.179832000
1	-5.854819000	8.510705000	-5.799685000		1	5.135144000	-0.333695000	-4.190344000
1	-5.474041000	9.929274000	-4.803223000		1	2.834541000	-1.015703000	-7.776258000
1	-5.797069000	8.361928000	-4.036294000		1	4.965660000	-1.220527000	-6.479506000
6	-3.829190000	8.497174000	-4.976763000		7	3.611265000	1.541817000	-3.220890000
6	-3.572010000	7.009971000	-5.109997000		8	3.288704000	2.686844000	-3.519321000
6	-3.445385000	6.193068000	-3.978159000		8	4.398159000	1.259822000	-2.314804000
6	-3.482551000	6.393591000	-6.367475000					
6	-3.236262000	4.816758000	-4.086617000					
6	-3.274684000	5.021050000	-6.496647000					
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8	-2.941655000	2.883752000	-5.522691000					
1	-2.842560000	2.431411000	-4.643362000					
1	-3.326937000	8.875972000	-4.077436000					
1	-3.382826000	9.025099000	-5.829499000					
1	-3.499557000	6.638538000	-2.987158000					
1	-3.570294000	7.000758000	-7.266649000					
1	-3.129859000	4.203807000	-3.196161000					
1	-3.198959000	4.556249000	-7.475792000					
8	0.983269000	3.550002000	-0.517578000					
8	1.965008000	5.479785000	-1.117127000					
6	1.979283000	4.363171000	-0.563083000					
6	3.232843000	3.917769000	0.209253000					
1	3.015457000	4.097732000	1.272738000					
1	3.350549000	2.833521000	0.099981000					
6	4.509147000	4.660936000	-0.189214000					
1	4.275947000	5.726613000	-0.270522000					
1	4.817968000	4.350337000	-1.197152000					
6	5.657259000	4.495723000	0.820440000					
1	5.369104000	4.923454000	1.786076000					
1	6.538187000	5.056576000	0.4766675000					
6	6.117825000	3.071981000	1.101632000					
8	6.403560000	2.695322000	2.258715000					
7	6.236308000	2.250600000	0.041362000					
1	5.900260000	2.563958000	-0.860505000					
6	6.713879000	0.875936000	0.128407000					
1	6.118424000	0.270035000	-0.557658000					
1	6.526475000	0.521370000	1.143526000					
6	8.214623000	0.735028000	-0.201454000					
1	8.486811000	-0.315136000	-0.035523000					
1	8.787883000	1.334674000	0.514860000					
6	8.561214000	1.141240000	-1.618674000					
6	8.2766676000	0.286336000	-2.695706000					
6	9.143693000	2.385998000	-1.893714000					
6	8.565788000	0.664936000	-4.007840000					
6	9.435326000	2.769436000	-3.205970000					
6	9.146543000	1.910017000	-4.267797000					

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6	-3.302597000	-0.219387000	3.210903000	1	-0.226272000	4.935628000	-0.568801000
8	-3.792469000	0.928548000	2.860098000	6	-2.513769000	7.200199000	-0.006994000
8	-3.704126000	-0.891977000	4.181097000	6	-1.272726000	6.832037000	-0.611234000
1	-1.196500000	-1.923760000	3.868170000	6	-2.929047000	8.544739000	-0.077554000
1	-2.130005000	-2.836621000	2.694118000	6	-0.447409000	7.765107000	-1.253962000
1	-1.402311000	0.122481000	2.326944000	6	-2.117378000	9.470772000	-0.725186000
1	-2.489609000	-0.792618000	1.322947000	6	-0.885519000	9.085233000	-1.302118000
16	1.886390000	-5.280499000	-1.100196000	1	-3.869899000	8.858704000	0.369726000
1	3.048181000	-5.657381000	-1.681290000	1	-2.428276000	10.511151000	-0.781247000
8	1.892249000	-1.115987000	-2.060088000	1	-0.269682000	9.835048000	-1.792308000
7	3.675634000	1.565953000	3.364676000	1	0.502051000	7.447853000	-1.673400000
1	4.608447000	1.824033000	3.059607000	6	-5.059379000	5.948131000	3.918506000
1	2.929278000	2.208025000	3.118663000	8	-5.913405000	5.062028000	3.750701000
6	3.450986000	0.743505000	4.421496000	7	-5.096610000	6.828182000	4.941133000
8	2.319399000	0.551213000	4.876820000	1	-4.299715000	7.443232000	5.056936000
6	4.661569000	0.010882000	5.004653000	6	-6.148652000	6.857799000	5.954677000
1	4.399704000	-0.236345000	6.036321000	1	-6.384503000	7.908028000	6.155852000
1	4.772749000	-0.939570000	4.466537000	1	-7.033651000	6.404058000	5.503295000
6	6.002686000	0.765621000	4.975152000	6	-5.775530000	6.164499000	7.276303000
1	6.329376000	0.975417000	3.953336000	1	-4.904097000	6.673757000	7.706849000
1	6.764906000	0.118012000	5.425240000	1	-6.604721000	6.327282000	7.978770000
6	5.965343000	2.039027000	5.816639000	6	-5.466288000	4.663138000	7.179091000
8	5.671516000	2.017174000	7.014057000	1	-5.111183000	4.313721000	8.156610000
7	6.291557000	3.194578000	5.171672000	1	-4.642789000	4.498351000	6.473661000
1	6.474725000	3.181206000	4.168417000	6	-6.674438000	3.808138000	6.764693000
6	6.386158000	4.438577000	5.910667000	1	-7.504041000	3.959791000	7.462327000
1	6.918615000	4.275922000	6.850687000	1	-7.036267000	4.094692000	5.774621000
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8	4.976118000	5.820468000	7.292030000	6	-5.758037000	1.702056000	5.772670000
7	4.031408000	4.926832000	5.421858000	7	-5.527354000	2.263385000	4.585865000
1	4.128655000	4.298306000	4.632233000	1	-5.720748000	3.245884000	4.396601000
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1	3.353837000	7.437715000	6.178278000	1	-4.824178000	-0.077908000	5.270115000
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6	2.222913000	8.159338000	1.827807000	1	-7.051550000	3.669651000	-2.028526000
6	3.545579000	8.411752000	1.454112000	1	-6.087948000	3.783343000	-3.490521000
1	5.083142000	7.654635000	4.395934000	6	-6.347255000	1.758782000	-2.788850000
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1	5.604028000	8.431608000	2.102665000	1	-6.109561000	1.308213000	-3.757263000
1	1.418004000	8.303447000	1.112230000	7	-5.130391000	1.664437000	-1.975441000
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6	1.752414000	4.750055000	4.679605000	6	-5.118006000	1.522587000	-0.642761000
8	2.177896000	4.104045000	3.717435000	7	-3.992615000	1.211922000	-0.008025000
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1	0.123716000	5.566204000	5.625825000	1	-6.996537000	2.259610000	-0.281781000
6	-0.573876000	4.489872000	3.972756000	7	-6.267806000	1.654373000	0.068042000
1	-0.140251000	4.605213000	2.970505000	1	-3.953097000	1.160271000	1.018758000
6	-0.973479000	2.990976000	4.077746000	1	-3.188518000	0.857608000	-0.550475000
1	-0.033229000	2.424408000	4.076280000	6	-5.599791000	8.694421000	-4.698607000
8	-1.690479000	2.701927000	2.869188000	1	-6.028348000	8.338850000	-5.643142000
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6	-1.756640000	2.639715000	5.339491000	1	-6.038007000	8.099094000	-3.888985000
1	-1.174980000	2.904213000	6.228946000	6	-4.066180000	8.565556000	-4.707156000
1	-1.957451000	1.563583000	5.378531000	6	-3.595645000	7.138430000	-4.897944000
1	-2.714836000	3.168572000	5.375011000	6	-3.489197000	6.261559000	-3.809159000
6	-1.741499000	5.492636000	4.077083000	6	-3.285612000	6.633825000	-6.169371000
8	-1.652695000	6.527924000	4.748468000	6	-3.089775000	4.934686000	-3.973338000
7	-2.820543000	5.162100000	3.337433000	6	-2.882580000	5.311632000	-6.353709000
1	-2.744475000	4.279205000	2.832305000	6	-2.779781000	4.448568000	-5.253701000
6	-3.861614000	6.111275000	2.966396000	8	-2.367665000	3.170489000	-5.473245000
1	-3.439144000	7.113570000	3.084174000	1	-2.351770000	2.664387000	-4.618314000
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6	-3.068135000	6.001207000	0.572564000	1	-3.353674000	7.290515000	-7.034875000
6	-2.166862000	4.995004000	0.287846000	1	-3.000246000	4.276130000	-3.114238000
7	-1.098847000	5.478439000	-0.428019000	1	-2.635508000	4.934371000	-7.342237000
1	-2.192927000	3.950459000	0.569573000	8	1.145357000	3.783578000	-0.281961000

8	2.172305000	5.623339000	-1.072272000	6	6.050311000	-5.661022000	2.103249000
6	2.159070000	4.564573000	-0.411555000	6	5.311873000	-5.436280000	0.878937000
6	3.409315000	4.159921000	0.387168000	6	5.127559000	-5.436254000	-1.582348000
1	3.237980000	4.484404000	1.423832000	6	5.676526000	-5.659009000	-2.901654000
1	3.465877000	3.066064000	0.412676000	6	4.684234000	-5.378995000	-3.791401000
6	4.711501000	4.761750000	-0.139898000	6	3.530130000	-4.981392000	-3.015321000
1	4.579251000	5.841500000	-0.258250000	6	1.193843000	-4.194670000	-2.838664000
1	4.913624000	4.370290000	-1.144240000	6	-0.060406000	-3.787977000	-3.433658000
6	5.912970000	4.520990000	0.792355000	6	-0.890672000	-3.449866000	-2.402394000
1	5.746385000	5.016119000	1.754143000	6	-0.143719000	-3.657881000	-1.182560000
1	6.817663000	4.964999000	0.353468000	6	-0.655178000	-3.441034000	0.095004000
6	6.226084000	3.064590000	1.108629000	6	2.818207000	-4.605614000	3.255827000
8	6.413997000	2.676403000	2.282124000	6	5.829703000	-5.627107000	-0.396489000
7	6.317403000	2.217428000	0.064804000	6	2.308888000	-4.604212000	-3.563781000
1	6.083539000	2.547945000	-0.866446000	1	-1.679509000	-3.089244000	0.158524000
6	6.680129000	0.810765000	0.207132000	1	2.894435000	-4.618361000	4.338822000
1	6.108405000	0.240062000	-0.529577000	1	6.860830000	-5.958489000	-0.473382000
1	6.370495000	0.479759000	1.199961000	1	2.219119000	-4.627721000	-4.645862000
6	8.190371000	0.552095000	0.020876000	1	0.443337000	-3.729388000	4.568257000
1	8.363777000	-0.514323000	0.212917000	1	5.387766000	-5.430844000	4.194906000
1	8.736094000	1.112248000	0.788669000	1	7.080775000	-5.990890000	2.148802000
6	8.701687000	0.921081000	-1.356123000	1	6.688745000	-5.989004000	-3.099822000
6	8.453986000	0.086720000	-2.457838000	1	4.711437000	-5.429739000	-4.872833000
6	9.405159000	2.114270000	-1.571150000	1	-0.269052000	-3.788812000	-4.496766000
6	8.897699000	0.434184000	-3.735371000	1	-1.917717000	-3.109020000	-2.446690000
6	9.850307000	2.467339000	-2.848174000	6	-1.870113000	-2.849831000	2.944602000
6	9.597486000	1.628355000	-3.935245000	6	-1.979019000	-1.341482000	2.647496000
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7	0.647487000	1.243028000	-1.293049000	1	-1.103075000	-0.821927000	3.061925000
1	-0.014763000	0.796413000	-0.644098000	1	-1.951397000	-1.151297000	1.569389000
1	1.221133000	0.441755000	-1.686592000	16	1.771335000	-6.878845000	-0.075548000
1	1.208227000	1.958796000	-0.788092000	1	2.948944000	-7.497378000	-0.321204000
6	-0.203107000	1.978800000	-2.280392000	8	3.131906000	-2.926212000	-0.186158000
1	-0.443917000	2.918098000	-1.772788000	7	2.827275000	1.391660000	1.802326000
6	-1.567371000	1.257503000	-2.384590000	1	3.761575000	1.531464000	1.430732000
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8	-1.800506000	0.402070000	-1.491346000	6	2.544943000	0.356205000	2.639590000
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1	-0.171468000	2.976571000	-4.140353000	6	3.564170000	-0.778673000	2.696650000
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6	1.120965000	1.323924000	-4.450479000	1	3.437361000	-1.405299000	1.803342000
6	0.320294000	0.602930000	-5.317090000	6	5.039172000	-0.341214000	2.793193000
1	-0.757269000	0.618322000	-5.400663000	1	5.365562000	0.182963000	1.890822000
7	1.076468000	-0.163194000	-6.155723000	1	5.652017000	-1.247853000	2.869025000
1	0.718905000	-0.780561000	-6.869657000	6	5.329287000	0.486686000	4.043117000
6	2.405586000	0.041518000	-5.876186000	8	5.077188000	0.070450000	5.175660000
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6	3.811653000	1.257770000	-4.348788000	1	6.008898000	2.048225000	2.874635000
6	4.925784000	0.753004000	-5.025709000	6	6.298032000	2.546015000	4.942017000
6	3.508922000	-0.483688000	-6.544557000	1	6.720566000	1.928552000	5.737085000
6	4.778598000	-0.104226000	-6.118671000	1	7.072857000	3.240272000	4.598812000
1	2.662387000	-0.974598000	-2.632668000	6	5.173899000	3.369604000	5.593885000
1	5.911126000	1.009834000	-4.658727000	8	5.208892000	3.645896000	6.794315000
1	3.375358000	-1.171666000	-7.373122000	7	4.201374000	3.806891000	4.757855000
1	5.660196000	-0.493425000	-6.616784000	1	4.169134000	3.482466000	3.797175000
7	4.099546000	2.006845000	-3.141409000	6	2.995380000	4.455682000	5.239815000
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26	2.603507000	-4.484071000	-0.152458000	6	3.596052000	6.878093000	4.518606000
7	1.319247000	-4.117737000	1.372524000	6	4.946740000	7.106924000	4.218539000
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7	3.823548000	-5.028835000	-1.677741000	6	5.313459000	7.971054000	3.183741000
7	1.114943000	-4.107447000	-1.474137000	6	2.981149000	8.400825000	2.721710000
6	0.033694000	-3.648832000	1.282606000	6	4.330803000	8.619401000	2.431208000
6	-0.517897000	-3.416287000	2.614230000	1	5.715018000	6.613640000	4.808887000
6	0.470364000	-3.766108000	3.485669000	1	1.565326000	7.379525000	3.983688000
6	1.608589000	-4.195194000	2.707297000	1	6.365589000	8.142266000	2.970563000
6	3.943999000	-4.982849000	2.532486000	1	2.211593000	8.902684000	2.141327000
6	5.201185000	-5.380812000	3.129448000	1	4.611670000	9.288748000	1.623175000

6	1.930638000	4.278012000	4.147913000	6	-4.481467000	1.565592000	-0.324257000
8	2.246906000	3.986535000	2.988104000	7	-3.214382000	1.212081000	-0.058774000
7	0.650412000	4.437790000	4.544037000	1	-5.160609000	0.714189000	1.382375000
1	0.455499000	4.816434000	5.461811000	1	-6.406808000	1.410256000	0.391862000
6	-0.469016000	4.279624000	3.635540000	7	-5.452486000	1.102021000	0.488338000
1	-0.071381000	4.362030000	2.618507000	1	-3.060473000	0.824977000	0.874487000
6	-1.073731000	2.855514000	3.762259000	1	-2.462540000	1.794062000	-0.454566000
1	-0.233277000	2.157023000	3.650502000	6	-8.369037000	7.578511000	-5.559941000
8	-1.968310000	2.701422000	2.656421000	1	-8.759228000	6.777760000	-6.198995000
1	-2.454527000	1.849886000	2.747956000	1	-9.033878000	8.445185000	-5.657279000
6	-1.764246000	2.603274000	5.103828000	1	-8.416271000	7.229317000	-4.521656000
1	-1.063782000	2.741709000	5.934760000	6	-6.925278000	7.942043000	-5.952767000
1	-2.133277000	1.573359000	5.153856000	6	-5.963942000	6.776794000	-5.835585000
1	-2.616348000	3.277764000	5.242837000	6	-5.278652000	6.515812000	-4.641168000
6	-1.451996000	5.452444000	3.831567000	6	-5.749497000	5.898371000	-6.909013000
8	-1.154188000	6.432404000	4.519475000	6	-4.417581000	5.424245000	-4.510983000
7	-2.615269000	5.319137000	3.152100000	6	-4.895097000	4.802996000	-6.799018000
1	-2.774179000	4.426189000	2.684152000	6	-4.222078000	4.552769000	-5.594106000
6	-3.574664000	6.393344000	2.994387000	8	-3.400566000	3.470382000	-5.532597000
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6	-3.726801000	6.792665000	1.492651000	1	-6.580223000	8.768107000	-5.317608000
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1	-4.128289000	5.920795000	0.962201000	1	-5.410593000	7.184817000	-3.792750000
6	-2.451412000	7.250946000	0.851680000	1	-6.259418000	6.076847000	-7.853923000
6	-1.574792000	6.471561000	0.123964000	1	-3.886484000	5.248283000	-3.579713000
7	-0.495064000	7.216397000	-0.288482000	1	-4.734696000	4.132013000	-7.638248000
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1	0.296770000	6.876324000	-0.853478000	8	3.214476000	7.771097000	-1.077329000
6	-1.871063000	8.570846000	0.894625000	6	2.841119000	6.592599000	-1.152464000
6	-0.643584000	8.504697000	0.170552000	6	3.677670000	5.479591000	-0.492732000
6	-2.255611000	9.802835000	1.458678000	1	3.251660000	5.322632000	0.510256000
6	0.197589000	9.614884000	0.011919000	1	3.530165000	4.537798000	-1.034358000
6	-1.427944000	10.909147000	1.298170000	6	5.169528000	5.800259000	-0.370088000
6	-0.210867000	10.815088000	0.586023000	1	5.276256000	6.808079000	0.040881000
1	-3.186672000	9.892123000	2.014323000	1	5.624554000	5.836205000	-1.369865000
1	-1.717234000	11.863507000	1.731083000	6	5.938394000	4.826132000	0.543308000
1	0.416387000	11.696926000	0.484071000	1	5.559982000	4.898861000	1.567120000
1	1.135404000	9.520588000	-0.529612000	1	6.998821000	5.113445000	0.572375000
6	-4.943056000	5.949978000	3.524313000	6	5.870782000	3.350410000	0.164941000
8	-5.423107000	4.849810000	3.205119000	8	5.613173000	2.471738000	1.009712000
7	-5.600124000	6.847172000	4.287203000	7	6.118362000	3.044929000	-1.127079000
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6	-6.973608000	6.672588000	4.758393000	6	6.174786000	1.682808000	-1.647983000
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1	-7.477953000	6.016678000	4.044955000	1	5.626151000	1.048817000	-0.949609000
6	-7.079953000	6.126475000	6.192301000	6	7.616606000	1.152579000	-1.810002000
1	-6.544075000	6.805454000	6.867061000	1	7.545505000	0.101732000	-2.116331000
1	-8.138099000	6.171692000	6.485584000	1	8.103764000	1.171081000	-0.828201000
6	-6.549575000	4.699093000	6.399804000	6	8.435489000	1.931221000	-2.818085000
1	-6.567721000	4.470430000	7.472892000	6	8.399302000	1.597160000	-4.180958000
1	-5.500893000	4.635452000	6.085958000	6	9.220790000	3.024476000	-2.422511000
6	-7.371694000	3.632975000	5.658975000	6	9.120120000	2.335504000	-5.121627000
1	-8.422780000	3.690729000	5.961383000	6	9.942893000	3.767293000	-3.360576000
1	-7.341168000	3.793301000	4.579462000	6	9.893683000	3.425959000	-4.713928000
7	-6.927978000	2.265328000	5.929430000	1	7.807202000	0.744026000	-4.505358000
1	-7.203919000	1.865277000	6.816047000	1	9.273074000	3.290575000	-1.369340000
6	-6.009065000	1.573662000	5.224173000	1	9.082142000	2.056032000	-6.171287000
7	-5.425393000	2.085361000	4.139354000	1	10.547236000	4.608901000	-3.032139000
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7	-5.689608000	0.331581000	5.613601000	1	0.572694000	3.405144000	-1.279569000
1	-6.262384000	-0.140834000	6.298032000	1	1.663354000	3.121355000	-2.502123000
1	-5.011760000	-0.236104000	5.068549000	1	1.395842000	4.773509000	-1.966685000
6	-7.730410000	4.747220000	-1.396171000	6	-0.217507000	3.848098000	-3.096461000
1	-7.939656000	5.667490000	-0.840552000	1	-0.444442000	4.908606000	-3.246583000
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6	-6.374083000	4.161674000	-0.991204000	8	-1.249624000	2.938457000	-1.141102000
1	-6.351168000	3.973673000	0.090242000	6	0.088313000	3.203288000	-4.463708000
1	-5.576266000	4.886035000	-1.197390000	1	-0.827890000	3.265344000	-5.058708000
6	-6.055985000	2.863167000	-1.749199000	1	0.829789000	3.812789000	-4.988418000
1	-6.840737000	2.113175000	-1.589056000	6	0.581544000	1.782591000	-4.363867000
1	-6.037107000	3.058915000	-2.825468000	6	-0.150159000	0.680604000	-3.924622000
7	-4.752796000	2.293788000	-1.411297000	1	-1.183458000	0.621956000	-3.614031000
1	-3.944238000	2.571285000	-1.988089000	7	0.644543000	-0.429983000	-3.929057000

1	0.354401000	-1.355226000	-3.625021000		6	5.407443000	0.275015000	3.937843000
6	1.908118000	-0.090655000	-4.363337000		8	5.164511000	-0.145722000	5.070751000
6	1.892163000	1.297510000	-4.645628000		7	5.990525000	1.490231000	3.724551000
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6	4.288457000	1.107421000	-5.183960000		6	6.413558000	2.310995000	4.842877000
6	3.058248000	-0.884336000	-4.475762000		1	6.864656000	1.681159000	5.612468000
6	4.248749000	-0.240715000	-4.879307000		1	7.173384000	3.015729000	4.488049000
1	3.214074000	2.990953000	-5.034565000		6	5.307713000	3.116897000	5.547255000
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1	3.045444000	-1.941177000	-4.229713000		7	4.309371000	3.565369000	4.748246000
1	5.163735000	-0.824305000	-4.929373000		1	4.247295000	3.240617000	3.789463000
7	2.679168000	2.174575000	-7.000861000		6	3.109730000	4.198316000	5.265783000
8	3.035305000	1.331945000	-7.806312000		1	2.759395000	3.624959000	6.133667000
8	2.015257000	3.172742000	-7.251245000		6	3.331283000	5.657647000	5.765534000
					1	4.090327000	5.588788000	6.549751000
⁴Int4_{B,C4-endo}								
26	2.508462000	-4.864538000	0.026734000		6	3.745660000	6.661316000	4.713426000
7	1.200416000	-4.349885000	1.485158000		6	5.102409000	6.907221000	4.456564000
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6	-0.053351000	-3.817628000	1.326860000		6	4.523656000	8.551155000	2.776226000
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6	0.308090000	-3.833419000	3.545936000		1	1.726347000	7.210520000	4.180193000
6	1.444208000	-4.366845000	2.831598000		1	6.547062000	8.028043000	3.316806000
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6	4.997946000	-6.064430000	-1.266869000		7	0.771567000	4.303315000	4.552857000
6	5.580610000	-6.368523000	-2.554682000		1	0.586861000	4.679505000	5.474070000
6	4.656271000	-6.024650000	-3.494027000		6	-0.350177000	4.223050000	3.635986000
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6	1.235562000	-4.543919000	-2.726195000		6	-0.996072000	2.812389000	3.691407000
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6	-0.815979000	-3.665858000	-2.397144000		8	-1.898209000	2.741064000	2.584249000
6	-0.142199000	-3.907868000	-1.140469000		1	-2.384906000	1.885282000	2.618852000
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1	2.313256000	-5.071865000	-4.476546000		1	-2.648297000	4.506670000	2.683497000
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1	6.782952000	-6.580192000	2.554136000		6	-3.531565000	6.962697000	1.642175000
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16	1.538381000	-7.233576000	0.195498000		1	-2.744520000	9.950551000	2.434464000
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7	2.934755000	1.252305000	1.735778000		1	1.444260000	9.522521000	-0.315668000
1	3.877738000	1.383366000	1.384122000		6	-4.768844000	6.070084000	3.626313000
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1	3.465397000	-1.588601000	1.718728000		1	-7.306572000	6.271697000	4.102089000
6	5.094707000	-0.544201000	2.687465000		6	-6.970227000	6.165372000	6.259183000
1	5.426015000	-0.026889000	1.782644000		1	-6.430130000	6.754392000	7.010745000
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7	-6.983501000	2.341093000	5.648022000	1	7.854795000	2.042699000	-4.982401000
1	-7.351807000	1.885046000	6.471806000	1	9.151325000	4.488249000	-1.693767000
6	-6.044767000	1.654991000	4.962147000	1	8.374233000	3.879342000	-6.556215000
7	-5.348056000	2.211377000	3.970184000	1	9.665737000	6.330989000	-3.264003000
1	-5.354553000	3.214404000	3.786629000	1	9.279215000	6.036870000	-5.705478000
1	-4.667657000	1.626218000	3.463555000	7	0.947789000	3.866382000	-2.248762000
7	-5.824070000	0.372829000	5.280255000	1	0.535952000	3.529338000	-1.359177000
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6	-0.090436000	2.311288000	-3.373128000	8	2.126351000	-1.043391000	-2.192585000
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1	-0.525486000	1.416521000	-5.259168000	6	4.804208000	0.052958000	5.053300000
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6	1.199797000	2.645094000	-5.559428000	1	4.930049000	-0.902101000	4.526559000
6	0.715608000	3.836141000	-6.095880000	6	6.120104000	0.847741000	4.976817000
1	-0.269402000	4.274229000	-6.012724000	1	6.412126000	1.053340000	3.943597000
7	1.703022000	4.431707000	-6.829385000	1	6.914000000	0.230631000	5.414638000
1	1.598346000	5.289378000	-7.353101000	6	6.062984000	2.130494000	5.802427000
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8	1.901988000	-1.126881000	-2.074864000	1	-0.280530000	9.835992000	-1.805966000
7	3.703693000	1.571406000	3.355133000	1	0.499385000	7.451862000	-1.680879000
1	4.633003000	1.840022000	3.048089000	6	-5.056972000	5.946974000	3.918672000
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6	-5.775520000	6.164501000	7.276319000	6	8.184707000	0.527953000	0.015729000
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1	6.056414000	1.765517000	-2.241011000	1	6.623532000	-6.558587000	-0.331414000	
1	6.063491000	1.132199000	-0.586240000	1	2.002466000	-5.325006000	-4.555093000	
6	8.039792000	1.611278000	-1.341829000	1	0.383415000	-3.629984000	4.575411000	
1	8.178570000	0.577659000	-1.684233000	1	5.251878000	-5.561750000	4.291409000	
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6	8.761694000	2.566640000	-2.270016000	1	6.410277000	-6.801993000	-2.942947000	
6	8.664478000	2.421239000	-3.663178000	1	4.440164000	-6.284548000	-4.736818000	
6	9.519163000	3.632114000	-1.763760000	1	-0.428614000	-4.322688000	-4.453869000	
6	9.305936000	3.313399000	-4.523745000	1	-2.031745000	-3.444864000	-2.443713000	
6	10.163773000	4.527811000	-2.621705000	6	-1.924600000	-2.816005000	2.903945000	
6	10.059064000	4.371110000	-4.005167000	6	-2.012487000	-1.330764000	2.500835000	
1	8.079178000	1.602538000	-4.075809000	6	-3.258386000	-0.618683000	3.033049000	
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1	1.769231000	2.616061000	-2.659472000	16	1.538375000	-7.233550000	0.195505000	
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1	-0.393552000	4.263630000	-3.466966000	7	2.919084000	1.295120000	1.690951000	
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1	-0.833594000	2.572549000	-5.143819000	6	3.584431000	-0.923887000	2.524158000	
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6	2.836214000	0.782069000	-5.418043000	1	6.083422000	1.839842000	2.746547000	
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7	0.768972000	4.310743000	4.557160000	1	-5.205603000	0.978681000	1.261751000
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6	1.464547000	-1.041702000	-4.462691000	8	5.134966000	-0.167827000	5.015484000
6	1.607662000	0.329335000	-4.779118000	7	5.970856000	1.485687000	3.696357000
6	2.836912000	0.786452000	-5.420777000	1	6.083979000	1.840194000	2.746793000
6	3.709930000	-0.285235000	-5.930249000	6	6.397583000	2.287592000	4.826782000
6	2.402528000	-2.023421000	-4.817907000	1	6.839494000	1.643189000	5.589645000
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1	6.153638000	-0.912142000	2.096893000	1	-7.156043000	-0.390055000	6.651522000
1	6.925884000	-2.336553000	2.772388000	1	-8.434923000	-1.382651000	5.969430000
6	5.904589000	-1.205274000	4.241461000	6	-6.433059000	-2.062435000	5.498141000
8	5.770849000	-1.966173000	5.201881000	1	-6.298715000	-2.629641000	6.427887000
7	5.993544000	0.147530000	4.392387000	1	-5.453903000	-1.636105000	5.250306000
1	5.993854000	0.744921000	3.566385000	6	-6.864097000	-3.036033000	4.391486000
6	5.982326000	0.742206000	5.715814000	1	-7.843466000	-3.465598000	4.627756000
1	6.578220000	0.131828000	6.397123000	1	-6.962980000	-2.523131000	3.432759000
1	6.440857000	1.735008000	5.654217000	7	-5.940215000	-4.156321000	4.217641000
6	4.598745000	0.895294000	6.373529000	1	-5.985610000	-4.891779000	4.910381000
8	4.470410000	0.845141000	7.597850000	6	-4.865203000	-4.173540000	3.401475000
7	3.577118000	1.147656000	5.521510000	7	-4.585631000	-3.158285000	2.584994000
1	3.728203000	1.079884000	4.520549000	1	-5.011714000	-2.237420000	2.686432000
6	2.185313000	1.172081000	5.931505000	1	-3.750951000	-3.240333000	1.982971000
1	1.993664000	0.311396000	6.585100000	7	-4.076374000	-5.257866000	3.393144000
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1	2.456145000	2.458868000	7.611258000	1	-3.255190000	-5.320894000	2.759769000
1	0.774393000	2.287612000	7.129993000	6	-7.953612000	0.052560000	-2.415894000
6	1.860655000	3.754143000	5.994759000	1	-8.584134000	0.589885000	-1.699734000
6	3.034434000	4.521831000	6.009603000	1	-8.357410000	-0.961730000	-2.522744000
6	0.752155000	4.237513000	5.280685000	1	-8.048049000	0.554220000	-3.386513000
6	3.103208000	5.738347000	5.326522000	6	-6.494801000	0.024028000	-1.943793000
6	0.818959000	5.451082000	4.592479000	1	-6.427333000	-0.462677000	-0.962779000
6	1.995300000	6.205833000	4.614234000	1	-6.119833000	1.047180000	-1.815417000
1	3.894885000	4.168382000	6.572397000	6	-5.580085000	-0.709444000	-2.937954000
1	-0.171254000	3.662227000	5.267058000	1	-5.967531000	-1.714810000	-3.147715000
1	4.018858000	6.323410000	5.356470000	1	-5.573444000	-0.185310000	-3.898237000
1	-0.047184000	5.809614000	4.042356000	7	-4.184253000	-0.798875000	-2.509524000
1	2.045275000	7.152653000	4.083410000	1	-3.531827000	-0.069539000	-2.831204000
6	1.352680000	1.006866000	4.648868000	6	-3.707892000	-1.662094000	-1.604031000
8	1.872258000	1.128320000	3.532011000	7	-2.443261000	-1.581550000	-1.194128000
7	0.048778000	0.703503000	4.815391000	1	-4.031167000	-3.316763000	-0.484565000

1	-5.321660000	-2.935247000	-1.560967000	6	2.725804000	0.935650000	-6.846720000
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1	-2.152503000	-2.220693000	-0.448344000	6	4.342491000	3.326132000	-7.416781000
1	-1.876983000	-0.743041000	-1.390559000	6	4.716261000	2.052956000	-7.909989000
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1	-8.453836000	6.184523000	-3.719636000	1	4.327539000	-0.050085000	-8.006909000
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8	-6.157191000	-0.609385000	3.336598000	8	5.885031000	1.347444000	2.656774000
7	-5.712320000	0.597770000	5.222820000	7	6.302462000	2.551265000	0.785678000
1	-5.055611000	1.250464000	5.636917000	1	5.984028000	3.287155000	0.167555000
6	-6.697716000	-0.047152000	6.088619000	6	7.446153000	1.756742000	0.347383000
1	-7.190529000	0.738026000	6.672229000	1	7.108530000	0.956186000	-0.323336000
1	-7.450821000	-0.487042000	5.431647000	1	7.873998000	1.283637000	1.233668000
6	-6.117734000	-1.096686000	7.054833000	6	8.501472000	2.626055000	-0.356514000
1	-5.402442000	-0.602715000	7.724362000	1	9.326669000	1.962224000	-0.643432000
1	-6.942014000	-1.448760000	7.690159000	1	8.906371000	3.349942000	0.360036000
6	-5.419779000	-2.293493000	6.392127000	6	7.975263000	3.356104000	-1.578484000
1	-4.954928000	-2.907945000	7.173057000	6	7.615555000	2.650802000	-2.738976000

6	7.817967000	4.749426000	-1.568526000
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6	7.322792000	5.425456000	-2.687842000
6	6.974572000	4.712974000	-3.836206000
1	7.721929000	1.568325000	-2.766650000
1	8.094990000	5.311121000	-0.679111000
1	6.848633000	2.759335000	-4.746993000
1	7.213656000	6.506435000	-2.660903000
1	6.597745000	5.237902000	-4.710046000
7	0.797221000	-0.270183000	-2.718220000
1	0.343269000	-1.106613000	-2.316649000
1	1.691475000	-0.596561000	-3.212304000
1	1.027206000	0.396954000	-1.945161000
6	-0.242191000	0.358590000	-3.600441000
1	-0.472443000	1.332262000	-3.160388000
6	-1.542647000	-0.470440000	-3.475242000
8	-2.581285000	-0.004657000	-4.031743000
8	-1.486218000	-1.516138000	-2.779873000
6	0.231951000	0.543327000	-5.049713000
1	-0.642311000	0.810356000	-5.649564000
1	0.578524000	-0.421814000	-5.432916000
6	1.308653000	1.595970000	-5.194638000
6	1.640688000	2.506262000	-4.208237000
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6	4.095666000	3.462114000	-6.655484000
6	4.326452000	2.901271000	-7.908291000
1	3.080689000	-0.850473000	-4.778840000
1	3.676816000	1.436200000	-9.358188000
1	4.703322000	4.281977000	-6.284644000
1	5.125369000	3.280891000	-8.536763000
7	1.622633000	0.365237000	-8.239337000
8	2.096453000	-0.299807000	-9.169317000
8	0.456816000	0.245573000	-7.850653000