

Supporting Information

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

Savvas Louka,^{§,⊥,‡} Sarah M. Barry,^{#,‡,†} Derren J. Heyes,^{§,&} M. Qadri E. Mubarak,^{§,⊥} Hafiz Saqib Ali,^{§,&} Lona Alkhalaf,[#] Andrew W. Munro,^{§,&} Nigel S. Scrutton,^{*,§,&} Gregory L. Challis^{*,§,#,¥} and Sam P. de Visser^{*,§,⊥}

[§] The Manchester Institute of Biotechnology, The University of Manchester, 131 Princess Street, Manchester M1 7DN, United Kingdom

[⊥] Department of Chemical Engineering and Analytical Science, The University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom

[&] Department of Chemistry, The University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom

[#] Department of Chemistry, University of Warwick, Coventry CV4 7AL, United Kingdom

[§] Department of Biochemistry and Molecular Biology, Monash University, Clayton VIC 3800, Australia

[¥] ARC Centre for Excellence in Innovations in Peptide and Protein Science, Monash University, Clayton, VIC 3800, Australia

Corresponding author: sam.devisser@manchester.ac.uk

Part I: Experimental data.

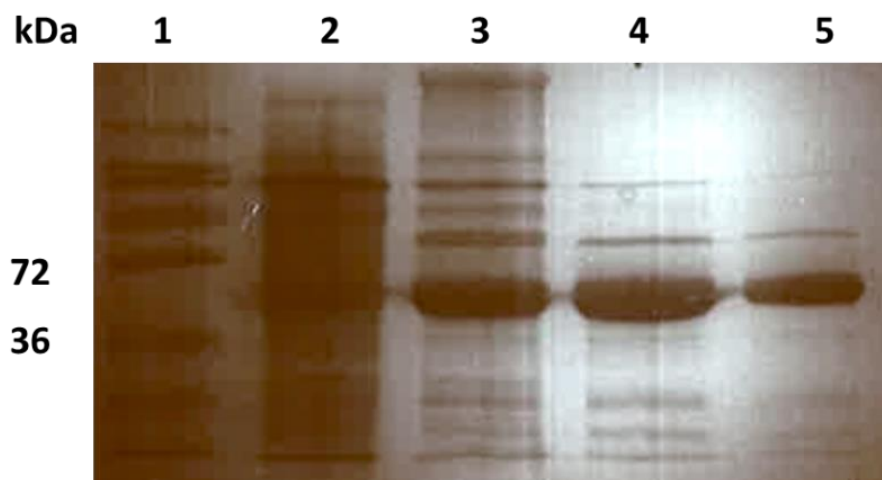


Figure S1: Representative SDS-PAGE of purified TxtE.

Lane 1: molecular size markers;

Lane 2: soluble protein;

Lane 3: after passing the sample through a Ni²⁺-IDA resin;

Lane 4: after passing the sample through a Ni²⁺-IDA resin using an FPLC instrument;

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

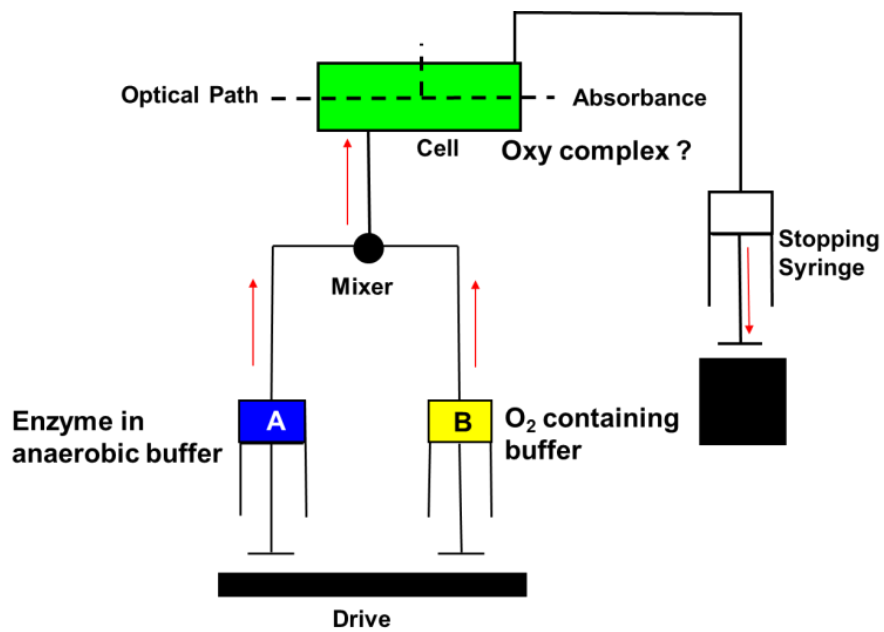


Figure S2: Diagram of stopped-flow apparatus for single mixing experiments. The scheme shows the mixing of enzyme against O_2 but also applies to NO .

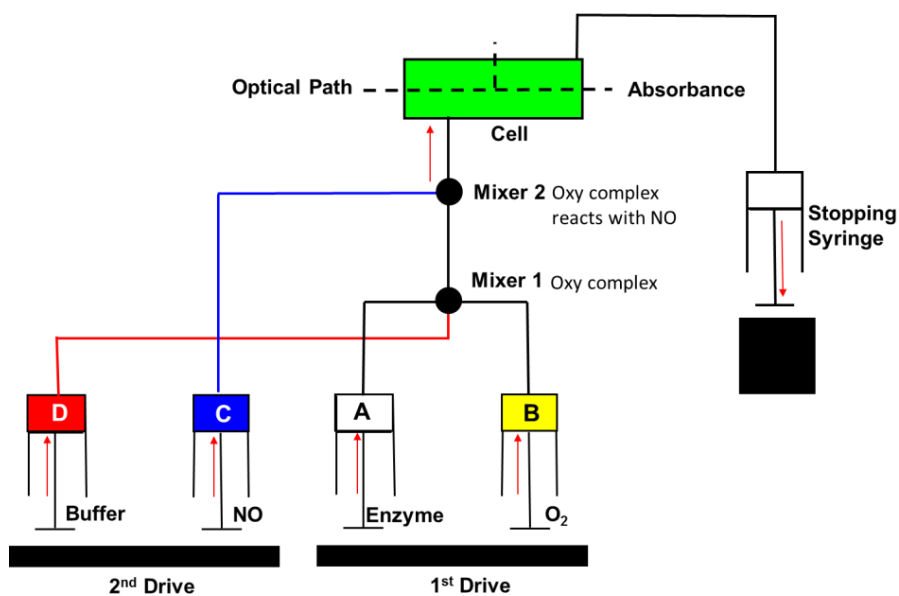


Figure S3: Diagram of stopped-flow apparatus for double mixing experiments. The enzyme is initially mixed against the first gas (in this case O₂ to form the oxy-complex), aged for a defined time delay and then mixed against the second gas (in this case NO). The order of mixing of the two gases can be varied in different stopped-slow experiments.

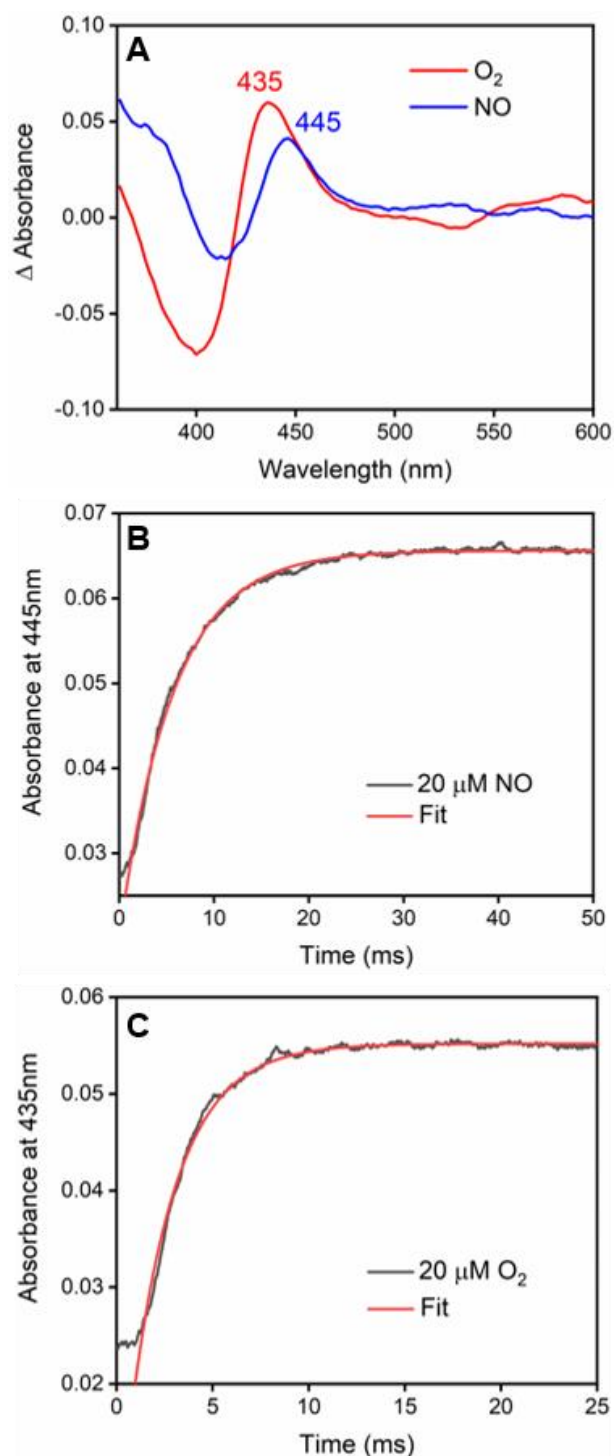


Figure S4: Examples of rapid mixing stopped-flow data to illustrate the rates of NO and O₂ binding to TxtE. A) Absorbance difference spectra measured after 50 ms from stopped-flow photodiode array experiments. A TxtE sample mixed against anaerobic buffer was used as a baseline. The maximum increases 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 μ M NO (B) and 20 μ M O₂ (C).

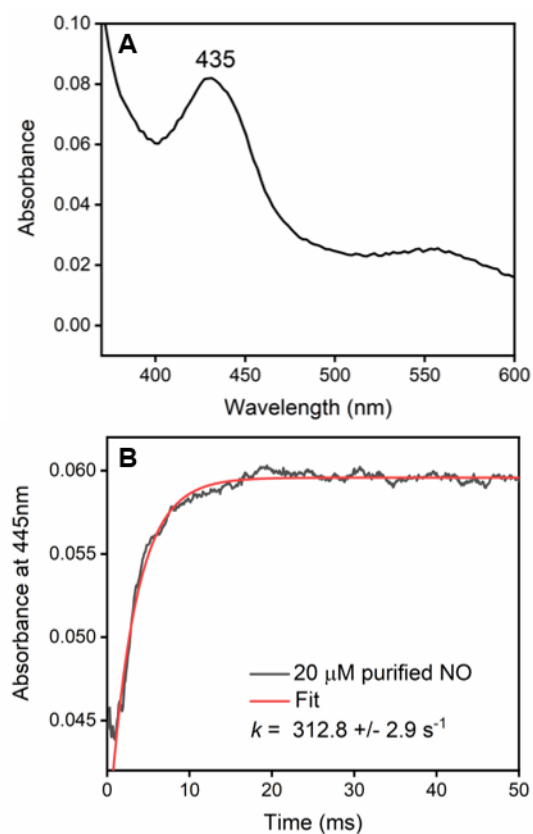


Figure S5: Rapid mixing stopped-flow data to illustrate binding of re-purified NO to TxtE. A) Absorbance spectra measured after 50 ms from stopped-flow photodiode array experiments. B) Example of kinetic transients at 445 nm are shown for binding of 20 μ M NO.

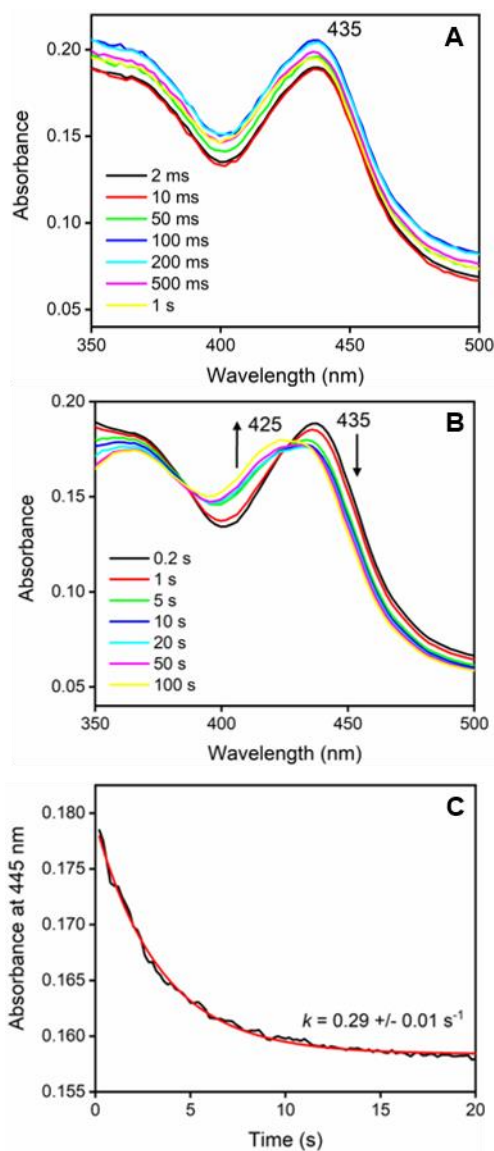


Figure S6: Representative double mixing stopped-flow measurements where TxtE was first mixed with 20 μM NO, aged for 50 ms and then mixed with 20 μM O₂, prior to data collection. A) Spectral changes over 1 s at selected time points show only the formation of the iron(II)-NO species at 435 nm. B) Spectral 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.

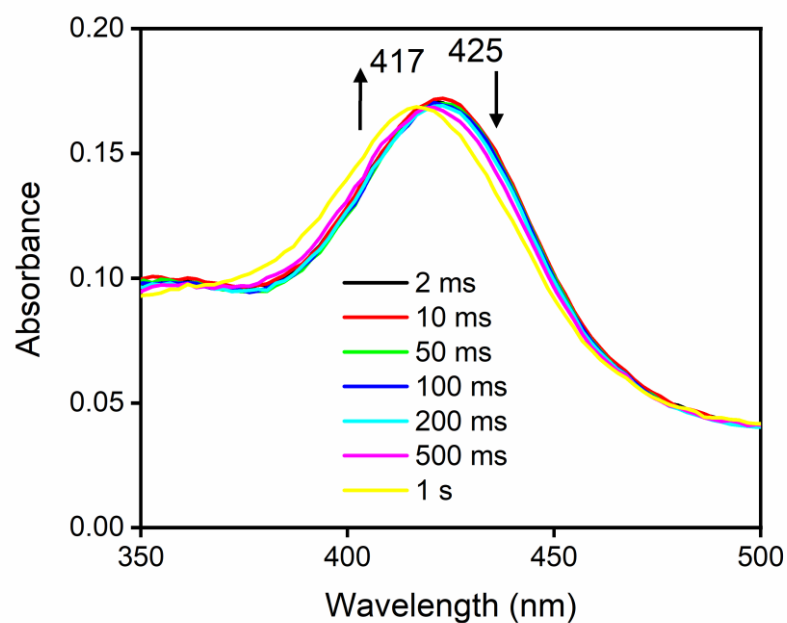


Figure S7: Representative double mixing stopped-flow measurements where TxtE was first mixed with 20 μM O_2 , aged for 50 ms and then mixed with anaerobic buffer, prior to data collection. Spectral changes over 1 s at selected time points show decay of the iron(III)-superoxo species at 425 nm and a simultaneous increase at 417 nm.

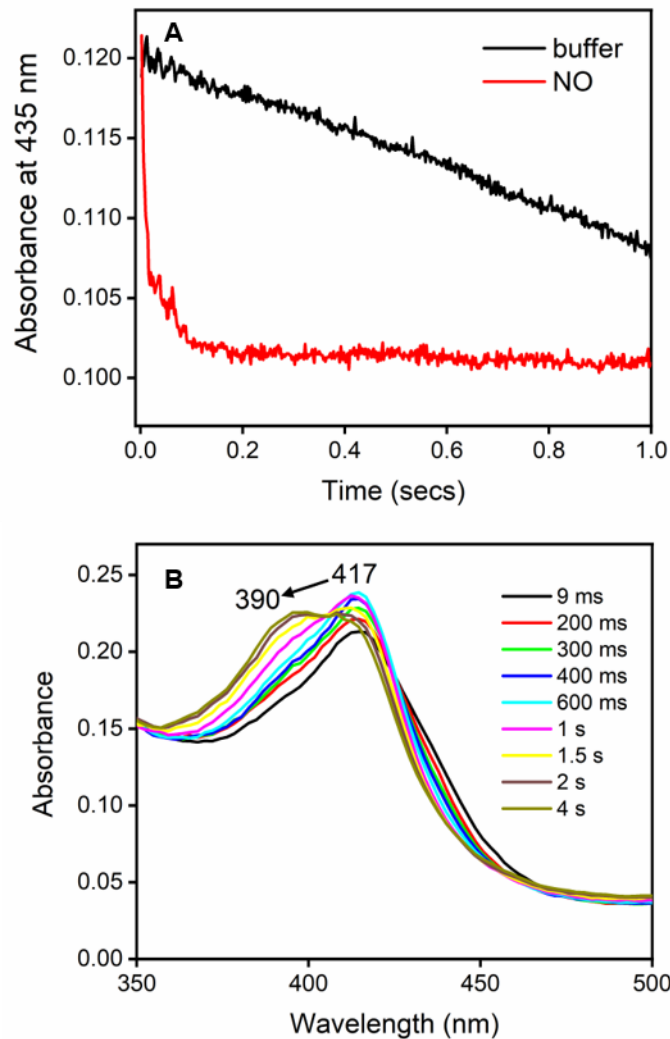


Figure S8: Double mixing stopped-flow measurements where TxtE was first mixed with 20 μM O_2 , aged for 50 ms and then mixed with either anaerobic buffer or 20 μM NO. A) Representative transients at 435 nm from double mixing stopped-flow measurements that show the disappearance of the iron(III)-superoxo 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 417nm absorbing species to substrate-bound heme peak at 390 nm.

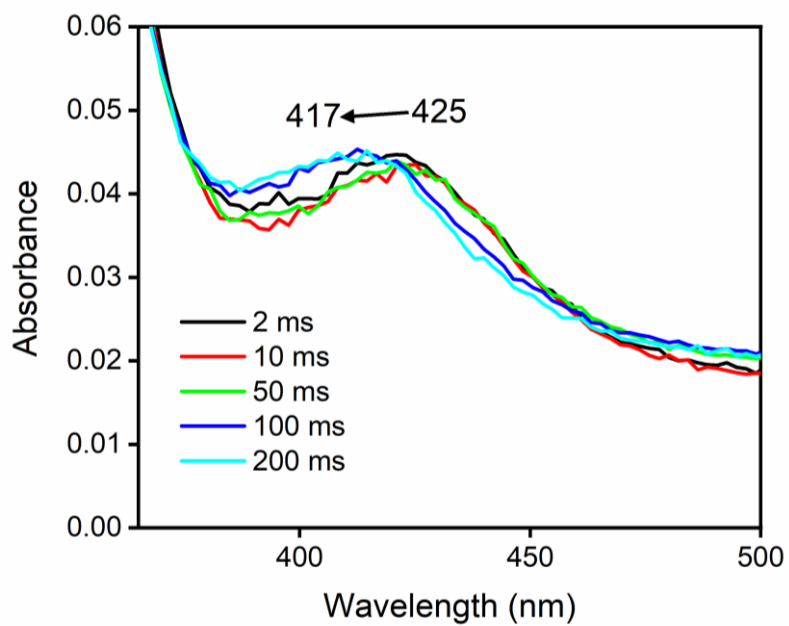


Figure S9: Representative double mixing stopped-flow measurements where 20 μM O_2 was first mixed with 20 μM NO , aged for 50 ms and then mixed with TxtE, prior to data collection. Spectral changes over 200 ms at selected time points show decay of the iron(III)-superoxo species at 425 nm and a simultaneous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

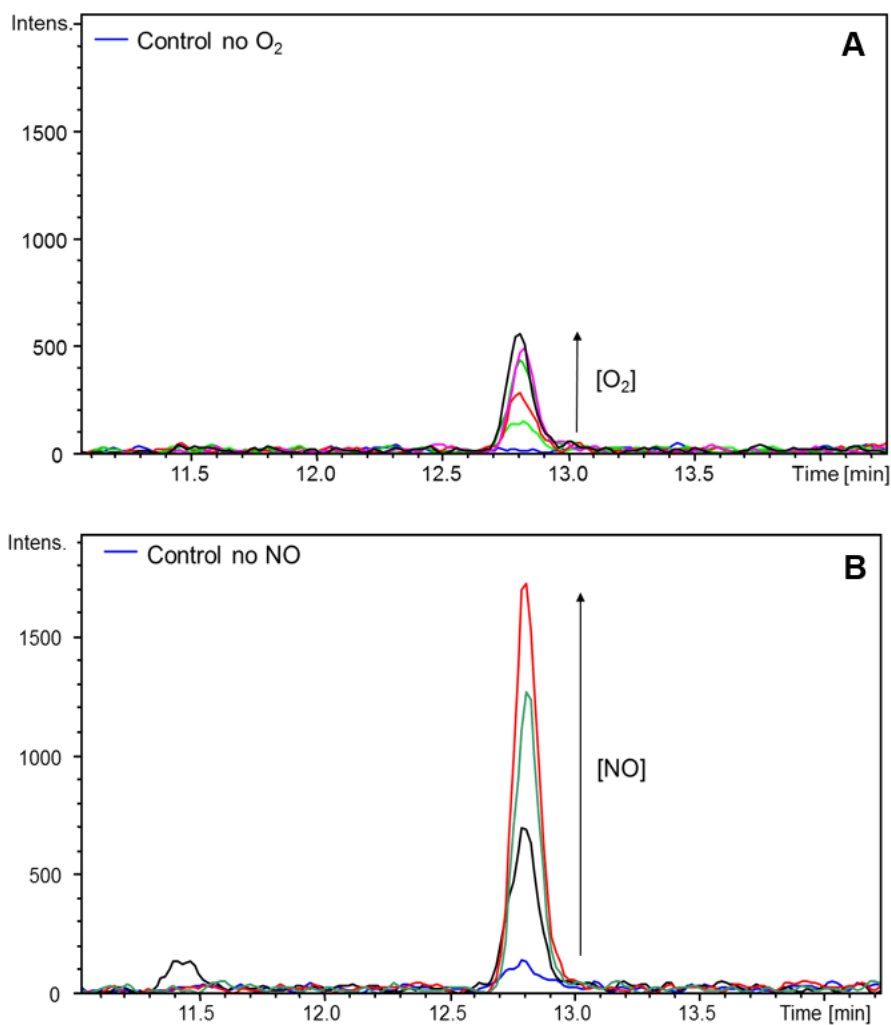
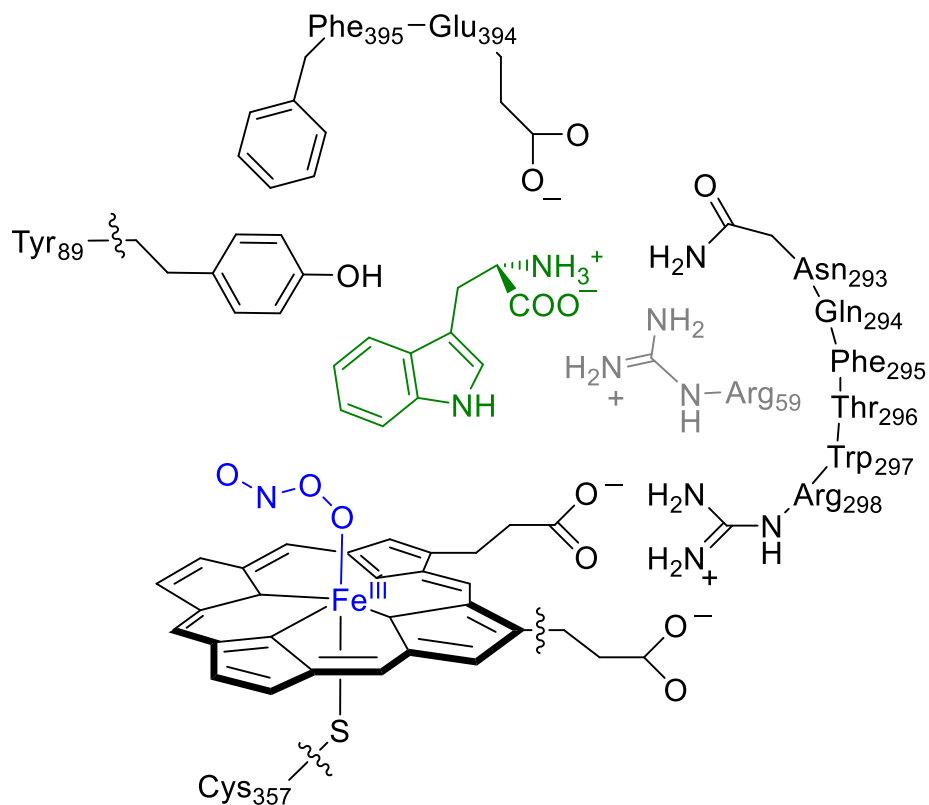
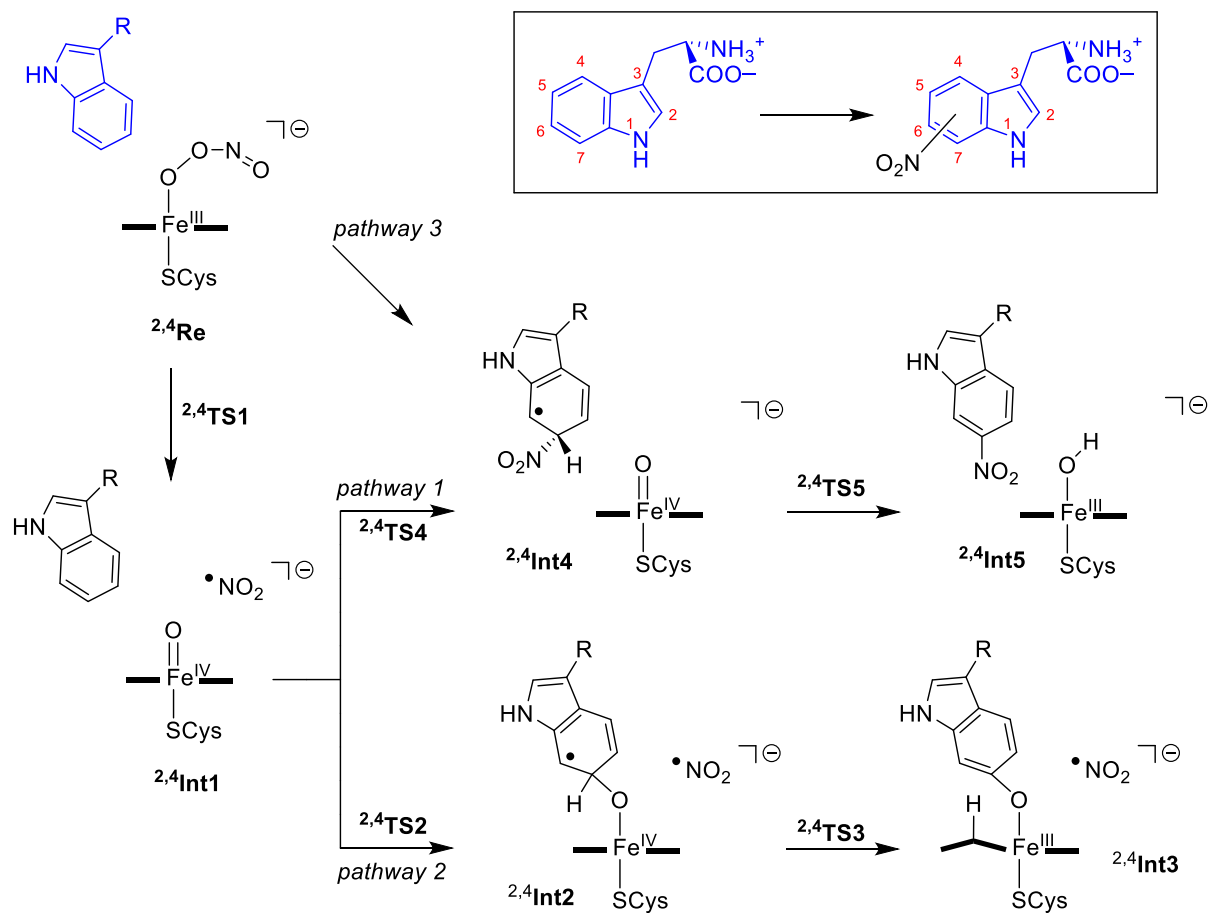


Figure S10: A) Representative mass spectral analysis of samples following double mixing experiments of TxtE iron(II)-NO complex reacted with buffers containing increasing concentrations of O₂ (0, 2, 5, 10, 20 and 100 μ M). **B)** Representative mass spectral analysis of samples following double mixing experiments of TxtE iron(III)-superoxo complex reacted with buffers containing increasing concentrations of NO (0, 20, 40 and 100 μ M). The data are LC-HRMS extracted ion chromatograms at m/z 250.0800 \pm 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.

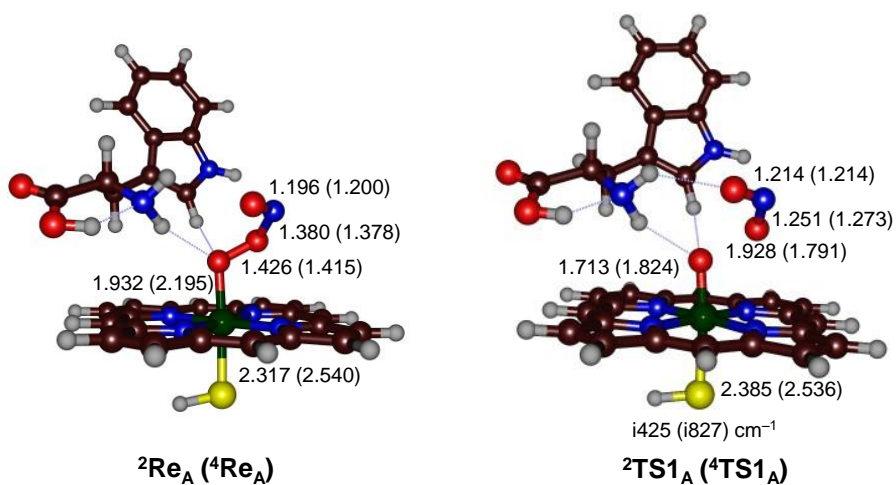


Figure S11: UB3LYP/BS1 optimized geometries of ${}^2,4\text{Re}_A$ and ${}^2,4\text{TS1}_A$ as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

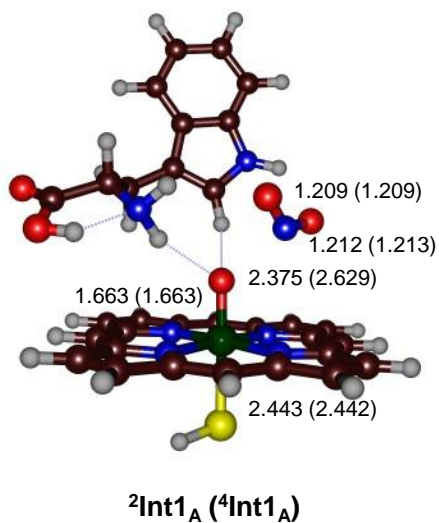


Figure S12: UB3LYP/BS1 optimized geometries of ${}^2,4\text{Int1}_A$ as obtained in Gaussian-09. Bond lengths are in angstroms.

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

	E	ZPE	G	E
	[BS1,au]	[BS1,au]	[BS1,au]	[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 peroxyxynitrite as calculated with B3LYP with model A in Gaussian-09.

	ΔE	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$	ΔG
	BS1	BS1	BS1	BS2	BS2	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

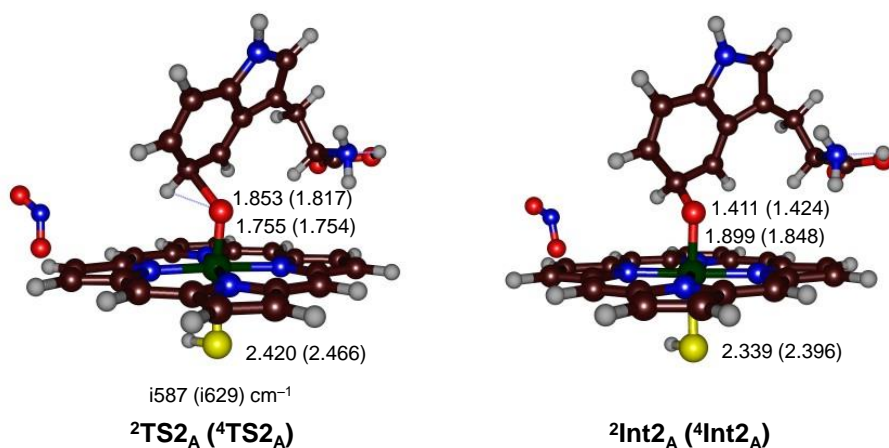


Figure S13: UB3LYP/BS1 optimized geometries of ^{2,4}TS_{2A} and ^{2,4}Int_{2A} as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

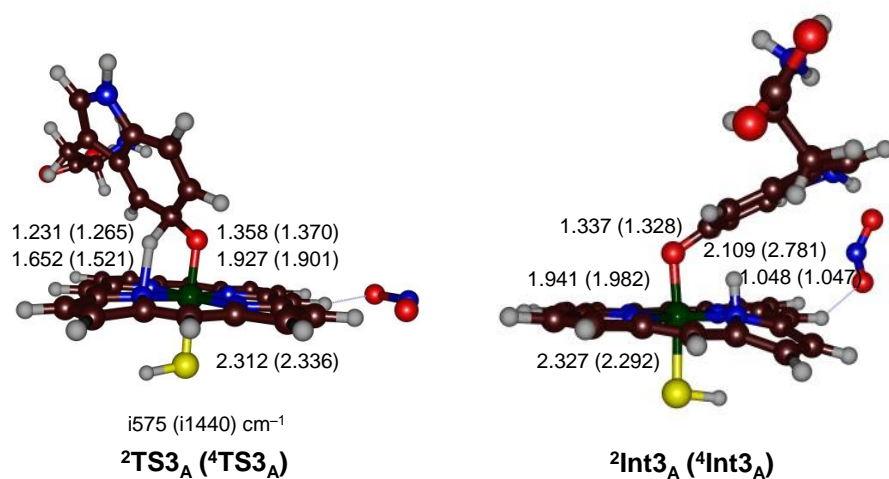


Figure S14: UB3LYP/BS1 optimized geometries of ^{2,4}TS_{3A} and ^{2,4}Int_{3A} as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

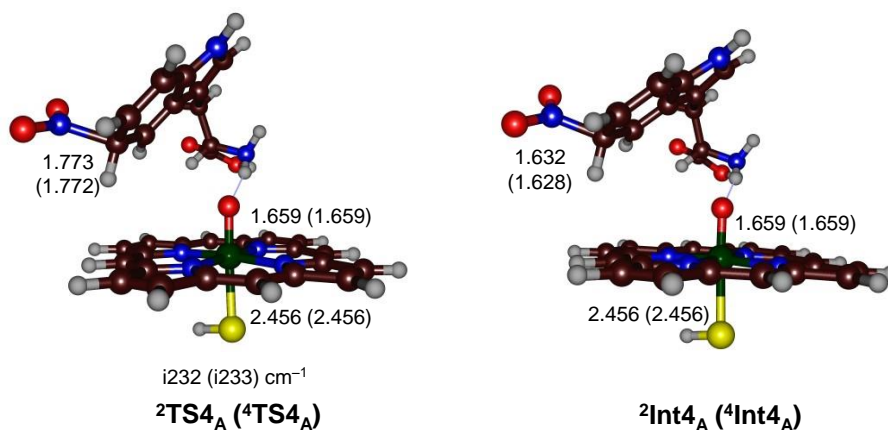


Figure S15: UB3LYP/BS1 optimized geometries of ^{2,4}TS_{4A} and ^{2,4}Int_{4A} as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

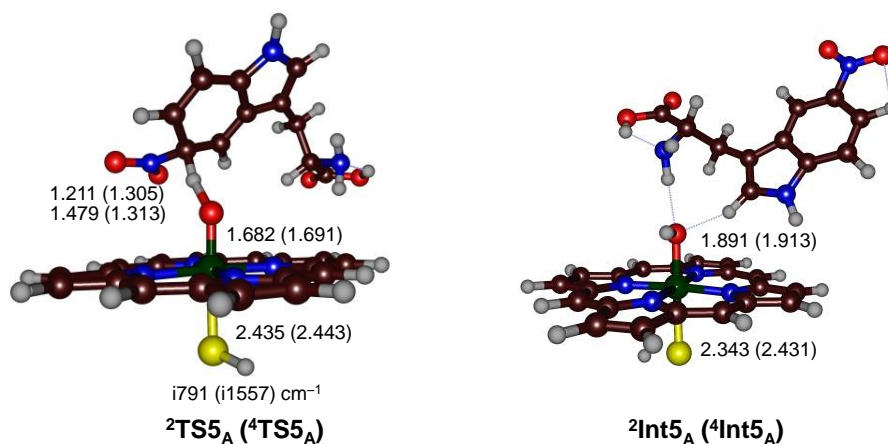


Figure S16: UB3LYP/BS1 optimized geometries of ^{2,4}TS_{5A} and ^{2,4}Int_{5A} as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wave numbers.

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	ZPE	G	E
	[BS1,au]	[BS1,au]	[BS1,au]	[BS2,au]
² TS2 _A	-2477.291661	0.515360	-2476.855971	-2477.933385
² Int2 _A	-2477.313338	0.516972	-2476.875642	-2477.967220
² TS3 _A	-2477.301674	0.512808	-2476.866745	-2477.968688
² Int3 _A	-2477.370838	0.519961	-2476.923404	-2478.014560
⁴ TS2 _A	-2477.289667	0.514911	-2476.855535	-2477.922144
⁴ Int2 _A	-2477.306212	0.515710	-2476.871496	-2477.937934
⁴ TS3 _A	-2477.274705	0.510352	-2476.841094	-2477.910412
⁴ Int3 _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	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$	ΔG
	BS1	BS1	BS1	BS2	BS2	BS2
² TS2 _A	40.12	38.10	35.90	27.85	25.83	23.63
² Int2 _A	26.52	25.51	23.56	6.62	5.60	3.66
² TS3 _A	33.84	30.21	29.14	5.70	2.07	1.00
² Int3 _A	-9.56	-8.70	-6.41	-23.09	-22.23	-19.94
⁴ TS2 _A	41.37	39.07	36.18	34.90	32.60	29.71
⁴ Int2 _A	30.99	29.19	26.16	25.00	23.19	20.17
⁴ TS3 _A	50.76	45.60	45.24	42.27	37.10	36.74
⁴ Int3 _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	ZPE	G	E
	[BS1,au]	[BS1,au]	[BS1,au]	[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	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$	ΔG
	BS1	BS1	BS1	BS2	BS2	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 peroxyxynitrite 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 TS2 _A	1.05	0.57	-0.63	-0.18	-0.06	0.25	1.00
² Int2 _A	1.00	0.08	-0.58	-0.09	0.03	0.56	1.00
² TS3 _A	0.98	0.05	-0.23	-0.05	0.05	0.20	1.00
² Int3 _A	0.99	0.06	0.00	-0.07	0.03	-0.01	1.00
⁴ TS2 _A	0.95	0.64	0.69	0.00	0.26	0.46	3.00
⁴ Int2 _A	0.94	0.17	0.73	0.05	0.18	0.93	3.00
⁴ TS3 _A	0.98	0.07	0.70	0.80	0.06	0.40	3.00
⁴ Int3 _A	1.04	0.03	0.84	1.03	0.03	0.03	3.00

Charges:

	Fe	O38	NO2	Por	SH	Trp	Total
² TS2 _A	0.35	-0.49	-0.34	-0.49	-0.20	0.17	-1.00
² Int2 _A	0.27	-0.56	-0.38	-0.58	-0.14	0.38	-1.00
² TS3 _A	0.25	-0.57	-0.64	-0.49	-0.11	0.57	-1.00
² Int3 _A	0.26	-0.58	-0.75	-0.31	-0.13	0.53	-1.00
⁴ TS2 _A	0.38	-0.50	-0.28	-0.54	-0.17	0.10	-1.00
⁴ Int2 _A	0.32	-0.56	-0.24	-0.52	-0.14	0.14	-1.00
⁴ TS3 _A	0.27	-0.58	-0.27	-0.71	-0.15	0.44	-1.00
⁴ Int3 _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

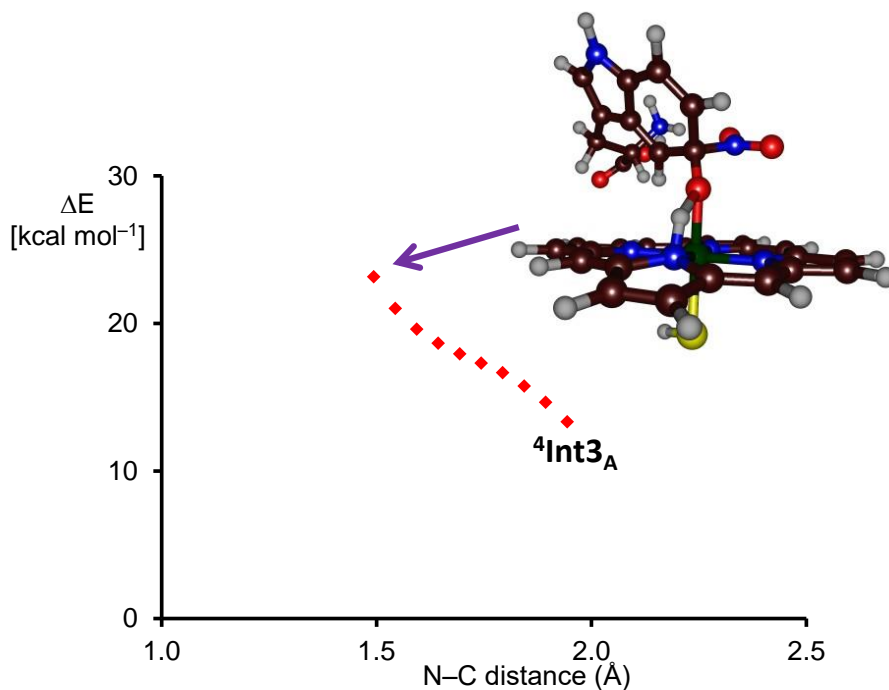


Figure S17: UB3LYP/BS1 geometry scan for NO₂ attack on the *ipso*-carbon atom of the substrate in ⁴Int3_A as obtained in Gaussian-09. All points refer to a full geometry optimization with fixed C–N distance. Energies are relative to ⁴Re_A.

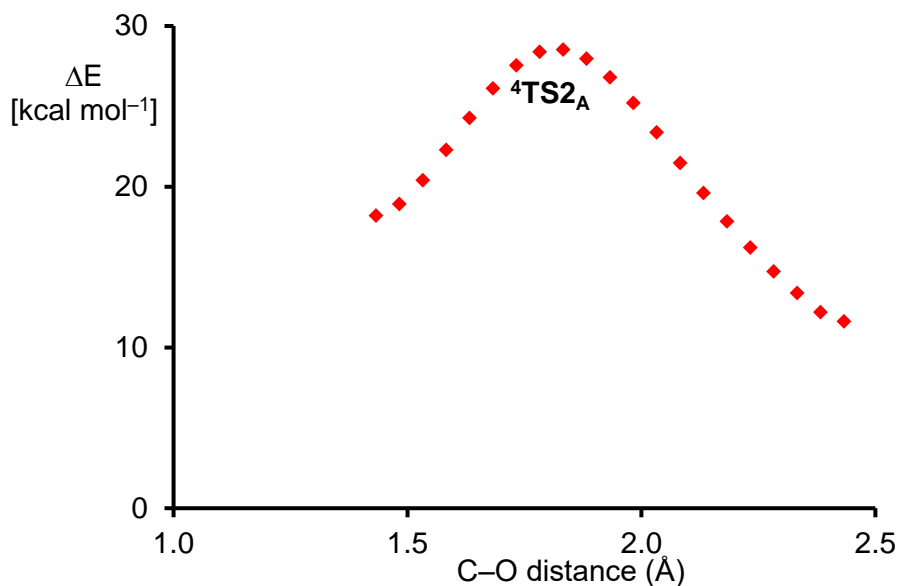


Figure S18: UB3LYP/BS1 geometry scan for electrophilic attack on the exo atom of the substrate starting from ⁴Int1_A as obtained in Gaussian-09. All points refer to a full geometry optimization with fixed C–O distance. Energies are relative to ⁴Re_A.

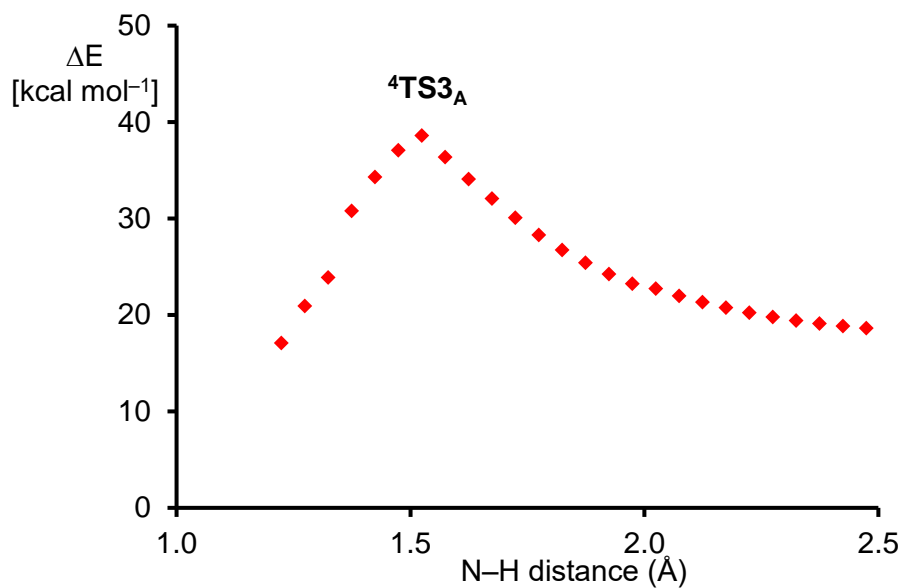


Figure S19: UB3LYP/BS1 geometry scan for proton transfer from the *ipso*-C–H bond of substrate in ⁴Int_{2A} as obtained in Gaussian-09. All points refer to a full geometry optimization with fixed H–N distance. Energies are relative to ⁴Re_A.

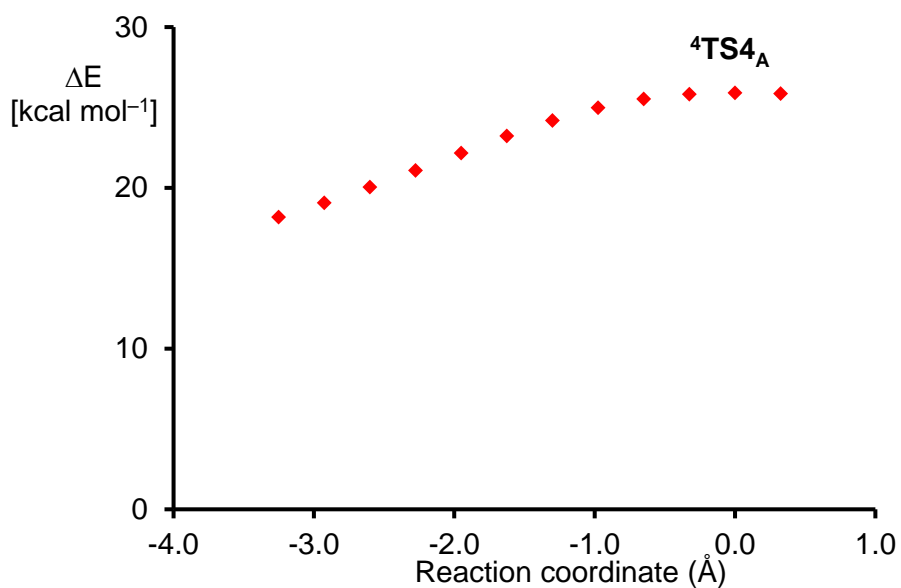


Figure S20: UB3LYP/BS1 calculated intrinsic reaction coordinate scan for NO₂ transfer to substrate in ⁴Int_{1A} around ⁴TS_{4A} as obtained in Gaussian-09. Energies are relative to ⁴Int_{1A}.

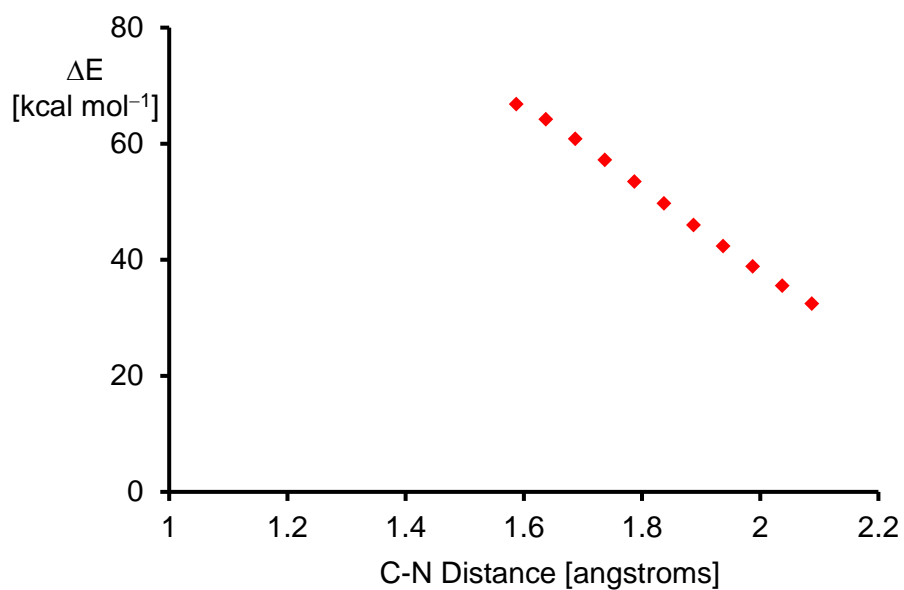
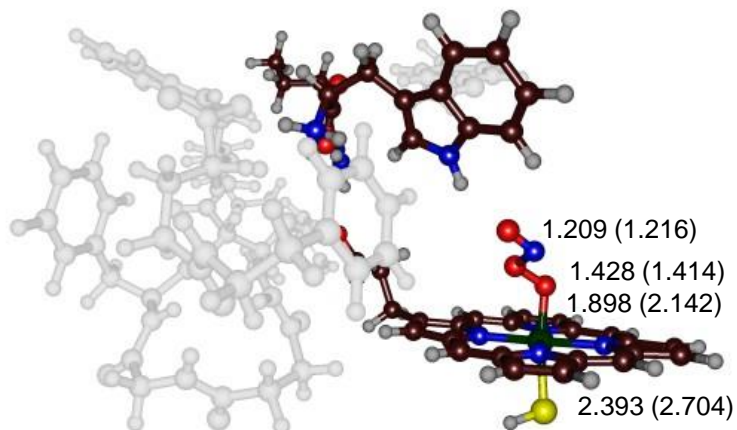


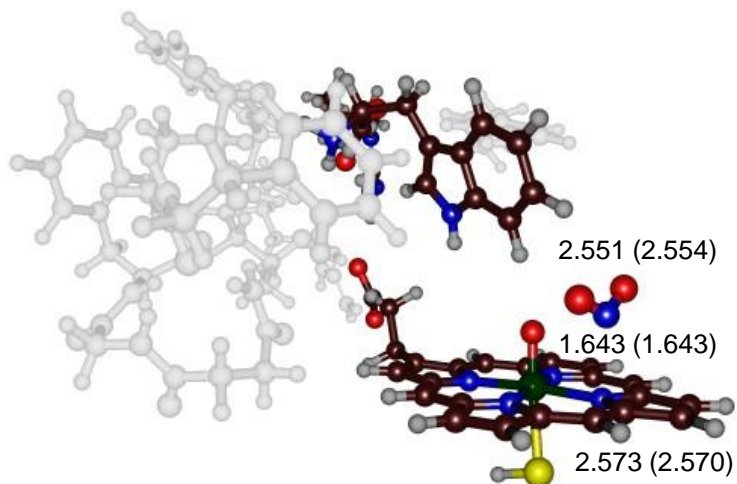
Figure S21: UB3LYP/BS1 calculated constraint geometry scan for direct attack of peroxytrite on the substrate in ⁴Re_A as obtained in Gaussian-09. Energies are relative to ⁴Re_A.

Large model B Data.



${}^2\text{Re}_B$ (${}^4\text{Re}_B$)

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



${}^2\text{Int1}_B$ (${}^4\text{Int1}_B$)

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

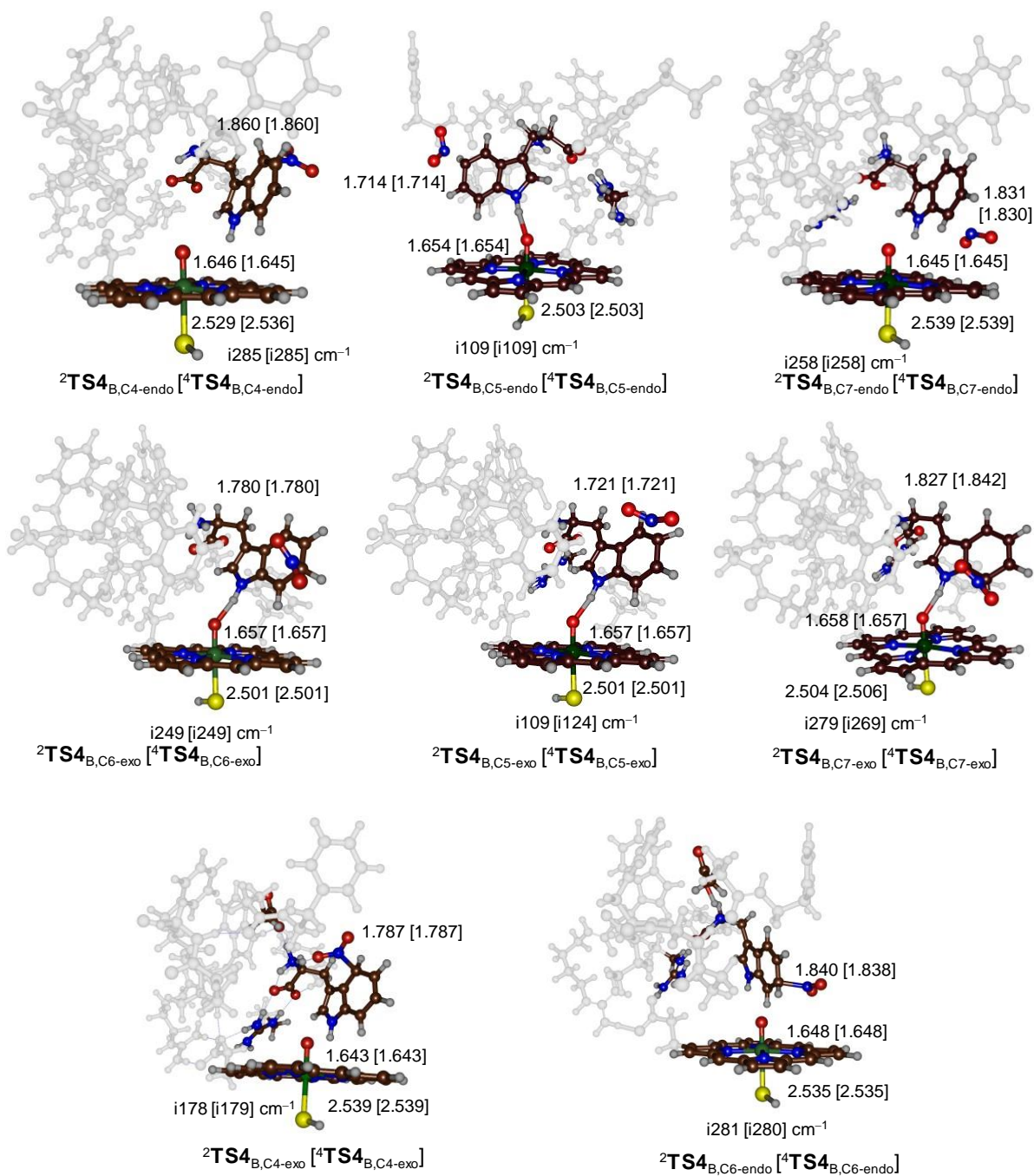


Figure S24: UB3LYP/BS1 optimized transition state geometries for NO₂ attack on L-Trp substrate via ${}^2,{}^4\text{TS4}_{\text{B}}$. N–C bond formation barriers calculated for attack on the C⁴, C⁵, C⁶ and C⁷-positions. Bond lengths are in angstroms and the imaginary frequency in the transition state in cm⁻¹.

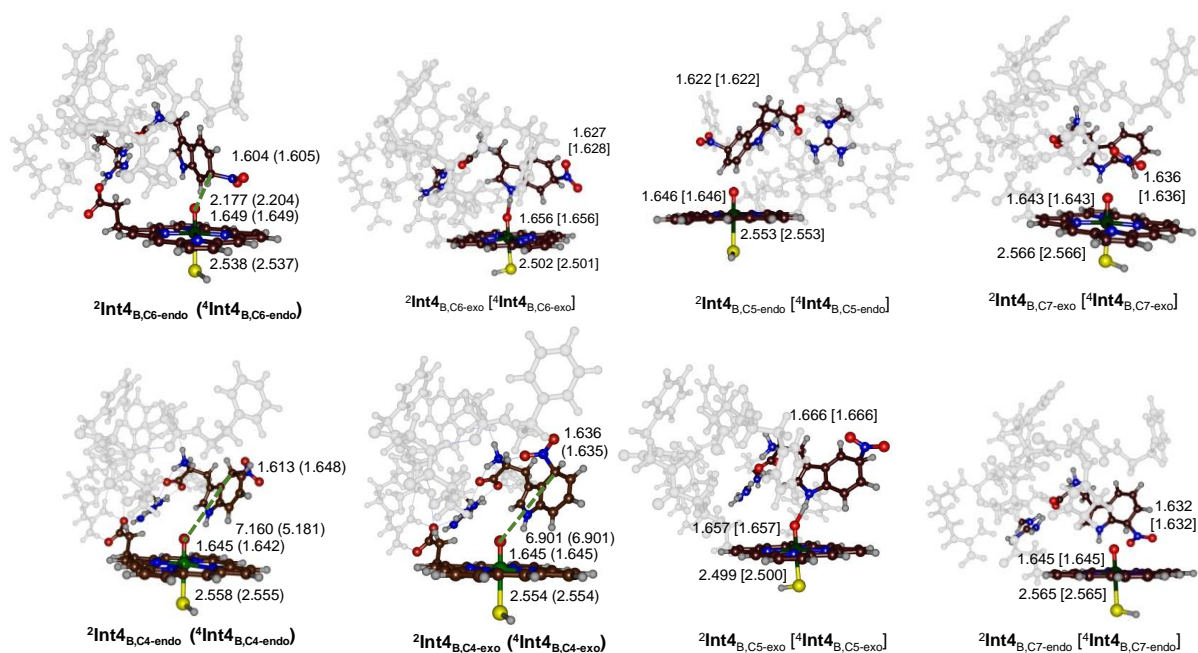


Figure S25: UB3LYP/BS1 optimized transition state geometries for NO₂ attack on L-Trp substrate via ^{2,4}Int4_B. N–C bond formation calculated for attack on the C⁴, C⁵, C⁶ and C⁷-positions. Bond lengths are in angstroms.

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 Re _B	-6677.060921	2.049469	-6675.212340	-6678.806670	0.375488
² TS1 _B	-6677.052201	2.049078	-6675.204844	-6678.800153	0.374037
² Int1 _B	-6677.056943	2.047748	-6675.215182	-6678.805779	0.379619
⁴ Re _B	-6677.045210	2.047408	-6675.202362	-6678.795184	0.375934
⁴ TS1 _B	-6677.030813	2.047526	-6675.185986	-6678.779820	0.371348
⁴ Int1 _B	-6677.056916	2.047740	-6675.216449	-6678.805556	0.379652
Pathway C4-endo:					
² TS4 _{B,C4-endo}	-6677.049204	2.049851	-6675.202993	-6678.796562	0.376604
² Int4 _{B,C4-endo}	-6677.049140	2.050807	-6675.202181	-6678.797819	0.370501
² TS5 _{B,C4-endo}	-6677.045271	2.047227	-6675.195421	-6678.786938	0.412531
² Int5 _{B,C4-endo}	-6677.148981	2.053599	-6675.292449	-6678.889153	0.408725
⁴ TS4 _{B,C4-endo}	-6677.063982	2.049926	-6675.218339	-6678.811947	0.376650
⁴ Int4 _{B,C4-endo}	-6677.066903	2.050787	-6675.216600	-6678.810851	0.374258
⁴ Int5 _{B,C4-endo}	-6677.091156	2.049539	-6675.239285	-6678.830437	0.409153
Pathway C4-oxo:					
² TS4 _{B,C4-oxo}	-6677.071584	2.050842	-6675.221058	-6678.815380	0.377088
² Int4 _{B,C4-oxo}	-6677.070616	2.051379	-6675.219694	-6678.814071	0.376689
² Int5 _{B,C4-oxo}	-6677.158908	2.052011	-6675.308455	-6678.901643	0.401059
⁴ TS4 _{B,C4-oxo}	-6677.071572	2.050842	-6675.221707	-6678.815366	0.377051
⁴ Int4 _{B,C4-oxo}	-6677.070613	2.051357	-6675.220457	-6678.814071	0.376705
⁴ Int5 _{B,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
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-endo:						
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-exo:						
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	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}
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}	$\rho_{\text{Subs}(\text{NO}_2)}$	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 Int5 _{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

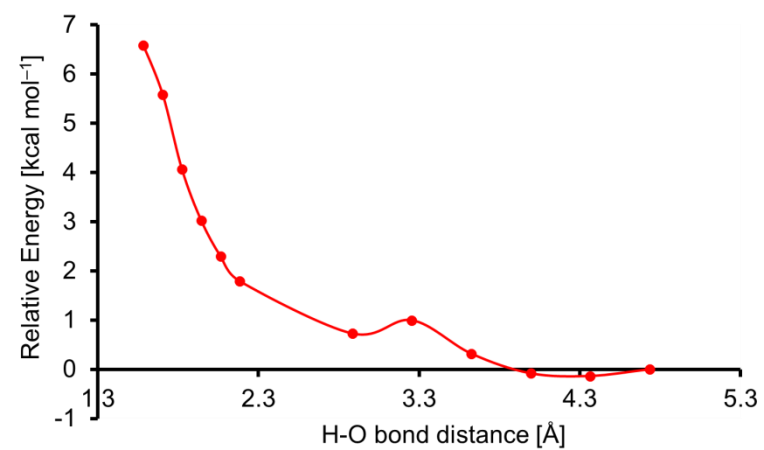


Figure S26: UB3LYP/BS1 geometry scan for proton transfer for Pathway C4-exo between the substrate to apical oxo of P450, as obtained in Gaussian-09. All points refer to a full geometry optimization. Energies are relative to ²Int4_{C4-oxo}.

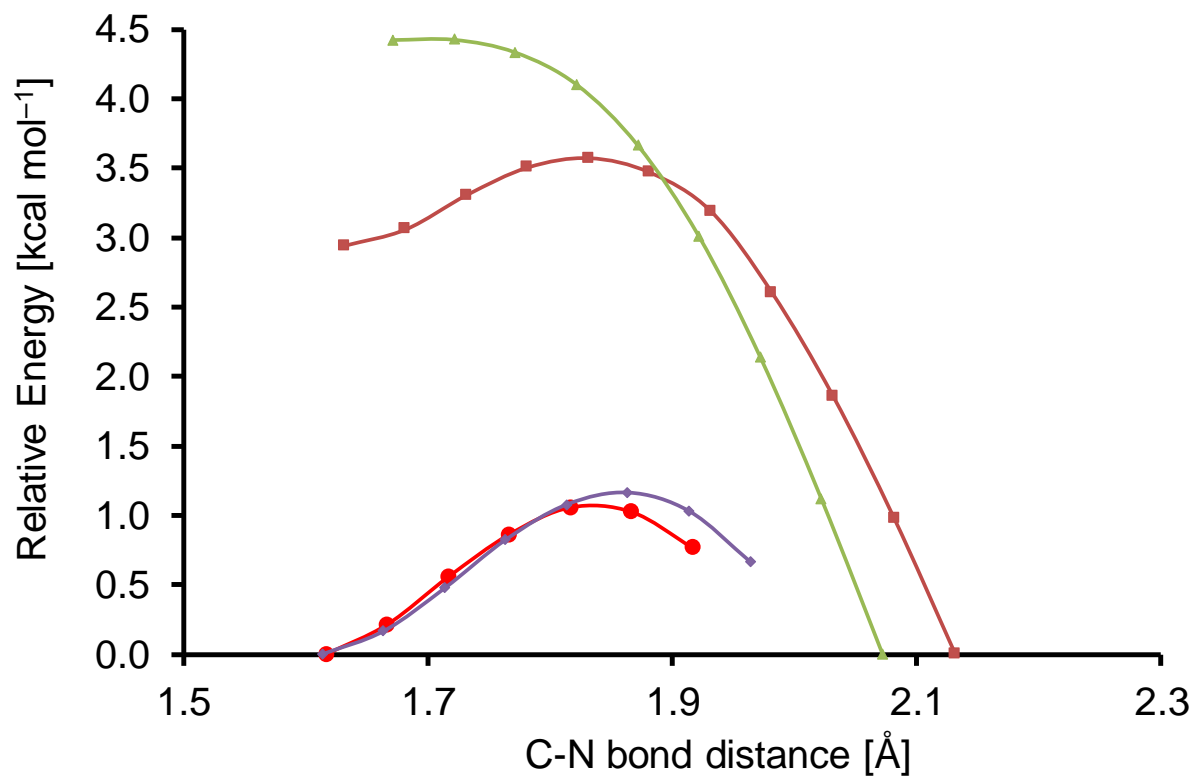


Figure S27: UB3LYP/BS1 geometry scan for NO₂ attack on a carbon position, -C⁴ (in purple), -C⁵ (in green), -C⁶ (in red), -C⁷ (in wine-red), of L-Trp substrate starting from ^{4,2}Int1_B as obtained in Gaussian-09. All points refer to a full geometry optimization. Energies are relative to ²Re.

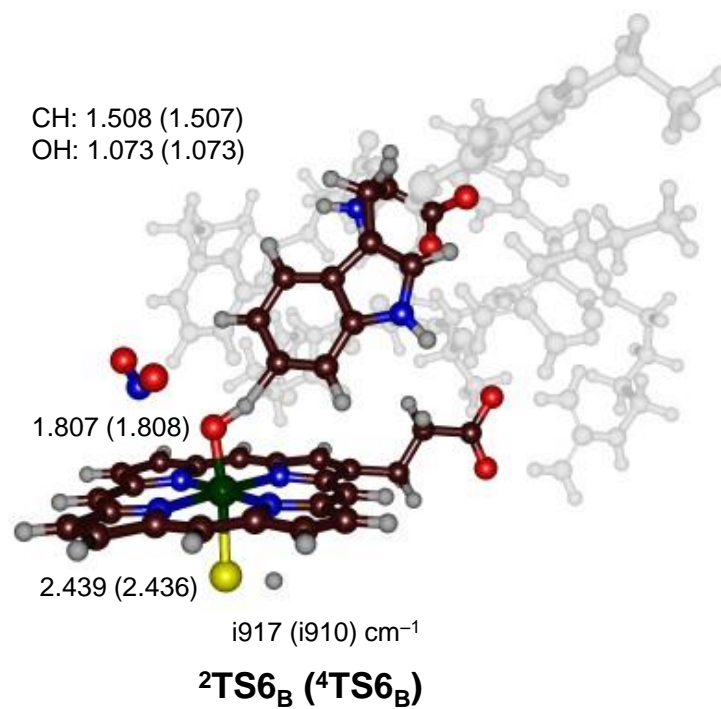


Figure S28: UB3LYP/BS1 optimized geometries of transition states ^{4,2}TS_{6B} for direct hydrogen atom abstraction from L-Trp from ^{4,2}Int1_B as obtained in Gaussian-09. Bond lengths are in angstroms and the imaginary frequency in wavenumbers.

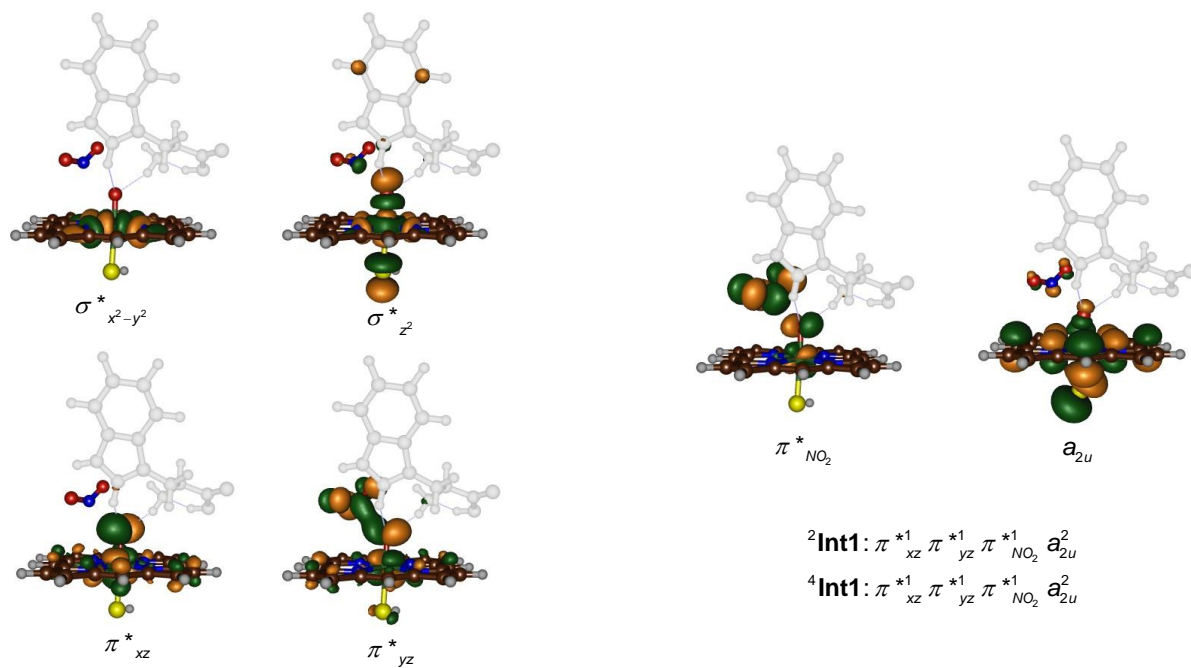


Figure S29: High-lying occupied and low-lying virtual orbitals of ${}^4,2\text{Int1}_B$ as obtained in Gaussian-09.

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_{NO2}	ρ_{Subs}	$\rho_{\text{Subs(NO}_2)}$	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_{NO2}	ρ_{Subs}	$\rho_{\text{Subs(NO}_2)}$	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:

²Re_A:

26	0.394425000	0.130821000	0.203226000
7	0.362866000	-1.135833000	-1.373441000
7	-0.296076000	1.643572000	-0.941584000
7	1.127074000	-1.379214000	1.340969000
7	0.464854000	1.402287000	1.775644000
6	0.746683000	-2.449377000	-1.408179000
6	-0.562825000	2.930696000	-0.560388000
6	-0.046222000	-0.820522000	-2.640222000
6	-0.626741000	1.555919000	-2.265887000
6	1.404843000	-2.664241000	0.957310000
6	0.103959000	2.721302000	1.803125000
6	1.440019000	-1.296846000	2.671187000
6	0.870093000	1.084741000	3.043013000
6	0.576722000	-2.985334000	-2.741160000
6	-1.075953000	3.685595000	-1.681605000
6	0.081785000	-1.973572000	-3.504961000
6	-1.115689000	2.831806000	-2.740819000
6	1.910477000	-3.421531000	2.081088000
6	0.289158000	3.260658000	3.131566000
6	1.931262000	-2.571911000	3.145165000
6	0.765800000	2.244196000	3.901928000
1	0.826813000	-3.997562000	-3.032699000
1	-1.360491000	4.730212000	-1.643914000
1	-0.170583000	-1.984248000	-4.558412000
1	-1.438074000	3.028788000	-3.756130000
1	2.208822000	-4.461876000	2.039414000
1	0.076184000	4.283679000	3.417716000
1	2.251670000	-2.770377000	4.160768000
1	1.026631000	2.257940000	4.953452000
6	1.233265000	-3.173792000	-0.325703000
6	-0.378533000	3.443817000	0.717880000
6	1.324663000	-0.160233000	3.464266000
6	-0.510582000	0.420467000	-3.059312000
1	1.514399000	-4.207597000	-0.500529000
1	-0.632657000	4.487254000	0.881697000
1	1.615481000	-0.253834000	4.506986000
1	-0.804254000	0.512610000	-4.101234000
8	2.230433000	0.502193000	-0.269175000
16	-1.782623000	-0.435035000	0.757867000
1	-1.668187000	-1.775856000	0.619375000
6	5.245934000	-2.198420000	-1.323948000
6	4.975873000	-3.660735000	-1.762234000
7	4.188085000	-1.342138000	-1.877138000
8	3.926723000	-3.775591000	-2.582611000
8	5.656814000	-4.601969000	-1.406543000
1	6.204198000	-1.924869000	-1.784153000
1	4.552251000	-0.527293000	-2.359982000
1	3.541781000	-0.970316000	-1.176966000
6	5.414251000	-2.135237000	0.214194000
6	5.900948000	-0.806749000	0.713895000
1	6.103011000	-2.938420000	0.498244000
1	4.447514000	-2.376251000	0.673870000
6	5.111609000	0.245939000	1.107889000
7	5.903870000	1.321129000	1.465631000
6	7.231169000	0.990864000	1.294518000
6	7.267404000	-0.355074000	0.822592000
1	4.032200000	0.316348000	1.135380000
6	8.394623000	1.734633000	1.515881000
6	8.517713000	-0.949209000	0.576567000
6	9.676895000	-0.211688000	0.794716000
6	9.616211000	1.118357000	1.258640000
1	5.546397000	2.228151000	1.721395000
1	8.347625000	2.760320000	1.874833000
1	10.537923000	1.672465000	1.419305000
1	8.576529000	-1.974601000	0.218796000
1	10.646717000	-0.665403000	0.604798000
1	3.599129000	-2.824784000	-2.655395000

8	2.570138000	1.886164000	-0.222224000
7	3.111083000	2.392800000	-1.385990000
8	3.227863000	1.627738000	-2.297525000

⁴Re_A:

26	0.303950000	0.085358000	0.223202000
7	0.268609000	-1.141056000	-1.376542000
7	-0.365221000	1.613272000	-0.929388000
7	1.137687000	-1.400067000	1.331623000
7	0.383552000	1.324955000	1.816337000
6	0.675523000	-2.450583000	-1.419854000
6	-0.654702000	2.885715000	-0.513914000
6	-0.124749000	-0.815187000	-2.649399000
6	-0.690289000	1.554665000	-2.257672000
6	1.410547000	-2.677680000	0.922913000
6	-0.005516000	2.637676000	1.853986000
6	1.483165000	-1.332860000	2.654890000
6	0.832033000	1.012974000	3.072793000
6	0.517109000	-2.973060000	-2.755402000
6	-1.169778000	3.660672000	-1.618969000
6	0.019033000	-1.958549000	-3.516989000
6	-1.190536000	2.835187000	-2.701525000
6	1.958418000	-3.442695000	2.020376000
6	0.190383000	3.170202000	3.180237000
6	2.003389000	-2.607115000	3.094903000
6	0.711570000	2.162292000	3.936279000
1	0.782775000	-3.978818000	-3.054998000
1	-1.470278000	4.699418000	-1.556210000
1	-0.219568000	-1.963011000	-4.573492000
1	-1.510936000	3.054784000	-3.712613000
1	2.265116000	-4.479200000	1.955860000
1	-0.039854000	4.186273000	3.476812000
1	2.353114000	-2.816983000	4.098252000
1	0.996556000	2.180604000	4.981197000
6	1.198250000	-3.176952000	-0.356059000
6	-0.494779000	3.369602000	0.777375000
6	1.344666000	-0.217284000	3.470647000
6	-0.579823000	0.430365000	-3.065474000
1	1.492690000	-4.202753000	-0.551396000
1	-0.766385000	4.405059000	0.960642000
1	1.661637000	-0.313269000	4.504993000
1	-0.864089000	0.533701000	-4.108454000
8	2.394387000	0.553925000	-0.253784000
16	-2.049095000	-0.557017000	0.931086000
1	-2.338023000	-1.283919000	-0.173460000
6	5.268891000	-2.168460000	-1.241682000
6	4.967947000	-3.648108000	-1.598493000
7	4.216847000	-1.328226000	-1.829695000
8	3.892757000	-3.782955000	-2.380747000
8	5.645195000	-4.581743000	-1.215556000
1	6.231175000	-1.939356000	-1.717870000
1	4.584544000	-0.598032000	-2.430663000
1	3.619373000	-0.839398000	-1.152483000
6	5.448305000	-2.027695000	0.289651000
6	5.997914000	-0.698268000	0.718469000
1	6.104282000	-2.843148000	0.613361000
1	4.475238000	-2.202875000	0.765431000
6	5.259621000	0.422429000	1.011410000
7	6.104158000	1.469736000	1.331723000
6	7.414259000	1.051441000	1.236953000
6	7.384783000	-0.322588000	0.852952000
1	4.183687000	0.551396000	0.981212000
6	8.611920000	1.738730000	1.457787000
6	8.604952000	-1.003079000	0.694808000
6	9.798322000	-0.321794000	0.912324000
6	9.802507000	1.036852000	1.288992000
1	5.795483000	2.410178000	1.521157000
1	8.614314000	2.786651000	1.749651000
1	10.749933000	1.545311000	1.451280000
1	8.614447000	-2.050861000	0.403404000
1	10.744916000	-0.842880000	0.789719000
1	3.584621000	-2.823420000	-2.481997000
8	2.652927000	1.935573000	-0.415277000
7	3.040110000	2.333910000	-1.676191000
8	3.117405000	1.467960000	-2.503724000

² 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	2.123942000
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

⁴ TS1A:			
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
6	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	-4.402574000	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

Int1A:			7	0.202757000	-1.215381000	-1.480273000	
26	0.507756000	0.038586000	0.187520000	7	-0.110154000	1.573042000	-0.919797000
7	0.308960000	-1.215840000	-1.389825000	7	1.023951000	-1.676346000	1.223675000
7	-0.145879000	1.577406000	-0.948768000	7	0.635927000	1.094481000	1.808495000
7	1.053883000	-1.535464000	1.352344000	6	0.437046000	-2.560738000	-1.570248000
7	0.521009000	1.247282000	1.806729000	6	-0.230847000	2.852422000	-0.455989000
6	0.632719000	-2.546113000	-1.424267000	6	-0.168081000	-0.800391000	-2.731102000
6	-0.339265000	2.870112000	-0.546004000	6	-0.447519000	1.604247000	-2.243531000
6	-0.051967000	-0.870545000	-2.663266000	6	1.143032000	-2.958301000	0.761399000
6	-0.464306000	1.531969000	-2.277782000	6	0.413906000	2.441809000	1.892146000
6	1.270635000	-2.821822000	0.943593000	6	1.377428000	-1.705109000	2.544246000
6	0.245376000	2.586060000	1.832591000	6	1.034767000	0.686177000	3.051381000
6	1.347339000	-1.495172000	2.685879000	6	0.190136000	-3.017259000	-2.919219000
6	0.880991000	0.897330000	3.079943000	6	-0.657667000	3.728989000	-1.525422000
6	0.456111000	-3.064037000	-2.762095000	6	-0.186950000	-1.924690000	-3.639054000
6	-0.787903000	3.674473000	-1.661300000	6	-0.792240000	2.954136000	-2.635693000
6	0.027063000	-2.024508000	-3.529800000	6	1.597685000	-3.829374000	1.823985000
6	-0.866543000	2.843863000	-2.735888000	6	0.672258000	2.901392000	3.238012000
6	1.721553000	-3.627390000	2.058970000	6	1.741452000	-3.051438000	2.930833000
6	0.429770000	3.102881000	3.169347000	6	1.057887000	1.811925000	3.256727000
6	1.766189000	-2.803654000	3.140949000	1	0.304296000	-4.041571000	-3.9251888000
6	0.823762000	2.054734000	3.943680000	1	-0.827312000	4.793587000	-1.418496000
1	0.655819000	-4.087083000	-3.054678000	1	-0.449703000	-1.864351000	-4.688283000
1	-1.011779000	4.732950000	-1.606190000	1	-1.096349000	3.247609000	-3.633226000
1	-0.207691000	-2.017355000	-4.587272000	1	1.783121000	-4.890283000	1.712398000
1	-1.167553000	3.075896000	-3.750316000	1	0.568662000	3.927762000	3.568668000
1	1.966978000	-4.680389000	1.997884000	1	2.064443000	-3.341409000	3.923196000
1	0.273620000	4.135469000	3.457189000	1	1.337510000	1.755570000	5.002629000
1	2.055355000	-3.038708000	4.157996000	6	0.871041000	-3.379942000	-3.379942000
1	1.059540000	2.045625000	5.000924000	6	0.011138000	3.265377000	0.847691000
6	1.081215000	-3.301677000	-0.346696000	6	1.382544000	-0.613195000	3.402903000
6	-0.155044000	3.350790000	0.743217000	6	-0.477283000	0.505832000	-3.093680000
6	1.265657000	-0.370886000	3.497577000	1	1.035360000	-4.428072000	-0.761869000
6	-0.422742000	0.401521000	-3.082830000	1	-0.123432000	4.320073000	1.069851000
1	1.315112000	-4.344780000	-0.534005000	1	1.685071000	-0.788052000	4.431324000
1	-0.343591000	4.406372000	0.915793000	1	-0.762415000	0.681361000	-4.127152000
1	1.529185000	-0.491303000	4.544412000	8	2.092727000	0.232110000	-0.276687000
1	-0.695322000	0.521997000	-4.127374000	16	-1.823745000	-0.361090000	0.796518000
8	2.107225000	0.323662000	-0.168140000	1	-2.269786000	-0.935625000	-0.344435000
16	-1.809157000	-0.417872000	0.814419000	6	5.167058000	-2.313363000	-0.818986000
1	-2.017740000	-1.485498000	0.010317000	6	4.878437000	-3.829043000	-0.941520000
6	5.142204000	-2.216263000	-1.174318000	7	4.135895000	-1.580142000	-1.567757000
6	4.839035000	-3.693057000	-1.525207000	8	3.932272000	-4.109225000	-1.846959000
7	4.094859000	-1.371797000	-1.765884000	8	5.470786000	-4.680628000	-0.310708000
8	3.862192000	-3.826128000	-2.431197000	1	6.126090000	-2.162353000	-1.333212000
8	5.443271000	-4.634738000	-1.053473000	1	4.522422000	-0.772277000	-2.047904000
1	6.086787000	-1.986774000	-1.685890000	1	3.395960000	-1.200904000	-0.965279000
1	4.468279000	-0.498584000	-2.126805000	6	5.350094000	-1.901771000	0.662306000
1	3.375619000	-1.091486000	-1.091279000	6	5.832141000	-0.488025000	0.813650000
6	5.370551000	-2.050482000	0.348692000	1	6.046216000	-2.612712000	1.120219000
6	5.857397000	-0.679613000	0.719677000	1	4.389163000	-2.030541000	1.175938000
1	6.079530000	-2.824290000	0.662186000	6	5.033268000	0.627981000	0.866330000
1	4.425827000	-2.267331000	0.862934000	7	5.812139000	1.767922000	0.930645000
6	5.061151000	0.409390000	0.977965000	6	7.143108000	1.413151000	0.888713000
7	5.843535000	1.524803000	1.211499000	6	7.194918000	-0.012521000	0.827392000
6	7.172884000	1.185038000	1.080471000	1	3.952641000	0.693565000	0.839602000
6	7.220837000	-0.209981000	0.780773000	6	8.299022000	2.200143000	0.910596000
1	3.979935000	0.475913000	0.988259000	6	8.453212000	-0.639189000	0.796169000
6	8.330188000	1.959853000	1.207899000	6	9.604477000	0.141613000	0.816994000
6	8.476954000	-0.820190000	0.617434000	6	9.528694000	1.548496000	0.871144000
6	9.629743000	-0.051706000	0.743479000	1	5.436109000	2.698301000	0.822668000
6	9.557467000	1.326339000	1.033229000	1	8.239304000	3.285253000	0.955558000
1	5.470397000	2.459850000	1.277648000	1	10.444604000	2.134569000	0.884439000
1	8.273430000	3.022035000	1.434969000	1	8.525403000	-1.723702000	0.754653000
1	10.474464000	1.903705000	1.124104000	1	10.580062000	-0.338232000	0.790693000
1	8.545761000	-1.882329000	0.393678000	1	3.641022000	-3.197607000	-2.153733000
1	10.603694000	-0.518505000	0.616224000	8	3.356060000	3.136159000	-0.473141000
1	3.567470000	-2.877879000	-2.584876000	7	3.129178000	2.375783000	-1.390746000
8	3.346046000	3.051326000	-0.150256000	8	3.884089000	1.886648000	-2.198264000
7	3.084702000	2.295434000	-1.060270000				
8	3.751480000	1.974647000	-2.016799000				

Int1A:
26 0.507528000 -0.046551000 0.142960000

²TS2A:

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	3.566110000	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	-3.6111379000	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	0.4331037000
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	1.214209000
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

²Int2A:

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	3.999475000	0.508837000	-4.308408000
1	1.653868000	4.821535000	-2.461137000
1	2.187912000	-4.878748000	0.502224000
1	-1.651633000	2.688739000	3.872835000
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	2.250330000	-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

⁴ TS2A:			
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

⁴ Int2A:			
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	0.250503000
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	0.250501000
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	3.090950000	-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	-4.637105000
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	-4.1834857000
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	-0.636631000	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

²TS4A:

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

⁴TS4A:

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

² Int4A:			
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

⁴ Int4A:			
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	-4.774875000
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

² TS5A:			
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

⁴ TS5A:			
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	0.710006000	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:			
26	1.374842000	-0.553541000	-1.042298000
7	1.326712000	-1.097535000	-2.982561000
7	0.385737000	1.171773000	-1.453939000
7	2.383215000	-2.252957000	-0.616524000
7	1.435682000	0.011772000	0.916264000
6	1.880632000	-2.209073000	-3.551191000
6	0.025809000	2.168255000	-0.584978000
6	0.742557000	-0.391469000	-3.995667000
6	-0.082018000	1.544065000	-2.684796000
6	2.793253000	-3.218679000	-1.492149000
6	0.967960000	1.172531000	1.469840000
6	2.786144000	-2.660947000	0.625148000
6	1.983424000	-0.716447000	1.936657000
6	1.635444000	-2.213320000	-4.978708000
6	-0.691073000	3.208165000	-1.290375000
6	0.925834000	-1.086297000	-5.254159000
6	-0.760979000	2.818831000	-2.593095000
6	3.482746000	-4.276890000	-0.783411000
6	1.241901000	1.191139000	2.889113000
6	3.475005000	-3.932265000	0.532446000
6	1.868869000	0.012877000	3.181470000
1	1.972972000	-2.983875000	-5.661114000
1	-1.085062000	4.107323000	-0.831985000
1	0.558236000	-0.736353000	-6.211263000
1	-1.222614000	3.333609000	-3.427144000
1	3.909619000	-5.156733000	-1.249330000
1	0.963917000	1.992827000	3.563117000
1	3.896562000	-4.468743000	1.373838000
1	2.207911000	-0.350367000	4.144747000
6	2.568933000	-3.203660000	-2.865431000
6	0.307790000	2.184790000	0.777092000
6	2.599671000	-1.958967000	1.811053000
6	0.080710000	0.824815000	-3.865007000
1	2.955018000	-4.037141000	-3.445408000
1	-0.025231000	3.047503000	1.347430000
1	2.986753000	-2.412227000	2.719513000
1	-0.339126000	1.257930000	-4.768835000
8	3.024029000	0.319814000	-1.349148000
16	-0.689450000	-1.602403000	-0.683501000
1	-0.372261000	-2.829954000	-1.156457000
6	6.905546000	0.776038000	-2.039385000
6	7.607109000	0.141529000	-3.267891000
7	5.581032000	1.262467000	-2.457887000
8	6.945775000	0.351390000	-4.410802000
8	8.660178000	-0.457800000	-3.200508000
1	7.522268000	1.645305000	-1.773909000
1	5.396627000	2.187613000	-2.082060000
1	4.792775000	0.670269000	-2.150266000
6	6.924127000	-0.209248000	-0.847644000
6	6.447657000	0.379266000	0.450592000
1	7.947235000	-0.587798000	-0.754629000
1	6.296930000	-1.070928000	-1.109474000
6	5.134501000	0.495368000	0.834405000
7	5.056983000	1.090707000	2.082855000
6	6.316264000	1.362750000	2.542351000
6	7.234320000	0.932728000	1.527417000
1	4.238469000	0.231005000	0.275396000
6	6.746079000	1.939830000	3.745411000
6	8.604939000	1.100383000	1.746117000
6	9.013200000	1.679689000	2.946950000
6	8.107777000	2.098892000	3.944274000
1	4.188894000	1.212165000	2.589798000
1	6.034219000	2.256939000	4.502725000
1	8.498682000	2.539883000	4.851873000
1	9.348601000	0.794939000	1.019484000
1	2.801711000	1.253716000	-1.195792000
1	6.126813000	0.846160000	-4.102546000
8	11.233831000	1.499082000	2.314455000
7	10.439619000	1.862336000	3.187807000
8	10.789731000	2.374291000	4.258375000

⁴ Int5A:			
26	1.436713000	-0.617310000	-1.053266000
7	1.208319000	-1.156235000	-2.949351000
7	0.436015000	1.267443000	-1.477111000
7	2.484442000	-2.434033000	-0.639721000
7	1.533439000	-0.112190000	0.878759000
6	1.703532000	-2.302789000	-3.520223000
6	0.095533000	2.211810000	-0.563552000
6	0.619147000	-0.412437000	-3.943150000
6	-0.091918000	1.630599000	-2.672033000
6	2.769694000	-3.405652000	-1.537812000
6	1.083891000	1.061257000	1.435598000
6	2.924665000	-2.844216000	0.574915000
6	2.126468000	-0.852900000	1.871868000
6	1.394962000	-2.293648000	-4.933643000
6	-0.669109000	3.263489000	-1.217229000
6	0.727212000	-1.133527000	-5.193124000
6	-0.786497000	2.901576000	-2.528601000
6	3.456606000	-4.502088000	-0.867284000
6	1.405319000	1.061249000	2.845186000
6	3.552394000	-4.152837000	0.447425000
6	2.044153000	-0.119589000	3.114574000
1	1.669642000	-3.078303000	-5.628259000
1	-1.070670000	4.145251000	-0.731284000
1	0.345825000	-0.778532000	-6.143073000
1	-1.302074000	3.430624000	-3.321800000
1	3.807342000	-5.410129000	-1.343588000
1	1.149956000	1.856486000	3.535947000
1	3.997062000	-4.718982000	-1.257460000
1	2.418818000	-0.476185000	4.066951000
6	2.409345000	-3.334790000	-2.887427000
6	0.423891000	2.120295000	0.791946000
6	2.758379000	-2.099834000	1.745163000
6	0.014206000	0.846822000	-3.826568000
1	2.701465000	-4.167518000	-3.522257000
1	0.122984000	2.946961000	1.431041000
1	3.160293000	-2.522160000	2.662648000
1	-0.422176000	1.247461000	-4.738274000
8	3.087027000	0.266777000	-1.443878000
16	-0.696909000	-1.633979000	-0.483327000
1	-1.019919000	-2.069367000	-1.722109000
6	6.999624000	0.793502000	-2.015519000
6	7.730568000	0.125767000	-3.207126000
7	5.677747000	1.251049000	-2.473777000
8	7.106589000	0.317336000	-4.375245000
8	8.775826000	-0.479909000	-3.096686000
1	7.599390000	1.681231000	-1.772666000
1	5.455925000	2.161109000	-2.080818000
1	4.903811000	0.630739000	-2.189252000
6	7.003617000	-0.142873000	-0.785752000
6	6.476454000	0.491053000	0.471216000
1	8.030156000	-0.496410000	-0.645538000
1	6.401860000	-1.027634000	-1.030587000
6	5.149258000	0.645688000	0.790144000
7	5.029079000	1.273475000	2.019255000
6	6.271569000	1.527588000	2.530955000
6	7.225066000	1.054877000	1.569557000
1	4.270073000	0.384104000	0.203000000
6	6.658416000	2.124692000	3.738894000
6	8.587573000	1.201394000	1.846196000
6	8.953220000	1.802084000	3.050242000
6	8.012640000	2.262403000	3.995637000
1	4.143619000	1.396800000	2.495026000
1	5.919704000	2.474093000	4.455161000
1	8.371333000	2.717923000	4.909328000
1	9.356986000	0.863725000	1.161887000
1	2.771172000	1.168143000	-1.629026000
1	6.281862000	0.821574000	-4.106330000
8	11.195882000	1.563754000	2.523423000
7	10.370728000	1.964104000	3.350716000
8	10.682748000	2.496888000	4.422889000

Large model structures:

⁴FeOO+NO:

26	-2.580902000	-4.949569000	-4.292668000
7	-2.915750000	-4.448410000	-2.360324000
7	-2.236514000	-6.866019000	-3.785016000
7	-2.169814000	-5.421045000	-6.217587000
7	-2.831274000	-3.003484000	-4.793787000
6	-3.284906000	-3.229964000	-1.852818000
6	-3.550501000	-3.332031000	-0.423323000
6	-3.306752000	-4.633836000	-0.098643000
6	-2.918617000	-5.318947000	-1.307932000
6	-2.304358000	-7.383645000	-2.521249000
6	-1.998963000	-8.797765000	-2.544941000
6	-1.744057000	-9.121579000	-3.841308000
6	-1.893151000	-7.904429000	-4.608035000
6	-1.843510000	-6.648153000	-6.726567000
6	-1.643782000	-6.560981000	-8.155755000
6	-1.847714000	-5.259920000	-8.498142000
6	-2.172819000	-4.554873000	-7.277658000
6	-2.742054000	-2.480899000	-6.056314000
6	-3.021612000	-1.062886000	-6.027422000
6	-3.294484000	-0.745101000	-4.727117000
6	-3.174616000	-1.967914000	-3.968524000
6	-3.398134000	-2.064228000	-2.597708000
6	-2.626778000	-6.676362000	-1.370498000
6	-1.715676000	-7.815778000	-5.982972000
6	-2.435594000	-3.192611000	-7.211680000
1	-3.683546000	-1.152650000	-2.081218000
1	-2.655313000	-7.232595000	-0.437764000
1	-1.446750000	-8.723966000	-6.514767000
1	-2.399256000	-2.634279000	-8.142994000
1	-3.403286000	-5.103887000	0.873553000
1	-1.981178000	-9.438688000	-1.671751000
1	-1.471686000	-10.083672000	-4.258086000
1	-1.374233000	-7.394281000	-8.793284000
1	-1.781449000	-4.800143000	-9.476805000
1	-3.024913000	-0.414164000	-6.895394000
1	-3.538767000	0.221268000	-4.304032000
6	-4.039237000	-2.244687000	0.491160000
6	-2.935922000	-1.293790000	1.031453000
6	-3.509864000	-0.388154000	2.115340000
8	-3.605458000	0.883781000	1.872141000
8	-3.891060000	-0.912362000	3.185195000
1	-4.524629000	-2.705236000	1.358548000
1	-4.804807000	-1.641605000	-0.016275000
1	-2.139712000	-1.899940000	1.476330000
1	-2.504974000	-0.698435000	0.221480000
16	-4.857891000	-5.341889000	-4.595605000
1	-4.755094000	-6.488344000	-5.307032000
6	5.535536000	0.430375000	2.556962000
6	5.607967000	0.961923000	3.991018000
8	5.116293000	0.340178000	4.928809000
6	4.099958000	0.096279000	2.103464000
6	3.243187000	1.186764000	1.461257000
8	2.033387000	0.959690000	1.276952000
7	3.832994000	2.308374000	1.019988000
7	6.274190000	2.142512000	4.169897000
6	6.517979000	2.650239000	5.508113000
6	5.294770000	3.208242000	6.254171000
8	5.316173000	3.378412000	7.472411000
7	4.263293000	3.524426000	5.447632000
6	2.930389000	3.855538000	5.886744000
6	2.060302000	3.700842000	4.622633000
8	2.553879000	3.352147000	3.553064000
6	2.835288000	5.238639000	6.594150000
6	3.399130000	6.397376000	5.804037000
6	4.760630000	6.719278000	5.908880000
6	2.590861000	7.161198000	4.951811000
6	5.301952000	7.772837000	5.171078000
6	3.128781000	8.216051000	4.211547000
6	4.487043000	8.522070000	4.318167000
7	0.725785000	3.903489000	4.766218000
6	-0.137029000	3.938236000	3.599107000
6	-1.203081000	5.012028000	3.879431000

8	-1.219270000	5.639384000	4.943266000
6	-0.699704000	2.523152000	3.279068000
8	-1.434271000	2.620447000	2.038590000
6	-1.558485000	1.956354000	4.405121000
7	-2.078118000	5.244568000	2.871885000
6	-2.936242000	6.406141000	2.865427000
6	-4.384006000	6.022466000	3.158446000
8	-4.889484000	4.958904000	2.758035000
6	-2.858071000	7.155845000	1.493483000
6	-1.496590000	7.680479000	1.182158000
6	-0.558815000	7.058979000	0.379816000
6	-0.873436000	8.879087000	1.676926000
7	0.597984000	7.784142000	0.336729000
6	0.444719000	8.899554000	1.125442000
6	-1.278595000	9.942923000	2.503555000
6	1.341489000	9.941941000	1.390509000
6	-0.389251000	10.979767000	2.764679000
6	0.910430000	10.977886000	2.214489000
7	-5.123959000	6.943465000	3.817460000
6	-6.543032000	6.764239000	4.094107000
6	-6.826537000	6.289337000	5.533819000
6	-6.258141000	4.905961000	5.897131000
6	-7.030070000	3.749087000	5.243382000
7	-6.487262000	2.422856000	5.530612000
6	-5.653896000	1.722091000	4.718218000
7	-5.167416000	2.263385000	3.604903000
7	-5.333019000	0.462329000	5.033085000
1	3.538586000	-0.293613000	2.958013000
1	4.124006000	-0.715770000	1.365911000
1	4.773460000	2.536149000	1.307911000
1	3.244615000	3.115760000	0.742282000
1	6.059341000	1.086612000	1.853626000
1	6.103220000	-0.508196000	2.575841000
1	6.651998000	2.650746000	3.372189000
1	6.919872000	1.858997000	6.148473000
1	7.269327000	3.443869000	5.440851000
1	4.319837000	3.278764000	4.464278000
1	2.587582000	3.105253000	6.615433000
1	3.385651000	5.124657000	7.532580000
1	1.786986000	5.430106000	6.858291000
1	5.389438000	6.141369000	6.581682000
1	1.529962000	6.934299000	4.868131000
1	6.358214000	8.013771000	5.268915000
1	2.487412000	8.796498000	3.555659000
1	4.905524000	9.345200000	3.744111000
1	0.370200000	4.435699000	5.554207000
1	0.456569000	4.255304000	2.731038000
1	0.174409000	1.881724000	3.115346000
1	-0.975260000	1.914276000	5.329883000
1	-1.895518000	0.941592000	4.172304000
1	-2.442832000	2.581365000	4.577065000
1	-2.156787000	1.944030000	2.017291000
1	-2.045905000	4.621778000	2.070619000
1	-2.568549000	7.065395000	3.657101000
1	-3.602309000	7.963827000	1.516813000
1	-3.177413000	6.454073000	0.715031000
1	-0.669743000	6.159472000	-0.212175000
1	-2.280001000	9.963987000	2.932338000
1	-0.696510000	11.806044000	3.401492000
1	2.338668000	9.930732000	0.959403000
1	1.584092000	11.802056000	2.435788000
1	1.512262000	7.420302000	-0.025201000
1	-4.662145000	7.776822000	4.157507000
1	-6.926149000	6.057459000	3.356504000
1	-7.049543000	7.721231000	3.924613000
1	-6.416441000	7.032037000	6.229820000
1	-7.915423000	6.298615000	5.686669000
1	-6.295157000	4.781397000	6.987243000
1	-5.199943000	4.849423000	5.618203000
1	-8.072911000	3.758432000	5.583723000
1	-7.052929000	3.861684000	4.157245000
1	-6.648288000	2.038586000	6.450997000
1	-5.084905000	3.273932000	3.493935000
1	-4.539337000	1.683703000	2.988523000
1	-5.931196000	-0.057085000	5.660091000

1	-4.733653000	-0.084844000	4.358077000	6	-1.419716000	3.458336000	-1.594363000
6	-7.148024000	7.828233000	-0.284893000	8	-1.882508000	4.626533000	-1.747389000
6	-5.938338000	6.891796000	-0.182028000	6	0.971411000	3.110263000	-2.483521000
6	-6.044480000	5.647975000	-1.079064000	6	0.805950000	1.787183000	-3.178875000
7	-4.982889000	4.657066000	-0.846830000	6	-0.148899000	1.455296000	-4.114917000
6	-5.159153000	3.501279000	-0.191360000	6	1.539215000	0.568390000	-2.908499000
7	-4.364518000	2.463309000	-0.380159000	7	-0.051032000	0.124605000	-4.448040000
7	-6.235532000	3.393111000	0.658415000	6	0.953428000	-0.458289000	-3.701689000
1	-7.013977000	8.708367000	0.353623000	6	2.627639000	0.236509000	-2.076550000
1	-8.073857000	7.325304000	0.022858000	6	1.376819000	-1.790437000	-3.651676000
1	-5.817562000	6.568148000	0.857407000	6	3.064061000	-1.084036000	-2.037704000
1	-5.026637000	7.439974000	-0.443358000	6	2.436099000	-2.089419000	-2.803442000
1	-7.002730000	5.142727000	-0.922482000	8	-2.065229000	2.378139000	-1.705861000
1	-5.995310000	5.929751000	-2.135067000	1	0.739679000	3.947219000	-3.153159000
1	-4.099721000	4.754192000	-1.352350000	1	2.005834000	3.259200000	-2.153328000
1	-4.244793000	1.766715000	0.365250000	1	-0.899073000	2.074653000	-4.587635000
1	-3.576331000	2.495448000	-1.069069000	1	3.118019000	0.996190000	-1.473135000
1	-6.280798000	2.503222000	1.141764000	1	3.899617000	-1.351002000	-1.394102000
1	-6.304626000	4.172970000	1.305030000	1	0.887999000	-2.568062000	-4.230300000
1	-7.293091000	8.185037000	-1.311627000	1	2.764772000	-3.122236000	-2.803442000
6	-8.555019000	2.165242000	-3.902891000	1	0.453998000	4.150131000	-0.663286000
6	-7.788940000	2.496889000	-5.197969000	1	-0.470127000	2.230331000	0.489190000
6	-6.561030000	3.342117000	-4.933895000	1	-0.192703000	1.287285000	-0.863021000
6	-5.412362000	2.769899000	-4.370127000	1	1.085563000	1.859687000	0.072243000
6	-6.547390000	4.723915000	-5.164013000	1	-0.750317000	-0.380120000	-4.979032000
6	-4.309348000	3.538717000	-4.005201000	7	2.150856000	-5.307739000	-4.110335000
6	-5.453667000	5.513664000	-4.805772000	8	0.011035000	-5.040772000	-3.137936000
6	-4.335656000	4.931477000	-4.189726000	8	1.941750000	-4.992600000	-5.219413000
8	-3.336753000	5.752648000	-3.775012000				
1	-8.458401000	3.020299000	-5.892960000				
1	-7.501644000	1.558221000	-5.690009000	⁴ Re _B :			
1	-5.381804000	1.695017000	-4.202307000	26	-1.555555000	-4.511456000	-4.281126000
1	-7.414658000	5.197475000	-5.6221534000	7	-2.287204000	-4.191792000	-2.417039000
1	-3.445014000	3.067415000	-3.545825000	7	-1.031406000	-6.392200000	-3.759780000
1	-5.454158000	6.586628000	-4.977856000	7	-0.771690000	-4.809759000	-6.124301000
1	-2.712067000	5.272011000	-3.176214000	7	-1.951417000	-2.586414000	-4.760341000
1	-7.918439000	1.610864000	-3.204488000	6	-2.840609000	-3.034708000	-1.933344000
1	-9.440969000	1.552430000	-4.110536000	6	-3.256878000	-3.216369000	-0.551375000
1	-8.883257000	3.082309000	-3.398821000	6	-2.928605000	-4.502371000	-0.231493000
6	6.994001000	5.915234000	1.497102000	6	-2.324141000	-5.099219000	-1.394416000
6	7.489265000	4.527484000	1.127953000	6	-1.256784000	-6.998727000	-2.552917000
8	7.257180000	3.516312000	1.806424000	6	-0.797489000	-8.367241000	-2.593438000
6	5.751297000	6.353185000	0.680525000	6	-0.300035000	-8.577941000	-3.842709000
6	4.670011000	5.278646000	0.700792000	6	-0.454018000	-7.337946000	-4.566791000
6	3.270995000	5.663387000	0.180200000	6	-0.210581000	-5.964405000	-6.600781000
8	3.086257000	6.854734000	-0.180637000	6	0.234839000	-5.772850000	-7.959447000
8	2.421060000	4.720107000	0.190247000	6	-0.055273000	-4.482687000	-8.289940000
7	8.195714000	4.445020000	-0.025147000	6	-0.679162000	-3.887013000	-7.133605000
6	8.662921000	3.181251000	-0.572884000	6	-1.701445000	-1.970625000	-5.959253000
6	8.748424000	3.219938000	-2.109124000	6	-2.152660000	-0.600428000	-5.913094000
6	7.402328000	3.359449000	-2.788991000	6	-2.678967000	-0.403176000	-4.671926000
6	6.552161000	2.250132000	-2.898730000	6	-2.550915000	-1.653150000	-3.960503000
6	6.959539000	4.591844000	-3.286163000	6	-2.972163000	-1.852117000	-2.649665000
6	5.290004000	2.367525000	-3.479615000	6	-1.854229000	-6.406123000	-1.448869000
6	5.693178000	4.718479000	-3.863036000	6	-0.068774000	-7.149072000	-5.886395000
6	4.855486000	3.606539000	-3.958058000	6	-1.112872000	-2.567799000	-7.066744000
1	5.361516000	7.283710000	1.104633000	1	-3.428949000	-1.002798000	-2.151874000
1	6.033019000	6.580375000	-0.355948000	1	-1.960709000	-7.011546000	-0.553724000
1	4.525319000	4.820546000	1.729236000	1	0.390534000	-7.989375000	-6.398370000
1	5.007981000	4.415730000	0.114692000	1	-0.975595000	-1.952294000	-7.950894000
1	6.736104000	5.887187000	2.560297000	1	-3.081787000	-5.008994000	0.714492000
1	9.239107000	2.292451000	-2.430290000	1	-0.853586000	-9.060238000	-1.763014000
1	9.414659000	4.039904000	-2.413191000	1	0.138499000	-9.479525000	-4.252252000
1	6.881959000	1.282367000	-2.525527000	1	0.714960000	-6.532748000	-8.563689000
1	7.613561000	5.460947000	-3.229429000	1	0.136953000	-3.965310000	-9.221916000
1	4.642499000	1.498573000	-3.548736000	1	-2.063871000	0.108272000	-6.727053000
1	5.361608000	5.684995000	-4.232823000	1	-3.095063000	0.500687000	-4.250527000
1	3.866900000	3.697479000	-4.398285000	6	-3.895601000	-2.194460000	0.344092000
1	7.972231000	2.400698000	-0.244390000	6	-2.902153000	-1.145646000	0.907505000
1	8.298967000	5.280352000	-0.584517000	6	-3.559673000	-0.287928000	1.982675000
1	9.650716000	2.935420000	-0.156350000	8	-3.640498000	0.991911000	1.778411000
1	7.807291000	6.643374000	1.371612000	8	-3.999245000	-0.849591000	3.008802000
8	-0.634243000	-4.560313000	-4.155141000	1	-4.356826000	-2.704037000	1.196540000
7	0.149186000	2.097520000	-0.334573000	1	-4.702493000	-1.670400000	-0.186850000
6	0.069179000	3.301533000	-1.231648000	1	-2.061469000	-1.677682000	1.368161000
				1	-2.505261000	-0.512887000	0.108301000

16	-3.882834000	-5.241745000	-5.016866000	1	-1.004258000	1.900900000	5.295131000
1	-3.687133000	-4.999389000	-6.334120000	1	-1.871436000	0.915414000	4.108067000
6	5.802690000	0.405712000	2.507653000	1	-2.460899000	2.543256000	4.500978000
6	5.754674000	0.930244000	3.944371000	1	-2.122500000	1.978180000	1.969204000
8	5.271713000	0.266390000	4.856825000	1	-2.041674000	4.564504000	2.066935000
6	4.434248000	-0.057028000	1.975092000	1	-2.573800000	7.056729000	3.566144000
6	3.442993000	0.996590000	1.487443000	1	-3.603274000	7.864997000	1.394041000
8	2.250849000	0.672122000	1.333129000	1	-3.233237000	6.307157000	0.665915000
7	3.909595000	2.209222000	1.157187000	1	-0.676904000	5.914641000	-0.265052000
7	6.311795000	2.163325000	4.156563000	1	-2.269609000	9.888325000	2.690007000
6	6.517979000	2.650239000	5.508113000	1	-0.660286000	11.726343000	3.082549000
6	5.286748000	3.195835000	6.244099000	1	2.355108000	9.698171000	0.737920000
8	5.308252000	3.385865000	7.459930000	1	1.623442000	11.645508000	2.127729000
7	4.248151000	3.483633000	5.436959000	1	1.503312000	7.174545000	-0.135858000
6	2.921927000	3.828847000	5.885315000	1	-4.642062000	7.743360000	4.162513000
6	2.039432000	3.665106000	4.633830000	1	-6.940418000	6.075223000	3.347168000
8	2.514459000	3.277093000	3.570310000	1	-7.033096000	7.732665000	3.943046000
6	2.842434000	5.221838000	6.575851000	1	-6.390901000	6.992112000	6.232861000
6	3.385080000	6.373403000	5.760131000	1	-7.913217000	6.308167000	5.689819000
6	4.747018000	6.702107000	5.833308000	1	-6.336027000	4.724159000	6.953172000
6	2.556179000	7.127018000	4.918223000	1	-5.236356000	4.790821000	5.587917000
6	5.268242000	7.751634000	5.075485000	1	-8.137267000	3.775154000	5.525875000
6	3.073911000	8.177494000	4.157485000	1	-7.109985000	3.876047000	4.104724000
6	4.432709000	8.490239000	4.233396000	1	-6.799083000	1.984703000	6.353883000
7	0.709968000	3.902790000	4.776879000	1	-5.119124000	3.301050000	3.498838000
6	-0.137029000	3.938236000	3.599107000	1	-4.557481000	1.729002000	2.957743000
6	-1.216636000	5.000377000	3.868309000	1	-6.094899000	-0.100604000	5.500305000
8	-1.232916000	5.654398000	4.915436000	1	-4.854262000	-0.093760000	4.243041000
6	-0.676560000	2.520881000	3.256277000	6	-7.148024000	7.828233000	-0.284893000
8	-1.369067000	2.615891000	1.991657000	6	-5.940483000	6.888245000	-0.257727000
6	-1.560205000	1.935826000	4.353372000	6	-6.133824000	5.611703000	-1.088475000
7	-2.104294000	5.193770000	2.862327000	7	-4.982473000	4.702776000	-1.015496000
6	-2.953457000	6.361617000	2.811545000	6	-4.973300000	3.538531000	-0.352062000
6	-4.403403000	6.004397000	3.127492000	7	-4.063060000	2.604249000	-0.556540000
8	-4.931696000	4.954708000	2.718136000	7	-5.978979000	3.296533000	0.555505000
6	-2.880002000	7.038196000	1.401950000	1	-6.956479000	8.725319000	0.314001000
6	-1.512079000	7.516979000	1.049528000	1	-8.047372000	7.342098000	0.115225000
6	-0.579063000	6.846236000	0.278869000	1	-5.722671000	6.603887000	0.776576000
6	-0.875094000	8.730589000	1.486362000	1	-5.054105000	7.416588000	-0.627393000
7	0.583465000	7.557237000	0.201773000	1	-7.021573000	5.061452000	-0.761798000
6	0.442913000	8.708648000	0.937680000	1	-6.277308000	5.858854000	-2.144753000
6	-1.267900000	9.834893000	2.264670000	1	-4.222734000	4.885957000	-1.677253000
6	1.355951000	9.746783000	1.161387000	1	-3.927187000	1.890868000	0.169784000
6	-0.363851000	10.868711000	2.483113000	1	-3.303332000	2.631739000	-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	6.497705000	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	0.537246000
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

${}^2\text{Re}_B$							
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	1	2.092552000	6.092457000	6.295511000
6	0.394220000	-2.851910000	0.683514000	6	3.691703000	6.908017000	5.113461000
6	0.911039000	-3.753946000	-0.317139000	6	5.055962000	7.231025000	5.155196000
6	2.700251000	-4.520269000	-1.832729000	6	2.863042000	7.604706000	4.221126000
6	4.049119000	-4.460727000	-2.348212000	6	5.582089000	8.222399000	4.323631000
6	4.110712000	-5.339953000	-3.387252000	6	3.385179000	8.596245000	3.387807000
6	2.802365000	-5.944336000	-3.501779000	6	4.747134000	8.907683000	3.436850000
6	1.234911000	-7.548770000	-4.550574000	1	5.705676000	6.709636000	5.853982000
6	0.937130000	-8.590974000	-5.508288000	1	1.800187000	7.373760000	4.188559000
6	-0.347362000	-8.981835000	-5.276898000	1	6.640494000	8.465330000	4.375215000
6	-0.836601000	-8.172641000	-4.183420000	1	2.729194000	9.128811000	2.705057000
6	-2.603597000	-7.456080000	-2.620243000	1	5.152179000	9.683280000	2.792323000
6	-3.954957000	-7.504978000	-2.110750000	6	2.247254000	4.232343000	4.223728000
6	-4.050224000	-6.531399000	-1.162400000	8	2.729350000	4.235239000	3.085134000
6	-2.753624000	-5.894918000	-1.084887000	7	0.932133000	4.063724000	4.482928000
6	-2.457148000	-4.838512000	-0.226177000	1	0.616559000	4.252571000	5.426285000
6	2.221338000	-3.742985000	-0.783086000	6	-0.080918000	4.122616000	3.449378000
6	2.468939000	-6.914763000	-4.440660000	1	0.438573000	4.316406000	2.505571000
6	-2.116236000	-8.260556000	-3.644301000	6	-0.800577000	2.757429000	3.291212000
1	-3.270832000	-4.476875000	0.393903000	1	-0.000293000	2.014431000	3.159378000
1	2.913382000	-3.047871000	-0.317025000	8	-1.571525000	2.853153000	2.094508000
1	3.245734000	-7.218265000	-5.136247000	1	-2.185964000	2.082814000	2.027248000
1	-2.792064000	-8.995335000	-4.071430000	6	-1.654910000	2.368644000	4.499178000
1	0.978914000	-2.094171000	1.194400000	1	-1.046235000	2.303820000	5.407991000
1	4.830196000	-3.819671000	-1.958548000	1	-2.111674000	1.386864000	4.336918000
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1	1.633389000	-8.964012000	-6.249235000	6	-0.983241000	5.341854000	3.735177000
1	-0.925620000	-9.740536000	-5.789523000	8	-0.691135000	6.159250000	4.613961000
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6	-1.926035000	-2.392924000	1.705262000	6	-2.945767000	6.590812000	2.965880000
6	-2.392948000	-1.046022000	1.112269000	1	-2.596144000	7.236184000	3.774845000
6	-3.434772000	-0.309231000	1.963464000	6	-2.932400000	7.372549000	1.615431000
8	-3.544875000	0.963057000	1.770657000	1	-3.642785000	8.204121000	1.703808000
8	-4.130353000	-0.955434000	2.777215000	1	-3.336778000	6.692945000	0.858602000
1	-1.465137000	-2.201389000	2.682117000	6	-1.595697000	7.871588000	1.161641000
1	-2.807332000	-3.009969000	1.902278000	6	-0.715390000	7.165647000	0.369620000
1	-1.539778000	-0.378416000	0.950063000	7	0.392698000	7.921393000	0.079284000
1	-2.840183000	-1.210465000	0.121409000	1	-0.811564000	6.155964000	-0.007879000
16	0.760054000	-7.743023000	-0.826271000	1	1.169922000	7.607186000	-0.523005000
1	1.538549000	-7.035955000	0.024855000	6	-0.987331000	9.160018000	1.382366000
8	-0.577687000	-4.726537000	-3.554875000	6	0.258131000	9.150015000	0.683107000
7	3.762214000	1.806918000	1.801397000	6	-1.359594000	10.326484000	2.078387000
1	4.733268000	2.073131000	1.666154000	6	1.121808000	10.253824000	0.670742000
1	3.101197000	2.573772000	1.876808000	6	-0.507421000	11.425852000	2.064119000
6	3.384493000	0.610497000	2.318563000	6	0.722803000	11.389285000	1.369478000
8	2.209132000	0.355823000	2.603275000	1	-2.301014000	10.370429000	2.621999000
6	4.474810000	-0.447250000	2.497642000	1	-0.788072000	12.329515000	2.599481000
1	4.108961000	-1.133129000	3.265298000	1	1.368363000	12.263726000	1.382362000
1	4.548666000	-1.019264000	1.563489000	1	2.068266000	10.198831000	0.139950000
6	5.872490000	0.069280000	2.882389000	6	-4.378339000	6.118021000	3.224125000
1	6.307290000	0.687694000	2.092993000	8	-4.791966000	5.043249000	2.759503000
1	6.532462000	-0.799257000	2.999536000	7	-5.167649000	6.978046000	3.896040000
6	5.877304000	0.797422000	4.225737000	1	-4.749982000	7.816082000	4.279094000
8	5.428367000	0.279836000	5.249878000	6	-6.604577000	6.787316000	4.074927000
7	6.436385000	2.041668000	4.225998000	1	-7.069927000	7.777053000	4.037637000
1	6.713346000	2.459152000	3.339435000	1	-6.970442000	6.220602000	3.215190000
6	6.601234000	2.779770000	5.464661000	6	-6.973058000	6.108236000	5.400130000
1	6.963664000	2.111416000	6.248846000	1	-6.492372000	6.666764000	6.213092000
1	7.354847000	3.557921000	5.304178000	1	-8.055363000	6.233452000	5.548144000
6	5.335541000	3.449747000	6.029792000	6	-6.618282000	4.622817000	5.540288000
8	5.195633000	3.609800000	7.243203000	1	-6.744939000	4.326726000	6.588875000
				1	-5.564031000	4.456702000	5.294033000

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	-6.689891000	8.360964000	5.141025000
1	4.177624000	-1.306040000	1.891411000	1	-6.898199000	6.805338000	4.336820000
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
1	6.941807000	1.842698000	6.349702000	1	-7.062906000	4.537871000	4.714142000
1	7.298231000	3.269298000	5.362008000	7	-6.684787000	2.855421000	5.875092000
6	5.327040000	3.207763000	6.207663000	1	-6.915382000	2.392105000	6.743882000
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
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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
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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
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8	-1.640027000	3.089346000	2.454355000	1	-7.250126000	-0.569387000	-6.277548000
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1	6.823274000	8.384262000	4.913902000	1	-5.612113000	6.259584000	-2.266807000
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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
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6	-0.951473000	5.365171000	3.719146000	6	-5.730507000	1.866966000	-6.378299000
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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
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1	2.224072000	10.190153000	0.520124000	1	7.600107000	6.219068000	1.898974000
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1	-6.961119000	6.220026000	3.214859000	1	9.552912000	2.846086000	-0.023197000
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1	-6.495449000	6.667328000	6.214553000	1	9.554829000	2.571717000	-2.413221000
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1	-5.464567000	-0.187951000	3.702683000	1	1.684758000	4.931988000	-0.868794000
6	-7.104654000	7.773255000	-0.293235000	6	0.522753000	4.554148000	-2.596705000
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1	-1.962737000	-3.502744000	0.122868000	1	-2.513250000	3.199746000	5.206070000
1	3.051931000	-4.169091000	4.013191000	6	-1.290122000	5.438795000	3.937704000
1	6.548776000	-6.357489000	-0.853850000	8	-0.952638000	6.351491000	4.695841000
1	1.478859000	-5.865079000	-4.696444000	7	-2.459243000	5.404370000	3.255262000
1	0.616015000	-3.248766000	4.319940000	1	-2.655195000	4.557494000	2.720879000
1	5.532417000	-4.993186000	3.766201000	6	-3.368614000	6.529440000	3.177406000
1	7.025184000	-5.913713000	1.694489000	1	-2.959909000	7.308989000	3.824279000
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6	-1.875743000	-2.724240000	2.809384000	6	-1.333817000	6.713111000	0.349656000
6	-2.047672000	-1.270155000	2.328909000	7	-0.209532000	7.419897000	-0.004903000
6	-3.270474000	-0.559052000	2.915292000	1	-1.456561000	5.686616000	0.026901000
8	-3.570000000	0.592126000	2.398172000	1	0.571003000	7.063254000	-0.576042000
8	-3.895894000	-1.080785000	3.859480000	6	-1.520104000	8.771090000	1.254398000
1	-1.991493000	-2.741088000	3.897168000	6	-0.289499000	8.681846000	0.537465000
1	-2.694420000	-3.334274000	2.406128000	6	-1.839023000	9.982741000	1.897932000
1	-1.160437000	-0.681757000	2.602173000	6	0.616203000	9.749078000	0.460605000
1	-2.106496000	-1.219430000	1.235016000	6	-0.947226000	11.047289000	1.818602000
16	1.538390000	-7.233562000	0.195505000	6	0.270515000	10.930238000	1.110818000
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7	2.978213000	1.556042000	1.500944000	1	0.948613000	11.779029000	1.073464000
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6	-1.875128000	-2.726518000	2.819184000	7	-0.217811000	7.387416000	-0.021905000
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1	3.938954000	1.704196000	1.162703000	6	-4.766897000	6.097327000	3.643720000
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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
8	2.730242000	-2.824711000	-5.558330000	6	2.795601000	6.955598000	5.371493000
				1	3.510497000	7.264503000	6.138882000
				1	1.798796000	7.238805000	5.730024000
				6	3.090766000	7.643377000	4.058488000

²TSS_{B,C6-endo}

26 2.616516000 -4.383647000 -1.230999000

6	4.408609000	7.962963000	3.699536000	1	-9.130779000	4.383162000	-1.686130000
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6	4.688408000	8.573173000	2.474400000	6	-6.971082000	4.526196000	-1.384396000
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6	3.650842000	8.876425000	1.589113000	1	-6.149499000	5.187262000	-1.686603000
1	5.217844000	7.741662000	4.390889000	6	-6.633991000	3.094128000	-1.828802000
1	1.025905000	7.742275000	3.437423000	1	-7.440052000	2.400657000	-1.559681000
1	5.715826000	8.815316000	2.214358000	1	-6.552772000	3.058421000	-2.919859000
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
6	1.899031000	4.797122000	4.296989000	6	-5.196645000	1.955971000	-0.137542000
8	2.313582000	4.239275000	3.273989000	7	-3.988197000	1.517439000	0.202341000
7	0.583873000	4.910626000	4.584667000	1	-6.068604000	1.422786000	1.626466000
1	0.281455000	5.544994000	5.315623000	1	-7.093196000	2.249082000	0.555300000
6	-0.436851000	4.531982000	3.624451000	7	-6.260393000	1.689292000	0.666157000
1	-0.014812000	4.643909000	2.618344000	1	-3.795981000	1.093332000	1.115392000
6	-0.834153000	3.038913000	3.758580000	1	-3.172707000	1.782113000	-0.371484000
1	0.105550000	2.468529000	3.770960000	6	-6.024456000	10.474966000	-3.936183000
8	-1.566848000	2.735156000	2.570652000	1	-6.637365000	10.188777000	-4.799057000
1	-2.044403000	1.873416000	2.673806000	1	-6.164144000	11.548494000	-0.202341000
6	-1.609356000	2.720144000	5.037737000	1	-6.407209000	9.935468000	-3.061888000
1	-1.023735000	3.004467000	5.918854000	6	-4.540514000	10.143411000	-4.180082000
1	-1.811129000	1.646219000	5.100954000	6	-4.286607000	8.669736000	-4.428490000
1	-2.567912000	3.249761000	5.064700000	6	-3.981990000	7.797517000	-3.374718000
6	-1.599092000	5.537852000	3.744159000	6	-4.370481000	8.121366000	-5.717806000
8	-1.482846000	6.570451000	4.412733000	6	-3.767214000	6.434098000	-3.588211000
7	-2.701455000	5.206977000	3.034969000	6	-4.159372000	6.763188000	-5.951117000
1	-2.678182000	4.300332000	2.564796000	6	-3.853105000	5.904623000	-4.885144000
6	-3.801253000	6.124284000	2.796704000	8	-3.649784000	4.586771000	-5.161154000
1	-3.515607000	7.077239000	3.247774000	1	-3.418705000	4.092278000	-4.333605000
6	-4.043046000	6.307731000	1.268187000	1	-3.954077000	10.473025000	-3.312869000
1	-4.872978000	7.015213000	1.143870000	1	-4.182371000	10.727502000	-5.037926000
1	-4.393050000	5.344973000	0.877539000	1	-3.895833000	8.188002000	-2.362900000
6	-2.832111000	6.769187000	0.513660000	1	-4.598578000	8.771682000	-6.560451000
6	-1.864349000	5.955528000	-0.041634000	1	-3.520702000	5.782754000	-2.754515000
7	-0.870413000	6.708437000	-0.618712000	1	-4.219024000	6.352703000	-6.955349000
1	-1.811781000	4.874154000	-0.064915000	8	1.379640000	5.470077000	-7.108576000
1	-0.031244000	6.328412000	-1.086762000	8	2.818023000	7.172535000	-1.466680000
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6	-1.167664000	8.039404000	-0.446712000	6	3.436706000	5.036589000	-0.537226000
6	-2.929986000	9.398364000	0.550833000	1	3.157765000	5.137347000	0.523148000
6	-0.457437000	9.175892000	-0.857749000	1	3.217703000	3.998313000	-0.808532000
6	-2.232106000	10.528538000	0.136852000	6	4.927741000	5.353341000	-0.703752000
6	-1.005388000	10.418945000	-0.556832000	1	5.048702000	6.440085000	-0.663580000
1	-3.869242000	9.501863000	1.089883000	1	5.264948000	5.057015000	-1.707785000
1	-2.631259000	11.515698000	0.355827000	6	5.831179000	4.737211000	0.379072000
1	-0.481560000	11.321859000	-0.859337000	1	5.577479000	5.158848000	1.357187000
1	0.489671000	9.071785000	-1.380902000	1	6.878284000	5.010586000	0.185482000
6	-5.085156000	5.581613000	3.439758000	6	5.793685000	3.223720000	0.559628000
8	-5.517024000	4.457301000	3.137397000	8	5.937510000	2.713725000	1.689340000
7	-5.721618000	6.408997000	4.293201000	7	5.621518000	2.469113000	-0.544564000
1	-5.288415000	7.297172000	4.508942000	1	5.547140000	2.940446000	-1.436072000
6	-7.030540000	6.126652000	4.883901000	6	5.582311000	1.008855000	-0.541295000
1	-7.572186000	7.076293000	4.934735000	1	4.758877000	0.687443000	-1.187778000
1	-7.567514000	5.481146000	4.184535000	1	5.352366000	0.694783000	0.477523000
6	-6.973845000	5.503876000	6.289659000	6	6.901398000	0.353314000	-1.004831000
1	-6.398154000	6.169614000	6.944402000	1	6.813383000	-0.722943000	-0.812029000
1	-7.998712000	5.492382000	6.686189000	1	7.715965000	0.729944000	-0.374926000
6	-6.377219000	4.089820000	6.371879000	6	7.207332000	0.591808000	-2.468209000
1	-6.269593000	3.814161000	7.428306000	6	6.691737000	-0.267966000	-3.451361000
1	-5.368603000	4.082408000	5.942584000	6	7.975065000	1.690982000	-2.880418000
6	-7.240755000	3.025473000	5.676153000	6	6.928405000	-0.031727000	-4.807210000
1	-8.253561000	3.030131000	6.091545000	6	8.215992000	1.929992000	-4.236566000
1	-7.333752000	3.231189000	4.607340000	6	7.691431000	1.070329000	-5.204391000
7	-6.727602000	1.662924000	5.837067000	1	6.104229000	-1.134319000	-3.155751000
1	-6.956114000	1.187857000	6.699822000	1	8.392809000	2.360900000	-2.132246000
6	-5.804250000	1.077588000	5.050126000	1	6.516162000	-0.712335000	-5.547090000
7	-5.351546000	1.681287000	3.939304000	1	8.816443000	2.785644000	-4.534918000
1	-5.456946000	2.689145000	3.816862000	1	7.879659000	1.254040000	-6.258849000
1	-4.508721000	1.253200000	3.502823000	7	0.506142000	3.074146000	-2.223881000
7	-5.360090000	-0.147970000	5.345022000	1	0.094306000	2.617459000	-1.389923000
1	-5.746272000	-0.655868000	6.127634000	1	1.152918000	2.413324000	-2.659214000
1	-4.633954000	-0.613826000	4.763106000	1	1.021779000	3.988829000	-1.931836000
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6	-2.410104000	-4.545887000	-0.356724000	6	-1.650022000	2.394810000	4.452519000
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1	-3.212061000	-4.193326000	0.282692000	6	-0.987384000	5.377017000	3.731173000
1	3.003948000	-2.893614000	-0.403895000	8	-0.705906000	6.184806000	4.622234000
1	3.316516000	-7.017344000	-5.265797000	7	-2.058848000	5.487232000	2.917989000
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1	4.922968000	-3.714439000	-1.995602000	1	-2.614412000	7.261862000	3.777747000
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1	1.632771000	-8.641622000	-6.471042000	1	-3.651481000	8.241531000	1.707918000
1	-0.975784000	-9.284516000	-6.091952000	1	-3.331733000	6.739515000	0.851559000
1	-4.731163000	-7.730246000	-2.759292000	6	-1.598003000	7.922824000	1.178715000
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6	-1.810887000	-2.196820000	1.647068000	7	0.399967000	7.990839000	0.114593000
6	-2.382653000	-0.906608000	1.023822000	1	-0.800633000	6.224865000	-0.007905000
6	-3.431092000	-0.208083000	1.895498000	1	1.183406000	7.688261000	-0.485930000
8	-3.574199000	1.062907000	1.717198000	6	-0.993461000	9.208810000	1.422988000
8	-4.098886000	-0.880479000	2.710405000	6	0.257938000	9.210511000	0.734443000
1	-1.299671000	-1.939011000	2.582220000	6	-1.373154000	10.364694000	2.132535000
1	-2.644724000	-2.848773000	1.923474000	6	1.120138000	10.315487000	0.744897000
1	-1.580045000	-0.195948000	0.800349000	6	-0.522371000	11.465204000	2.141183000
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7	3.760597000	1.846689000	1.771164000	1	2.071076000	10.269399000	0.221161000
1	4.731795000	2.117769000	1.647366000	6	-4.384179000	6.133170000	3.209623000
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6	3.380924000	0.632741000	2.241899000	7	-5.182973000	6.983590000	3.883068000
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6	6.307089000	0.720781000	2.040733000	1	-6.487361000	6.674277000	6.204749000
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1	3.946188000	5.590023000	7.187171000	1	-5.007707000	0.349783000	4.628327000
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6	3.282980000	8.443518000	3.704205000	1	-6.040611000	5.606123000	0.054992000
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1	5.829763000	6.447833000	5.839660000	6	-5.793416000	4.646209000	-1.876288000
1	1.768290000	7.279180000	4.699983000	1	-6.635940000	3.948679000	-1.791734000
1	6.631024000	8.177814000	4.257119000	1	-5.741371000	4.937424000	-2.929985000
1	2.566052000	9.006640000	3.112505000	7	-4.549384000	3.940236000	-1.577787000
1	4.998889000	9.464800000	2.885108000	1	-3.705352000	4.197433000	-2.121107000
6	2.178145000	4.158667000	4.557895000	6	-4.405155000	3.005578000	-0.634003000
8	2.601690000	3.942045000	3.416341000	7	-3.230604000	2.392609000	-0.464356000
7	0.867409000	4.327102000	4.837270000	1	-5.213601000	2.015357000	0.926739000
1	0.597366000	4.682780000	5.746303000	1	-6.253121000	3.196532000	0.231970000
6	-0.150211000	4.376713000	3.803984000	7	-5.452269000	2.592747000	0.123222000
1	0.353915000	4.589427000	2.855122000	1	-3.130633000	1.850515000	0.394325000
6	-0.844746000	2.997324000	3.639766000	1	-2.383994000	2.772188000	-0.918718000
1	-0.036363000	2.266122000	3.492681000	6	-7.557076000	0.102412000	-5.467632000
8	-1.627176000	3.085285000	2.445443000	1	-7.248112000	-0.576904000	-6.270499000
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6	-1.672750000	2.588211000	4.857643000	1	-6.929274000	-0.107724000	-4.594025000
1	-1.045021000	2.553399000	5.754434000	6	-7.416219000	1.571835000	-5.905411000
1	-2.100492000	1.590312000	4.714887000	6	-5.996154000	1.947697000	-6.276698000
1	-2.495570000	3.291131000	5.028833000	6	-5.097374000	2.428537000	-5.315035000
6	-1.088653000	5.566163000	4.101983000	6	-5.520297000	1.792085000	-7.587421000
8	-0.834563000	6.371108000	5.003475000	6	-3.774515000	2.740832000	-5.633850000
7	-2.150060000	5.665524000	3.269912000	6	-4.201577000	2.091468000	-7.925924000
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6	-3.001027000	6.838866000	3.202182000	8	-2.038590000	2.847768000	-7.331728000
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6	-1.789853000	7.757643000	1.143307000	1	-6.193876000	1.427516000	-8.360554000
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7	0.172262000	7.668847000	0.016597000	1	-3.840977000	1.964325000	-8.942619000
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1	0.938259000	7.319961000	-0.578638000	8	3.789095000	8.079822000	-0.562443000
6	-1.098827000	9.010101000	1.325513000	6	3.397224000	6.927995000	-6.804577000
6	0.128727000	8.911980000	0.606124000	6	4.152799000	5.719645000	-0.219650000
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6	1.067383000	9.952731000	0.574095000	1	4.445973000	5.050392000	-1.039952000
6	-0.460576000	11.243680000	1.979759000	6	5.351051000	6.103764000	0.653690000
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1	-2.311706000	10.315126000	2.573381000	1	6.170574000	6.488234000	0.030866000
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6	-4.411420000	6.518871000	3.713371000	6	6.475164000	3.742980000	0.986664000
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6	-1.526104000	8.751317000	1.233502000	6	3.080357000	6.672741000	-0.864096000
6	-0.296160000	8.658376000	0.515947000	6	3.973774000	5.562630000	-0.282648000
6	-1.845543000	9.966829000	1.869463000	1	3.548756000	5.300944000	0.698543000
6	0.608581000	9.725890000	0.431396000	1	3.882509000	4.661193000	-0.901169000
6	-0.954708000	11.031557000	1.782490000	6	5.442935000	5.958296000	-0.119766000
6	0.262491000	10.910885000	1.074357000	1	5.492160000	6.921769000	0.395249000
1	-2.775646000	10.075282000	2.423366000	1	5.893262000	6.124172000	-1.108237000
1	-1.193704000	11.972957000	2.271024000	6	6.268593000	4.935137000	0.685735000
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8	-5.287056000	5.049418000	3.231919000	8	5.898868000	2.542909000	0.852463000
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6	-0.277440000	11.007421000	1.392067000	6	5.164872000	5.738523000	0.378457000
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1	-2.142206000	10.202641000	2.110080000	1	6.015382000	6.039954000	-0.248551000
1	-0.424659000	11.969931000	1.875656000	6	5.582143000	4.713906000	1.445207000
1	1.639065000	11.577055000	0.563574000	1	4.711492000	4.433024000	2.046243000
1	2.036325000	9.372629000	-0.563440000	1	6.287409000	5.190738000	2.141702000
6	-4.362379000	6.643479000	3.583867000	6	6.250664000	3.415710000	1.013182000
8	-5.021420000	5.649351000	3.238404000	8	6.126278000	2.377426000	1.694779000
7	-4.830301000	7.575384000	4.439198000	7	7.035375000	3.456994000	-0.082864000
1	-4.219238000	8.339762000	4.695520000	1	7.107248000	4.335015000	-0.579756000
6	-6.178629000	7.560458000	5.004860000	6	7.899483000	2.362829000	-0.515486000
1	-6.535719000	8.594931000	5.028176000	1	7.803850000	1.576446000	0.234180000
1	-6.813007000	7.009945000	4.306348000	1	8.938287000	2.715027000	-0.501334000

6	-2.972983000	6.920268000	2.999456000	8	-2.151722000	0.605981000	-6.530022000
1	-2.493479000	7.750321000	3.523726000	1	-1.620407000	1.111265000	-5.889064000
6	-3.106856000	7.255905000	1.484989000	1	-7.928965000	0.965726000	-4.362516000
1	-3.798528000	8.104364000	1.393506000	1	-8.213432000	-0.141310000	-5.699080000
1	-3.593805000	6.402795000	0.997878000	1	-5.591974000	1.552538000	-3.678026000
6	-1.799532000	7.562555000	0.817296000	1	-6.316414000	-1.055716000	-7.013117000
6	-1.053728000	6.706643000	0.032637000	1	-3.249008000	1.829232000	-4.387472000
7	0.105931000	7.319975000	-0.381470000	1	-3.947073000	-0.807299000	-7.712901000
1	-1.262468000	5.685073000	-0.260420000	8	2.227525000	6.175988000	-1.925404000
1	0.827495000	6.907313000	-0.988008000	8	3.768417000	7.613837000	-1.161993000
6	-1.046393000	8.789771000	0.898121000	6	3.300553000	6.470028000	-1.258903000
6	0.143821000	8.594982000	0.136786000	6	3.972273000	5.299036000	-0.514326000
6	-1.247945000	10.031817000	1.531287000	1	3.197222000	4.830150000	0.108535000
6	1.125164000	9.587581000	0.007433000	1	4.269897000	4.532157000	-1.243373000
6	-0.281417000	11.023184000	1.399732000	6	5.150890000	5.727810000	0.365231000
6	0.895738000	10.801151000	0.649589000	1	4.867226000	6.644131000	0.890335000
1	-2.146032000	10.217113000	2.116652000	1	6.005509000	6.019221000	-0.260891000
1	-0.428444000	11.984710000	1.885334000	6	5.554681000	4.698757000	1.433168000
1	1.634978000	11.594372000	0.572029000	1	4.679068000	4.424391000	2.029776000
1	2.031735000	9.392151000	-0.559594000	1	6.260377000	5.170350000	2.132888000
6	-4.367450000	6.653001000	3.581936000	6	6.217035000	3.396258000	1.004191000
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7	-4.845344000	7.587519000	4.428736000	7	7.027023000	3.439456000	-0.073577000
1	-4.241048000	8.358397000	4.681613000	1	7.121065000	4.322531000	-0.557778000
6	-6.193584000	7.563642000	4.993825000	6	7.901576000	2.346791000	-0.488810000
1	-6.559676000	8.595035000	5.012311000	1	7.782734000	1.554369000	0.251365000
1	-6.823159000	7.004339000	4.297942000	1	8.939706000	2.698291000	-0.441180000
6	-6.264820000	6.975867000	6.413580000	6	7.615509000	1.822281000	-1.906930000
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1	-5.847869000	5.223800000	7.598858000	6	6.001558000	-0.055908000	-1.355043000
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7	-6.634487000	3.136054000	6.032877000	1	6.742999000	-0.457929000	-0.667639000
1	-6.869467000	2.725195000	6.926285000	1	5.524678000	2.497967000	-3.541113000
6	-5.846229000	2.398224000	5.223116000	1	4.591236000	-1.634946000	-0.960963000
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6	-4.461237000	2.721418000	-0.480233000	1	0.605395000	-0.992520000	-3.766869000
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6	-7.570347000	0.038331000	-4.827929000	7	4.067556000	-0.727447000	-7.384533000
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				² TSS _{B,C6-exo}			
				26	-0.056698000	-5.668246000	-1.671739000
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6	4.041377000	-6.817311000	-1.288196000	6	2.275274000	3.960153000	4.015702000
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7	3.543469000	1.782164000	1.094965000	1	1.345652000	9.922963000	-0.029174000
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6	3.340964000	0.487554000	1.413396000	7	-4.871026000	7.053431000	5.254359000
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1	6.662580000	-0.659025000	1.415115000	1	-7.184151000	6.372221000	7.686455000
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6	3.888206000	6.535078000	4.920804000	1	-8.832799000	2.211879000	-2.967972000
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8	5.197206000	0.019015000	5.821921000	1	-5.849713000	5.206348000	7.599110000
7	6.145504000	1.648532000	4.548359000	1	-4.913313000	5.285168000	6.114521000
1	6.331435000	1.985473000	3.604804000	6	-6.938174000	4.556406000	5.859354000
6	6.466304000	2.480071000	5.692872000	1	-7.931676000	4.726908000	6.286740000
1	6.821781000	1.852690000	6.512663000	1	-7.012243000	4.767551000	4.7920157000
1	7.274510000	3.163226000	5.410093000	7	-6.647891000	3.130804000	6.021179000
6	5.313620000	3.322512000	6.267894000	1	-6.885455000	2.715219000	6.911714000
8	5.288744000	3.621468000	7.463093000	6	-5.862440000	2.394716000	5.207051000
7	4.394499000	3.751243000	5.370857000	7	-5.317800000	2.913614000	4.107533000
1	4.410398000	3.395212000	4.421342000	1	-5.278678000	3.917548000	3.932114000
6	3.173507000	4.433209000	5.759574000	1	-4.723755000	2.305669000	3.518883000
1	2.751562000	3.922305000	6.634424000	7	-5.640838000	1.104587000	5.500015000
6	3.391592000	5.918629000	6.180132000	1	-6.209855000	0.643739000	6.195532000
1	4.103973000	5.888418000	7.009539000	1	-5.075378000	0.513543000	4.862320000
1	2.445147000	6.292297000	6.589587000	6	-7.301776000	6.290840000	-1.671224000
6	3.883385000	6.846874000	5.092210000	1	-7.412163000	7.251252000	-1.156823000
6	5.257224000	7.042095000	4.886743000	1	-8.187988000	5.685540000	-1.444406000
6	2.977567000	7.544211000	4.277089000	1	-7.299100000	6.487684000	-2.750026000
6	5.716577000	7.906919000	3.890554000	6	-6.016070000	5.581441000	-1.234884000
6	3.433194000	8.407385000	3.277649000	1	-6.023992000	5.425111000	-0.147690000
6	4.804885000	8.591558000	3.082001000	1	-5.144780000	6.212147000	-1.450542000
1	5.970330000	6.522096000	5.521624000	6	-5.830079000	4.233058000	-1.948941000
1	1.907919000	7.415933000	4.430087000	1	-6.691825000	3.577319000	-1.772714000
1	6.784897000	8.052485000	3.752161000	1	-5.783493000	4.390094000	-3.030955000
1	2.718879000	8.939075000	2.654416000	7	-4.601536000	3.535835000	-1.575791000
1	5.159575000	9.268098000	2.309137000	1	-3.755943000	3.703304000	-2.350038000
6	2.192378000	4.284500000	4.587153000	6	-4.456701000	2.749424000	-0.504294000
8	2.579717000	3.924244000	3.469039000	7	-3.275111000	2.186492000	-0.238030000
7	0.897010000	4.546515000	4.862063000	1	-5.278442000	1.966032000	1.167874000
1	0.651664000	5.017845000	5.724486000	1	-6.338260000	3.000217000	0.284481000
6	-0.126851000	4.506322000	3.835011000	7	-5.504717000	2.433189000	0.293844000
1	0.372036000	4.623944000	2.866841000	1	-3.180214000	1.761553000	0.686459000
6	-0.830263000	3.122408000	3.802178000	1	-2.426927000	2.531633000	-0.715948000
1	-0.028884000	2.373460000	3.728302000	6	-7.749510000	-1.148198000	-3.762518000
8	-1.607348000	3.103367000	2.601449000	1	-7.434715000	-2.094684000	-4.217084000
1	-2.296325000	2.400971000	2.654875000	1	-8.792576000	-1.255744000	-3.441507000
6	-1.664305000	2.834499000	5.050030000	1	-7.134321000	-0.985645000	-2.869769000
1	-1.039495000	2.882794000	5.948257000	6	-7.594513000	0.018307000	-4.755582000
1	-2.092957000	1.827954000	4.999601000	6	-6.168635000	0.212552000	-5.230139000
1	-2.487024000	3.550767000	5.152505000	6	-5.270861000	1.021016000	-4.519740000
6	-1.055489000	5.723179000	4.020352000	6	-5.688619000	-0.434798000	-6.378781000
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	-2.827480000
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	-0.623862000	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	1.0282185000	-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	3.631690000
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

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26	0.496306000	-3.879921000	-2.325698000	1	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	6	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	1	5.198137000	9.349397000	2.172258000
6	3.390494000	-4.805537000	-2.642839000	6	2.245219000	4.427525000	4.587328000
6	2.082899000	-4.872543000	-4.734151000	8	2.628414000	4.038202000	3.477405000
6	1.964064000	-5.114971000	-6.153185000	7	0.950953000	4.699116000	4.855951000
6	0.672673000	-4.839004000	-6.492193000	1	0.701996000	5.190125000	5.706284000
6	0.002510000	-4.426374000	-5.281145000	6	-0.069881000	4.623451000	3.828041000
6	-1.992349000	-3.628396000	-4.066648000	1	0.429055000	4.730655000	2.858674000
6	-3.386642000	-3.248494000	-4.015627000	6	-0.750332000	3.227967000	3.819020000
6	-3.657537000	-2.927017000	-2.720633000	1	0.061818000	2.489475000	3.763174000
6	-2.428019000	-3.107469000	-1.980540000	8	-1.520378000	3.174514000	2.614880000
6	-2.294697000	-2.879796000	-0.614371000	1	-2.181832000	2.446267000	2.669369000
				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	5.827274000	3.986613000	6	-5.817842000	-0.592294000	-6.147487000
8	-0.775774000	6.736950000	4.786581000	6	-4.067985000	1.045118000	-4.725963000
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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
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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	6.025040000
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	0.042580000
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
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7	-6.530205000	3.147138000	6.018194000	1	6.697598000	-0.355557000	-0.584997000
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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
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1	-4.884993000	0.546909000	4.919239000	1	1.774087000	4.723713000	-2.340666000
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6	-4.418659000	2.699103000	-0.446632000	1	0.597667000	-1.040781000	-3.788830000
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1	7.548628000	3.891370000	4.948208000	7	-6.345322000	2.142793000	5.795460000
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6	-0.355316000	8.665242000	0.183945000	6	3.653879000	5.637965000	-0.804337000
6	-1.709639000	9.921303000	1.777296000	1	3.002793000	5.054423000	-0.138384000
6	0.536714000	9.734390000	0.025972000	1	4.006466000	4.930151000	-1.567563000

1	0.752673000	4.745191000	5.531211000	1	-6.304137000	2.650911000	0.208670000
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⁴Int6_{B,HAT}							
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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
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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	3.403670000	-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
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1	-3.910445000	4.130722000	-2.037130000	7	-2.159448000	0.232456000	-3.938989000
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7	-3.194765000	2.322242000	-0.479963000	6	-0.963646000	-0.293246000	-4.367384000
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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
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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				
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1	-6.975896000	7.266617000	-6.816822000				
1	-7.730783000	6.496314000	-8.206324000				
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6	2.745902000	6.730829000	-1.479122000				
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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				
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6	6.387150000	1.527398000	-2.345932000				
6	6.729205000	0.278309000	-1.802990000				
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Model B system – C7

²TS4_{B,C7-endo}

26	2.512545000	-4.553530000	-0.180364000
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6	5.227457000	-5.492652000	0.845788000
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6	4.588554000	-5.436209000	-3.823416000
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6	-3.236082000	-0.644982000	3.202160000
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1	-2.729977000	-3.364150000	2.369754000
1	-1.118520000	-0.845079000	3.061061000
1	-1.950294000	-1.148912000	1.553261000
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6	5.028497000	-0.508004000	2.989807000
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6	5.320397000	0.348120000	4.220309000
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8	2.335646000	3.896970000	3.023589000
7	0.713755000	4.416798000	4.532037000
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6	-1.017115000	2.851588000	3.730405000
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6	-1.730583000	2.617624000	5.063202000
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1	0.372212000	6.817868000	-1.002179000
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6	-0.480020000	8.445140000	0.097132000
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6	0.405828000	9.523413000	-0.035391000
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1	0.721245000	11.575317000	0.509055000
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6	-4.834658000	6.001739000	3.452355000
8	-5.334330000	4.909286000	3.137018000
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7	2.935806000	1.274432000	1.708634000	1	1.419589000	9.464986000	-0.389432000
1	3.879313000	1.405663000	1.358385000	6	-4.775216000	6.063543000	3.622283000
1	2.415043000	2.131227000	1.871326000	8	-5.318416000	5.020256000	3.221879000
6	2.613657000	0.219488000	2.506901000	7	-5.382116000	6.936182000	4.452267000
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8	5.151530000	-0.164192000	5.043488000	1	-6.620286000	4.373116000	7.403493000
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6	6.404591000	2.294870000	4.848962000	1	-8.404928000	3.837444000	5.701360000
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6	5.299967000	3.104362000	5.550823000	1	-7.350935000	1.883600000	6.472699000
8	5.369870000	3.355235000	6.755090000	6	-6.044763000	1.654992000	4.962165000
7	4.307362000	3.560951000	4.749237000	7	-5.349681000	2.211670000	3.969238000
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6	3.109728000	4.198279000	5.265727000	1	-4.668021000	1.627561000	3.463139000
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6	3.740678000	6.659221000	4.698603000	1	-7.733920000	6.311306000	-0.749542000
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6	1.937898000	-6.737073000	-5.455100000	8	2.514922000	4.115439000	3.356921000
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6	5.521400000	7.906957000	3.689514000	6	-6.250359000	4.751803000	-0.932511000
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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	-7.534770000
1	-2.054326000	1.515910000	4.948609000	6	-6.233542000	6.494945000	-6.484732000
1	-2.498966000	3.220737000	5.148637000	6	-5.555888000	6.495678000	-5.258064000
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
1	-2.631623000	4.550215000	2.679149000	6	-4.231595000	4.578002000	-5.917325000
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

6	3.61000000	8.49797200	3.19076700	1	-5.85086800	5.37559000	-0.08949900
6	4.98030400	8.67373100	2.97830500	1	-5.00680800	6.14323400	-1.42650800
1	6.16286200	6.66776300	5.46233800	6	-5.69426200	4.15257000	-1.87424500
1	2.09291600	7.54048300	4.38198900	1	-6.54842800	3.49663500	-1.66471100
1	6.96495600	8.14869200	3.64590300	1	-5.67472400	4.29097300	-2.95956000
1	2.89125400	9.01445600	2.55982200	7	-4.45394200	3.46710300	-1.51900600
1	5.32973200	9.32914500	2.18511900	1	-3.62643100	3.61215800	-2.12514300
6	2.38532900	4.41288700	4.61223400	6	-4.28146500	2.69617700	-0.44076900
8	2.77306200	4.02297300	3.50424400	7	-3.09760600	2.12733600	-0.20119500
7	1.08962300	4.68309900	4.87639600	1	-5.05804900	1.94437300	1.26614400
1	0.83733700	5.17396100	5.72584100	1	-6.12713500	2.98981100	0.41339400
6	0.07216000	4.60709400	3.84522700	7	-5.30865800	2.40108600	0.39361700
1	0.57307200	4.72119600	2.87757700	1	-2.97424300	1.72601200	0.73109200
6	-0.60141900	3.20832100	3.82731600	1	-2.26244700	2.44283100	-0.72137400
1	0.21491700	2.47437300	3.77248800	6	-7.84738500	-1.31267200	-3.50399200
8	-1.36479900	3.15539300	2.61883100	1	-7.55077200	-2.25352000	-3.98186400
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6	-1.43990600	2.92157400	5.07250500	1	-7.21981600	-1.17766200	-2.61524200
1	-0.82346200	2.99973800	5.97445800	6	-7.68773700	-0.12772700	-4.47434700
1	-1.84439300	1.90454700	5.03611400	6	-6.26592700	0.05688100	-4.96530500
1	-2.27974900	3.61998600	5.15674300	6	-5.35213200	0.85563700	-4.26422300
6	-0.88333900	5.80583800	4.00634000	6	-5.80690400	-0.58874000	-6.12361200
8	-0.64534500	6.71547400	4.80720500	6	-4.03061900	1.00874100	-4.68846600
7	-1.94159500	5.78457800	3.16525700	6	-4.49051000	-0.45338700	-6.56199500
1	-2.05960100	4.93414100	2.61326600	6	-3.59378900	0.34512900	-5.84088600
6	-2.81448000	6.92261300	2.94605300	8	-2.31635200	0.44704100	-6.31743400
1	-2.34393200	7.77664500	3.43915500	1	-1.76690100	0.95583500	-5.69489600
6	-2.96318400	7.20342200	1.42237100	1	-8.02515600	0.78977700	-3.97488300
1	-3.66006000	8.04476900	1.30711200	1	-8.35522800	-0.27772800	-5.33275600
1	-3.45060000	6.33136500	0.97113100	1	-5.67621900	1.37554500	-3.36514900
6	-1.66398300	7.49070900	0.73014100	1	-6.49320900	-1.20852600	-6.69726900
6	-0.93056800	6.61446900	-0.04392100	1	-3.34968500	1.65674100	-4.14045300
7	0.22313800	7.21592400	-0.49099400	1	-4.14396900	-0.95607400	-7.46030800
1	-1.14451000	5.58632000	-0.30894900	8	2.34487200	6.07066600	-2.04420700
1	0.93694400	6.78799100	-1.09584300	8	3.88720800	7.54989300	-1.36759900
6	-0.90880500	8.71875600	0.76840100	6	3.41786000	6.40237500	-1.39609200
6	0.26935000	8.50395000	-0.00609400	6	4.08992800	5.28083500	-0.57844600
6	-1.10054900	9.97658500	1.37283100	1	3.31215100	4.84128000	0.06205000
6	1.24792300	9.49299900	-0.17709500	1	4.40136500	4.47556000	-1.25886400
6	-0.13614500	10.96382100	1.20123800	6	5.25627200	5.77275900	0.28515800
6	1.02862500	10.72243500	0.43783800	1	4.95327400	6.71002800	0.76049100
1	-1.98957700	10.17713200	1.96690300	1	6.10881500	6.04746700	-0.35102400
1	-0.27550500	11.93742600	1.66450600	6	5.67301200	4.80974000	1.40828100
1	1.76605700	11.51347300	0.32753500	1	4.79867200	4.54387100	2.01046700
1	2.14474400	9.28455700	-0.75502000	1	6.35866500	5.33400800	2.09009000
6	-4.20145900	6.65459300	3.54777200	6	6.37120800	3.50338400	1.05614200
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1	-4.06508400	8.36148900	4.64391100	1	7.25411800	4.35483500	-0.56079100
6	-6.01147300	7.56106500	4.98295000	6	8.05795200	2.39337100	-0.38758900
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1	-5.62414700	5.24125800	7.60031500	6	6.05520000	0.01304800	-1.04715800
1	-4.69713500	5.32010800	6.11002100	6	5.43029100	1.54834000	-2.79269500
6	-6.70987500	6.55287700	5.87370900	6	4.81836400	-0.62357500	-1.16015900
1	-7.70414600	4.70970600	6.30444700	6	4.19588000	0.90354100	-2.91900400
1	-6.79335800	4.75076800	4.80263500	6	3.88143900	-0.18311400	-2.10044600
7	-6.39223400	3.13462600	6.05102100	1	6.78153100	-0.35544500	-0.32588600
1	-6.61651200	2.72700300	6.94868600	1	5.66895900	2.38699400	-3.44337800
6	-5.58849700	2.40665000	5.24735300	1	4.58883100	-1.47772700	-0.52876800
7	-5.06606200	2.91945600	4.13388200	1	3.49651400	1.22346200	-3.68640700
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1	-4.45148300	2.31779800	3.56023900	7	1.38180900	3.73285000	-2.68696500
7	-5.32663700	1.12970900	5.56258500	1	1.01801700	3.26179300	-1.83831100
1	-5.86270200	0.66933000	6.28389200	1	2.02577100	3.09547600	-3.16110500
1	-4.74098700	0.54291900	4.93928100	1	1.89768500	4.64791800	-2.38209100
6	-7.16891800	6.20813000	-1.59666600	6	0.15932500	4.03758900	-3.50671900
1	-7.27166600	7.17689900	-1.09654600	1	0.11036000	5.12598800	-3.59931100
1	-8.04637600	5.60284700	-1.33801800	6	-1.08746300	3.59599700	-2.68867800
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1	3.026885000	-3.733840000	1.382266000	8	-0.642045000	6.708923000	4.806365000
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1	5.151487000	-4.572746000	0.082253000	1	-2.341328000	7.770631000	3.442057000
1	5.638807000	-5.278994000	-2.493461000	6	-2.957944000	7.199661000	1.423931000
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1	-4.054727000	-3.370880000	-4.831876000	6	-1.656509000	7.486229000	0.735632000
1	-4.538549000	-2.679003000	-2.254039000	6	-0.918165000	6.608155000	-0.031663000
6	-1.899842000	-2.111566000	2.380961000	7	0.237043000	7.209438000	-0.475087000
6	-2.070677000	-0.608661000	2.101168000	1	-1.129548000	5.578826000	-0.294120000
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8	-3.418554000	1.313008000	2.523415000	6	-0.903012000	8.715278000	0.773355000
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1	-1.621113000	-2.255725000	3.429643000	6	-1.099411000	9.974939000	1.372442000
1	-2.863726000	-2.617225000	2.244428000	6	1.257525000	9.488917000	-0.163785000
1	-1.120680000	-0.089678000	2.291641000	6	-0.135412000	10.962808000	1.202313000
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16	-0.010568000	-6.275793000	-1.912998000	1	-1.991677000	10.176356000	1.961346000
1	-0.701243000	-6.087161000	-0.765965000	1	-0.278358000	11.937843000	1.661469000
8	0.947350000	-2.315226000	-2.760834000	1	1.770549000	11.511795000	0.336427000
7	3.422498000	1.424836000	2.392634000	1	2.157594000	9.279351000	-0.736182000
1	4.394140000	1.605602000	2.157627000	6	-4.201015000	6.651973000	3.547418000
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6	3.040848000	0.365983000	3.151650000	7	-4.668465000	7.584905000	4.401822000
8	1.901105000	0.263918000	3.617791000	1	-4.062469000	8.357472000	4.645489000
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6	5.531651000	-0.285036000	3.558205000	6	-6.066141000	6.981936000	6.407263000
1	5.917227000	0.231187000	2.674766000	1	-5.401043000	7.571349000	7.050511000
1	6.151029000	-1.180434000	3.692745000	1	-7.084165000	7.140395000	6.789401000
6	5.714841000	0.557416000	4.819657000	6	-5.691907000	5.496692000	6.536501000
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
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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
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1	6.161381000	6.676473000	5.480343000	6	-5.668817000	4.173097000	-1.887258000
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1	0.573653000	4.714764000	2.876191000	1	-2.971113000	1.732962000	0.727871000
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1	-0.820884000	2.989413000	5.972625000	6	-7.708205000	-0.107656000	-4.452217000
1	-1.843727000	1.896800000	5.033395000	6	-6.292622000	0.098691000	-4.951975000
1	-2.277299000	3.612468000	5.157219000	6	-5.379002000	0.890270000	-4.242597000

6	-5.838780000	-0.520618000	-6.126470000
6	-4.062633000	1.062350000	-4.675175000
6	-4.527465000	-0.366130000	-6.573513000
6	-3.631173000	0.425708000	-5.844692000
8	-2.359333000	0.549022000	-6.330629000
1	-1.807206000	1.043416000	-5.699086000
1	-8.049119000	0.796832000	-3.931840000
1	-8.382254000	-0.247130000	-5.307254000
1	-5.699182000	1.388745000	-3.330129000
1	-6.525154000	-1.134814000	-6.706024000
1	-3.380693000	1.703761000	-4.120699000
1	-4.184652000	-0.848576000	-7.484252000
8	2.367995000	6.053186000	-2.008095000
8	3.897810000	7.546336000	-1.332082000
6	3.437493000	6.395110000	-1.359791000
6	4.117326000	5.279165000	-0.541816000
1	3.342528000	4.834170000	0.098516000
1	4.434170000	4.476426000	-1.222709000
6	5.280323000	5.777804000	0.321973000
1	4.971729000	6.711738000	0.800199000
1	6.130969000	6.059193000	-0.313882000
6	5.702749000	4.812929000	1.441187000
1	4.831443000	4.548655000	2.048355000
1	6.395480000	5.333349000	2.118680000
6	6.391167000	3.504857000	1.077327000
8	6.261056000	2.493969000	1.798085000
7	7.198321000	3.508092000	-0.002801000
1	7.273297000	4.364515000	-0.535674000
6	8.057952000	2.393371000	-0.387589000
1	7.946617000	1.633779000	0.387075000
1	9.100070000	2.735640000	-0.374620000
6	7.736473000	1.816266000	-1.776798000
1	8.517823000	1.075929000	-1.998934000
1	7.843388000	2.607376000	-2.529484000
6	6.369497000	1.173098000	-1.905570000
6	6.000504000	0.089859000	-1.092689000
6	5.456517000	1.618378000	-2.870827000
6	4.756595000	-0.526422000	-1.237873000
6	4.216425000	0.992034000	-3.030632000
6	3.857763000	-0.080685000	-2.211608000
1	6.696700000	-0.284994000	-0.345593000
1	5.729251000	2.447235000	-3.520703000
1	4.492867000	-1.369671000	-0.605104000
1	3.544715000	1.317233000	-3.821407000
1	2.903517000	-0.583038000	-2.344472000
7	1.420629000	3.707605000	-2.645980000
1	1.042372000	3.237600000	-1.803056000
1	2.065919000	3.066822000	-3.114025000
1	1.936837000	4.619896000	-2.335791000
6	0.210466000	4.031164000	-3.477207000
1	0.175436000	5.120963000	-3.559901000
6	-1.049888000	3.597450000	-2.675113000
8	-2.159114000	3.821954000	-3.213014000
8	-0.823692000	3.080544000	-1.540541000
6	0.268680000	3.451371000	-4.897151000
1	-0.673568000	3.749278000	-5.373113000
1	1.062594000	3.968191000	-5.451927000
6	0.479863000	1.961953000	-5.012582000
6	0.342122000	0.973153000	-4.050820000
1	0.056958000	1.048260000	-3.010734000
7	0.634149000	-0.255637000	-4.596852000
1	0.695978000	-1.124441000	-4.035057000
6	0.962029000	-0.095325000	-5.911209000
6	0.878297000	1.279778000	-6.220537000
6	1.095689000	1.715465000	-7.548707000
6	1.350662000	0.750999000	-8.543571000
6	1.339518000	-1.098506000	-6.881919000
6	1.417970000	-0.600675000	-8.252517000
1	1.033269000	2.767696000	-7.809481000
1	1.469130000	1.075047000	-9.573962000
1	0.926840000	-2.099881000	-6.753993000
1	1.597119000	-1.323963000	-9.040311000
7	3.051088000	-1.657888000	-6.492330000
8	3.539542000	-1.319289000	-5.427832000
8	3.581645000	-2.363239000	-7.337558000

⁴Int4_{B,C7-exo}

26	2.605252000	-4.900043000	0.212696000
7	1.201694000	-4.398586000	1.582842000
7	3.813653000	-5.584272000	1.682188000
7	3.924816000	-5.570853000	-1.171057000
7	1.327827000	-4.364941000	-1.269888000
6	-0.019734000	-3.820342000	1.349261000
6	-0.691169000	-3.520535000	2.609450000
6	0.165071000	-3.933191000	3.587107000
6	1.338403000	-4.473833000	2.942336000
6	3.584143000	-5.499361000	3.028473000
6	4.714407000	-6.030891000	3.759876000
6	5.625639000	-6.434427000	2.832975000
6	5.053672000	-6.147348000	1.534795000
6	5.148773000	-6.137117000	-0.931931000
6	5.824623000	-6.407185000	-2.181385000
6	4.993390000	-5.987156000	-3.174915000
6	3.809287000	-5.461888000	-2.532402000
6	1.573935000	-4.414245000	-2.616798000
6	0.452829000	-3.863515000	-3.345151000
6	-0.470383000	-3.482123000	-2.412681000
6	0.091264000	-3.799964000	-1.118931000
6	-0.548608000	-3.554351000	0.093505000
6	2.437034000	-4.985951000	3.622868000
6	5.680643000	-6.413447000	0.323752000
6	2.722687000	-4.924455000	-3.212973000
1	-1.537493000	-3.110385000	0.045408000
1	2.396965000	-4.981463000	4.707832000
1	6.666772000	-6.866487000	0.359659000
1	2.771948000	-4.907152000	-4.297689000
1	0.022757000	-3.877615000	4.659870000
1	4.780650000	-6.079367000	4.839610000
1	6.597866000	-6.884260000	2.991558000
1	6.806276000	-6.856546000	-2.266063000
1	5.149530000	-6.019640000	-4.246038000
1	0.386384000	-3.804201000	-4.424710000
1	-1.449052000	-3.045445000	-2.570703000
6	-2.032453000	-2.867608000	2.788582000
6	-2.039163000	-1.353698000	2.493740000
6	-3.291305000	-0.635275000	3.004795000
8	-3.542515000	0.530257000	2.495606000
8	-3.985168000	-1.167252000	3.894193000
1	-2.359308000	-3.011473000	3.822313000
1	-2.786621000	-3.356755000	2.157449000
1	-1.171276000	-0.878703000	2.973463000
1	-1.928410000	-1.154310000	1.422350000
16	1.538379000	-7.233557000	0.195502000
1	2.673021000	-7.939677000	-0.011882000
8	3.287226000	-3.405741000	0.257867000
7	2.890840000	1.222939000	1.770966000
1	3.823172000	1.335868000	1.387043000
1	2.368842000	2.084327000	1.899032000
6	2.578541000	0.200141000	2.612634000
8	1.518823000	0.179962000	3.249565000
6	3.573963000	-0.953672000	2.699431000
1	3.323502000	-1.509230000	3.606266000
1	3.407881000	-1.628568000	1.848532000
6	5.060839000	-0.550355000	2.733865000
1	5.369554000	-0.056763000	1.807842000
1	5.654748000	-1.469249000	2.810301000
6	5.408165000	0.295367000	3.956650000
8	5.193508000	-0.099139000	5.104886000
7	5.986857000	1.504683000	3.703121000
1	6.070492000	1.829032000	2.739880000
6	6.429723000	2.350081000	4.795095000
1	6.914841000	1.741295000	5.560968000
1	7.165391000	3.062053000	4.405713000
6	5.329395000	3.147036000	5.518762000
8	5.426571000	3.414649000	6.717641000
7	4.308679000	3.573744000	4.736821000
1	4.235252000	3.242446000	3.781017000
6	3.109728000	4.198279000	5.265727000
1	2.764256000	3.618229000	6.131317000
6	3.327288000	5.655668000	5.772875000

1	4.085684000	5.585024000	6.557352000	1	-5.151588000	-0.201909000	4.728039000
1	2.398515000	5.981101000	6.257052000	6	-7.598913000	5.379350000	-1.308407000
6	3.741691000	6.664244000	4.725567000	1	-7.740530000	6.306983000	-0.744012000
6	5.098710000	6.912312000	4.472165000	1	-8.456492000	4.727251000	-1.102002000
6	2.780252000	7.384697000	3.999249000	1	-7.617606000	5.629626000	-2.375965000
6	5.487991000	7.852875000	3.515523000	6	-6.276846000	4.703694000	-0.923570000
6	3.165755000	8.323094000	3.039303000	1	-6.255823000	4.499066000	0.155010000
6	4.521540000	8.560594000	2.795663000	1	-5.438849000	5.382150000	-1.127412000
1	5.853474000	6.373390000	5.039682000	6	-6.042351000	3.398525000	-1.702370000
1	1.722837000	7.213061000	4.190400000	1	-6.856859000	2.685259000	-1.525468000
1	6.544466000	8.037553000	3.338201000	1	-6.047244000	3.605617000	-2.776959000
1	2.409046000	8.871692000	2.484797000	7	-4.757212000	2.763730000	-1.411979000
1	4.820979000	9.293847000	2.051717000	1	-3.954379000	3.007203000	-2.011643000
6	2.042467000	4.101561000	4.162947000	6	-4.498887000	1.937833000	-0.393525000
8	2.348703000	3.825721000	2.996373000	7	-3.246185000	1.498226000	-0.196614000
7	0.768984000	4.307260000	4.559724000	1	-5.178525000	0.989184000	1.261640000
1	0.586410000	4.681392000	5.482103000	1	-6.409384000	1.829925000	0.369642000
6	-0.353296000	4.227864000	3.643876000	7	-5.471128000	1.465503000	0.412117000
1	0.044044000	4.351629000	2.630790000	1	-3.084644000	1.014825000	0.689423000
6	-1.000596000	2.818072000	3.699054000	1	-2.474514000	2.068706000	-0.569510000
1	-0.181792000	2.100543000	3.551582000	6	-8.716207000	6.935032000	-6.256527000
8	-1.900180000	2.747741000	2.589430000	1	-8.996109000	6.030981000	-6.809829000
1	-2.385501000	1.891158000	2.620862000	1	-9.465192000	7.707860000	-6.466877000
6	-1.696551000	2.518993000	5.028254000	1	-8.762591000	6.698776000	-5.186854000
1	-0.990019000	2.590724000	5.862432000	6	-7.305807000	7.409056000	-6.653896000
1	-2.098735000	1.500391000	5.024860000	6	-6.232330000	6.373683000	-6.386061000
1	-2.526193000	3.212231000	5.205908000	6	-5.536373000	6.341886000	-5.170027000
6	-1.301895000	5.415499000	3.907710000	6	-5.922213000	5.386153000	-7.334147000
8	-0.978904000	6.339150000	4.659560000	6	-4.575135000	5.365405000	-4.898181000
7	-2.464805000	5.364598000	3.215724000	6	-4.968533000	4.402116000	-7.081335000
1	-2.649074000	4.509817000	2.689984000	6	-4.287990000	4.378912000	-5.854776000
6	-3.382776000	6.482705000	3.120055000	8	-3.371369000	3.396088000	-5.649130000
1	-2.964695000	7.283860000	3.733631000	1	-3.018172000	3.443511000	-4.725253000
6	-3.527544000	6.964934000	1.642241000	1	-7.071355000	8.331223000	-6.106788000
1	-4.258904000	7.784527000	1.632632000	1	-7.306056000	7.671762000	-7.719815000
1	-3.973728000	6.140939000	1.072809000	1	-5.740742000	7.101737000	-4.417898000
6	-2.241054000	7.395451000	1.005801000	1	-6.437778000	5.387295000	-8.292734000
6	-1.444864000	6.632624000	0.175683000	1	-4.035828000	5.368523000	-3.954952000
7	-0.331892000	7.341624000	-0.210098000	1	-4.737249000	3.643320000	-7.823642000
1	-1.590136000	5.616088000	-0.169132000	8	1.799175000	6.350795000	-1.802587000
1	0.409217000	7.008042000	-0.842903000	8	3.291030000	7.791996000	-0.948547000
6	-1.571674000	8.665283000	1.145848000	6	2.886947000	6.639355000	-1.153928000
6	-0.376625000	8.588621000	0.370708000	6	3.649930000	5.435944000	-0.569613000
6	-1.851523000	9.859637000	1.838148000	1	3.028326000	5.038990000	0.247521000
6	0.534189000	9.650649000	0.284178000	1	3.698685000	4.640344000	-1.323897000
6	-0.955891000	10.919988000	1.748298000	6	5.045048000	5.763647000	-0.503282000
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
1	-1.163950000	11.845244000	2.279871000	6	5.644687000	4.649491000	0.842197000
1	0.910887000	11.659177000	0.940115000	1	4.995655000	4.474174000	1.705782000
1	1.447878000	9.542552000	-0.294583000	1	6.614020000	4.978349000	1.243408000
6	-4.771262000	6.073073000	3.624322000	6	5.876763000	3.285351000	0.200643000
8	-5.308100000	5.027942000	3.220287000	8	5.748289000	2.232207000	0.855127000
7	-5.384870000	6.942165000	4.453314000	7	6.258315000	3.271467000	-1.093976000
1	-4.869641000	7.759567000	4.752887000	1	6.403185000	4.158385000	-1.556631000
6	-6.779854000	6.822631000	4.881079000	6	6.604168000	2.055179000	-1.822908000
1	-7.198465000	7.833606000	4.904754000	1	6.286546000	2.184766000	-2.862309000
1	-7.309190000	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
7	-1.338956000	-4.251825000	-0.185911000
7	0.260736000	-5.494919000	-2.213421000
7	-2.041673000	-5.697501000	-3.893630000
7	-3.624881000	-4.393610000	-1.896918000
6	-2.242587000	-3.650361000	0.652575000
6	-1.597522000	-3.266701000	1.903487000
6	-0.296052000	-3.655321000	1.781062000
6	-0.142079000	-4.263186000	0.480898000
6	1.233538000	-5.340573000	-1.263433000
6	2.490602000	-5.867030000	-1.750621000
6	2.257006000	-6.339246000	-3.006486000
6	0.857586000	-6.104255000	-3.285758000
6	-1.129538000	-6.273984000	-4.739242000
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8	-5.200468000	4.833099000	4.017413000	8	5.965305000	2.037316000	0.880183000
7	-5.061868000	6.848995000	5.064265000	7	6.230750000	1.932813000	-1.375720000
1	-4.526124000	7.700996000	5.167043000	1	6.382906000	2.463309000	-2.224195000
6	-6.261355000	6.687321000	5.885738000	6	6.089093000	0.485281000	-1.506984000
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	1.637863000	-4.950349000
1	-6.614418000	3.781253000	5.835274000	6	8.385217000	1.138652000	-6.057352000
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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
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7	-4.644013000	0.382985000	6.472532000	1	0.554118000	1.542267000	-1.662293000
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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
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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
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7	-3.283665000	0.966362000	0.376971000	6	-0.411081000	-0.940374000	-6.067312000
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1	-6.379325000	1.421470000	0.9744417000	6	1.366716000	-0.514342000	-4.467136000
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6	-0.869124000	2.379583000	5.559704000	1	-8.404291000	4.861240000	-6.243612000
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6	-0.443886000	5.344206000	4.539467000	6	-5.294728000	3.013468000	-7.466325000
8	0.085010000	6.206273000	5.246588000	6	-4.294989000	3.933179000	-5.035496000
7	-1.707371000	5.418260000	4.060868000	6	-4.359145000	2.248637000	-6.771253000
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6	-1.072749000	6.524476000	0.934087000	1	-3.898367000	4.294524000	-4.090602000
7	0.007583000	7.142368000	0.348333000	1	-4.005474000	1.300798000	-7.167114000
1	-1.313618000	5.498426000	0.682824000	8	1.980094000	5.742645000	-1.118052000
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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
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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
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6	0.979495000	10.739930000	0.610431000	1	4.919476000	6.592083000	0.891267000
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6	-4.318870000	6.659043000	3.567874000	6	6.284725000	3.352779000	1.051448000
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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	8.665228000	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
1	-0.299668000	4.283440000	3.777260000	7	-4.420019000	1.918239000	0.568848000
6	0.132843000	4.239406000	2.772332000	1	-1.980083000	2.470298000	1.054505000
6	-0.979169000	2.912237000	4.037066000	1	-1.572262000	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

6	-5.996190000	5.086769000	-7.488170000
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6	-4.121297000	4.505588000	-6.067053000
8	-3.018218000	3.734566000	-5.870762000
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1	-7.593621000	7.859454000	-6.383968000
1	-7.820034000	7.018938000	-7.911881000
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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	3.744986000	-3.000975000
8	-1.998926000	4.071481000	-3.411912000
8	-0.503975000	3.577492000	-1.806670000
6	-0.036465000	2.186055000	-4.892873000
1	-0.655659000	2.495871000	-5.739974000
1	0.910798000	1.827038000	-5.317236000
6	-0.767130000	1.123424000	-4.118465000
6	-2.134205000	0.971770000	-4.142119000
1	-2.857068000	1.435015000	-4.798571000
7	-2.535619000	0.154312000	-3.106720000
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6	-1.440089000	-0.224073000	-2.376145000
6	-0.283105000	0.308161000	-3.018734000
6	0.979994000	0.001907000	-2.512486000
6	1.072772000	-0.888088000	-1.338658000
6	-1.378554000	-0.835250000	-1.097543000
6	-0.160157000	-1.046390000	-0.531752000
1	1.896497000	0.301974000	-3.004900000
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1	-2.291779000	-1.078077000	-0.564253000
1	-0.056105000	-1.477527000	0.453315000
7	2.311260000	-0.623961000	-0.497223000
8	2.382186000	-1.166125000	0.601199000
8	3.216345000	0.052290000	-0.992280000

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26	0.439647000	-3.912257000	-2.333099000
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7	-1.480218000	-3.583085000	-2.879396000
6	-1.254693000	-3.062215000	0.059520000
6	-1.165350000	-2.753207000	1.482135000
6	0.120813000	-3.031905000	1.840042000
6	0.810022000	-3.498818000	0.660349000
6	2.846983000	-4.278473000	-0.497740000
6	4.241631000	-4.665160000	-0.500787000
6	4.550763000	-5.004460000	-1.782660000
6	3.345818000	-4.826203000	-2.562307000
6	2.093477000	-4.927934000	-4.685829000
6	2.013694000	-5.185643000	-6.104905000
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6	0.028322000	-4.490247000	-5.294593000
6	-2.002596000	-3.690373000	-4.142306000
6	-3.988870000	-3.314470000	-4.133424000
6	-3.707467000	-2.985323000	-2.848793000
6	-2.498724000	-3.155915000	-2.073014000
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6	3.247462000	-5.080985000	-3.923991000
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1	2.696474000	-3.826171000	1.570440000
1	4.140924000	-5.426565000	-4.434830000
1	-1.855034000	-4.145972000	-6.208029000
1	0.582107000	-2.901597000	2.811642000
1	4.880249000	-4.671763000	0.373691000
1	5.497344000	-5.346501000	-2.182194000
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1	0.288210000	-4.986770000	-7.467473000
1	-4.038872000	-3.301613000	-5.006457000
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6	-2.251800000	-2.143816000	-2.323221000
6	-2.391666000	-0.637908000	2.042387000
6	-3.461751000	0.095584000	2.849641000
8	-3.688317000	1.317406000	2.473320000
8	-4.030177000	-0.458565000	3.809192000
1	-2.024882000	-2.293350000	3.383605000
1	-3.214524000	-2.637091000	2.140254000
1	-1.434254000	-0.136432000	2.241664000
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16	-0.180253000	-6.302708000	-1.936692000
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7	3.273014000	1.303256000	2.350900000
1	4.244992000	1.470093000	2.107403000
1	2.696409000	2.136429000	2.410348000
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8	1.747150000	0.157292000	3.584673000
6	3.905282000	-0.875834000	3.306808000
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1	3.848432000	-1.540877000	2.435204000
6	5.366815000	-0.434589000	3.506747000
1	5.758756000	0.082406000	2.626617000
1	5.977062000	-1.336553000	3.638472000
6	5.554132000	0.400640000	4.772166000
8	5.200194000	-0.009224000	5.879283000
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6	6.477951000	2.447279000	5.743708000
1	6.826120000	1.823194000	6.569120000
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6	5.325307000	3.297596000	6.307035000
8	5.294822000	3.603591000	7.500340000
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6	3.193906000	4.415949000	5.780567000
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6	3.418075000	5.903620000	6.189967000

1	4.127150000	5.876572000	7.022328000	1	-5.068693000	0.544069000	4.869930000
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6	3.919000000	6.820159000	5.096305000	1	-7.369388000	7.275406000	-1.184944000
6	5.294663000	7.005568000	4.894011000	1	-8.158611000	5.715293000	-1.466462000
6	3.020130000	7.515796000	4.272085000	1	-7.261517000	6.503944000	-2.774675000
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6	3.484281000	8.367347000	3.266633000	1	-5.998408000	5.441575000	-0.166508000
6	4.857702000	8.541518000	3.074002000	1	-5.110875000	6.215036000	-1.471796000
1	6.002499000	6.487064000	5.535966000	6	-5.813410000	4.240064000	-1.962607000
1	1.949230000	7.395196000	4.422570000	1	-6.681683000	3.593282000	-1.785252000
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1	5.219006000	9.208978000	2.296331000	1	-3.743575000	3.691023000	-2.156550000
6	2.216706000	4.263087000	4.605253000	6	-4.456592000	2.751967000	-0.507474000
8	2.606973000	3.893012000	3.491422000	7	-3.280848000	2.180078000	-0.235333000
7	0.921332000	4.533121000	4.872857000	1	-5.289565000	1.987427000	1.167875000
1	0.674831000	5.012857000	5.730389000	1	-6.336677000	3.026173000	0.276527000
6	-0.097763000	4.494681000	3.840827000	7	-5.509670000	2.449710000	0.289980000
1	0.406071000	4.607231000	2.874566000	1	-3.190791000	1.762737000	0.693499000
6	-0.808147000	3.114253000	3.808281000	1	-2.428831000	2.517543000	-0.712560000
1	-0.010178000	2.361120000	3.739885000	6	-7.826005000	-1.151923000	-3.886395000
8	-1.579835000	3.095924000	2.603990000	1	-7.508513000	-2.097937000	-4.340117000
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6	-1.648638000	2.833295000	5.053309000	1	-7.240585000	-1.008092000	-2.970700000
1	-1.027038000	2.880862000	5.953789000	6	-7.619426000	0.022650000	-4.860355000
1	-2.081800000	1.828647000	5.003606000	6	-6.174619000	0.201710000	-5.280167000
1	-2.468354000	3.553650000	5.151036000	6	-5.295348000	0.998006000	-4.533945000
6	-1.021055000	5.716806000	4.018739000	6	-5.658393000	-0.449133000	-6.411035000
8	-0.758846000	6.606560000	4.834335000	6	-3.952886000	1.143935000	-4.888221000
7	-2.079158000	5.739752000	3.177541000	6	-4.319842000	-0.321427000	-6.779373000
1	-2.225947000	4.901000000	2.615026000	6	-3.458226000	0.474688000	-6.014186000
6	-2.920923000	6.905589000	2.983553000	8	-2.156924000	0.570837000	-6.422409000
1	-2.431394000	7.732789000	3.503047000	1	-1.636860000	1.061316000	-5.759735000
6	-3.050446000	7.234320000	1.467393000	1	-7.980978000	0.945207000	-4.387723000
1	-3.734002000	8.088711000	1.370673000	1	-8.243392000	-0.136630000	-5.749231000
1	-3.545075000	6.383353000	0.984365000	1	-5.663709000	1.522416000	-3.654626000
6	-1.739438000	7.525662000	0.799930000	1	-6.316269000	-1.067648000	-7.018410000
6	-0.997786000	6.658416000	0.023695000	1	-3.301229000	1.790336000	-4.304070000
7	0.167289000	7.260162000	-0.392039000	1	-3.928784000	-0.828792000	-7.656548000
1	-1.213397000	5.636373000	-0.262747000	8	2.287666000	6.085144000	-1.910990000
1	0.889247000	6.836473000	-0.990948000	8	3.827037000	7.535890000	-1.168543000
6	-0.977593000	8.747904000	0.873540000	6	3.362188000	6.389455000	-1.252673000
6	0.213008000	8.538758000	0.116671000	6	4.042076000	5.228337000	-0.499783000
6	-1.171876000	9.996146000	1.496749000	1	3.269539000	4.755719000	0.123270000
1	1.201693000	9.523401000	-0.017875000	1	4.348449000	4.460539000	-1.224225000
6	-0.197979000	10.979561000	1.360089000	6	5.214439000	5.673220000	0.380626000
6	0.979305000	10.743434000	0.614431000	1	4.923208000	6.593863000	0.893948000
1	-2.070094000	10.192292000	2.078379000	1	6.070889000	5.962375000	-0.244039000
1	-0.339331000	11.945805000	1.837964000	6	5.618475000	4.659072000	1.462381000
1	1.724340000	11.530795000	0.532598000	1	4.741613000	4.388460000	2.059132000
1	2.108120000	9.316996000	-0.581227000	1	6.319467000	5.141209000	2.159585000
6	-4.318633000	6.659534000	3.568088000	6	6.286127000	3.353478000	1.052461000
8	-4.986278000	5.670331000	3.225023000	8	6.149294000	2.323678000	1.744740000
7	-4.778965000	7.598022000	4.420410000	7	7.083972000	3.378456000	-0.034543000
1	-4.161252000	8.357614000	4.674982000	1	7.167687000	4.250861000	-0.539583000
6	-6.127731000	7.596483000	4.985301000	6	7.950761000	2.276029000	-0.440471000
1	-6.476661000	8.633853000	5.003744000	1	7.826027000	1.492712000	0.307907000
1	-6.765873000	7.047742000	4.288848000	1	8.992265000	2.617939000	-0.396015000
6	-6.210451000	7.009625000	6.405084000	6	7.660536000	1.742706000	-1.853311000
1	-5.537928000	7.578997000	7.058541000	1	8.454731000	1.018452000	-2.083839000
1	-7.227990000	7.188603000	6.779324000	1	7.774075000	2.558229000	-2.578426000
6	-5.871639000	5.515209000	6.526481000	6	6.304331000	1.088461000	-2.032726000
1	-5.814137000	5.252261000	7.590131000	6	5.907315000	0.010285000	-1.225909000
1	-4.878929000	5.318654000	6.104171000	6	5.432675000	1.516514000	-3.042523000
6	-6.908322000	4.600678000	5.854613000	6	4.673691000	-0.613141000	-1.417392000
1	-7.900126000	4.778252000	6.283053000	6	4.201192000	0.885655000	-3.247916000
1	-6.983248000	4.807920000	4.784705000	6	3.813234000	-0.179148000	-2.430907000
7	-6.625397000	3.174150000	6.021629000	1	6.571234000	-0.353703000	-0.445008000
1	-6.863201000	2.763598000	6.914427000	1	5.728828000	2.337434000	-3.691926000
6	-5.845913000	2.430602000	5.208564000	1	4.386228000	-1.449141000	-0.784955000
7	-5.301371000	2.942099000	4.105567000	1	3.564192000	1.212541000	-4.065934000
1	-5.256077000	3.945171000	3.926515000	1	2.860842000	-0.679637000	-2.582609000
1	-4.710921000	2.328658000	3.518834000	7	1.283163000	3.765128000	-2.548293000
7	-5.630412000	1.140333000	5.505899000	1	0.878650000	3.314806000	-1.707080000
1	-6.199880000	0.684851000	6.204584000	1	1.916640000	3.099361000	-2.998686000

6	-3.066275000	-4.692287000	-2.171859000	8	-1.876615000	2.692732000	2.939007000
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6	-1.988480000	-4.118534000	0.015042000	6	-1.697642000	2.834922000	5.373482000
6	2.463706000	-4.431845000	1.867879000	1	-1.002415000	3.012489000	6.200982000
6	4.113757000	-6.152549000	-2.354314000	1	-2.121749000	1.834220000	5.507587000
6	-0.344363000	-5.828266000	-4.220048000	1	-2.514586000	3.562497000	5.433812000
1	-2.966135000	-3.814311000	0.374931000	6	-1.221006000	5.535795000	3.820890000
1	2.911456000	-4.220255000	2.833810000	8	-0.886430000	6.556755000	4.427377000
1	5.081380000	-6.477216000	-2.724538000	7	-2.364456000	5.412104000	3.108343000
1	-0.794614000	-6.054003000	-5.181858000	1	-2.589479000	4.488829000	2.742039000
1	0.633307000	-3.257554000	3.718737000	6	-3.281927000	6.510965000	2.878605000
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1	6.173319000	-6.013731000	-0.378733000	6	-3.430804000	6.820976000	1.355718000
1	4.040708000	-6.985084000	-5.089316000	1	-4.145655000	7.649895000	1.259434000
1	1.542737000	-6.803122000	-6.135070000	1	-3.899863000	5.947848000	0.886365000
1	-3.163000000	-5.362140000	-4.273037000	6	-2.141195000	7.144323000	0.658482000
1	-4.079804000	-4.429674000	-1.895005000	6	-1.422358000	6.290611000	-0.151626000
6	-2.179225000	-2.818183000	2.902792000	7	-0.283407000	6.904422000	-0.616990000
6	-2.217742000	-1.285202000	2.723043000	1	-1.639858000	5.276543000	-0.451645000
6	-3.367624000	-0.555009000	3.427101000	1	0.412909000	6.477015000	-1.238529000
8	-3.587387000	0.657820000	3.024091000	6	-1.393695000	8.377915000	0.698126000
8	-4.005561000	-1.103977000	4.346208000	6	-0.233131000	8.184954000	-0.110916000
1	-2.156583000	-3.040710000	3.974884000	6	-1.581300000	9.626864000	1.321372000
1	-3.111688000	-3.250752000	2.521712000	6	0.729146000	9.186880000	-0.295443000
1	-1.282282000	-0.850686000	3.104514000	6	-0.633927000	10.627956000	1.133459000
1	-2.251419000	-1.018099000	1.662090000	6	0.512053000	10.408282000	0.336851000
16	0.505786000	-7.398713000	-0.451474000	1	-2.455899000	9.810570000	1.941821000
1	1.533078000	-7.597668000	0.405710000	1	-0.772240000	11.595014000	1.610645000
8	1.472698000	-3.451987000	-1.763936000	1	1.237688000	11.208577000	0.215456000
7	2.865223000	1.149342000	2.615583000	1	1.614605000	8.991062000	-0.894291000
1	3.777996000	1.189973000	2.175459000	6	-4.656563000	6.146322000	3.455859000
1	2.312211000	1.998249000	2.572396000	8	-5.166014000	5.038288000	3.225260000
6	2.506831000	0.191466000	3.498819000	7	-5.276059000	7.109109000	4.169336000
8	1.414452000	0.201165000	4.082796000	1	-4.778894000	7.973697000	4.338038000
6	3.508314000	-0.938985000	3.733833000	6	-6.639902000	6.995726000	4.685708000
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1	3.322099000	-1.709269000	2.976453000	1	-7.176329000	6.305082000	4.030801000
6	4.996158000	-0.545245000	3.694531000	6	-6.718008000	6.551349000	6.156702000
1	5.292773000	-0.181691000	2.706965000	1	-6.126963000	7.248586000	6.763286000
1	5.590056000	-1.447297000	3.887293000	1	-7.760907000	6.666875000	6.483503000
6	5.358932000	0.454831000	4.789715000	6	-6.245301000	5.116752000	6.445200000
8	5.118074000	0.231741000	5.978225000	1	-6.191506000	4.974686000	7.531840000
7	5.987142000	1.593061000	4.377601000	1	-5.229352000	4.969579000	6.060454000
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1	2.444722000	6.491881000	6.082739000	6	-7.597284000	3.810453000	-2.254316000
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6	3.381670000	8.207745000	2.527615000	1	-6.314282000	3.947300000	-0.510658000
6	4.751052000	8.373486000	2.300235000	1	-5.766590000	4.908850000	-1.877265000
1	5.946506000	6.604221000	4.952334000	6	-5.265466000	2.822513000	-2.039649000
1	1.871623000	7.346663000	3.800369000	1	-5.684607000	1.839736000	-1.787961000
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8	2.420619000	3.922341000	3.206032000	7	-2.245592000	2.526259000	0.061488000
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1	0.595414000	4.949340000	5.575898000	1	-5.398249000	1.883340000	0.351355000
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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

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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				
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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				
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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				
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6	-0.076716000	2.197624000	-4.908540000				
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6	-0.767582000	1.123421000	-4.113728000				
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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				
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Model B system – C4

²TS4_{B,C4-endo}

26	2.601809000	-4.490955000	-0.150338000
7	1.315748000	-4.122207000	1.372215000
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6	2.314001000	-4.608377000	-3.562428000
1	-1.679601000	-3.090314000	0.152918000
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1	5.377130000	-5.442894000	4.202171000
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1	6.691198000	-5.999278000	-3.090471000
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1	-1.913872000	-3.111025000	-2.452740000
6	-1.875818000	-2.853220000	2.939228000
6	-1.981729000	-1.344006000	2.645247000
6	-3.224270000	-0.672336000	3.234965000
8	-3.576656000	0.452288000	2.692675000
8	-3.809858000	-1.188951000	4.206524000
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1	-2.664706000	-3.382628000	2.388104000
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16	1.771335000	-6.878845000	-0.075548000
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8	3.133499000	-2.933717000	-0.182462000
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1	3.301010000	-1.390191000	3.566692000
1	3.436586000	-1.408269000	1.806726000
6	5.038397000	-0.343119000	2.795379000
1	5.364421000	0.180583000	1.892597000
1	5.651518000	-1.249531000	2.871621000
6	5.328554000	0.485603000	4.044784000
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7	5.907086000	1.702826000	3.828873000
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1	7.072585000	3.239214000	4.598665000
6	5.173852000	3.369524000	5.594061000
8	5.209075000	3.646297000	6.794367000
7	4.201376000	3.806790000	4.757949000
1	4.168769000	3.481635000	3.797523000
6	2.995380000	4.455682000	5.239815000

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6	3.595710000	6.878038000	4.517992000
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6	2.617555000	7.539395000	3.758610000
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6	1.930545000	4.277358000	4.148048000
8	2.246748000	3.984807000	2.988483000
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6	-7.953612000	0.052560000	-2.415894000	6	-0.093743000	2.309897000	-3.371673000
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1	-8.324695000	-0.971342000	-2.546910000	6	-1.166469000	1.408434000	-2.718626000
1	-8.048442000	0.568512000	-3.378984000	8	-2.282309000	1.345516000	-3.317840000
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6	-5.550202000	-0.626584000	-2.914691000	1	0.922171000	0.772729000	-4.514295000
1	-5.906558000	-1.637451000	-3.151947000	6	1.197649000	2.641462000	-5.557661000
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7	-4.159653000	-0.687408000	-2.465229000	1	-0.269456000	4.272135000	-6.012242000
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6	-3.674780000	-1.560863000	-1.573971000	1	1.599920000	5.284399000	-7.352410000
7	-2.416455000	-1.463069000	-1.147986000	6	2.834860000	3.640164000	-6.805653000
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1	4.219615000	4.682722000	-8.128530000	7	4.005712000	4.933169000	5.445472000
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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	4.338622000
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
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6	8.701687000	0.921081000	-1.356123000	1	6.688745000	-5.989004000	-3.099822000
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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
1	7.909151000	-0.843547000	-2.311833000	6	-3.222455000	-0.670951000	3.265160000
1	9.608907000	2.771153000	-0.728681000	8	-3.576192000	0.452737000	2.693172000
1	8.703493000	-0.230463000	-4.573443000	8	-3.807539000	-1.187520000	4.208404000
1	10.395580000	3.396627000	-2.991681000	1	-2.074651000	-3.005755000	4.007860000
1	9.945232000	1.898954000	-4.928623000	1	-2.659489000	-3.381682000	2.396528000
7	0.647487000	1.243028000	-1.293049000	1	-1.103075000	-0.821927000	3.061925000
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1	4.895291000	-4.236857000	-5.855838000	1	-3.434508000	7.110452000	3.085780000
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1	-2.389000000	-3.755494000	-4.573169000	1	-5.025626000	6.621555000	1.225264000
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6	-1.417682000	-1.980191000	2.817816000	6	-3.063304000	5.999912000	0.573808000
6	-2.131678000	-0.699564000	2.355848000	6	-2.158969000	4.995859000	0.291361000
6	-3.298081000	-0.222998000	3.217258000	7	-1.093402000	5.480717000	-0.427315000
8	-3.791254000	0.923182000	2.866053000	1	-2.181074000	3.952052000	0.576068000
8	-3.693493000	-0.894133000	4.190831000	1	-0.219491000	4.940662000	-0.567488000
1	-1.170646000	-1.892941000	3.880722000	6	-2.513459000	7.198994000	-0.009895000
1	-2.098528000	-2.835929000	2.725960000	6	-1.271891000	6.833257000	-0.614436000
1	-1.411352000	0.126232000	2.307365000	6	-2.933429000	8.541875000	-0.084114000
1	-2.499741000	-0.816010000	1.329574000	6	-0.450519000	7.767132000	-1.261012000
16	1.886398000	-5.280547000	-1.100189000	6	-2.125689000	9.468678000	-0.735526000
1	3.075208000	-5.641012000	-1.634100000	6	-0.893217000	9.085595000	-1.312742000
8	1.901988000	-1.126881000	-2.074864000	1	-3.874858000	8.853994000	0.363228000
7	3.703693000	1.571406000	3.355133000	1	-2.440249000	10.507789000	-0.794488000
1	4.633003000	1.840022000	3.048089000	1	-0.280530000	9.835992000	-1.805966000
1	2.949566000	2.204808000	3.110440000	1	0.499385000	7.451862000	-1.680879000
6	3.489743000	0.745484000	4.411473000	6	-5.056972000	5.946974000	3.918672000
8	2.360677000	0.539976000	4.867586000	8	-5.911483000	5.061415000	3.750406000
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				1	-4.297577000	7.442343000	5.057050000

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1	6.313610000	-6.599786000	-1.615516000	7	-2.728436000	5.244306000	2.950255000
1	0.848588000	-5.612577000	-4.758611000	1	-2.787171000	4.304997000	2.554777000
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7	6.011379000	2.370495000	4.315366000	1	-5.473096000	4.646972000	5.938966000
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6	6.397128000		2.286734000		4.826708000	
1	6.838560000		1.642001000		5.589577000	
1	7.165699000		2.988228000		4.484439000	
6	5.297210000		3.094924000		5.537678000	
8	5.369941000		3.334558000		6.744136000	
7	4.305390000		3.562834000		4.741803000	
1	4.241790000		3.250059000		3.779023000	
6	3.109724000		4.198280000		5.265722000	
1	2.760103000		3.622073000		6.131901000	
6	3.338365000		5.654425000		5.771354000	
1	4.101097000		5.579792000		6.551569000	

1	2.414428000	5.984378000	6.261837000	6	-7.598906000	5.379347000	-1.308404000
6	3.750299000	6.661739000	4.721706000	1	-7.738260000	6.307007000	-0.743502000
6	5.106376000	6.909099000	4.462949000	1	-8.459394000	4.730301000	-1.104481000
6	2.786486000	7.382083000	3.998280000	1	-7.614279000	5.630658000	-2.375763000
6	5.492397000	7.849126000	3.504365000	6	-6.280368000	4.698441000	-0.921346000
6	3.168644000	8.319432000	3.036066000	1	-6.262483000	4.492675000	0.157097000
6	4.523603000	8.556538000	2.787474000	1	-5.439294000	5.373825000	-1.122564000
1	5.863364000	6.370234000	5.027575000	6	-6.049640000	3.393322000	-1.701210000
1	1.729670000	7.211062000	4.193259000	1	-6.867360000	2.683068000	-1.527282000
1	6.548263000	8.033346000	3.323035000	1	-6.050779000	3.601845000	-2.775536000
1	2.409996000	8.867186000	2.483393000	7	-4.768112000	2.752480000	-1.408120000
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6	2.043540000	4.108623000	4.161530000	6	-4.517539000	1.921297000	-0.392184000
8	2.352458000	3.841290000	2.993874000	7	-3.268668000	1.470590000	-0.195456000
7	0.768972000	4.310743000	4.557160000	1	-5.205603000	0.978681000	1.261751000
1	0.584400000	4.678834000	5.481587000	1	-6.426881000	1.834539000	0.375462000
6	-0.352528000	4.233091000	3.639614000	7	-5.495085000	1.452766000	0.410270000
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1	-0.174714000	2.107326000	3.535564000	6	-8.716204000	6.935031000	-6.256526000
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6	-1.689118000	2.513553000	5.017183000	1	-8.770276000	6.684333000	-5.190499000
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1	-2.088769000	1.493957000	5.010443000	6	-6.226123000	6.392155000	-6.373297000
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6	-1.304712000	5.417279000	3.907343000	6	-5.897719000	5.423061000	-7.334134000
8	-0.983511000	6.340171000	4.660810000	6	-4.571491000	5.376620000	-4.887086000
7	-2.468158000	5.364250000	3.216316000	6	-4.936059000	4.444871000	-7.088711000
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6	-3.387434000	6.481147000	3.118528000	8	-3.339283000	3.433179000	-5.660217000
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6	-0.381879000	8.558943000	0.351271000	6	3.681937000	5.381458000	-0.558059000
6	-1.854960000	9.850977000	1.802814000	1	3.091285000	4.967970000	0.273825000
6	0.532992000	9.616771000	0.255972000	1	3.742120000	4.585263000	-1.310697000
6	-0.955247000	10.907032000	1.703732000	6	5.074548000	5.764642000	-0.051643000
6	0.229647000	10.789172000	0.942221000	1	4.988732000	6.678779000	0.542114000
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1	-1.160954000	11.838622000	2.225144000	6	5.726673000	4.686292000	0.831556000
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1	1.447341000	9.497553000	-0.319245000	1	6.706288000	5.039797000	1.183439000
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1	-8.035746000	6.241442000	6.516593000	1	8.358471000	1.448530000	-0.724731000
6	-6.518995000	4.699406000	6.359269000	6	9.027845000	2.625972000	-2.401398000
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7	-5.353271000	2.212064000	3.966660000	1	10.997568000	5.297441000	-1.590729000
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6	4.674081000	-2.753026000	-0.615786000	1	-0.932317000	-2.321567000	5.150556000
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6	1.838747000	4.612277000	4.212263000	6	-4.446843000	1.170796000	-0.221531000
8	2.219369000	4.145195000	3.131854000	7	-3.176223000	0.987790000	0.142160000
7	0.535663000	4.778158000	4.521355000	1	-5.124511000	0.361866000	1.505566000
1	0.275750000	5.318995000	5.336734000	1	-6.357454000	0.637948000	0.327590000
6	-0.525946000	4.439160000	3.592568000	7	-5.420558000	0.824394000	0.652121000
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6	-1.017262000	2.985829000	3.828782000	1	-2.429799000	1.505901000	-0.344531000
1	-0.121086000	2.350775000	3.813168000	6	-6.100932000	9.430019000	-4.684066000
8	-1.847019000	2.663321000	2.708805000	1	-6.674607000	9.018471000	-5.522868000
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6	-1.737586000	2.794343000	5.164153000	1	-6.449338000	8.937646000	-3.768628000
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1	-2.024005000	1.745249000	5.294402000	6	-4.213454000	7.744654000	-5.002855000
1	-2.645283000	3.405359000	5.218344000	6	-3.876982000	6.988429000	-3.872115000
6	-1.611192000	5.532683000	3.656236000	6	-4.217805000	7.086940000	-6.242753000
8	-1.424990000	6.586664000	4.271502000	6	-3.558099000	5.632322000	-3.963912000
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1	-4.288832000	5.436163000	0.716809000	1	-3.854273000	7.466169000	-2.894461000
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6	-1.773615000	6.029914000	-0.204817000	1	-3.295676000	5.070417000	-3.072184000
7	-0.723714000	6.774927000	-0.686713000	1	-3.898426000	5.238930000	-7.322124000
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6	-2.178949000	8.185065000	0.324954000	6	2.616873000	6.241782000	-1.382752000
6	-0.938632000	8.097476000	-0.374980000	6	3.483457000	5.236871000	-0.600140000
6	-2.625449000	9.451440000	0.750961000	1	2.904485000	4.957986000	0.293622000
6	-0.144241000	9.221370000	-0.642282000	1	3.585503000	4.316962000	-1.189503000
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6	-0.614537000	10.456138000	-0.205239000	1	4.719995000	6.770465000	0.249591000
1	-3.567280000	9.557036000	1.285149000	1	5.496390000	5.909930000	-1.052446000
1	-2.182588000	11.551538000	0.805745000	6	5.550701000	4.901461000	0.890016000
1	-0.024931000	11.349660000	-0.393773000	1	4.941311000	4.873204000	1.798709000
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6	-5.098657000	5.739091000	3.262551000	6	5.845419000	3.448642000	0.532277000
8	-5.511061000	4.585557000	3.060093000	8	5.796395000	2.547492000	1.395146000
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6	6.170288000	-2.964504000	-7.330246000	6	-0.842766000	0.528523000	3.683964000
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6	0.644211000	-3.682672000	-4.960826000	8	-1.537025000	-0.959068000	1.963973000
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6	3.103208000	5.738347000	5.326522000	6	-6.494801000	0.024028000	-1.943793000
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7	-3.181344000	0.462981000	3.257416000	6	-3.600981000	4.356313000	-5.925338000
1	-2.820631000	0.002241000	2.421785000	6	-3.297614000	3.248618000	-5.118456000
6	-4.466955000	1.145408000	3.200495000	8	-3.071892000	2.055457000	-5.728724000
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6	-2.740488000	1.522161000	0.224434000	1	-2.993508000	2.573858000	-3.089834000
7	-1.794650000	2.439984000	-0.172142000	1	-3.639402000	4.223887000	-7.003081000
1	-2.639553000	0.484011000	-0.064199000	8	0.862563000	1.797844000	-0.935034000
1	-0.878283000	2.210616000	-0.587404000	8	1.820601000	3.812993000	-1.237470000
6	-3.344564000	3.514840000	1.086601000	6	1.725606000	2.712569000	-0.656256000
6	-2.128855000	3.668224000	0.354904000	6	2.699441000	2.370960000	0.487523000
6	-3.902975000	4.645533000	1.714019000	1	2.127396000	1.902666000	1.297703000
6	-1.465354000	4.898178000	0.249735000	1	3.380680000	1.590803000	0.115511000
6	-3.250656000	5.869681000	1.608285000	6	3.488693000	3.570445000	1.018480000
6	-2.041612000	5.994233000	0.886201000	1	2.785271000	4.334308000	1.369054000
1	-4.832003000	4.566724000	2.274373000	1	4.037685000	4.042994000	0.194531000
1	-3.674923000	6.747661000	2.088745000	6	4.421082000	3.226187000	2.195794000
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6	-5.532476000	0.291489000	3.920058000	6	5.583825000	2.288903000	1.892822000
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7	-5.712320000	0.597770000	5.222820000	7	6.302462000	2.551265000	0.785678000
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