

Electronic Supporting Information

How external perturbations affect the chemoselectivity of substrate activation by cytochrome P450 OleT_{JE}

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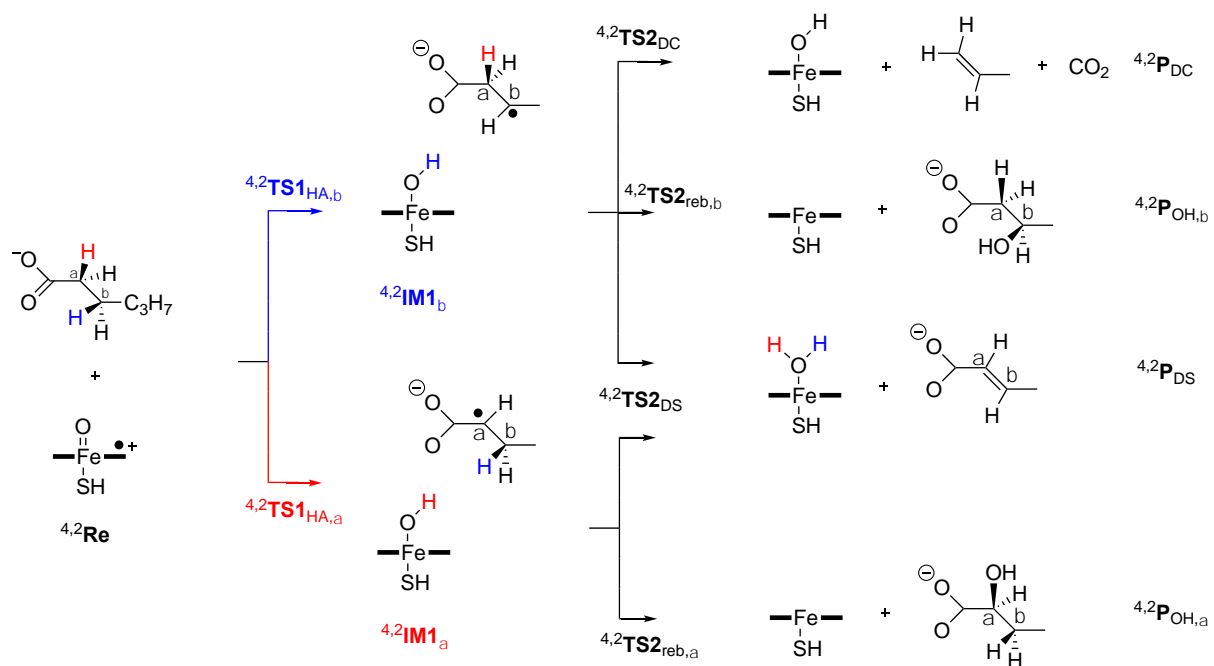
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Scheme S1: Reaction mechanism with definition of labels for substrate activation by P450 CpdI leading to various products.

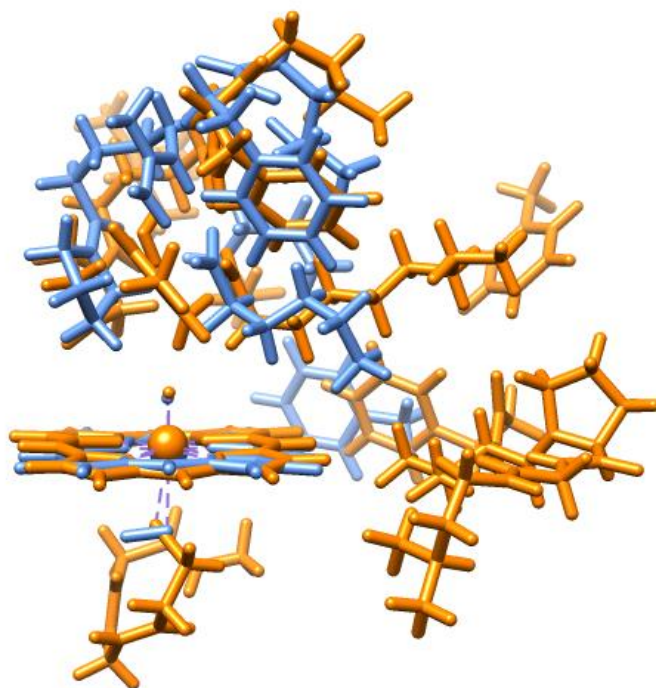


Fig. S1: Overlay of the optimized geometries of ${}^2\text{Re}_A$ (in blue) and ${}^2\text{Re}_B$ (in amber).

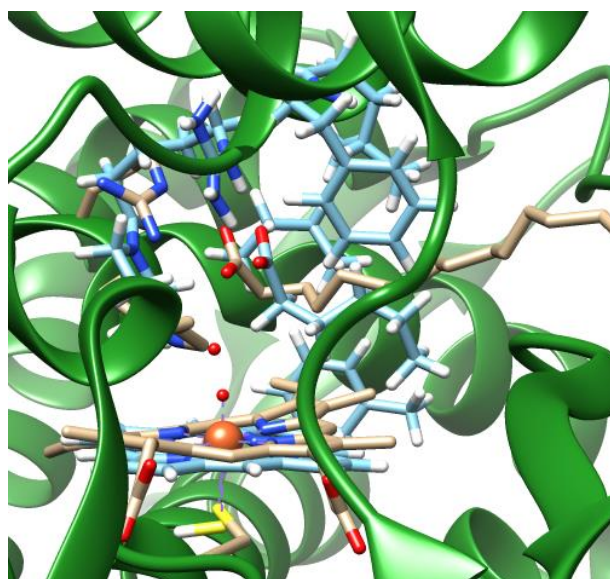


Fig. S2: Overlay of the optimized geometry of ${}^2\text{Re}_A$ (with light blue carbon atoms) with the crystal structure coordinates (4L40 pdb, green chains and grey carbon atoms).

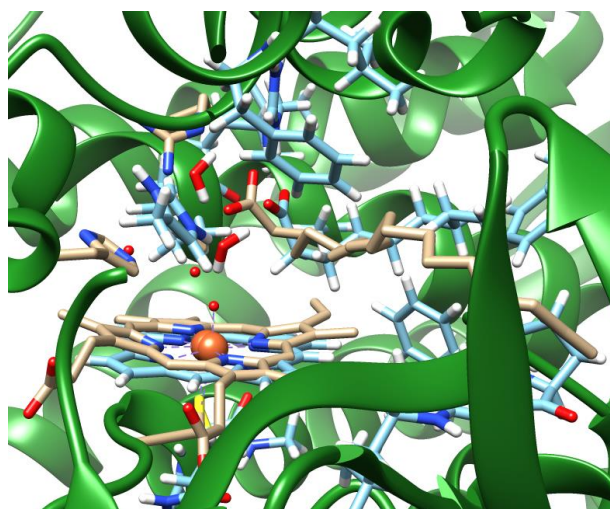


Fig. S3: Overlay of the optimized geometry of ${}^2\text{Re}_B$ (with light blue carbon atoms) with the crystal structure coordinates (4L40 pdb, green chains and grey carbon atoms).

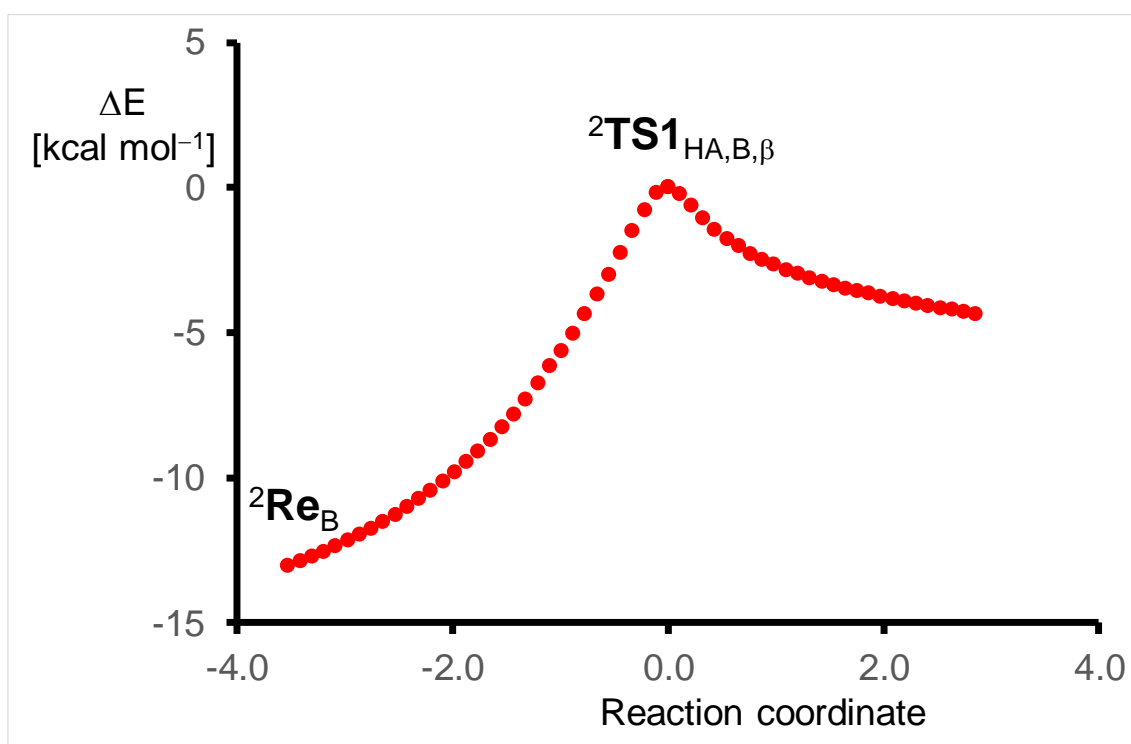


Fig. S4: UB3LYP/BSG1 calculated intrinsic reaction coordinate scan from ${}^2\text{TS1}_{\text{HA,B},\beta}$ in the direction of reactants and products. As can be seen, the scan falls back ${}^2\text{Re}_B$ in one direction. Energies are relative to the transition state structure.

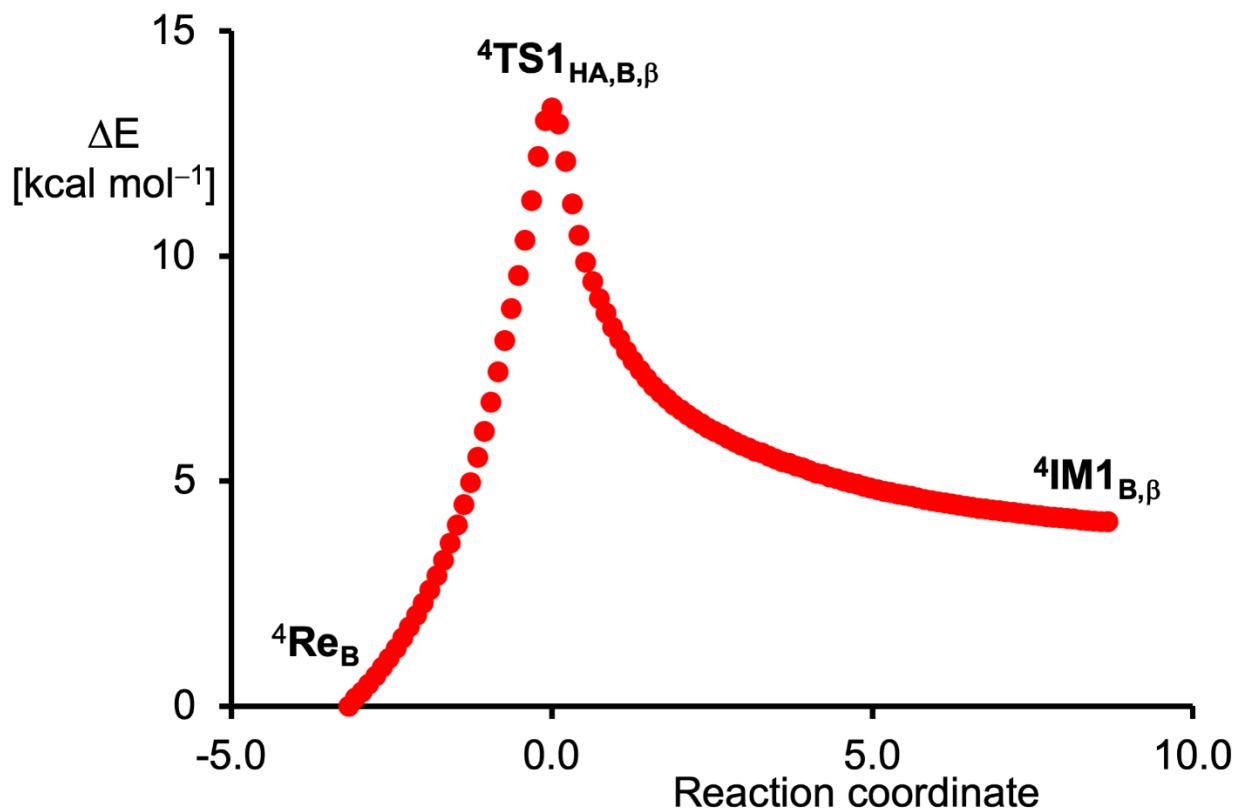


Fig. S5: UB3LYP/BSG1 calculated intrinsic reaction coordinate scan from ${}^4\text{TS1}_{\text{HA,B},\beta}$ in the direction of reactants and products. As can be seen, the scan falls back ${}^4\text{Re}_B$ in one direction. Energies are relative to the transition state structure.

Model A data:**Table S1: Absolute (free) energies (in au) of optimized geometries of local minima and transition states for the pathway of substrate activation by $^{2,4}\text{Re}_A$ as calculated in Gaussian-09.**

Structure	E [BSG1, au]	ZPE [au]	G [au]	E [BSG2, au]
$^2\text{Re}_A$	-3765.657348	1.371386	-3764.424599	-3766.600343
$^4\text{Re}_A$	-3765.657291	1.371421	-3764.425384	-3766.600171
$^2\text{TS1}_{\text{HA,A},\alpha}$	-3765.632924	1.366115	-3764.409439	-3766.578722
$^2\text{IM1}_{\text{A},\alpha}$	-3765.649347	1.369673	-3764.423993	-3766.599322
$^4\text{TS1}_{\text{HA,A},\alpha}$	-3765.630742	1.365570	-3764.406169	-3766.573767
$^4\text{IM1}_{\text{A},\alpha}$	-3765.647699	1.368373	-3764.423039	-3766.590810
$^2\text{TS1}_{\text{HA,A},\beta}$	-3765.627131	1.364774	-3764.400671	-3766.563006
$^2\text{IM1}_{\text{A},\beta}$	-3765.648742	1.367759	-3764.426105	-3766.591303
$^2\text{IM1}'_{\text{A},\beta}$	-3765.640601	1.367238	-3764.415450	-3766.566766
$^4\text{TS1}_{\text{HA,A},\beta}$	-3765.624701	1.364872	-3764.397397	-3766.560096
$^4\text{IM1}_{\text{A},\beta}$	-3765.653842	1.369020	-3764.428662	-3766.601867
$^2\text{P}_{\text{DC},\text{A}}$	-3765.687229	1.367841	-3764.462894	-3766.660498
$^4\text{TS2}_{\text{DC},\text{A}}$	-3765.627447	1.365577	-3764.397872	-3766.580140
$^4\text{P}_{\text{DC},\text{A}}$	-3765.631598	1.363429	-3764.416785	-3766.602147
$^2\text{P}_{\text{OH},\text{A},\beta}$	-3765.740006	1.373697	-3764.504858	-3766.679672
$^4\text{TS2}_{\text{reb,A},\beta}$	-3765.645349	1.367878	-3764.419207	-3766.594022
$^4\text{P}_{\text{OH},\text{A},\beta}$	-3765.743298	1.373942	-3764.514604	-3766.685640
$^2\text{TS2}_{\text{DS},\text{A}}$	-3765.648076	1.367078	-3764.417294	-3766.593016
$^2\text{P}_{\text{DS},\text{A}}$	-3765.735566	1.372113	-3764.505171	-3766.677398
$^4\text{TS2}_{\text{DS},\text{A}}$	-3765.642144	1.366380	-3764.416121	-3766.590635
$^4\text{P}_{\text{DS},\text{A}}$	-3765.715214	1.369543	-3764.489519	-3766.659426

Table S2: Relative (free) energies (in kcal mol⁻¹) of optimized geometries of local minima and transition states for the pathway of substrate activation by ^{2,4}Re_A as calculated in Gaussian-09.

Structure	ΔE	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$	ΔG
	[BSG1]	[BSG1]	[BSG1]	[BSG2]	[BSG2]	[BSG2]
² Re _A	0.00	0.00	0.00	0.00	0.00	0.00
⁴ Re _A	0.04	0.06	-0.49	0.11	0.13	-0.42
² TS1 _{HA,A,α}	15.33	12.02	9.51	13.57	10.26	7.75
² IM1 _{A,α}	5.02	3.95	0.38	0.64	-0.43	-4.00
⁴ TS1 _{HA,A,α}	16.70	13.05	11.57	16.68	13.03	11.55
⁴ IM1 _{A,α}	6.06	4.16	0.98	5.98	4.09	0.91
² TS1 _{HA,A,β}	18.96	14.81	15.02	23.43	19.28	19.48
² IM1 _{A,β}	5.40	3.12	-0.95	5.67	3.40	-0.67
² IM1' _{A,β}	10.51	7.91	5.74	21.07	18.47	16.30
⁴ TS1 _{HA,A,β}	20.49	16.40	17.07	25.26	21.17	21.84
⁴ IM1 _{A,β}	2.20	0.72	-2.55	-0.96	-2.44	-5.71
² P _{DC,A}	-18.75	-20.97	-24.03	-37.75	-39.97	-43.03
⁴ TS2 _{DC,A}	18.76	15.12	16.77	12.68	9.03	10.69
⁴ P _{DC,A}	16.16	11.17	4.90	-1.13	-6.12	-12.39
² P _{OH,A,β}	-51.87	-50.42	-50.36	-49.78	-48.33	-48.27
⁴ TS2 _{reb,A,β}	7.53	5.33	3.38	3.97	1.77	-0.18
⁴ P _{OH,A,β}	-53.93	-52.33	-56.48	-53.52	-51.92	-56.07
² TS2 _{DS,A}	5.82	3.12	4.58	4.60	1.89	3.36
² P _{DS,A}	-49.08	-48.63	-50.56	-48.35	-47.90	-49.83
⁴ TS2 _{DS,A}	9.54	6.40	5.32	6.09	2.95	1.87
⁴ P _{DS,A}	-36.31	-37.47	-40.74	-37.07	-38.23	-41.50

Table S3: Group spin densities and charges of optimized geometries of local minima and transition states for the pathway of substrate activation by $^{2,4}\text{Re}_A$ as calculated in Gaussian-09 at B3LYP/BSG1 level of theory.

(a) Spin densities

Spin	Fe	O	Por	SH	Protein	SubH	Total
$^2\text{Re}_A$	1.21	0.87	-0.52	-0.57	0.00	0.00	1.00
$^4\text{Re}_A$	1.09	0.92	0.46	0.52	0.00	0.00	3.00
$^2\text{TS1}_{\text{HA,A},\alpha}$	1.68	-0.03	-0.16	-0.05	0.00	-0.44	1.00
$^2\text{IM1}_{\text{A},\alpha}$	1.75	0.24	-0.11	0.12	0.04	-1.04	1.00
$^4\text{TS1}_{\text{HA,A},\alpha}$	1.11	0.66	0.31	0.43	-0.02	0.51	3.00
$^4\text{IM1}_{\text{A},\alpha}$	1.77	0.23	-0.11	0.11	-0.05	1.04	3.00
$^2\text{TS1}_{\text{HA,A},\beta}$	1.01	0.52	-0.54	-0.36	0.00	0.36	1.00
$^2\text{IM1}_{\text{A},\beta}$	0.89	0.14	0.45	0.31	-0.01	-0.77	1.00
$^2\text{IM1}'_{\text{A},\beta}$	1.01	0.08	-0.53	-0.36	0.03	0.76	1.00
$^4\text{TS1}_{\text{HA,A},\beta}$	0.96	0.65	0.41	0.45	0.01	0.52	3.00
$^4\text{IM1}_{\text{A},\beta}$	1.79	0.24	-0.11	0.09	0.01	0.98	3.00
$^2\text{P}_{\text{DC,A}}$	0.97	0.07	-0.08	0.04	0.00	0.00	1.00
$^4\text{TS2}_{\text{DC,A}}$	2.83	0.11	0.05	0.00	0.00	0.01	3.00
$^4\text{P}_{\text{DC,A}}$	0.92	0.11	1.82	0.15	0.00	0.00	3.00
$^2\text{P}_{\text{OH,A},\beta}$	1.21	0.00	-0.13	-0.08	0.00	0.00	1.00
$^4\text{TS2}_{\text{reb,A},\beta}$	2.02	0.12	-0.12	0.13	0.03	0.82	3.00
$^4\text{P}_{\text{OH,A},\beta}$	2.49	0.00	0.04	0.47	0.00	0.00	3.00
$^2\text{TS2}_{\text{DS,A}}$	1.06	0.01	-0.35	-0.33	0.05	0.56	1.00
$^2\text{P}_{\text{DS,A}}$	1.07	0.00	-0.08	0.01	0.00	0.00	1.00
$^4\text{TS2}_{\text{DS,A}}$	2.32	0.04	-0.11	0.10	0.07	0.58	3.00
$^4\text{P}_{\text{DS,A}}$	3.09	0.01	0.05	-0.15	0.00	0.00	3.00

(b) Charges

Charge	Fe	O	Por	SH	Protein	SubH	Total
$^2\text{Re}_A$	0.48	-0.41	-0.05	-0.04	0.82	-0.81	0.00
$^4\text{Re}_A$	0.47	-0.40	-0.04	-0.04	0.82	-0.81	0.00
$^2\text{TS1}_{\text{HA,A},\alpha}$	0.43	-0.56	-0.24	-0.02	0.87	-0.48	0.00
$^2\text{IM1}_{\text{A},\alpha}$	0.39	-0.67	-0.24	0.05	0.82	-0.34	0.00
$^4\text{TS1}_{\text{HA,A},\alpha}$	0.40	-0.59	-0.14	0.01	0.84	-0.52	0.00
$^4\text{IM1}_{\text{A},\alpha}$	0.40	-0.68	-0.22	0.05	0.81	-0.36	0.00
$^2\text{TS1}_{\text{HA,A},\beta}$	0.37	-0.58	-0.11	-0.05	0.84	-0.46	0.00
$^2\text{IM1}_{\text{A},\beta}$	0.32	-0.70	-0.14	-0.06	0.85	-0.25	0.00
$^2\text{IM1}'_{\text{A},\beta}$	0.39	-0.63	-0.25	-0.05	0.89	-0.34	0.00
$^4\text{TS1}_{\text{HA,A},\beta}$	0.40	-0.60	-0.14	-0.02	0.83	-0.48	0.00
$^4\text{IM1}_{\text{A},\beta}$	0.41	-0.68	-0.23	0.04	0.81	-0.35	0.00
$^2\text{P}_{\text{DC,A}}$	0.28	-0.73	-0.62	-0.18	1.06	0.20	0.00
$^4\text{TS2}_{\text{DC,A}}$	0.41	-0.77	-0.69	-0.20	1.02	0.24	0.00
$^4\text{P}_{\text{DC,A}}$	0.29	-0.73	-0.70	-0.14	1.06	0.22	0.00
$^2\text{P}_{\text{OH,A},\beta}$	0.27	-0.64	-0.36	0.01	0.82	-0.12	0.00
$^4\text{TS2}_{\text{reb,A},\beta}$	0.42	-0.68	-0.28	-0.03	0.85	-0.28	0.00
$^4\text{P}_{\text{OH,A},\beta}$	0.45	-0.64	-0.37	-0.15	0.83	-0.11	0.00
$^2\text{TS2}_{\text{DS,A}}$	0.34	-0.71	-0.26	-0.08	0.92	-0.22	0.00
$^2\text{P}_{\text{DS,A}}$	0.23	-0.73	-0.44	0.01	1.10	-0.16	0.00
$^4\text{TS2}_{\text{DS,A}}$	0.45	-0.71	-0.32	-0.09	0.93	-0.27	0.00
$^4\text{P}_{\text{DS,A}}$	0.44	-0.74	-0.59	-0.03	1.08	-0.17	0.00

Model B data:

Table S4: Absolute (free) energies (au) of optimized geometries for substrate activation by $^{4,2}\text{Re}_B$ as calculated at the UB3LYP level of theory in the quartet spin state. Uncorrected vibrational energies and entropies.

	E_{BSG1}	$E_{\text{BSG1+ZPE}}$	G_{BSG1}	E_{BSG2}	$E_{\text{BSG2+ZPE}}$	G_{BSG2}	E_{Disp}	$E_{\text{Disp+ZPE}}$	G_{Disp}
$^4\text{Re}_B$	-6657.56226	-6654.94439	-6655.19763	-6660.83135	-6658.21347	-6658.46672	-6661.24313	-6658.62830	-6658.71265
$^4\text{TS1}_{\text{HA,B},\alpha}$	-6657.54574	-6654.93431	-6655.19422	-6660.80133	-6658.18990	-6658.44981	-6661.21103	-6658.60262	-6658.68369
$^4\text{TS1}_{\text{HA,B},\beta}$	-6657.54247	-6654.93199	-6655.18737	-6660.79413	-6658.18365	-6658.43904	-6661.21855	-6658.61102	-6658.69420
$^4\text{IM1}_{\text{B},\alpha}$	-6657.56843	-6654.95332	-6655.21095	-6660.82771	-6658.21260	-6658.47023	-6661.23448	-6658.62249	-6658.70428
$^4\text{IM1}_{\text{B},\beta}$	-6657.55910	-6654.94498	-6655.20103	-6660.81719	-6658.20307	-6658.45913	-6661.23827	-6658.62723	-6658.71183
$^4\text{TS2}_{\text{reb,B},\alpha}$	-6657.55860	-6654.94138	-6655.19478	-6660.82365	-6658.20643	-6658.45983	-6661.23869	-6658.62450	-6658.70976
$^4\text{TS2}_{\text{DS,B},\beta}$	-6657.54913	-6654.93718	-6655.18811	-6660.80739	-6658.19543	-6658.44637	-6661.22929	-6658.62010	-6658.71145
$^4\text{TS2}_{\text{DC,B}}$	-6657.51711	-6654.90634	-6655.15661	-6660.78080	-6658.17003	-6658.42030	-6661.22929	-6658.62148	-6658.70655
$^4\text{P}_{\text{OH,B},\alpha}$	-6657.61571	-6654.99456	-6655.24444	-6660.88148	-6658.26034	-6658.51022	-6661.29266	-6658.67458	-6658.75988
$^4\text{P}_{\text{OH,B},\beta}$	-6657.64954	-6655.02625	-6655.27912	-6660.90861	-6658.28531	-6658.53818	-6661.33182	-6658.71170	-6658.79424
$^4\text{P}_{\text{DS,B}}$	-6657.64091	-6655.02165	-6655.27339	-6660.89960	-6658.28034	-6658.53208	-6661.31379	-6658.69750	-6658.78805
$^4\text{P}_{\text{DC,B}}$	-6657.58879	-6654.97722	-6655.25324	-6660.88705	-6658.27548	-6658.55150	-6658.27548	-6658.55150	-6661.30435
$^2\text{Re}_B$	-6657.56260	-6654.94476	-6655.19717	-6660.83182	-6658.21397	-6658.46638	-6661.24358	-6658.62867	-6658.71477
$^2\text{TS1}_{\text{HA,B},\alpha}$	-6657.54761	-6654.93580	-6655.19256	-6660.80335	-6658.19154	-6658.44830	-6661.21353	-6658.60482	-6658.68494
$^2\text{TS1}_{\text{HA,B},\beta}$	-6657.54441	-6654.93382	-6655.18823	-6660.79617	-6658.18558	-6658.43999	-6661.22058	-6658.61294	-6658.69542
$^2\text{IM1}_{\text{B},\alpha}$	-6657.56884	-6654.95384	-6655.21127	-6660.82796	-6658.21297	-6658.47039	-6661.23490	-6658.62301	-6658.70427
$^2\text{IM1}_{\text{B},\beta}$	-6657.55989	-6654.94583	-6655.20084	-6660.81813	-6658.20407	-6658.45909	-6661.23957	-6658.62861	-6658.71241

Table S5: Relative (free) energies (kcal mol^{-1}) of optimized geometries for substrate activation by $^{4,2}\text{Re}_B$ as calculated at the UB3LYP level of theory in the quartet spin state. Uncorrected vibrational energies and enthalpies.

	ΔE_{BSG1}	$\Delta E_{\text{BSG1+ZPE}}$	ΔG_{BSG1}	ΔE_{BSG2}	$\Delta E_{\text{BSG2+ZPE}}$	ΔG_{BSG2}	E_{Disp}	$E_{\text{Disp+ZPE}}$	G_{Disp}
$^4\text{Re}_B$	0.21	0.23	-0.29	0.29	0.31	-0.21	0.28	0.24	1.33
$^4\text{TS1}_{\text{HA,B},\alpha}$	10.58	6.56	1.85	19.13	15.11	10.40	20.43	16.35	19.50
$^4\text{TS1}_{\text{HA,B},\beta}$	12.63	8.01	6.15	23.65	19.03	17.16	15.71	11.08	12.91
$^4\text{IM1}_{\text{B},\alpha}$	-3.66	-5.37	-8.65	2.58	0.86	-2.41	5.71	3.88	6.58
$^4\text{IM1}_{\text{B},\beta}$	2.20	-0.14	-2.43	9.18	6.84	4.55	3.33	0.90	1.84
$^4\text{TS2}_{\text{reb,B},\alpha}$	2.51	2.12	1.50	5.12	4.73	4.11	3.07	2.62	3.14
$^4\text{TS2}_{\text{DS,B},\beta}$	8.45	4.76	5.68	15.33	11.63	12.56	8.97	5.38	2.08
$^4\text{TS2}_{\text{DC,B}}$	28.54	24.11	25.45	32.01	27.58	28.92	8.97	4.51	5.16
$^4\text{P}_{\text{OH,B},\alpha}$	-33.33	-31.25	-29.67	-31.17	-29.09	-27.51	-30.80	-28.80	-28.31
$^4\text{P}_{\text{OH,B},\beta}$	-54.56	-51.14	-51.43	-48.19	-44.77	-45.06	-55.37	-52.10	-49.87
$^4\text{P}_{\text{DS,B}}$	-49.14	-48.25	-47.83	-42.53	-41.64	-41.23	-44.06	-43.19	-45.99
$^4\text{P}_{\text{DC,B}}$	-16.43	-20.37	-35.19	-34.66	-38.60	-53.41	-38.14	-42.07	-56.89
$^2\text{Re}_B$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$^2\text{TS1}_{\text{HA,B},\alpha}$	9.41	5.62	2.89	17.87	14.08	11.35	18.86	14.97	18.72
$^2\text{TS1}_{\text{HA,B},\beta}$	11.41	6.86	5.61	22.37	17.82	16.56	14.43	9.87	12.14
$^2\text{IM1}_{\text{B},\alpha}$	-3.91	-5.70	-8.85	2.42	0.63	-2.52	5.45	3.55	6.59
$^2\text{IM1}_{\text{B},\beta}$	1.70	-0.67	-2.31	8.59	6.21	4.58	2.52	0.04	1.48

Table S6: Group spin densities of optimized geometries for substrate activation by $^4\text{Re}_B$ as calculated at the UB3LYP/BSG1 level of theory in the quartet spin state.

System	Fe	O	Porphyrin	Substrate	Amino Acids	Total
$^4\text{Re}_B$	1.20	0.82	0.33	0.00	0.65	3.00
$^4\text{TS1}_{\text{HA,B},\alpha}$	1.01	0.56	0.47	0.46	0.50	3.00
$^4\text{TS1}_{\text{HA,B},\beta}$	0.98	0.53	0.43	0.51	0.55	3.00
$^4\text{IM1}_{\text{B},\alpha}$	0.98	0.08	0.51	0.99	0.44	3.00
$^4\text{IM1}_{\text{B},\beta}$	0.98	0.08	0.49	0.98	0.47	3.00
$^4\text{TS2}_{\text{reb,B},\alpha}$	2.33	-0.02	-0.09	0.76	0.03	3.00
$^4\text{TS2}_{\text{DS,B},\beta}$	2.53	-0.06	-0.09	0.55	0.07	3.00
$^4\text{TS2}_{\text{DC,B}}$	0.98	0.07	0.50	0.95	0.49	3.00
$^4\text{P}_{\text{OH,B},\alpha}$	2.50	0.00	0.04	-0.00	0.46	3.00
$^4\text{P}_{\text{OH,B},\beta}$	2.52	0.00	0.05	-0.00	0.44	3.00
$^4\text{P}_{\text{DS,B}}$	2.51	0.00	0.05	-0.00	0.44	3.00
$^4\text{P}_{\text{DC,B}}$	2.64	0.00	-0.05	0.00	0.42	3.00

Table S7: Group charges of optimized geometries for substrate activation by $^4\text{Re}_B$ as calculated at the UB3LYP/BSG1 level of theory in the quartet spin state.

System	Fe	O	Porphyrin	Substrate	Amino Acids	Total
$^4\text{Re}_B$	0.52	-0.45	-0.17	-0.62	1.67	1.00
$^4\text{TS1}_{\text{HA,B},\alpha}$	0.48	-0.62	-0.13	-0.37	1.64	1.00
$^4\text{TS1}_{\text{HA,B},\beta}$	0.48	-0.63	-0.18	-0.32	1.65	1.00
$^4\text{IM1}_{\text{B},\alpha}$	0.43	-0.73	-0.12	-0.21	1.64	1.00
$^4\text{IM1}_{\text{B},\beta}$	0.41	-0.73	-0.13	-0.22	1.67	1.00
$^4\text{TS2}_{\text{reb,B},\alpha}$	0.43	-0.67	-0.33	-0.09	1.66	1.00
$^4\text{TS2}_{\text{DS,B},\beta}$	0.48	-0.68	-0.37	-0.02	1.59	1.00
$^4\text{TS2}_{\text{DC,B}}$	0.44	-0.73	-0.12	-0.26	1.68	1.00
$^4\text{P}_{\text{OH,B},\alpha}$	0.60	-0.68	-0.41	0.12	1.38	1.00
$^4\text{P}_{\text{OH,B},\beta}$	0.52	-0.70	-0.43	0.17	1.44	1.00
$^4\text{P}_{\text{DS,B}}$	0.55	-0.79	-0.43	0.24	1.43	1.00
$^4\text{P}_{\text{DC,B}}$	0.40	-0.74	-0.12	-0.25	1.71	1.00

Table S8: Group spin densities of optimized geometries for substrate activation by $^4\text{Re}_B$ as calculated at the UB3LYP/BSG1 level of theory in the doublet spin state.

System	Fe	O	Porphyrin	Substrate	Amino Acids	Total
$^2\text{Re}_B$	1.32	0.80	-0.42	0.00	-0.70	1.00
$^2\text{TS1}_{\text{HA,B},\alpha}$	1.10	0.53	-0.55	0.44	-0.52	1.00
$^2\text{TS1}_{\text{HA,B},\beta}$	1.08	0.49	-0.50	0.49	-0.57	1.00
$^2\text{IM1}_{\text{B},\alpha}$	1.07	0.06	-0.60	0.99	-0.51	1.00
$^2\text{IM1}_{\text{B},\beta}$	1.08	0.05	-0.57	0.94	-0.49	1.00

Table S9: Group charges of optimized geometries for substrate activation by $^4\text{Re}_B$ as calculated at the UB3LYP/BSG1 level of theory in the doublet spin state.

System	Fe	O	Porphyrin	Substrate	Amino Acids	Total
$^2\text{Re}_B$	0.52	-0.46	-0.11	-0.62	1.67	1.00
$^2\text{TS1}_{\text{HA,B},\alpha}$	0.46	-0.62	-0.13	-0.37	1.65	1.00
$^2\text{TS1}_{\text{HA,B},\beta}$	0.47	-0.63	-0.18	-0.31	1.65	1.00
$^2\text{IM1}_{\text{B},\alpha}$	0.43	-0.73	-0.12	-0.21	1.64	1.00
$^2\text{IM1}_{\text{B},\beta}$	0.41	-0.73	-0.14	-0.19	1.66	1.00

Cartesian Coordinates of model B optimized structures.

⁴ ReB				H	3.82318100	2.66836600	-9.54725600
C	5.72507800	7.49505500	1.97845600	H	2.98545500	0.84214500	-8.10054400
C	6.25997500	6.36904700	1.04659200	H	4.58653000	-0.70183400	-6.97084900
C	5.47734900	6.14806900	-0.27117500	H	7.03631500	-0.38489700	-7.31300600
C	5.56872200	7.36447600	-1.21302800	H	7.86861200	1.44386900	-8.76098000
C	5.99871200	4.87871800	-0.97510300	C	-3.79350500	9.19927300	-2.25225300
C	4.38956200	7.15115200	2.60278300	C	-2.29093700	9.28151300	-1.87484700
O	3.29086400	7.33497200	1.99549400	C	-1.35328700	8.73463100	-2.96895200
H	5.60492700	8.42475200	1.41512200	C	0.09157600	8.56195300	-2.47383200
H	7.30295400	6.61195100	0.79927600	N	0.18709400	7.43975400	-1.52464100
H	6.28174400	5.42692300	1.61168300	C	1.02669400	7.36682000	-0.48771700
H	4.41963800	5.98399100	-0.02107700	N	1.90944800	8.34875600	-0.19814900
H	5.02455700	7.17137400	-2.14444100	N	0.99514200	6.28173100	0.32834100
H	5.14203100	8.26952400	-0.76565300	C	-4.22172700	7.75407700	-2.44757000
H	6.61346800	7.57667100	-1.47549400	O	-4.17393200	7.21784700	-3.58827800
H	5.44595800	4.69050600	-1.90250100	H	-3.96658700	9.71927500	-3.19852700
H	5.88862000	3.99737400	-0.33275400	H	-2.12050400	8.72408000	-0.94354900
H	7.06050200	4.98196600	-1.23488400	H	-2.03675000	10.33047200	-1.66664200
N	4.42279400	6.60285300	3.84435400	H	-1.72378600	7.77549900	-3.34894800
C	3.22846800	6.15696200	4.56742200	H	-1.34334500	9.42317100	-3.82351600
C	3.21804500	4.63362900	4.83031200	H	0.76365200	8.38610400	-3.32442700
C	3.29349400	3.78655200	3.57323500	H	0.41252700	9.48846200	-1.97991700
C	2.23919300	3.77330500	2.64096000	H	-0.34731100	6.56882500	-1.75327900
C	2.32651700	3.01083400	1.46992100	H	2.00590300	9.15434800	-0.79033600
C	3.47158100	2.24241100	1.21856600	H	2.54401900	8.22118500	0.59147800
C	4.52259000	2.23923200	2.14191100	H	0.44802900	5.43271600	0.08322700
C	4.43259400	3.00900100	3.30887900	H	1.72062900	6.20810600	1.03317300
H	5.32231200	6.46834100	4.28492500	N	-4.56368100	7.03286000	-1.34278800
H	2.37347900	6.45093200	3.95553500	C	-4.79602300	5.57034800	-1.44594000
H	4.05269000	4.37639300	5.49625500	C	-5.25292100	5.16241800	-0.03127300
H	2.29831400	4.40968300	5.39052100	C	-4.67568200	6.25741000	0.89577100
H	1.34022900	4.35897500	2.82211400	C	-4.73495600	7.53618500	0.03858300
H	1.50605100	3.02598800	0.75849100	H	-3.86121900	5.08567300	-1.75025600
H	3.54202700	1.65143500	0.31118900	H	-6.34765300	5.16475800	0.02397600
H	5.40890300	1.64031800	1.95733500	H	-4.90997500	4.15818500	0.23343200
H	5.25143000	3.00035000	4.02386800	H	-5.24203300	6.36397800	1.82647400
C	0.02924100	1.62925700	7.42290100	H	-3.63776200	6.03516300	1.16730700
C	-0.46861000	2.16649100	6.11997500	H	-3.95110900	8.24996600	0.30469600
N	-0.73227900	3.53143700	5.91829700	H	-5.70577100	8.04212200	0.14665700
C	-1.14537400	3.74536000	4.64450400	C	-2.77689100	5.55136100	-7.25180600
N	-1.16075100	2.55943800	4.02530900	C	-2.50756800	5.01404500	-5.83807400
C	-0.74729400	1.56866900	4.91379500	H	-2.81159500	6.64683100	-7.26206000
H	0.99370800	2.07133600	7.69978400	H	-1.51418400	5.30718800	-5.47707600
H	0.16947400	0.54806500	7.35358500	H	-3.23598600	5.39906100	-5.11793700
H	-1.36117900	4.68820200	4.14564500	H	-2.54999600	3.91566900	-5.81766400
H	-0.67737500	0.53535200	4.62393900	C	2.30608800	-3.21850000	-7.86111000
H	-1.44472400	2.47206600	2.97578500	C	0.81003200	-3.17014700	-8.24408000
C	-3.45635800	13.42592600	-6.54339700	C	0.03870200	-1.91013900	-7.86693600
C	-3.56142500	12.02138300	-7.16950800	C	-1.27019500	-1.75435800	-8.36349400
C	-3.40204700	10.92885600	-6.08458800	C	-2.01926400	-0.60970100	-8.08051900
C	-3.65883100	9.49267700	-6.57282000	C	-1.47123500	0.40988100	-7.28919400
C	-2.54116300	11.85938000	-8.31356100	C	-0.17662500	0.26287100	-6.78159100
H	-2.46245300	13.57989000	-6.10061000	C	0.57432600	-0.88727200	-7.06608300
H	-4.57165700	11.91488600	-7.59757100	C	2.61439800	-3.33367300	-6.37357700
H	-2.38561000	11.00791200	-5.66344400	O	3.35904000	-2.50467900	-5.78178400
H	-4.09691700	11.15857600	-5.26202600	H	2.82509200	-2.32896300	-8.22635400
H	-4.63090800	9.42442100	-7.07881900	H	0.29271900	-4.04639700	-7.82467700
H	-2.89090000	9.16920600	-7.28542800	H	0.74814000	-3.29545800	-9.33357600
H	-3.67021300	8.77761300	-5.74139200	H	-1.69866100	-2.53372100	-8.98886400
H	-2.66968500	12.64568700	-9.06755200	H	-3.02088900	-0.50602700	-8.48617200
H	-2.64495800	10.89316700	-8.81884600	H	-2.03758300	1.31423600	-7.08824800
H	-1.51432900	11.93111200	-7.92846500	H	0.26003100	1.04805500	-6.17170800
C	6.41541000	3.28040700	-10.17807700	H	1.57602900	-0.97382900	-6.66060100
C	5.90657900	2.18609500	-9.26455200	N	2.05535100	-4.39433300	-5.72095700
C	4.52851700	2.00009600	-9.05988600	C	2.27132300	-4.67564900	-4.29089500
C	4.05515500	0.96857200	-8.24110600	C	0.92468800	-4.88431400	-3.54865500
C	4.95295900	0.09976900	-7.60578900	C	1.16093800	-5.25382200	-2.07171100
C	6.32871200	0.27973400	-7.80038500	C	0.03447600	-3.63390400	-3.66747300
C	6.79895800	1.31249900	-8.61886200	C	3.14101900	-5.94162900	-4.21742800
H	7.40893300	3.62728700	-9.87375900	O	2.64716500	-7.04074400	-4.57884500
H	5.74204300	4.14451800	-10.18310400	H	1.55413400	-5.10229100	-6.24214000

H	2.78166800	-3.80221500	-3.88324300	N	-3.90154600	-1.11448000	0.16686800
H	0.42293900	-5.73288800	-4.03474800	C	-2.85796100	-1.11660600	-2.06730300
H	1.70602900	-6.19529400	-1.96184400	C	-3.71357000	-0.20781000	-2.67138000
H	0.20217700	-5.37445600	-1.55355900	C	-3.68296300	0.14256700	-4.07632700
H	1.72664300	-4.47214900	-1.54809100	C	-4.73755600	0.98196300	-4.29844300
H	-0.94583100	-3.82651300	-3.21492200	C	-5.40235000	1.17027400	-3.02802400
H	-0.12609100	-3.34168000	-4.70965400	N	-4.76343500	0.44079300	-2.04231300
H	0.49255700	-2.78148200	-3.14677800	C	-6.52085500	1.97218600	-2.84559700
N	4.43859500	-5.82642800	-3.79892100	C	-7.13014100	2.21546900	-1.62451600
C	5.36554500	-6.97622600	-3.93181400	C	-8.24919100	3.11030100	-1.42932300
C	6.69313000	-6.30472300	-4.34229000	C	-8.54307400	3.09985900	-0.09440100
C	6.66599100	-4.97331800	-3.55873500	C	-7.62297700	2.17927000	0.53572400
C	5.18015900	-4.54390400	-3.57665100	N	-6.75990600	1.65015000	-0.41151400
C	5.54636100	-7.79836800	-2.64916400	C	-7.65742800	1.82214900	1.87626600
O	6.38840900	-8.72802800	-2.61248300	C	-6.88717700	0.82514600	2.44816400
H	4.97390000	-7.65692100	-4.69226700	C	-6.99679900	0.37988700	3.81813000
H	7.54873400	-6.93764200	-4.09991700	C	-6.09630400	-0.63335200	3.98974200
H	6.69083800	-6.11807900	-5.42202500	C	-5.40791700	-0.81229200	2.73207600
H	7.00333400	-5.13857600	-2.52898200	N	-5.91717100	0.07525300	1.78456000
H	7.31059500	-4.20821800	-4.00002100	Fe	-5.22338700	0.38422600	-0.08711700
H	4.96668400	-3.84252200	-4.38900600	H	-4.06167400	-2.32344400	3.35054800
H	4.87611900	-4.07869900	-2.63303000	H	-2.07795300	-1.55406000	-2.67990900
N	4.78394100	-7.46503300	-1.57721800	H	-6.94994300	2.42958300	-3.72799100
C	4.88428000	-8.19687700	-0.33055700	H	-8.38139000	2.32275700	2.51000400
C	4.04432800	-7.49370600	0.73083400	O	-0.51930700	3.96718500	-0.20933800
O	3.31171300	-6.51345300	0.44049100	C	-0.91993000	3.99616600	-1.46802500
H	4.11467100	-6.70618200	-1.60732000	O	-0.94825200	5.06630300	-2.15150800
H	4.53518600	-9.23245400	-0.45677000	C	-1.33753000	2.68315400	-2.10428300
N	4.14832400	-8.00473200	1.98790700	C	-0.19044900	1.64607300	-2.11763100
C	3.40237900	-7.47857300	3.13982600	C	1.04014900	2.08739800	-2.92915600
C	2.34917900	-8.45881500	3.68778300	C	2.16760000	1.03874000	-2.93366300
C	1.20559700	-8.83371600	2.71592700	C	3.41375500	1.48622900	-3.72140000
C	0.31004600	-9.91586600	3.35192500	C	4.56910000	0.46384600	-3.73046900
C	0.37053800	-7.60853100	2.29176600	C	5.24383900	0.25417700	-2.36034700
H	4.76062500	-8.79467700	2.14259400	C	6.46681900	-0.67487300	-2.43493500
H	2.94140000	-6.54693300	2.80618100	H	-1.67863700	2.89400300	-3.12140900
H	2.85551300	-9.37976700	4.01488500	H	-2.18716900	2.27394500	-1.54081400
H	1.91629500	-8.01017100	4.59519000	H	0.10915600	1.43264400	-1.08205800
H	1.66103500	-9.26219200	1.80997200	H	-0.57920700	0.70631700	-2.53190600
H	-0.47945200	-10.22940900	2.65940400	H	1.42964600	3.03290400	-2.52320300
H	-0.17384300	-9.53610900	4.26186300	H	0.73479000	2.30517600	-3.96359900
H	0.88965100	-10.80544500	3.62687000	H	2.44401600	0.81365500	-1.89231200
H	-0.46484100	-7.91850500	1.65263900	H	1.79192900	0.09610600	-3.36187400
H	0.96791100	-6.88533200	1.72732900	H	3.12105200	1.69432700	-4.76046000
H	-0.05314800	-7.10512400	3.17245100	H	3.77761500	2.44148400	-3.30952200
C	-8.01885800	-3.89620400	0.15037700	H	4.20106700	-0.49917800	-4.11328500
C	-6.74571000	-3.09056000	-0.13905300	H	5.32975900	0.80303800	-4.44779700
S	-7.14636500	-1.29051900	-0.57338700	H	5.55281500	1.23178400	-1.95795200
C	-8.98031600	-3.86217900	-1.02890900	H	4.51913500	-0.16070800	-1.64461000
O	-8.60265300	-4.12225900	-2.19908000	H	7.22752100	-0.26669800	-3.11177100
H	-8.50077300	-3.52501800	1.06175600	H	6.18385800	-1.66429900	-2.81579900
H	-6.07766400	-3.08459600	0.72655500	O	-1.39827000	5.42078600	2.37243000
H	-6.21060700	-3.50728300	-0.99598400	H	-1.72654900	4.63083900	1.88412600
N	-10.26620800	-3.48824100	-0.75350600	H	-0.84429600	5.95987800	1.77402800
C	-11.30315400	-3.44821200	-1.78493400	O	-1.89167400	2.67240200	1.55820600
C	-11.18915600	-2.30885500	-2.80600000	H	-2.72531100	2.27412000	1.19402700
O	-11.95411900	-2.29716300	-3.79324500	H	-1.27723600	3.00752600	0.81626300
H	-10.52005600	-3.26984500	0.19852400	O	-4.13267400	1.55576800	0.35155400
H	-11.28059600	-4.37474500	-2.36665300	H	-7.15807400	-2.57289900	-6.07215100
N	-10.22205800	-1.37161600	-2.58180600	H	-6.48122800	-3.20543000	-4.55084300
C	-9.87370000	-0.36387300	-3.57437900	H	-12.28011700	-3.38321300	-1.29912800
C	-8.56798800	-0.64119600	-4.32899600	H	-7.73808200	-4.94408900	0.32750600
O	-8.01077800	0.29227200	-4.96506500	H	-5.90061200	-1.20995100	4.88220700
H	-9.66164400	-1.42125200	-1.74048600	H	-2.13125000	-3.37414300	1.89329000
H	-9.78318900	0.62181900	-3.11053200	H	-0.63925000	4.25024400	6.61959800
H	-10.68948600	-0.32451500	-4.30379900	H	-0.67726200	1.82075300	8.23937100
N	-8.09442000	-1.91032800	-4.28640800	H	6.93152000	-0.81371600	-1.45131500
C	-6.90860900	-2.32407300	-5.03343400	H	3.16381800	6.69696800	5.52063000
H	-8.55666000	-2.61323900	-3.71811500	H	6.46493500	7.68773000	2.76516000
H	-6.17613600	-1.51518700	-5.04137000	H	-4.39432000	9.69852700	-1.48418100
C	-4.36295300	-1.69500600	2.51891500	H	-5.54226400	5.35760100	-2.21662100
C	-3.64792400	-1.81859400	1.33294400	H	-3.74215900	5.19533300	-7.63346600
C	-2.52396800	-2.70672200	1.14004300	H	-2.00220600	5.23281400	-7.96078100
C	-2.08944800	-2.53036600	-0.14383800	H	-3.61084600	14.20844300	-7.29581000
C	-2.95034200	-1.54109100	-0.75095800	H	-4.20279900	13.56653400	-5.75142800

H	2.75944000	-4.08319200	-8.36616500
H	4.11874800	-7.23078700	3.93344400
H	5.93408600	-8.26295400	-0.01530800
H	6.49817700	2.92751900	-11.21534200
H	-2.95811200	-0.22441900	-4.78849100
H	-5.06997400	1.42218000	-5.22534300
H	-8.73008000	3.66828800	-2.21915600
H	-9.31962800	3.64240400	0.42456700
H	-7.68531600	0.79227900	4.54121300
H	-1.27052000	-3.02216200	-0.64760200

4TS1_{HA,B, α}

C	4.33687300	9.76178000	1.18623200
C	5.36561900	9.05526600	0.25820300
C	4.79295800	8.39458000	-1.01847600
C	4.09723600	9.41282700	-1.94323400
C	5.92326800	7.66212300	-1.76961200
C	3.31042000	8.81124500	1.76596400
O	2.22060200	8.55186900	1.16959500
H	3.79825800	10.53439200	0.63095600
H	6.10994700	9.80807400	-0.03760800
H	5.90343400	8.29386500	0.84032600
H	4.04963000	7.64307100	-0.71543400
H	3.76523000	8.92693700	-2.86779700
H	3.21424200	9.85874600	-1.47259000
H	4.78455700	10.22284800	-2.22142200
H	5.53484100	7.15584400	-2.66031100
H	6.39777100	6.90597600	-1.13338300
H	6.69807800	8.36775000	-2.09699400
N	3.62413800	8.22854800	2.95053700
C	2.77187100	7.25225200	3.63767300
C	3.44195100	5.86797400	3.79344700
C	3.81390000	5.20565300	2.47986100
C	2.81865600	4.75814100	1.59091100
C	3.16263000	4.16753300	0.36873500
C	4.51183500	4.00748900	0.02387800
C	5.51021500	4.43987400	0.90339100
C	5.16093400	5.03831900	2.12092700
H	4.50954300	8.46422600	3.37765400
H	1.85425300	7.17305000	3.05154600
H	4.33616900	5.96799800	4.42332600
H	2.74024000	5.23458600	4.35573900
H	1.76777800	4.86560100	1.85294900
H	2.37884700	3.84300000	-0.30923300
H	4.78017200	3.54436300	-0.92013900
H	6.55693800	4.30959600	0.64686000
H	5.94175300	5.36635800	2.80247600
C	1.20346800	0.19697600	6.00446800
C	0.69506400	1.06975700	4.90701300
N	0.42821100	2.43753700	5.07788100
C	-0.01810300	2.97201600	3.91211700
N	-0.04469600	1.98991100	3.00631200
C	0.39011800	0.80683000	3.59325300
H	2.17558700	0.53896000	6.37940300
H	1.33211000	-0.82452300	5.63923200
H	-0.30439500	3.99669700	3.69865900
H	0.44955000	-0.11587800	3.04340100
H	-0.39217100	2.17290600	1.97280400
C	-9.63800800	11.75771100	-2.22935000
C	-9.88188200	10.24583700	-2.05197300
C	-8.61233800	9.54943700	-1.50361900
C	-8.79988100	8.07501200	-1.10909800
C	-10.36749400	9.61853200	-3.37367400
H	-8.84458400	11.93987900	-2.96701900
H	-10.67892600	10.11696600	-1.30121700
H	-7.81492400	9.63063200	-2.25979000
H	-8.26307300	10.11245600	-0.62455000
H	-9.60171900	7.96957300	-0.36648900
H	-9.06530500	7.45510800	-1.97317500
H	-7.88055400	7.66511400	-0.67568700
H	-11.26477600	10.13013800	-3.74156000
H	-10.61415200	8.55773000	-3.25823000
H	-9.59364700	9.70309000	-4.14893700
C	9.57994100	-0.50179400	-10.11996700
C	8.65744000	-1.08798400	-9.07279700

C	7.28542600	-0.78303500	-9.06766700
C	6.43668200	-1.30396200	-8.08421400
C	6.94266800	-2.14619900	-7.08494700
C	8.30836600	-2.45910900	-7.08382800
C	9.15466300	-1.93578800	-8.06731900
H	9.04982800	-0.31053200	-11.05912000
H	10.41816400	-1.17290800	-10.33596600
H	6.88136400	-0.13546800	-9.84148700
H	5.37904500	-1.05582900	-8.10028700
H	6.27973900	-2.55558600	-6.32859200
H	8.71337600	-3.11578100	-6.31931300
H	10.21163800	-2.18895600	-8.06013900
C	-4.56859300	9.35044900	0.01237500
C	-3.24385600	9.40821500	-0.79618100
C	-3.26323100	8.53840500	-2.06796200
C	-1.87949300	8.35791600	-2.72577700
N	-1.01104300	7.42006400	-1.99735300
C	-0.10364700	7.72078200	-1.06234000
N	0.20771600	8.99548900	-0.72444500
N	0.52999800	6.71946400	-0.40657500
C	-4.75496100	8.00819000	0.70169200
O	-5.39675200	7.07100000	0.14155200
H	-5.41907500	9.48886100	-0.66194500
H	-2.41641700	9.09635800	-0.14647000
H	-3.05029200	10.45430700	-1.07446700
H	-3.66685100	7.54551400	-1.83976700
H	-3.94092900	8.99175200	-2.80453500
H	-2.00489400	7.93569600	-3.72723000
H	-1.37745000	9.32616100	-2.86060800
H	-1.07961000	6.41544200	-2.29067000
H	-0.20748200	9.77771500	-1.19868000
H	0.95194400	9.14808200	-0.04386000
H	0.40801100	5.72877100	-0.71025100
H	1.30994200	6.96995600	0.19275500
N	-4.17192600	7.82841000	1.91784300
C	-4.28323300	6.53365100	2.63858300
C	-3.78324600	6.86503300	4.05494100
C	-2.75794600	7.99466000	3.81508800
C	-3.40328600	8.83363600	2.69456500
H	-3.64354200	5.78549800	2.15674800
H	-4.60908000	7.22584100	4.68011700
H	-3.34093400	5.99369500	4.54504000
H	-2.55210200	8.59048600	4.70890500
H	-1.81612800	7.55955800	3.46111800
H	-2.65947900	9.33499500	2.06957500
H	-4.07614800	9.59799400	3.10721800
C	-0.78622900	5.74477600	-7.21310500
C	-2.01243800	5.80882900	-6.29063700
H	0.04822900	6.32897900	-6.80645900
H	-1.78337000	5.41526200	-5.29363400
H	-2.36632700	6.84273300	-6.17882400
H	-2.84521300	5.22455100	-6.70215100
C	3.87496600	-4.75991500	-7.31216400
C	2.56892300	-4.83789900	-8.13200800
C	1.64159900	-3.63100900	-8.06071200
C	0.33456000	-3.75334300	-8.57026200
C	-0.54055200	-2.66390300	-8.58288600
C	-0.12486400	-1.42461100	-8.07711200
C	1.16636600	-1.29339700	-7.55686100
C	2.04378700	-2.38602800	-7.54845200
C	3.70596500	-4.58566100	-5.80868500
O	4.29248000	-3.66483900	-5.17694400
H	4.50276500	-3.93554200	-7.65779200
H	2.00159100	-5.73643600	-7.84962100
H	2.85627300	-5.00032400	-9.18116600
H	0.00615100	-4.70959800	-8.97002500
H	-1.53998600	-2.77877900	-8.99115400
H	-0.79762200	-0.57294800	-8.09452500
H	1.49782600	-0.33912100	-7.15845000
H	3.03485100	-2.26217700	-7.12704000
N	2.90750100	-5.49767300	-5.18165900
C	2.67784800	-5.51620400	-3.72651000
C	1.17323600	-5.69830500	-3.39542600
C	0.94811800	-5.71598100	-1.87151300
C	0.31915300	-4.60263400	-4.05952600

C	3.51464700	-6.68756500	-3.18017300	C	-3.31613800	-2.64866100	0.70692200
O	3.19510500	-7.86218800	-3.49816100	C	-2.69622500	-2.96026700	-0.47291300
H	2.54917800	-6.29095900	-5.69732100	C	-2.91252500	-1.84872200	-1.37193000
H	3.02352800	-4.55192400	-3.35200300	N	-3.65002800	-0.86281300	-0.73106400
H	0.87776400	-6.67880700	-3.79532700	C	-2.50337300	-1.80943800	-2.69898900
H	1.46748200	-6.53975200	-1.37419600	C	-2.81356100	-0.80102800	-3.60416400
H	-0.11931500	-5.83266400	-1.64888600	C	-2.58086100	-0.87129300	-5.03251300
H	1.28192900	-4.77454100	-1.41388500	C	-3.16736500	0.23362700	-5.58698300
H	-0.74417200	-4.78774100	-3.86187400	C	-3.71606900	1.00942200	-4.49659600
H	0.45981100	-4.56795300	-5.14359200	N	-3.49361300	0.36519300	-3.29452400
H	0.57522600	-3.61255900	-3.65840200	C	-4.30867600	2.26195300	-4.63821900
N	4.62197000	-6.41808200	-2.42286400	C	-4.67713000	3.08316800	-3.58100600
C	5.61765900	-7.48766400	-2.16303400	C	-5.12421700	4.45435000	-3.70212200
C	6.95876600	-6.72382700	-2.16370500	C	-5.32594600	4.92590800	-2.43466000
C	6.58263500	-5.35355100	-1.55889600	C	-5.04444000	3.83173200	-1.52833500
C	5.17744400	-5.05954600	-2.12929000	N	-4.63148300	2.71971900	-2.24282700
C	5.42161000	-8.25401100	-0.84920000	C	-5.28796100	3.87054600	-0.16005500
O	6.28626100	-9.08200400	-0.47153900	C	-5.24324400	2.76765600	0.68272600
H	5.54872700	-8.22985900	-2.96374300	C	-5.68398100	2.75542000	2.06089100
H	7.71788900	-7.26198400	-1.59317000	C	-5.53557600	1.47844800	2.52620000
H	7.31476800	-6.60563600	-3.19328300	C	-4.97403700	0.69419700	1.44878400
H	6.54524000	-5.42405600	-0.46536500	N	-4.82230300	1.49572600	0.31647100
H	7.29409400	-4.56446000	-1.81781600	Fe	-4.05826300	0.96735600	-1.47233200
H	5.22665000	-4.46965800	-3.05046100	H	-4.70545200	-1.12473800	2.49798400
H	4.54316400	-4.52961900	-1.41097000	H	-1.95034300	-2.66338200	-3.07598600
N	4.29447200	-8.00587000	-0.13815500	H	-4.46334300	2.62153000	-5.64866400
C	3.99277000	-8.74880400	1.06853900	H	-5.59343200	4.82845300	0.24908900
C	2.61364000	-8.33963800	1.57492900	O	0.11028800	4.08639700	-1.12491900
O	1.98031200	-7.38802400	1.04978900	C	-0.58063000	3.89965300	-2.23497500
H	3.60020800	-7.33729800	-0.44613700	O	-1.10678500	4.86256500	-2.88525500
H	4.02853400	-9.82850100	0.86914500	C	-0.78988100	2.49724500	-2.71024000
N	2.14281800	-9.06239500	2.62618100	C	0.35175600	1.50724700	-2.55242700
C	0.84025500	-8.81584500	3.26170900	C	1.52570800	1.77909600	-3.52451200
C	-0.16337200	-9.96666400	3.06409100	C	2.66189900	0.74888600	-3.38496600
C	-0.57023700	-10.26229200	1.60133400	C	3.82511300	1.00024300	-4.36316800
C	-1.48486900	-11.50295600	1.55246700	C	4.95545200	-0.04770300	-4.29563800
C	-1.24763100	-9.05300700	0.92559500	C	5.76967600	0.02353700	-2.98711400
H	2.69774800	-9.83362400	2.97293100	C	6.92405000	-1.03974800	-2.99172800
H	0.46273900	-7.88470200	2.83469800	H	-1.28986200	2.47435100	-3.67968200
H	0.25060200	-10.88300200	3.51207500	H	-1.72475500	2.01899500	-1.89886000
H	-1.06648700	-9.72429400	3.64508000	H	0.72360200	1.53846300	-1.52079300
H	0.34547100	-10.49620300	1.03687500	H	-0.02884200	0.49302900	-2.72773900
H	-1.74190000	-11.76004200	0.51866900	H	1.91946500	2.78939700	-3.34228900
H	-2.42204600	-11.31821200	2.09428600	H	1.14896700	1.77119900	-4.55766200
H	-1.00112500	-12.37644500	2.00656900	H	3.03165200	0.76204300	-2.34928700
H	-1.57775800	-9.31627400	-0.08624300	H	2.26087500	-0.26156700	-3.55838000
H	-0.56535800	-8.20101300	0.83931200	H	3.42195700	1.02130800	-5.38694400
H	-2.13458400	-8.73816200	1.49309900	H	4.24381100	2.00287900	-4.18096100
C	-8.45999600	-1.51660700	-1.31395100	H	4.53607300	-1.05369200	-4.44365400
C	-6.93685100	-1.33489800	-1.37375800	H	5.64392400	0.12031500	-5.13600000
S	-6.47570900	0.42210700	-1.91523800	H	6.17307800	0.98948400	-2.83174100
C	-9.12033600	-1.25618200	-2.65980800	H	5.11098500	-0.22842200	-2.13087500
O	-8.77490400	-1.86969300	-3.70082900	H	7.61425100	-0.84611900	-3.82164300
H	-8.88390700	-0.87155600	-0.53639300	H	6.54144200	-2.06066700	-3.11621800
H	-6.49062600	-1.51308100	-0.39159700	O	-0.92960500	5.09839000	2.07442100
H	-6.49248500	-2.02460700	-2.09558400	H	-1.18706800	4.28860800	1.55437500
N	-10.08895800	-0.29036900	-2.68103900	H	-0.64580000	5.79586200	1.44877000
C	-10.85789600	0.01797700	-3.88509400	O	-0.94495500	2.69447000	0.75305400
C	-10.11410400	0.77524300	-4.99061600	H	-1.66344000	2.19155700	0.23583500
O	-10.69298200	0.98373300	-6.07832000	H	-0.36567000	3.16450100	0.05196100
H	-10.30278600	0.20642000	-1.82913400	O	-2.42701600	1.53483300	-1.01649200
H	-11.20602100	-0.91287400	-4.34420600	H	-6.09384200	-1.44438100	-7.68314500
N	-8.82748800	1.14996500	-4.73153900	H	-6.88919700	-2.63648600	-6.61807800
C	-7.95868500	1.67806100	-5.77312100	H	-11.73938700	0.59884000	-3.60237600
C	-6.95684700	0.66693800	-6.34208800	H	-8.67613700	-2.55750400	-1.03581700
O	-5.99677900	1.08177700	-7.04705000	H	-5.77158200	1.09267600	3.50754800
H	-8.43061500	0.99454500	-3.81290700	H	-3.37673700	-3.24295300	1.60713600
H	-7.39112900	2.53437100	-5.40044300	H	0.54505300	2.94687300	5.94041400
H	-8.59604800	2.02083600	-6.59466200	H	0.50869200	0.16118800	6.85218300
N	-7.18211500	-0.64157300	-6.08026000	H	7.49818500	-1.00180200	-2.05792000
C	-6.34046000	-1.69317900	-6.64798300	H	2.50723700	7.64593100	4.62753300
H	-7.91318200	-0.91966000	-5.43247300	H	4.87907500	10.26372800	1.99751600
H	-5.40297400	-1.80540900	-6.09156500	H	-4.58863000	10.16732600	0.74221300
C	-4.55692900	-0.62297800	1.54710000	H	-5.31772500	6.18220500	2.60749800
C	-3.89499400	-1.33358200	0.54531000	H	-1.01244100	6.13764700	-8.21142400

H	-0.43650300	4.71271100	-7.33458200
H	-10.54278800	12.26679200	-2.58192500
H	-9.33350500	12.22607300	-1.28515700
H	4.44661400	-5.68206900	-7.48862200
H	1.00151000	-8.65044600	4.33479100
H	4.74786300	-8.55440300	1.84421100
H	10.00673400	0.45433800	-9.78664600
H	-2.05948000	-1.67263100	-5.53553600
H	-3.26316200	0.50461200	-6.62670300
H	-5.24128800	4.97694800	-4.63992300
H	-5.65090100	5.90197600	-2.10653100
H	-6.07546800	3.61564700	2.58375600
H	-2.15268100	-3.85901700	-0.72600600

⁴TS1_{HA,B,β}

C	4.87181500	10.01127400	-0.05024800
C	5.86288800	9.22121200	-0.95115500
C	5.24349900	8.48234900	-2.16138100
C	4.53511400	9.44283800	-3.13653500
C	6.34055300	7.67973400	-2.88967200
C	3.84870300	9.12008900	0.62251500
O	2.72166900	8.87078500	0.09421300
H	4.32949400	10.75131100	-0.64429100
H	6.61313200	9.93593300	-1.31834600
H	6.40149600	8.49206700	-0.32981800
H	4.49961900	7.76487700	-1.78486800
H	4.16346200	8.89575000	-4.01047600
H	3.67653400	9.94039800	-2.67271400
H	5.22676500	10.21577900	-3.49744800
H	5.91818100	7.11883300	-3.73102100
H	6.82051200	6.96199800	-2.21437600
H	7.11638100	8.34711600	-3.28760300
N	4.20809700	8.57415400	1.81076300
C	3.37121300	7.64141200	2.57369700
C	4.03768800	6.26191700	2.77213500
C	4.36123800	5.53321600	1.48035600
C	3.33577000	5.11427500	0.61185000
C	3.63690900	4.45339000	-0.58533400
C	4.97139200	4.18885300	-0.92486400
C	5.99812100	4.59377700	-0.06490800
C	5.69321400	5.26576500	1.12617100
H	5.12198000	8.79727500	2.18111500
H	2.43349200	7.54238400	2.02381700
H	4.95375200	6.38391500	3.36595300
H	3.35230700	5.66120700	3.38815700
H	2.29515100	5.29421200	0.87458500
H	2.83329500	4.15039200	-1.24993200
H	5.20294000	3.66353500	-1.84603100
H	7.03364200	4.38473100	-0.31548200
H	6.49629300	5.57298400	1.79157800
C	1.98653500	0.92161500	5.26668600
C	1.43555600	1.76956100	4.17035800
N	1.12054400	3.12792500	4.33692800
C	0.64331700	3.63823100	3.17208000
N	0.64576900	2.65101800	2.27249200
C	1.12790600	1.48758900	2.86115600
H	2.95203800	1.29709000	5.62659100
H	2.14330700	-0.09737600	4.90537000
H	0.31374300	4.64781000	2.95419900
H	1.21486100	0.56462800	2.31452400
H	0.26989600	2.80439300	1.24384200
C	-9.88987900	10.88952000	-2.58631000
C	-9.85598400	9.44015200	-2.06160100
C	-8.40040900	9.00413700	-1.76396300
C	-8.25886500	7.63998000	-1.06815200
C	-10.55959200	8.49053900	-3.05107700
H	-9.34541300	10.97078700	-3.53684100
H	-10.41067400	9.41113400	-1.10921300
H	-7.83658000	8.99533100	-2.71048500
H	-7.93220000	9.77575400	-1.13333700
H	-8.82817700	7.62035200	-0.12920600
H	-8.62971600	6.82382800	-1.69861500
H	-7.20945700	7.42870400	-0.83427700
H	-11.58386000	8.82590000	-3.25286600
H	-10.61528500	7.46630100	-2.66705700

H	-10.02257800	8.46308500	-4.00898100
C	6.06943200	4.13661700	-5.73237800
C	5.65035400	2.76332000	-5.25344400
C	4.55559400	2.10117100	-5.83591200
C	4.19083000	0.81397700	-5.42409700
C	4.91174300	0.15998300	-4.41449600
C	6.00134200	0.81393800	-3.82430100
C	6.36500100	2.10102400	-4.23906700
H	6.55197000	4.71164100	-4.93427200
H	5.21128900	4.71302400	-6.09513400
H	3.99107600	2.59562100	-6.62225800
H	3.34814600	0.31773500	-5.89686200
H	4.62973500	-0.84201000	-4.10241600
H	6.57151000	0.31884700	-3.04368800
H	7.22068500	2.59319800	-3.78293000
C	-4.10849200	9.73810500	-0.99886000
C	-2.81994100	9.81353800	-1.86500500
C	-2.82962800	8.81996200	-3.04384400
C	-1.45565000	8.61623500	-3.71515900
N	-0.58452900	7.69325000	-2.97203800
C	0.33915800	8.00807000	-2.06034600
N	0.67071800	9.28685500	-1.75838600
N	0.97381200	7.01493100	-1.39080700
C	-4.10018400	8.51105400	-0.10142900
O	-4.57401700	7.40714600	-0.50333900
H	-4.98657500	9.66145200	-1.64742200
H	-1.94992800	9.62430100	-1.22240900
H	-2.71222700	10.83643400	-2.25272300
H	-3.18975300	7.84276700	-2.70379000
H	-3.54102800	9.17397400	-3.80248000
H	-1.59588800	8.16498300	-4.70183800
H	-0.95041100	9.57733200	-3.88497800
H	-0.66621300	6.67898900	-3.23530100
H	0.25635000	10.06123300	-2.24610000
H	1.43014200	9.44721400	-1.09630900
H	0.83665800	6.02163800	-1.66818000
H	1.77192600	7.26877600	-0.81745700
N	-3.51942500	8.62293200	1.12327200
C	-3.43700000	7.46144100	2.04796900
C	-3.05335700	8.10152300	3.39410700
C	-2.22895900	9.34190800	2.98308600
C	-2.95138600	9.85686400	1.72292900
H	-2.66721100	6.76030200	1.70251300
H	-3.95132700	8.40940300	3.94341900
H	-2.48953500	7.41281600	4.02935600
H	-2.17654700	10.10304200	3.76661000
H	-1.20441600	9.04348500	2.72988900
H	-2.26966900	10.35796400	1.02980600
H	-3.75261000	10.56118900	1.98493600
C	-0.91871800	6.46290700	-7.97418900
C	-2.05787100	6.01068100	-7.04819400
H	-0.31430900	7.25099800	-7.50782900
H	-1.67149700	5.61970600	-6.09955400
H	-2.73820700	6.84402500	-6.82354400
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C	4.37031700	-3.49790100	-6.27322200
C	3.55831600	-3.84538000	-7.53709600
C	2.23327100	-3.11645100	-7.72343000
C	1.50759300	-3.33719800	-8.90994800
C	0.29647900	-2.68376200	-9.14743600
C	-0.21673100	-1.79031100	-8.19765400
C	0.49095500	-1.56470600	-7.01401900
C	1.70680400	-2.22290900	-6.77631000
C	3.78024100	-3.91780100	-4.93082400
O	3.76582100	-3.13032300	-3.94405100
H	4.54841300	-2.42105700	-6.21668800
H	3.37949700	-4.93035900	-7.58542300
H	4.19750800	-3.62833700	-8.40415300
H	1.90093700	-4.02497400	-9.65442100
H	-0.24407000	-2.86699700	-10.07076400
H	-1.15479700	-1.27633400	-8.38230700
H	0.09796000	-0.87900600	-6.26996900
H	2.23167700	-2.03765700	-5.84543100
N	3.32156400	-5.19810000	-4.84234400
C	2.84364200	-5.80970100	-3.58965600

C	1.38863400	-6.33513600	-3.70978200	H	-5.77168700	-2.32778000	-4.97917900
C	0.92139400	-6.93408000	-2.36955600	C	-3.66569800	-0.12011000	1.78989800
C	0.43303800	-5.21961000	-4.17138200	C	-3.24438500	-1.02331100	0.81447800
C	3.83556000	-6.94940900	-3.30081400	C	-2.80384900	-2.37405900	1.07934300
O	3.88276900	-7.92720100	-4.09154900	C	-2.41781800	-2.91154600	-0.11938300
H	3.41008600	-5.82736200	-5.62978700	C	-2.63598300	-1.89899700	-1.12718000
H	2.88097400	-5.02364600	-2.83510000	N	-3.14922200	-0.75133500	-0.53898200
H	1.39807300	-7.13539700	-4.46306300	C	-2.40812900	-2.07175700	-2.48672800
H	1.51569500	-7.79611700	-2.05350600	C	-2.69272600	-1.13543000	-3.47186500
H	-0.11730200	-7.27445700	-2.44690700	C	-2.63997500	-1.39537900	-4.89682900
H	0.96363300	-6.17826000	-1.57223200	C	-3.13492100	-0.28511000	-5.52315700
H	-0.58289100	-6.61777200	-4.27984900	C	-3.45461800	0.67326500	-4.48704800
H	0.73430400	-4.79211800	-5.13206000	N	-3.17330400	0.14330500	-3.24213600
H	0.40337000	-4.40370700	-3.43586300	C	-3.94079500	1.95639700	-4.72280300
N	4.69450300	-6.83157600	-2.24265000	C	-4.14401600	2.91921800	-3.74402000
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C	6.95231200	-6.83295300	-1.52136800	C	-4.55779400	4.92647500	-2.78046100
C	6.14904700	-5.89848500	-0.59027500	C	-4.24851200	3.93250900	-1.77495000
C	4.83733600	-5.63211700	-1.36149700	N	-3.98814000	2.71200900	-2.37973500
C	5.63682900	-8.98114800	-1.24904600	C	-4.31152200	4.16712000	-0.40660700
O	6.60747500	-9.71896900	-0.94943400	C	-4.21064800	3.18473700	0.56887900
H	6.11609600	-8.11071800	-3.12404100	C	-4.44519100	3.38868100	1.98277300
H	7.71051300	-7.42290000	-1.00347900	C	-4.31306300	2.17471200	2.59664200
H	7.43915800	-6.25829400	-2.31749000	C	-3.97166600	1.21331900	1.56985100
H	5.93716100	-6.40694200	0.35759100	N	-3.92954000	1.84590700	0.32947300
H	6.67770900	-4.96929500	-0.35967000	Fe	-3.45792800	1.01810600	-1.45958900
H	4.90407600	-4.72339400	-1.96971200	H	-3.71517400	-0.48180800	2.81212500
H	3.97525900	-5.53648800	-0.69401800	H	-2.02457200	-3.03401000	-2.81016500
N	4.37304800	-9.23250200	-0.83324400	H	-4.16736900	2.21585100	-5.74986500
C	4.05284400	-10.41532400	-0.06000900	H	-4.51438800	5.18911200	-0.10048000
C	2.55839400	-10.41066500	0.25011900	O	0.56928800	4.33031500	-2.09610400
O	1.82235600	-9.45722100	-0.11189800	C	-0.07788400	4.17773500	-3.22559600
H	3.59665700	-8.62996900	-1.07537900	O	-0.66696000	5.14163200	-3.81544800
H	4.32546600	-11.32419800	-0.61464600	C	-0.09037800	2.82446200	-3.93658200
N	2.10223100	-11.49027800	0.93768900	C	-0.00403900	1.54125300	-3.12227900
C	0.69458200	-11.67045000	1.32526200	C	1.28512300	1.22614000	-2.37740800
C	0.00749700	-12.84075300	0.59814900	C	1.30271500	-0.17693800	-1.74336100
C	-0.10122500	-12.70775000	-0.93912800	C	2.61687400	-0.47351900	-0.99561700
C	-0.68731900	-14.00276400	-1.53710400	C	2.72938100	-1.91610400	-0.46145600
C	-0.93349500	-11.48126100	-1.36448500	C	1.75167900	-2.25300000	0.68098800
H	2.75358900	-12.22692400	1.17459500	C	1.87853600	-3.70101700	1.18218900
H	0.19343800	-10.72412500	1.11339400	H	0.77229700	2.84760800	-4.62839700
H	0.54054600	-13.77323600	0.83977400	H	-0.98329700	2.81453800	-4.56664800
H	-1.00294600	-12.94875900	1.02113100	H	-0.97471000	1.53793300	-2.20131900
H	0.91678000	-12.58165100	-1.33933200	H	-0.35316300	0.68603300	-3.71329400
H	-0.72814800	-13.94623200	-2.63084500	H	1.47705500	1.98672900	-1.61256800
H	-1.70925300	-14.17216800	-1.17263000	H	2.12309800	1.30762400	-3.09314000
H	-0.08493000	-14.87876800	-1.26683400	H	0.44155000	-0.26988500	-1.06858400
H	-1.03976500	-11.45171200	-2.45533400	H	1.16798500	-0.93251400	-2.53207500
H	-0.46379700	-10.54262400	-1.05327000	H	3.45699200	-0.28505900	-1.67761600
H	-1.94321600	-11.52824300	-0.93368600	H	2.73368400	0.23862300	-0.16136500
C	-8.04547000	-0.81111600	-0.32303800	H	2.58212000	-2.61220600	-1.30005500
C	-6.53432000	-0.84960600	-0.58659000	H	3.75613900	-2.08493300	-0.10297800
S	-5.96746300	0.67911000	-1.55017200	H	1.94070100	-1.56297000	1.52101200
C	-8.84280200	-0.72304500	-1.61561500	H	0.71710200	-2.07356900	0.35906200
O	-8.66687000	-1.52994100	-2.56259800	H	2.90437300	-3.92136100	1.50429700
H	-8.28872000	0.02189100	0.34607600	H	1.61532900	-4.41364800	0.39008300
H	-5.97782800	-0.87946900	0.35425100	O	-0.36290400	5.63828000	1.25794700
H	-6.26682700	-1.72493400	-1.18348900	H	-0.63265000	4.80179200	0.78333800
N	-9.73963000	0.30641300	-1.70463000	H	-0.12927300	6.31450600	0.58998900
C	-10.62064800	0.47390100	-2.85878600	O	-0.39070500	3.22379700	0.03569400
C	-9.96051800	0.96981100	-4.15026200	H	-1.06803500	2.54620400	-0.34230400
O	-10.64436800	1.03740800	-5.19396700	H	0.10086000	3.60780100	-0.76600700
H	-9.81824000	0.95490900	-0.93554400	O	-1.73461600	1.49126500	-1.24728700
H	-11.08129700	-0.48701200	-3.10912000	H	-6.05303900	-1.80426800	-6.65407700
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C	-7.85542300	1.56478700	-5.28834200	H	-11.42231300	1.16780700	-2.59366800
C	-6.97870000	0.40417400	-5.77324300	H	-8.33675800	-1.74075700	0.18592200
O	-6.09001300	0.63001500	-6.63860800	H	-4.42990200	1.93802700	3.64455900
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H	-7.20285300	2.42638900	-5.12613200	H	1.22461300	3.64554500	5.19603500
H	-8.55869100	1.81308300	-6.08974600	H	1.30462500	0.86846500	6.12395400
N	-7.24078600	-0.82052200	-5.25705000	H	1.21237200	-3.89504100	2.03130000
C	-6.53739500	-2.02127200	-5.70091800	H	3.14320000	8.08481100	3.55169600
H	-7.91452300	-0.92417700	-4.50417700	H	5.44391300	10.55962000	0.70891600

H	-4.21395300	10.65416900	-0.40881300
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H	-1.30271700	6.85646700	-8.92279600
H	-0.24591300	5.62968300	-8.20919300
H	-10.91884100	11.22447800	-2.76254400
H	-9.42652800	11.58254100	-1.87297100
H	5.35763900	-3.97452600	-6.35836600
H	0.65158300	-11.83510700	2.40935200
H	4.63500400	-10.43532800	0.87184300
H	6.78675900	4.06739400	-6.56156100
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4IM1_{HA,B, α}

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C	4.85320300	8.68694800	-1.30888700
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C	6.00163100	7.99071900	-2.06716000
C	3.38107000	9.09584200	1.47595000
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H	3.80917500	10.82197800	0.32292000
H	6.13063500	10.16181200	-0.36544500
H	5.98897300	8.65461500	0.53655200
H	4.14673500	7.90929000	-0.98418300
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H	3.20697200	10.07555300	-1.75759800
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H	6.51357100	7.26101100	-1.42902100
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C	3.41370100	4.46136200	0.09999500
C	4.77013200	4.33190400	-0.22932300
C	5.74877300	4.78618600	0.66114300
C	5.37242500	5.37723500	1.87424100
H	4.60212700	8.79096200	3.07986700
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H	5.05927700	3.87595500	-1.17084000
H	6.80102900	4.67950500	0.41646000
H	6.13790400	5.72364000	2.56412900
C	1.54803400	0.09975300	5.24013600
C	1.00321200	1.04528900	4.22318000
N	0.74992400	2.39886500	4.49504600
C	0.26560400	3.01074100	3.38295500
N	0.20072100	2.09310000	2.41443500
C	0.64956100	0.87254100	2.90638800
H	2.53574900	0.41293900	5.59931100
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H	-0.18104800	2.35517500	1.39222400
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C	-9.77482900	10.18400200	-2.55613500
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H	-8.84679200	12.08563200	-3.10743900
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H	-10.74403500	10.04648700	-4.51122600
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C	7.90759900	0.47645300	-8.02178100
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C	5.79150200	-0.55068500	-7.37003500
C	6.45376100	-1.37771700	-6.45255800
C	7.84494600	-1.27255500	-6.32060900
C	8.56202200	-0.35453000	-7.09526100
H	9.58097900	1.81368600	-8.36362600
H	8.08191500	2.30927000	-9.16904000
H	5.98825100	1.00325200	-8.85258300
H	4.71334700	-0.62041100	-7.48438200
H	5.89471600	-2.08964400	-5.85213100
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C	-4.49881900	9.40238600	-0.05333000
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N	-0.93966200	7.56817600	-2.23887800
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N	0.69626900	6.91204900	-0.72619800
C	-4.65735700	8.05996900	0.64282700
O	-5.34600300	7.13348900	0.12170400
H	-5.37555300	9.53697200	-0.69358300
H	-2.35107700	9.17871700	-0.28550600
H	-3.03998300	10.51359900	-1.20779400
H	-3.59084300	7.57390700	-1.91500600
H	-3.98620900	8.99599900	-2.87287800
H	-2.05254100	8.05599800	-3.89964600
H	-1.44715700	9.46628500	-3.04921700
H	-0.91164200	6.58382500	-2.60314800
H	-0.26833200	9.94212200	-1.36892000
H	0.96199500	9.34816500	-0.26949300
H	0.63759900	5.92831200	-1.07195100
H	1.47767500	7.19066900	-0.14139400
N	-4.00099100	7.86827500	1.81920600
C	-4.07628200	6.56813400	2.53428100
C	-3.48089700	6.88088700	3.91753000
C	-2.46387400	8.00376400	3.61989000
C	-3.17690900	8.86030800	2.55505100
H	-3.47702400	5.82010100	2.00292900
H	-4.26015500	7.24168300	4.60001500
H	-3.01452600	6.00097200	4.36854600
H	-2.19141100	8.58806300	4.50350000
H	-1.55423700	7.56263500	3.19639800
H	-2.47285000	9.36550700	1.88901600
H	-3.81715000	9.62240400	3.02045300
C	-1.81893500	6.40539200	-7.44236500
C	-2.63469000	5.66657300	-6.37110800
H	-1.41201800	7.34784500	-7.05493600
H	-2.02235300	5.42589200	-5.49439200
H	-3.48623400	6.27243000	-6.03397400
H	-3.04080200	4.72673200	-6.76623500
C	3.86020100	-4.50339300	-7.19894900
C	2.57163900	-4.50798000	-8.04785300
C	1.66368300	-3.28963900	-7.92819000
C	0.49794500	-3.24361700	-8.71725900
C	-0.35785900	-2.14050400	-8.67785400
C	-0.06457200	-1.05406900	-7.84177200
C	1.08480500	-1.09085700	-7.04723200
C	1.94378600	-2.19873400	-7.08818000
C	3.67751700	-4.55172500	-5.68661700
O	4.25840900	-3.73225400	-4.92321700
H	4.46138800	-3.61755600	-7.41749600
H	1.98355400	-5.41309700	-7.83364300
H	2.87601100	-4.61054300	-9.09885100
H	0.26666500	-4.07803900	-9.37471000
H	-1.24553200	-2.12338600	-9.30261900
H	-0.72126900	-0.19034500	-7.81590300
H	1.32280900	-0.25560300	-6.39517300

H	2.82457800	-2.20363700	-6.45601400	N	-7.41489200	-0.95800300	-5.71017000
N	2.88084500	-5.54893200	-5.20483800	C	-6.53296600	-1.94703800	-6.32595700
C	2.65198100	-5.79053200	-3.76888300	H	-8.03949400	-1.27802500	-4.97577000
C	1.13833700	-5.85432900	-3.43361100	H	-5.61783700	-2.09373100	-5.74075500
C	0.92383700	-6.11071700	-1.92987900	C	-4.00191300	-0.40726500	1.58104100
C	0.41525200	-4.56990600	-3.87842300	C	-3.40140400	-1.09835100	0.52677400
C	3.34742300	-7.12717100	-3.45713400	C	-2.69149100	-2.35145500	0.65297300
O	2.87494600	-8.18581600	-3.94637900	C	-2.18769500	-2.65082100	-0.58476300
H	2.50791200	-6.24774900	-5.83446800	C	-2.60741900	-1.59481500	-1.47898500
H	3.10975000	-4.95150800	-3.24340800	N	-3.35085000	-0.65586000	-0.78086700
O	0.72750700	-6.70954600	-3.98836200	C	-2.36055800	-1.56843700	-2.84772500
H	1.34822600	-7.06208600	-1.59784800	C	-2.85998100	-0.62657600	-3.73941500
H	-0.14785800	-6.14102600	-1.70000800	C	-2.79232400	-0.73687900	-5.18252000
H	1.37180800	-5.31035300	-1.32517900	C	-3.53511200	0.29038700	-5.69776800
H	-0.66151500	-4.66560800	-3.68954400	C	-4.01881700	1.06217900	-4.57441800
H	0.55561500	-4.36639400	-4.94399800	N	-3.59998500	0.49143800	-3.38781200
H	0.78558800	-3.69952600	-3.31973800	C	-4.73134400	2.25566600	-4.67840000
N	4.49791200	-7.12027500	-2.71747100	C	-5.03729900	3.08371400	-3.60574700
C	5.34476600	-8.33760000	-2.65356600	C	-5.57166100	4.42520200	-3.70608700
C	6.77687900	-7.76379300	-2.60964900	C	-5.63659100	4.92935900	-2.43633900
C	6.60721700	-6.45887000	-1.80189600	C	-5.18801900	3.88168200	-1.54218300
C	5.23763100	-5.90465700	-2.25461500	N	-4.80579000	2.76833200	-2.27355500
C	5.07881600	-9.24607200	-1.44609400	C	-5.26215700	3.95303100	-0.15613400
O	5.82319700	-10.23283400	-1.22846300	C	-5.04182500	2.88625700	0.70858600
H	5.15357000	-8.94336600	-3.54387300	C	-5.31394200	2.89767100	2.13094600
H	7.47121900	-8.47315800	-2.15570300	C	-5.01809800	1.65291400	2.61244000
H	7.11775900	-7.54568200	-3.62801200	C	-4.53199900	0.87002500	1.49733400
H	6.59305300	-6.68142700	-0.72860700	N	-4.57732800	1.63592700	0.33279700
H	7.41138900	-5.74005900	-1.98158700	Fe	-4.03625400	1.08778200	-1.52857200
H	5.33843900	-5.19021700	-3.07824100	H	-3.99671400	-0.88404900	2.55613200
H	4.70163800	-5.41261200	-1.43627500	H	-1.78181400	-2.38691700	-3.26339500
N	4.02727900	-8.93682500	-0.64899200	H	-5.03037600	2.56594700	-5.67258200
C	3.66406800	-9.77428300	0.47606000	H	-5.56580300	4.90788100	0.26129200
C	2.44079200	-9.17521900	1.16342100	O	0.49444300	4.29448000	-1.59381200
O	1.94134900	-8.08823000	0.77360600	C	-0.05286500	4.16730400	-2.79338500
H	3.43369800	-8.13640900	-0.82609700	O	-0.70146500	5.12554900	-3.35787300
H	3.45175900	-10.79917100	0.14055800	C	0.06057900	2.89853100	-3.49886400
N	1.95218100	-9.89045800	2.21121400	C	0.80032100	1.71540500	-2.97169500
C	0.78623500	-9.47341000	3.00391600	C	2.29650100	1.69359900	-3.40991500
C	-0.42814300	-10.40652500	2.84514000	C	3.05084700	0.46845000	-2.86276100
C	-1.02397800	-10.50251500	1.42102800	C	4.54128800	0.45909400	-3.25330400
C	-2.14668700	-11.55912700	1.39129800	C	5.32245400	-0.77833700	-2.76461800
C	-1.53668500	-9.14210200	0.90662600	C	5.48109900	-0.86952600	-1.23445900
H	2.39665900	-10.76670900	2.45124800	C	6.34902500	-2.06086700	-0.79688700
O	0.54810900	-8.45656000	2.68631900	H	-0.35488600	2.87632500	-4.50262800
H	-0.14928500	-11.41586000	3.18449900	H	-2.07644900	2.21523600	-2.20263300
H	-1.20876500	-10.05650800	3.53787200	H	0.76223700	1.70717000	-1.87632800
H	-0.22497300	-10.84103900	0.74347100	H	0.32297000	0.79136600	-3.32533800
H	-2.54878000	-11.67511000	0.37837400	H	2.77793300	2.61609900	-3.05797800
H	-2.97625100	-11.26618300	2.04872700	H	2.35629600	1.70679500	-4.50748500
H	-1.78466200	-12.53950300	1.72428500	H	2.94923900	0.44865400	-1.76789400
H	-2.00066300	-9.25760500	-0.08005900	H	2.57468700	-0.45107100	-3.23636000
H	-0.72567100	-8.41322300	0.80799500	H	4.62352200	0.51427200	-4.34777800
H	-2.29756100	-8.73251200	1.58566800	H	5.02275300	1.36996300	-2.86206200
C	-8.08660600	-1.74162300	-0.78704300	H	4.83605000	-1.68937500	-3.14294500
C	-6.60110700	-1.43132100	-1.01517800	H	6.32228800	-0.75798600	-3.22134500
S	-6.37239100	0.32986200	-1.67935100	H	5.92809500	0.06479200	-0.86135300
C	-8.90057200	-1.61462500	-2.06588100	H	4.49319300	-0.94892500	-0.75833600
O	-8.59636500	-2.23873500	-3.11332000	H	7.35705900	-1.98973200	-1.22396600
H	-8.48777700	-1.09399600	0.00053900	H	5.91221700	-3.00844600	-1.13715500
H	-6.04363700	-1.51732000	-0.07904500	O	-0.70208300	5.24919900	1.69977700
H	-6.17167700	-2.11540700	-1.75081300	H	-0.95360400	4.45969300	1.14218200
N	-9.96721800	-0.75880000	-2.01971600	H	-0.41069700	5.96862000	1.10269700
C	-10.88896400	-0.59644600	-3.14243200	O	-0.73853900	2.93890800	0.24542700
C	-10.35699600	0.18066400	-4.35115100	H	-1.50125800	2.45313100	-0.28142700
O	-11.06898300	0.27536100	-5.37366600	H	-0.13815300	3.39432000	-0.43746100
H	-10.14497100	-0.24572200	-1.16911500	O	-2.35653600	1.85666500	-1.33591800
H	-11.17706700	-1.58141500	-3.52367100	H	-6.25345400	-1.59880100	-7.32221300
N	-9.09933700	0.70112500	-4.25083600	H	-7.06111000	-2.90030200	-6.40447100
C	-8.41192400	1.27288300	-5.39886800	H	-11.79527600	-0.10027300	-2.78641700
C	-7.36370300	0.35461000	-6.03758300	H	-8.17664300	-2.78046700	-0.44002900
O	-6.53448100	0.84418600	-6.85257500	H	-5.10629500	1.28995200	3.62633300
H	-8.59200700	0.62932600	-3.37762500	H	-2.59403600	-2.91705200	1.56839000
H	-7.91277700	2.20495900	-5.12237800	H	0.90325100	2.84952600	5.38393500
H	-9.16768500	1.50076200	-6.15761400	H	0.88627600	0.00961200	6.11004400

H	6.44992400	-2.10939400	0.29407500	H	-7.81527300	9.68926000	-1.92796000
H	2.62229700	7.92446100	4.34383100	H	-8.94120200	7.71056800	-0.80573000
H	4.90830900	10.59618100	1.68323400	H	-8.46609300	6.68237100	-2.16706800
H	-4.49382400	10.21871200	0.67788000	H	-7.22305400	7.41413700	-1.14343300
H	-5.11412800	6.22707700	2.56852300	H	-10.98260100	8.40205100	-4.58092000
H	-2.42982000	6.64470600	-8.32091800	H	-10.17730400	7.15254400	-3.62233700
H	-0.97151100	5.79872200	-7.78301700	H	-9.30770300	7.95197400	-4.94559000
H	-10.61770000	12.13750800	-3.08068600	C	6.54106700	4.20918300	-5.46518900
H	-9.70907800	12.13510600	-1.55720100	C	6.02725900	2.85833300	-5.01556800
H	4.46498700	-5.37387900	-7.49067200	C	4.91764400	2.26390800	-5.64121600
H	1.08096900	-9.43251200	4.06035500	C	4.46605800	0.99656100	-5.25351300
H	4.49952800	-9.84924600	1.18633400	C	5.11352400	0.29558300	-4.22620600
H	9.03119700	0.96582200	-9.81158600	C	6.21726300	0.88198800	-3.59279500
H	-2.26440400	-1.51276800	-5.71731400	C	6.66724800	2.14926500	-3.98272500
H	-3.77904800	0.50611500	-6.72607100	H	6.96481600	4.77778000	-4.62957600
H	-5.83283900	4.91020600	-4.63503400	H	5.74402200	4.81060100	-5.91539300
H	-5.96153800	5.90267900	-2.10024400	H	4.41013000	2.79503800	-6.44226600
H	-5.70200400	3.74788500	2.67196100	H	3.60901000	0.55602400	-5.75468400
H	-1.59984300	-3.50857700	-0.87783800	H	4.76458500	-0.69068600	-3.93252400
				H	6.73087500	0.34970500	-2.79755500
				H	7.53203900	2.58890200	-3.49152400
4IM1_{HA,B,β}				C	-4.15980500	9.65825700	-1.13956700
C	4.70384200	10.24661100	-0.03911400	C	-2.87526100	9.70087100	-2.01304700
C	5.80947200	9.49102100	-0.82902600	C	-2.86476600	8.63469400	-3.12699300
C	5.32445600	8.62753300	-2.01794200	C	-1.49084700	8.43229500	-3.80010400
C	4.60219700	9.46242000	-3.09345200	N	-0.58465300	7.57299600	-3.02253000
C	6.52262900	7.87238000	-2.62790400	C	0.31631700	7.96020600	-2.11438300
C	3.70604100	9.31341100	0.61547100	N	0.58732500	9.26266700	-1.85592300
O	2.60944400	9.00303600	0.05676600	N	0.98890700	7.02205200	-1.40589700
H	4.14863100	10.90922700	-0.70740900	C	-4.13264900	8.48160400	-0.17762500
H	6.51937600	10.24259100	-1.20225100	O	-4.61749200	7.35873200	-0.50785100
H	6.36836000	8.85045500	-0.13249500	H	-5.03988400	9.53828200	-1.77838200
H	4.61690900	7.87726900	-1.63477800	H	-2.00187600	9.56943500	-1.36122500
H	4.33331700	8.83403700	-3.95017900	H	-2.78774600	10.69883400	-2.46573600
H	3.67723200	9.90974100	-2.71339700	H	-3.19256400	7.66979900	-2.72442400
H	5.24835200	10.26995200	-3.46292300	H	-3.59301200	8.91969400	-3.89870000
H	6.19718000	7.22669700	-3.45134700	H	-1.62687900	7.92638500	-4.76039900
H	7.01460000	7.23972100	-1.88017700	H	-1.01457700	9.39711900	-4.02536100
H	7.26734900	8.57408800	-3.02604600	H	-0.60119100	6.55283300	-3.26920900
N	4.05486600	8.80135300	1.82179700	H	0.14894200	9.99979800	-2.37909400
C	3.23795200	7.84570600	2.57844000	H	1.32579900	9.48021500	-1.18642400
C	3.96412600	6.50776000	2.83983700	H	0.90621500	6.01310900	-1.65206500
C	4.36192300	5.75402100	1.58354100	H	1.76635100	7.33363800	-0.83262700
C	3.38528300	5.26557400	0.69526400	N	-3.52084900	8.65642300	1.02435500
C	3.75405200	4.57884000	-0.46812800	C	-3.40810300	7.54158600	2.00181000
C	5.10930600	4.35938500	-0.75305300	C	-2.99949600	8.24799500	3.30664200
C	6.08818300	4.83296100	0.12738800	C	-2.19691100	9.47490300	2.81905400
C	5.71525300	5.52945500	1.28456000	C	-2.95150300	9.92237900	1.55166700
H	4.94564000	9.07329800	2.21527500	H	-2.64184600	6.82880100	1.67210800
H	2.32771300	7.68472000	1.99798500	H	-3.88751100	8.57396800	3.86163900
H	4.85464900	6.69215500	3.45598200	H	-2.41477500	7.59492100	3.96034200
H	3.28943100	5.89400800	3.45497500	H	-2.13622500	10.27330800	3.56396500
H	2.32931700	5.40962300	0.91580000	H	-1.17461500	9.17543800	2.55815500
H	2.98463800	4.22157300	-1.14632100	H	-2.29025600	10.39561700	0.82043000
H	5.39434700	3.81549300	-1.64818100	H	-3.75397700	10.63115400	1.79744900
H	7.13942900	4.65872500	-0.08087200	C	-1.51414800	6.29248400	-7.96568900
H	6.48142600	5.89039200	1.96640700	C	-2.35050500	5.58778600	-6.88716100
C	2.12794000	0.98758900	5.22083200	H	-1.05912500	7.21417000	-7.58094300
C	1.54339200	1.82018900	4.13007900	H	-1.73990900	5.31491500	-6.01872400
N	1.20411800	3.17252600	4.29691100	H	-3.17004600	6.23121400	-6.53939500
C	0.70055400	3.66862800	3.13647400	H	-2.80388600	4.66967100	-7.28129900
N	0.70910200	2.67918100	2.23995700	C	4.32128400	-3.15901900	-6.24640300
C	1.22227500	1.52795900	2.82628500	C	3.49147200	-3.40059200	-7.52323300
H	3.09412500	1.38015700	5.56024400	C	2.13960300	-2.70271200	-7.60713200
H	2.29384800	-0.03106100	4.86263500	C	1.34400100	-2.91492500	-8.74946300
H	0.34863800	4.67079600	2.91988000	C	0.10796000	-2.28150700	-8.89580100
H	1.31921400	0.60500900	2.28147100	C	-0.36141600	-1.41913400	-7.89592700
H	0.31584600	2.82557100	1.20699100	C	0.41532300	-1.20333500	-6.75471100
C	-9.41328700	10.55813000	-3.89193400	C	1.65703600	-1.83944600	-6.60987400
C	-9.51967500	9.20207900	-3.16616900	C	3.74588600	-3.68746900	-4.93625700
C	-8.16561800	8.82666400	-2.51566800	O	3.74661100	-2.98469500	-3.88714600
C	-8.20093900	7.58644300	-1.60713100	H	4.50409000	-2.09130200	-6.10329700
C	-10.02638900	8.11114500	-4.13013200	H	3.34600300	-4.47975000	-7.68179900
H	-8.68099700	10.50466600	-4.70901100	H	4.10529700	-3.07349200	-8.37452500
H	-10.25800100	9.30885000	-2.35444600	H	1.70156800	-3.58075300	-9.53103100
H	-7.42298500	8.67607700	-3.31583900				

H	-0.48711700	-2.45789300	-9.78637100	H	-8.22664900	1.03804500	-2.77041800
H	-1.31991900	-0.92253700	-8.00870300	H	-7.33684600	2.11835900	-4.77591900
H	0.05960300	-0.54190500	-5.97096800	H	-8.70774000	1.44091400	-5.67285000
H	2.23583200	-1.66327100	-5.70989000	N	-7.34771800	-1.13072800	-4.72120400
N	3.28369200	-4.96888000	-4.95345100	C	-6.64457200	-2.35014200	-5.11122500
C	2.81027600	-5.69106300	-3.75949000	H	-8.00233700	-1.19548400	-3.94734200
C	1.35614400	-6.20567600	-3.93469200	H	-5.86627300	-2.61351800	-4.38592900
C	0.90010800	-6.99135800	-2.69107700	C	-3.65641200	0.02486500	2.22123400
C	0.39244400	-5.04171700	-4.23097900	C	-3.26332500	-0.93756700	1.29088800
C	3.80172700	-6.85191400	-3.57395800	C	-2.81431000	-2.26985700	1.62387900
O	3.86018500	-7.74534600	-4.45786800	C	-2.45041100	-2.87351800	0.44992400
H	3.36722200	-5.52772300	-5.79300400	C	-2.69088700	-1.91901100	-0.60860300
H	2.84510100	-4.97738300	-2.93603300	N	-3.19978500	-0.74375100	-0.07682100
H	1.36403900	-6.89372200	-4.79185200	C	-2.47575000	-2.16510000	-1.96061600
H	1.50358600	-7.88463800	-2.50865300	C	-2.77957000	-1.29182100	-2.99674500
H	-0.13681100	-7.32425500	-2.81208500	C	-2.74218800	-1.63444000	-4.40408700
H	0.94150300	-6.36485000	-1.78934200	C	-3.27071400	-0.57447300	-5.08778600
H	-0.62057300	-5.42709700	-4.39794500	C	-3.59332100	0.43849900	-4.10732300
H	0.69127600	-4.47640600	-5.11857900	N	-3.27969300	-0.00787400	-2.83692200
H	0.35601400	-4.34293100	-3.38379900	C	-4.10834500	1.69696800	-4.40858900
N	4.64231300	-6.84417000	-2.49439200	C	-4.30421400	2.71299500	-3.48314500
C	5.79449200	-7.77922600	-2.44622600	C	-4.68290200	4.07199700	-3.80280100
C	6.88198900	-6.95541600	-1.72290700	C	-4.69139000	4.77490700	-2.63001500
C	6.06894400	-6.09796100	-0.72856200	C	-4.35164600	3.84355000	-1.57538700
C	4.78669400	-5.73100800	-1.50692100	N	-4.11071000	2.58727500	-2.11320100
C	5.52855000	-9.10053000	-1.71288200	C	-4.36461000	4.16328900	-0.22355700
O	6.46537700	-9.91881200	-1.54508000	C	-4.22719100	3.24561200	0.81095800
H	6.07164300	-8.04662000	-3.46970100	C	-4.41175200	3.54346500	2.21626900
H	7.61590100	-7.60614300	-1.24400500	C	-4.26354600	2.37110500	2.90262200
H	7.40228200	-6.31660500	-2.44566900	C	-3.96180000	1.34410600	1.92819800
H	5.81923000	-6.68924900	0.16015800	N	-3.95738400	1.89601600	0.64974900
H	6.60800400	-5.20661400	-0.39550400	Fe	-3.57794200	0.95493800	-1.10249200
H	4.89279200	-4.77440600	-2.03045600	H	-3.67750900	-0.27344900	3.26465900
H	3.90961100	-5.67012800	-0.85534500	H	-2.08467700	-3.14027400	-2.23215300
N	4.27087600	-9.32638500	-1.26346200	H	-4.35806100	1.89225800	-5.44437700
C	3.91451800	-10.56827900	-0.60726800	H	-4.55478300	5.20371100	0.02304800
C	2.44875400	-10.49872100	-0.18738100	O	0.78663500	4.32810500	-2.07894100
O	1.76071100	-9.46724900	-0.40024700	C	0.30042600	4.14971400	-3.28274300
H	3.52368600	-8.65545000	-1.39180800	O	-0.41750500	5.01780500	-3.87662600
H	4.07785400	-11.42210100	-1.28009900	C	0.66953700	2.87093000	-4.05182600
N	1.96289300	-11.61138400	0.42294100	C	0.63111900	1.58271700	-3.28164800
C	0.57656700	-11.73604500	0.89863000	C	1.69731800	1.20990300	-2.29546000
C	-0.24556800	-12.78092900	0.12215200	C	1.62547900	-0.24979400	-1.80944700
C	-0.44878100	-12.49542000	-1.38442900	C	2.74592600	-0.59208600	-0.80975300
C	-1.18406600	-13.67750300	-2.04786100	C	2.76840100	-2.06652600	-0.35989500
C	-1.20000300	-11.17187700	-1.63328900	C	1.56151100	-2.48665000	0.50059600
H	2.57480800	-12.40797500	0.54139800	C	1.63870100	-3.94455500	0.98150100
H	0.13272100	-10.74221700	0.81555700	H	1.69779600	3.04527100	-4.42073300
H	0.22876300	-13.76752400	0.23861800	H	0.01623900	2.83019600	-4.92655300
H	-1.23040500	-12.85609300	0.60790500	H	-1.38361600	1.38378200	-1.91758700
H	0.54573700	-12.41389900	-1.84980700	H	-0.06124500	0.81018100	-3.61741700
H	-1.29455100	-13.51493300	-3.12606300	H	1.65669800	1.88489900	-1.42521600
H	-2.18953700	-13.79916400	-1.62336700	H	2.68859400	1.39365800	-2.74787300
H	-0.64214800	-14.62013000	-1.90275500	H	0.63980800	-0.42278100	-1.35494700
H	-1.37849100	-11.02962300	-2.70578000	H	1.70742500	-0.92739500	-2.67146200
H	-0.63142300	-10.30760900	-1.27477100	H	3.71171900	-0.34996200	-1.27463000
H	-2.17781800	-11.18071300	-1.13219000	H	2.66023100	0.06156600	0.07524100
C	-8.05245000	-0.83768300	0.22493500	H	2.83118500	-2.70247700	-1.25467000
C	-6.54520400	-0.88468700	-0.05889300	H	3.68903400	-2.25019200	0.21538900
S	-6.01497600	0.58737700	-1.12784700	H	1.49648700	-1.82048300	1.37721600
C	-8.87429400	-0.83382300	-1.05549500	H	0.62981400	-2.33826500	-0.06070400
O	-8.70890800	-1.69351600	-1.95677700	H	2.54680600	-4.12029800	1.57247000
H	-8.28914100	0.03441200	0.84477000	H	1.65711800	-4.63873300	0.13133300
H	-5.97732400	-0.85094400	0.87435800	O	-0.35925700	5.64222500	1.21687100
H	-6.28076800	-1.79384200	-0.60405100	H	-0.60046800	4.79398000	0.74465500
N	-9.78358500	0.18034600	-1.18629900	H	-0.12156500	6.31430100	0.54625200
C	-10.68924200	0.27185200	-2.32978900	O	-0.34750100	3.21865200	0.01412800
C	-10.06083900	0.70233500	-3.65979100	H	-1.04950000	2.51441500	-0.31919700
O	-10.76750800	0.71083500	-4.69035100	H	0.16473300	3.57336400	-0.78097100
H	-9.85586400	0.87061900	-0.45376300	O	-1.79028000	1.45489500	-1.02751600
H	-11.14181800	-0.70726400	-2.51637400	H	-6.17664500	-2.18265700	-6.08239000
N	-8.73400300	1.02242900	-3.64645600	H	-7.35500400	-3.17851900	-5.18392000
C	-7.98499900	1.24381200	-4.87451300	H	-11.49477300	0.96978500	-2.08813800
C	-7.10876300	0.06433900	-5.31224200	H	-8.32920500	-1.73501500	0.79622500
O	-6.24023300	0.24820200	-6.20791500	H	-4.34396400	2.20333400	3.96706100

H	-2.77938500	-2.67741400	2.62378700
H	1.31132300	3.69550400	5.15226900
H	1.46333900	0.92902500	6.09127800
H	0.77718400	-4.20972000	1.60574500
H	2.95080900	8.30125400	3.53514300
H	5.18029900	10.87562800	0.72370400
H	-4.27133800	10.60348600	-0.59813000
H	-4.36538500	7.01792300	2.07026400
H	-2.12367700	6.56290900	-8.83606600
H	-0.69994600	5.64842700	-8.31821200
H	-10.37571600	10.85273200	-4.32656000
H	-9.09492700	11.35325200	-3.20621600
H	5.30653700	-3.62740200	-6.38445500
H	0.59779600	-12.00326200	1.96278700
H	4.55599700	-10.73756700	0.26854900
H	7.33327500	4.10324000	-6.21885200
H	-2.38551900	-2.57396300	-4.79969000
H	-3.47207600	-0.47962100	-6.14313600
H	-4.88679400	4.42950900	-4.80129200
H	-4.91784600	5.81553000	-2.45144200
H	-4.64426700	4.52290900	2.60717600
H	-2.06439300	-3.87156400	0.30251500

⁴TS₂reb,B, α

C	4.44611100	10.02821700	0.92142200
C	5.54975700	9.26473300	0.13491400
C	5.07972200	8.49468600	-1.12254200
C	4.44183100	9.42267900	-2.17475700
C	6.27000200	7.72366500	-1.72813300
C	3.38895200	9.10706600	1.49265200
O	2.33953900	8.80482400	0.84507500
H	3.94453700	10.74431400	0.26554500
H	6.30869800	10.00154900	-0.16390800
H	6.04624600	8.55993400	0.81658800
H	4.32459900	7.75738300	-0.81277100
H	4.17994900	8.85710900	-3.07625800
H	3.52395400	9.89318400	-1.80553100
H	5.13972900	10.21685900	-2.47164600
H	5.95413500	7.14246900	-2.60162600
H	6.70404400	7.02808400	-1.00078000
H	7.05936600	8.41412700	-2.05310400
N	3.63118000	8.59334200	2.72442300
C	2.74531100	7.64461300	3.40859700
C	3.42643500	6.29009600	3.70849600
C	3.91349000	5.55236400	2.47515900
C	3.00160900	5.03273500	1.53711600
C	3.45419900	4.37461600	0.38669100
C	4.82960100	4.21655700	0.16668900
C	5.74545900	4.71807000	1.09767200
C	5.28787200	5.38544200	2.24107700
H	4.48696000	8.85990200	3.19207600
H	1.87922400	7.50587700	2.75880300
H	4.26655000	6.45224300	4.39702000
H	2.69478800	5.67931600	4.25685900
H	1.93065600	5.13420400	1.70499500
H	2.73581100	3.99907700	-0.33588600
H	5.18150900	3.70209200	-0.72170200
H	6.81152200	4.58913400	0.93845800
H	6.00449800	5.76829600	2.96339200
C	0.33751100	0.15971300	5.63070900
C	0.04815800	1.09024300	4.50145700
N	-0.07782200	2.47905000	4.66781100
C	-0.33355400	3.06898200	3.47263500
N	-0.37614000	2.10092400	2.55262000
C	-0.14468100	0.87146200	3.15880900
H	1.29799800	0.38666300	6.10871700
H	0.38734300	-0.86824400	5.26429600
H	-0.47723000	4.12160800	3.24840300
H	-0.13879100	-0.04671800	2.59878900
H	-0.57476900	2.32385100	1.50015100
C	-9.84409600	10.48560000	-3.28395100
C	-10.06276200	9.43254900	-2.17944800
C	-8.70551600	8.89852300	-1.65982300
C	-8.79693700	7.98799900	-0.42384700
C	-10.97890800	8.30106400	-2.68621500

H	-9.33273100	10.04143000	-4.14865900
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H	-8.20383200	8.35900700	-2.47900300
H	-8.06350500	9.76061800	-1.42094000
H	-9.30095500	8.50315400	0.40452700
H	-9.36036700	7.07245100	-0.63633000
H	-7.79791900	7.69256000	-0.08364500
H	-11.93226100	8.70347800	-3.04870100
H	-11.20453800	7.57181900	-1.90084900
H	-10.50534000	7.76421600	-3.51941800
C	8.51445400	1.33178900	-8.97912900
C	7.74331600	0.36581300	-8.10540500
C	6.34661900	0.25269100	-8.21211500
C	5.63631200	-0.66272100	-7.42661200
C	6.31039900	-1.48528000	-6.51378600
C	7.70284700	-1.37733500	-6.39769900
C	8.40964700	-0.46068700	-7.18333700
H	7.90080900	2.19346700	-9.26326500
H	8.84801300	0.84977200	-9.90838300
H	5.81395700	0.88621100	-8.91669400
H	4.55710300	-0.73503100	-7.52842000
H	5.75969800	-2.19632100	-5.90463100
H	8.23795100	-2.00839800	-5.69393100
H	9.48937600	-0.38423900	-7.08394200
C	-4.37811000	9.59958000	-0.51263200
C	-3.04822200	9.56200100	-1.31547200
C	-3.04866100	8.52375400	-2.45516700
C	-1.66822900	8.30279200	-3.11126100
N	-0.77482900	7.42674800	-2.33510400
C	0.11747500	7.79957900	-1.41137100
N	0.36619700	9.09660200	-1.11215500
N	0.79962600	6.85018700	-0.72443000
C	-4.50669400	8.39544500	0.40613600
O	-5.10878500	7.34846200	0.02725300
H	-5.22926000	9.57604000	-1.19945300
H	-2.22373500	9.35335700	-0.62194900
H	-2.86541700	10.56069800	-1.73824000
H	-3.42068400	7.55965500	-2.08952400
H	-3.74933800	8.85351300	-3.23459300
H	-1.80159900	7.80691100	-4.07712200
H	-1.17638500	9.26270700	-3.32394800
H	-0.79466600	6.41261600	-2.59563200
H	-0.09837200	9.84327100	-1.59787500
H	1.09773900	9.30585700	-0.43248700
H	0.78518200	5.85635600	-1.04047800
H	1.55167500	7.16453000	-0.11868700
N	-3.90200600	8.45604900	1.62368200
C	-3.92190300	7.29327400	2.54978700
C	-3.50563700	7.90372700	3.89946100
C	-2.57574400	9.06997300	3.49703900
C	-3.23358900	9.63834700	2.22386300
H	-3.20351700	6.53655300	2.20875300
H	-4.38337900	8.28664500	4.43388700
H	-3.01067500	7.17410000	4.54658100
H	-2.47211400	9.82754800	4.27896400
H	-1.57547900	8.68722700	3.26024000
H	-2.49996100	10.07393000	1.53966500
H	-3.97327300	10.41189300	2.47077900
C	-1.64732700	6.37421100	-7.20811900
C	-2.48430700	5.46478700	-6.29611600
H	-1.34128300	7.29192600	-6.68900000
H	-1.92347800	5.16414600	-5.40356100
H	-3.40101500	5.96945500	-5.96464200
H	-2.78924400	4.55323100	-6.82431700
C	3.72815200	-4.63691400	-7.19261000
C	2.41172300	-4.62729300	-7.99949200
C	1.54797700	-3.37541800	-7.89626600
C	0.41543700	-3.27404400	-8.72736700
C	-0.40146000	-2.14139100	-8.70053000
C	-0.10156800	-1.07970600	-7.83551400
C	1.01498000	-1.17135700	-6.99962900
C	1.83506400	-2.30882200	-7.02758800
C	3.59254000	-4.68619100	-5.67538200
O	4.16925200	-3.84771500	-4.92946200
H	4.33013300	-3.75657600	-7.43025700

H	1.80312100	-5.50454000	-7.73194100	C	-8.59819200	1.86725700	-5.22282200
H	2.67605400	-4.77615100	-9.05537500	C	-7.76664900	1.08044900	-6.24250500
H	0.18061400	-0.48791300	-9.40883300	C	-7.03389900	1.70124800	-7.06240100
H	-1.26188400	-2.08116100	-9.35993200	H	-8.26458600	0.87480100	-3.36499200
H	-0.72571400	-0.19181000	-7.82116900	H	-8.02461200	2.75242900	-4.93956500
H	1.25904200	-0.35490000	-6.32623900	H	-9.52100000	2.19822400	-5.71178300
H	2.69348600	-2.35380800	-6.36689500	N	-7.89794600	-0.26587800	-6.23316400
N	2.83845600	-5.70446000	-5.16970000	C	-7.23229700	-1.11012700	-7.22323800
C	2.65251800	-5.94491100	-3.72764400	H	-8.42709400	-0.73066500	-5.49973500
C	1.14918600	-6.03348200	-3.35284400	H	-6.18815600	-1.30762300	-6.95145600
C	0.97763200	-6.30029400	-1.84558800	C	-3.31656500	-0.18290100	1.25715100
C	0.39717700	-4.75736600	-3.77319500	C	-2.87681700	-0.83331000	0.11351100
C	3.37881900	-7.26731300	-3.42820400	C	-2.15236800	-2.08179400	0.09804800
O	2.91947100	-8.33437500	-3.91146600	C	-1.83289600	-2.35222900	-1.20575000
H	2.47251300	-6.41869200	-5.78617000	C	-2.38596600	-1.29044500	-2.01221400
H	3.10833400	-5.09566500	-3.21720900	N	-3.01274900	-0.36013200	-1.18714100
H	0.73631200	-6.89181800	-3.90127300	C	-2.37900800	-1.26844600	-3.39951400
H	1.42282200	-7.24837100	-1.53225600	C	-3.06021900	-0.33878600	-4.17196000
H	-0.08659200	-6.34450000	-1.58670400	C	-3.20645500	-0.40329800	-5.61087700
H	1.43213700	-5.49905400	-1.24718600	C	-4.01149200	0.63817000	-5.98440100
H	-0.67282000	-4.86587000	-3.55586000	C	-4.33533900	1.37605000	-4.78352600
H	0.50603400	-4.54869700	-4.84166600	N	-3.76132900	0.75282500	-3.68286000
H	0.77270000	-3.88400700	-3.22238700	C	-5.02703900	2.57731000	-4.76533500
N	4.53788600	-7.23859300	-2.70263100	C	-5.19168700	3.36403300	-3.63526800
C	5.40305400	-8.44304500	-2.64076600	C	-5.76613700	4.68842400	-3.62737200
C	6.82715400	-7.84781300	-2.61774300	C	-5.68358800	5.16469300	-2.34599500
C	6.64760800	-6.54076200	-1.81562600	C	-5.09306900	4.12044500	-1.54214400
C	5.26507300	-6.00918000	-2.25594000	N	-4.77819400	3.03137300	-2.34721300
C	5.16536700	-9.34554800	-1.42290000	C	-4.95931600	4.17581300	-0.16271700
O	5.91616100	-10.32990300	-1.21733400	C	-4.55107600	3.10811700	0.62120100
H	5.21041100	-9.05820000	-3.52408800	C	-4.58911800	3.08596000	2.06423200
H	7.53786800	-8.54379200	-2.16840000	C	-4.18896500	1.83944200	2.46373500
H	7.15220300	-7.63085500	-3.64153200	C	-3.86679400	1.09050600	1.27178000
H	6.64826100	-6.75705000	-0.74102200	N	-4.10384800	1.87753700	0.15282800
H	7.43922200	-5.81144900	-2.00828400	Fe	-3.91836500	1.32019400	-1.76417800
H	5.34638600	-5.29879500	-3.08527100	H	-3.17669300	-0.68396400	2.20890100
H	4.73163100	-5.51920500	-1.43477300	H	-1.86063800	-2.06925200	-3.91488200
N	4.13452400	-9.03091000	-0.60107800	H	-5.44536800	2.92230500	-5.70386600
C	3.80552100	-9.85672800	0.54304100	H	-5.23121900	5.10859800	0.31758500
C	2.61884600	-9.23710600	1.27483600	O	0.71124100	4.19159100	-1.50670900
O	2.10621100	-8.15583700	0.88619800	C	-0.00024400	3.94583600	-2.59013900
H	3.53743800	-8.23065600	-0.76710000	C	-0.71945300	4.84185000	-3.17300500
H	3.56503200	-10.88072000	0.22375300	C	-0.05300000	2.57678300	-3.10643400
N	2.17632600	-9.92899800	2.35812100	C	0.77782200	1.46152100	-2.58319800
C	1.04850300	-9.49208800	3.19426400	C	2.20207500	1.42926000	-3.21977200
C	-0.17525000	-10.42226600	3.10681800	C	3.04425700	0.25640900	-2.68490000
C	-0.83536300	-10.53985200	1.71293100	C	4.48566400	0.25252900	-3.22903200
C	-1.96686700	-11.58674800	1.75484600	C	5.33365500	-0.95228700	-2.77170300
C	-1.36015800	-9.18501700	1.19597600	C	5.61709200	-0.99723500	-1.25746200
H	2.62937200	-10.80137600	2.59625700	C	6.54677400	-2.15614400	-0.86171700
H	0.80025900	-8.47991600	2.86938400	H	-0.58924400	2.44805800	-4.04052500
H	0.11470900	-11.42700300	3.45035000	H	-2.37312200	3.06354000	-2.42278600
H	-0.92272900	-10.05706300	3.82775000	H	0.89279800	1.55525400	-1.49798100
H	-0.07049500	-10.89825500	1.00682700	H	0.27509500	0.50855800	-2.78603900
H	-2.41352300	-11.72114000	0.76306900	H	2.70613000	2.38062500	-3.00367500
H	-2.76446000	-11.27148300	2.44079800	H	2.11711100	1.35644600	-4.31320100
H	-1.59895700	-12.56295200	2.09375300	H	3.05961400	0.30428300	-1.58640500
H	-1.87347900	-9.31614300	0.23598800	H	2.55548200	-0.69379300	-2.94893000
H	-0.54846000	-8.46658500	1.04241700	H	4.45497600	0.26057900	-4.32748500
H	-2.08291300	-8.75393200	1.90281300	H	4.98728200	1.18628000	-2.92822700
C	-7.27882000	-2.26693400	-1.99235900	H	4.84008900	-1.88351600	-3.08632200
C	-5.99473400	-1.47683300	-2.31956900	H	6.29255900	-0.92312700	-3.30841800
S	-6.12134300	0.30156600	-1.64890600	H	6.06997100	-0.04324200	-0.94611000
C	-8.48450700	-1.74539300	-2.75515900	H	4.67350100	-1.08576800	-0.70022300
O	-8.68153700	-2.04369200	-3.96100600	H	7.51360100	-2.07604600	-1.37402700
H	-7.45546700	-2.25859300	-0.91101600	H	6.10584800	-3.12271800	-1.13742800
H	-5.13603700	-1.95275900	-1.84413500	O	-0.81080100	5.30320600	1.62696700
H	-5.83524300	-1.43534900	-3.39925500	H	-1.06931700	4.53596500	1.04863100
N	-9.30928600	-0.88691400	-2.08402100	H	-0.44376900	6.01225300	1.05951900
C	-10.50366600	-0.31632300	-2.70410100	O	-0.83408200	2.95142300	0.20258100
C	-10.25726700	0.64432600	-3.87281900	H	-1.49488700	2.60794500	-0.49869600
O	-11.21131000	0.95321700	-4.61880400	H	-0.06189600	3.34215100	-0.31651800
H	-9.07426000	-0.62593500	-1.13736200	O	-2.17048300	2.24499600	-1.91664300
H	-11.13350200	-1.11472400	-3.10760100	H	-7.24386400	-0.61154300	-8.19532800
N	-8.98273100	1.10331100	-4.04422800	H	-7.76545100	-2.06039300	-7.29036500

H	-11.07848000	0.20614800	-1.93445000
H	-7.12957000	-3.30704100	-2.30439300
H	-4.11240000	1.45103400	3.46921200
H	-1.92312400	-2.67013300	0.97506600
H	0.00893600	2.96697000	5.54608300
H	-0.44061700	0.19989900	6.40237400
H	6.73908000	-2.17036500	0.21772700
H	2.39563200	8.09552600	4.34625700
H	4.91849400	10.60063500	1.72966100
H	-4.43862200	10.53330600	0.05695800
H	-4.92019100	6.84843600	2.55836500
H	-2.20746600	6.67264900	-8.10211400
H	-0.73393900	5.86810500	-7.54226300
H	-10.79830500	10.89477900	-3.63608300
H	-9.23120600	11.32091100	-2.92292400
H	4.31272200	-5.51418100	-7.50433100
H	1.39047000	-9.43373100	4.23551600
H	4.66876900	-9.93900200	1.21816500
H	9.40921600	1.70648400	-8.47009000
H	-2.75287700	-1.15885900	-6.23554400
H	-4.38374400	0.89995200	-6.96322800
H	-6.15996200	5.18330300	-4.50294900
H	-5.98079900	6.12308700	-1.94757600
H	-4.91039100	3.91577300	2.67644400
H	-1.29181000	-3.20006100	-1.59936100

4TS2_{DS,B,β}

C	5.13268100	10.08269300	0.14208600
C	6.18502900	9.24458900	-0.63810800
C	5.66813700	8.50658200	-1.89643500
C	5.11876000	9.47744600	-2.95986600
C	6.79873500	7.63827900	-2.48493500
C	4.02886000	9.23127900	0.73350600
O	2.95239400	8.99044900	0.10476100
H	4.66936700	10.81817300	-0.52037900
H	6.99402600	9.92659300	-0.93575600
H	6.62910700	8.50855900	0.04679200
H	4.85334000	7.83321100	-1.59271400
H	4.81712600	8.93006900	-3.86017900
H	4.24085000	10.02609400	-2.60102600
H	5.88375800	10.20782900	-3.25476100
H	6.44559800	7.08281600	-3.36126600
H	7.16323900	6.91141600	-1.75006800
H	7.64682700	8.25929900	-2.80209500
N	4.26103500	8.70719400	1.96263000
C	3.33497600	7.81008600	2.66253000
C	3.94785400	6.42173800	2.95221500
C	4.36172500	5.64948600	1.71268400
C	3.39974300	5.19656200	0.79036600
C	3.78371700	4.48959900	-0.35566700
C	5.13819100	4.21478400	-0.59099800
C	6.10228500	4.65555200	0.32217700
C	5.71517600	5.37153000	1.46276900
H	5.13859200	8.92396200	2.41543700
H	2.45169100	7.71803300	2.02776500
H	4.81256500	6.53935300	3.61912000
H	3.19765000	5.85388600	3.52201800
H	2.34301300	5.38677500	0.96921900
H	3.02754800	4.15884900	-1.06088600
H	5.43370500	3.65455700	-1.47239600
H	7.15229400	4.43802900	0.15279300
H	6.46959100	5.70372100	2.17172300
C	1.22893000	0.92406800	5.16732900
C	0.81968600	1.81506700	4.04335300
N	0.66277200	3.20358600	4.18521700
C	0.29563200	3.75175700	2.99896900
N	0.21390800	2.75901100	2.10957600
C	0.52890900	1.55331200	2.72619200
H	2.21805200	1.19104100	5.55844700
H	1.28062300	-0.11104700	4.82183900
H	0.10045100	4.79035100	2.75843200
H	0.52403800	0.61921800	2.19221100
H	-0.08612900	2.93919800	1.07154100
C	-9.38999900	11.22906200	-3.29260800
C	-9.45438400	9.94255400	-2.44548500

C	-8.02894400	9.43968000	-2.10977800
C	-7.97219500	8.27535500	-1.10669300
C	-10.29894800	8.86817000	-3.15874400
H	-8.89823500	11.03573900	-4.25555200
H	-9.95105700	10.18839500	-1.49228200
H	-7.53128400	9.14406600	-3.04730900
H	-7.45036200	10.28557200	-1.70739700
H	-8.47509600	8.54353700	-0.16823200
H	-8.46141400	7.37704000	-1.49951900
H	-6.93474600	8.01068700	-0.87212100
H	-11.30199000	9.24799900	-3.38630100
H	-10.41651000	7.96625500	-2.54869200
H	-9.82999100	8.57546200	-4.10800500
C	7.98649400	3.38799700	-3.97454000
C	7.00063100	2.24228300	-3.88425700
C	5.71812700	2.34864400	-4.45295900
C	4.82211200	1.27387100	-4.41071100
C	5.18612400	0.06833000	-3.79422000
C	6.45810700	-0.04293700	-3.21815900
C	7.35333300	1.03217300	-3.26138900
H	8.76246500	3.31023100	-3.20562900
H	7.49003100	4.35849000	-3.85887800
H	5.42603100	3.27544300	-4.94031500
H	3.83984000	1.37642000	-4.86349900
H	4.49436200	-0.76915400	-3.76501700
H	6.75410200	-0.97011500	-2.73642100
H	8.33925700	0.93167300	-2.81512100
C	-3.67433500	9.97953000	-1.60152300
C	-2.32986800	9.95290200	-2.38098700
C	-2.26373200	8.83310500	-3.43939700
C	-0.86481900	8.62707000	-4.06441400
N	0.01113100	7.74141000	-3.28028700
C	0.82379300	8.08473300	-2.27408800
N	1.09546200	9.37310400	-1.95586100
N	1.39704400	7.11146500	-1.52975600
C	-3.73748000	8.87471400	-0.55916000
O	-4.21776800	7.73702500	-0.84127600
H	-4.50782300	9.82325400	-2.29279200
H	-1.50632700	9.84322400	-1.66348500
H	-2.19145400	10.92377000	-2.87787700
H	-2.59690400	7.88340400	-3.00508300
H	-2.96980600	9.07278800	-4.24627100
H	-0.97027500	8.14190700	-5.03870000
H	-0.37489200	9.59307000	-4.25486900
H	0.05465500	6.74390900	-3.59239000
H	0.76066300	10.12940500	-2.52677300
H	1.76857600	9.55498700	-1.21111800
H	1.24895000	6.11148700	-1.76896600
H	2.13461800	7.37572300	-0.88479100
N	-3.21124200	9.12891800	0.66921200
C	-3.19857100	8.08763100	1.73041300
C	-2.86997200	8.88002200	3.00876800
C	-2.01653500	10.06256600	2.49792700
C	-2.66758500	10.42471900	1.14887000
H	-2.43189700	7.33505100	1.50520000
H	-3.78983400	9.25276500	3.47511600
H	-2.34382300	8.26963200	3.74822300
H	-2.00198000	10.91105900	3.18768900
H	-0.98075800	9.73934900	2.33752300
H	-1.94695200	10.84086900	0.43930100
H	-3.47750100	11.15465600	1.28267400
C	-2.93077800	4.37807100	-7.31514600
C	-2.54623600	5.60334100	-6.47201100
H	-2.14331400	4.12923900	-8.03644000
H	-1.61815700	5.42796900	-5.91533300
H	-2.40012300	6.48552100	-7.10852200
H	-3.33322700	5.84244900	-5.74554000
C	2.29003300	-2.45254200	-6.08421800
C	2.69372300	-3.24279100	-7.36586900
C	1.63157100	-4.17835000	-7.92416500
C	1.76386000	-5.57693000	-7.83729700
C	0.77503400	-6.42223400	-8.36065000
C	-0.35473300	-5.88351800	-8.98365800
C	-0.49506100	-4.49230200	-9.08021500
C	0.48828800	-3.64996100	-8.55403800

C	2.41600500	-3.21090000	-4.76842800	H	-9.36121100	0.32482000	0.24388100
O	2.98270100	-2.68673600	-3.76700600	H	-11.56251800	-0.44101100	-1.47572300
H	1.25807300	-2.08985500	-6.19076200	N	-8.27398000	1.21557900	-3.01128800
H	3.61667800	-3.80100800	-7.16982100	C	-8.89648400	1.62310800	-4.35636400
H	2.94194900	-2.49874000	-8.13348900	C	-8.24847000	0.51630000	-5.19524700
H	2.63326100	-6.01302900	-7.35347600	O	-7.53993400	0.82984100	-6.19326700
H	0.89591800	-7.49753900	-8.28050300	H	-8.53319600	1.05319300	-2.33585000
H	-1.11651000	-6.53790800	-9.39487600	H	-8.20097700	2.46458600	-4.32416600
H	-1.36485900	-4.06668700	-9.57103300	H	-9.80875500	1.95055000	-4.86685900
H	0.37705800	-2.57210900	-8.64489700	N	-8.51244100	-0.76047200	-4.83411000
N	1.88016300	-4.46131700	-4.72649100	C	-8.03670200	-1.90137100	-5.61300500
C	2.01557300	-5.36869500	-3.57448800	H	-9.00721500	-0.95919000	-3.96776100
C	0.68541100	-6.11932900	-3.30059800	H	-7.08043500	-2.28314800	-5.23377600
C	0.83352500	-7.08748200	-2.11268500	C	-3.29832400	0.36150200	1.97315400
C	-0.46586100	-5.12608300	-3.05385400	C	-3.08571100	-0.58828600	0.98290500
C	3.14945500	-6.35114000	-3.92662800	C	-2.56678500	-1.92086200	1.20331900
O	2.99777800	-7.13474500	-4.90046000	C	-2.36748000	-2.48951700	-0.02498900
H	1.50941400	-4.86966300	-5.57725900	C	-2.79470400	-1.52947900	-1.02006200
H	2.26769600	-4.74710800	-2.71469900	N	-3.22609400	-0.37457700	-0.38134700
H	0.46271900	-6.71069800	-4.20010000	N	-2.88015100	-1.78742900	-2.38231300
H	1.57412900	-7.87033700	-2.29555500	C	-3.49682100	-0.95732800	-3.30841500
H	-0.11922600	-7.58931600	-1.91047500	C	-3.81572000	-1.31486700	-4.67444300
H	1.12463100	-6.55353300	-1.19788300	C	-4.56363000	-0.29597300	-5.20061100
H	-1.40514400	-5.66961900	-2.89859100	C	-4.67330400	0.72278700	-4.18005200
H	-0.59972400	-4.44262800	-3.89881000	N	-4.02292000	0.29544800	-3.03106400
H	-0.26904800	-4.52238200	-2.15702300	C	-5.24164400	1.97567800	-4.36324100
N	4.31310000	-6.30840300	-3.20948500	C	-5.16863400	3.00856400	-3.43764400
C	5.50787000	-7.04315600	-3.69559600	C	-5.54377700	4.38346600	-3.69223000
C	6.67605600	-6.12155200	-3.28203900	C	-5.18217900	5.11943200	-2.59731100
C	6.18406100	-5.50656400	-1.95368400	C	-4.62456900	4.19868600	-1.62998500
C	4.67083100	-5.28924800	-2.17313700	N	-4.60686900	2.91740500	-2.16923400
C	5.68728200	-8.44992700	-3.11009500	C	-4.27854100	4.53996600	-0.32951200
O	6.70086400	-9.12535900	-3.41250000	C	-3.94896800	3.62375400	0.66055700
H	5.42579200	-7.16902700	-4.77844800	C	-3.82807900	3.92730900	2.06702400
H	7.60721700	-6.68333100	-3.18761500	C	-3.63766500	2.74209400	2.72761100
H	6.81571300	-5.34155100	-4.03914800	C	-3.59564400	1.69650500	1.73198500
H	6.35438800	-6.20835000	-1.12890200	N	-3.79203200	2.25490700	0.47821500
H	6.69297700	-4.57097100	-1.70473800	Fe	-3.94567900	1.25807400	-1.26314600
H	4.45398000	-4.28527500	-2.55240600	H	-3.15536400	0.05427700	3.00329100
H	4.09497600	-5.44826800	-1.25576600	H	-2.51730100	-2.74765700	-2.73161600
N	4.73080800	-8.90521700	-2.26534900	H	-5.74468800	2.15629100	-5.30642800
C	4.79645400	-10.23707300	-1.69797400	H	-4.33946500	5.59241500	-0.07396600
C	3.59625600	-10.43871600	-0.77673700	O	0.87708500	4.42705800	-2.13917300
O	2.75799700	-9.51894500	-0.59189000	C	0.51079100	4.23118200	-3.38839300
H	3.92100900	-8.35028600	-2.01779900	O	0.27270700	5.19845900	-4.19997800
H	4.79845400	-10.99586500	-2.49321800	C	0.30747300	2.86834800	-3.90597900
N	3.51298400	-11.65880200	-0.18486500	C	0.36452300	1.63825200	-3.16781400
C	2.43072500	-12.04274400	0.73474200	C	1.46784900	1.38086100	-2.11204800
C	1.48451300	-13.11039500	0.15493800	C	1.47729400	-0.07226900	-1.60600700
C	0.68736400	-12.69141300	-1.10253400	C	2.63555000	-0.32425100	-0.61871000
C	-0.10013500	-13.89817400	-1.65183400	C	2.75086500	-1.78335400	-0.13240900
C	-0.25318300	-11.50041300	-0.82875700	C	1.63947900	-2.22410100	0.83886600
H	4.21791500	-12.35208300	-0.39783700	C	1.80028900	-3.67590000	1.31887300
H	1.89080800	-11.12517100	0.97610800	H	-0.08868900	2.85292700	-4.91872300
H	2.06705600	-14.01560100	-0.07520200	H	-2.29985800	2.58288500	-2.46771300
H	0.77764700	-13.39517100	0.94902000	H	-0.69657700	1.61682700	-2.54325800
H	1.41054100	-12.38220800	-1.87310500	H	0.25384900	0.77470700	-3.83610900
H	-0.63608600	-13.63152500	-2.56995300	H	1.35663900	2.06613900	-1.26930100
H	-0.84230100	-14.24542600	-0.92063100	H	2.44178200	1.60485400	-2.56927700
H	0.56418000	-14.74036400	-1.88131300	H	0.50946000	-0.30363900	-1.13771900
H	-0.84418500	-11.26685100	-1.72249000	H	1.59452100	-0.75988100	-2.45510800
H	0.30377000	-10.59850500	-0.55493200	H	3.57512100	-0.04458700	-1.11456800
H	-0.95619100	-11.73926300	-0.01885100	H	2.53640300	0.34738000	0.25067200
C	-7.80348800	-1.67947000	-0.17810700	H	2.75884300	-2.44368200	-1.01131800
C	-6.45534200	-1.24626100	-0.78802900	H	3.72210400	-1.91717200	0.36744800
S	-6.29898600	0.65177000	-0.80377100	H	1.64537000	-1.55217400	1.71409800
C	-8.98069300	-1.23834400	-1.03008000	H	0.65596000	-2.10518000	0.36469700
O	-9.26673000	-1.81340900	-2.11183300	H	2.76201500	-3.82065500	1.82694600
H	-7.88740100	-1.29804600	0.84561500	H	1.76537100	-4.37428200	0.47292200
H	-5.63454400	-1.65493800	-0.19667000	O	-0.36364300	5.83573900	1.03048600
H	-6.37503200	-1.60944400	-1.81564000	H	-0.70808700	5.04383000	0.53296900
N	-9.67986300	-0.15050000	-0.58770500	H	0.00207400	6.47623700	0.38811800
C	-10.84599900	0.36700800	-1.29918900	O	-0.57069500	3.42686600	-0.22380300
C	-10.57659900	0.98772000	-2.67399300	H	-1.25470700	2.83385600	-0.69943600
O	-11.54269000	1.23957700	-3.42696200	H	0.08101200	3.76324200	-0.92615800

C	-0.24120500	-1.75908600	-7.38807200	C	-11.13802800	0.55494600	-2.51273100
C	0.61501500	-1.42252800	-6.33567600	C	-10.54823500	0.97700400	-3.86309100
C	1.90205700	-1.97453100	-6.26657500	O	-11.28320100	0.97830700	-4.87297900
C	4.05708800	-3.87981100	-4.68934700	H	-10.25287500	1.17094900	-0.66693800
O	4.08297800	-3.25187300	-3.59349500	H	-11.59281100	-0.42677800	-2.67876300
H	4.74007800	-2.19278700	-5.76924200	N	-9.22206500	1.29693900	-3.88893900
H	3.69736100	-4.52931600	-7.49956500	C	-8.50626700	1.50858100	-5.13792300
H	4.32465000	-3.01234300	-8.08122900	C	-7.64371700	0.32473500	-5.59113800
H	1.80603700	-3.90423500	-9.06543500	O	-6.79910800	0.50224600	-6.51060200
H	-0.46388600	-2.93027500	-9.19066100	H	-8.69136200	1.31852000	-3.02689600
H	-1.23449700	-1.32470500	-7.44386500	H	-7.85549700	2.38404800	-5.06267300
H	0.29497700	-0.72656600	-5.56687200	H	-9.24943900	1.69941800	-5.91797000
H	2.54357500	-1.70634700	-5.43414300	N	-7.86822000	-0.86538200	-4.98581000
N	3.60667200	-5.16177600	-4.78250000	C	-7.18503300	-2.09130600	-5.39040500
C	3.16263600	-5.96632500	-3.63037400	H	-8.49878000	-0.92195100	-4.19174700
C	1.73146700	-6.52984600	-3.84048000	H	-6.41798900	-2.38063000	-4.66384600
C	1.30215000	-7.39205700	-2.63861100	C	-4.02625900	0.42949900	1.86852100
C	0.72138800	-5.39455900	-4.08829800	C	-3.60475600	-0.53174300	0.94861300
C	4.19954100	-7.09510800	-3.50014300	C	-3.09603900	-1.84005900	1.29318900
O	4.27189700	-7.96284100	-4.40823200	C	-2.71599700	-2.44059700	0.12283700
H	3.66669000	-5.65732400	-5.66244700	C	-3.01166900	-1.51142400	-0.94466000
H	3.16780600	-5.29716100	-2.76968400	N	-3.55946400	-0.35113500	-0.42065500
H	1.77324000	-7.17625200	-4.72859800	C	-2.83043500	-1.77542900	-2.29840200
H	1.95080400	-8.25908900	-2.48684300	C	-3.21096100	-0.94001500	-3.34090200
H	0.28565000	-7.77282400	-2.78881000	C	-3.22888200	-1.31948000	-4.73915000
H	1.29836100	-6.80342800	-1.71123700	C	-3.82136000	-0.29474600	-5.42467100
H	-0.27381400	-5.81281200	-4.27942000	C	-4.12531900	0.73576600	-4.45673600
H	0.99969900	-4.77509800	-4.94572000	N	-3.74550700	0.33041700	-3.19151300
H	0.64978800	-4.73997100	-3.20920800	C	-4.66152900	1.98404200	-4.76857500
N	5.06309900	-7.08373100	-2.43770900	C	-4.80668900	3.02596800	-3.86197700
C	6.24774000	-7.97756700	-2.43582100	C	-5.16097300	4.38824800	-4.19827000
C	7.32657200	-7.12895900	-1.72929700	C	-5.09983700	5.11841100	-3.04328000
C	6.51239800	-6.31890200	-0.69721300	C	-4.75220400	4.19873900	-1.97983400
C	5.19323200	-5.98920600	-1.42824500	N	-4.56215400	2.92698400	-2.49805000
C	6.04720900	-9.31701500	-1.71396200	C	-4.73466700	4.53561100	-0.63134700
O	7.02010000	-10.09572400	-1.56235200	C	-4.61320200	3.62784200	0.41461700
H	6.50411400	-8.21935000	-3.47101600	C	-4.78707100	3.94627400	1.81645400
H	8.09554700	-7.76156100	-1.28241600	C	-4.64970100	2.78133100	2.51838300
H	7.80404200	-6.46051100	-2.45507900	C	-4.35873800	1.73851100	1.55846300
H	6.31415000	-6.93292800	0.18905200	N	-4.36290700	2.27205200	0.27110400
H	7.02712000	-5.41257200	-0.36614200	Fe	-4.00698800	1.31663200	-1.46755000
H	5.24197200	-5.01697800	-1.93046500	H	-4.03436800	0.14575700	2.91614100
H	4.33590100	-5.98228000	-0.74816800	H	-2.41164900	-2.74031200	-2.56428400
N	4.80359900	-9.60304200	-1.25837000	H	-4.95564900	2.15113000	-5.79776800
C	4.50573800	-10.86622400	-0.61290800	H	-4.88312800	5.58474600	-0.39590000
C	3.03556900	-10.87434100	-0.20154200	O	0.66948300	4.36371800	-2.07215000
O	2.30023900	-9.87326000	-0.39952900	C	0.27599500	4.11512200	-3.27889700
H	4.02677900	-8.96439600	-1.37530500	O	-0.15662200	4.91794400	-4.14433200
H	4.71837200	-11.70595600	-1.28970900	C	0.78094000	2.02759600	-4.06677100
N	2.60017200	-12.01955700	0.38728700	C	0.63014600	1.06324700	-3.10421100
C	1.21932000	-12.21707700	0.85469800	C	1.64020500	0.77159000	-2.02771200
C	0.44720200	-13.27953000	0.05102900	C	1.77593700	-0.72794800	-1.68548300
C	0.23023600	-12.96636200	-1.44779700	C	2.75848500	-0.97968400	-0.52732800
C	-0.44657100	-14.16619000	-2.14088900	C	2.89950400	-2.46020100	-0.12113400
C	-0.58391800	-11.67506000	-1.66488000	C	1.65275500	-3.05103000	0.56492900
H	3.24830000	-12.78853400	0.49441900	C	1.84943300	-4.50516100	1.02116800
H	0.73198600	-11.24226200	0.79296000	H	1.76317600	2.45234100	-4.26172500
H	0.96821700	-14.24499700	0.14238800	H	0.05415400	2.15101600	-4.86305400
H	-0.53274500	-13.41420500	0.53373900	H	-1.90279200	1.95499000	-2.36384500
H	1.21957700	-12.82493800	-1.90980300	H	-0.31902100	0.53266900	-3.02212800
H	-0.56616500	-13.98220800	-3.21463700	H	1.34153100	1.30578100	-1.10759300
H	-1.44434700	-14.34784400	-1.71961500	H	2.62062900	1.17722100	-2.31377200
H	0.14134900	-15.08428400	-2.01938700	H	0.78076100	-1.12159900	-1.43258200
H	-0.77128900	-11.51673500	-2.73357500	H	2.12012400	-1.28348400	-2.56834400
H	-0.05607900	-10.79327800	-1.28746300	H	3.74544000	-0.59464200	-0.81950300
H	-1.55919600	-11.74158500	-1.16297400	H	2.44698200	-0.38888600	0.35183300
C	-8.42291900	-0.51941700	-0.02556200	H	3.15039600	-3.04685700	-1.01649900
C	-6.92309300	-0.55454500	-0.34864000	H	3.75378600	-2.56188200	0.56582300
S	-6.43431700	0.91772500	-1.43763400	H	1.39527900	-2.42919900	1.43821700
C	-9.28060300	-0.53322000	-1.28254300	H	0.78942200	-2.99460200	-0.11197000
O	-9.13637700	-1.40054300	-2.18018900	H	2.69509900	-4.58900800	1.71586500
H	-8.65071000	0.35513800	0.59397000	H	2.05472900	-5.16359200	0.16871600
H	-6.33288200	-0.51207400	0.57034700	O	-0.52371500	5.59018400	1.05629600
H	-6.66449700	-1.46424000	-0.89538600	H	-0.76207200	4.74049000	0.58383500
N	-10.19867500	0.47532700	-1.39581300	H	-0.25530900	6.25399300	0.39205600

O	-0.55906500	3.13970700	-0.10667300	H	0.97742300	2.55274300	7.70814700
H	-1.33797600	2.59063200	-0.55220500	H	0.30649000	6.18211700	3.69845200
H	0.04056400	3.48457700	-0.84062300	H	0.29444700	2.14828400	4.99038800
O	-2.22950200	1.85537100	-1.44845100	H	-0.07727700	3.81297500	2.96315300
H	-6.70804600	-1.91635400	-6.35590700	C	-10.68018400	6.45325500	1.14016500
H	-7.90948500	-2.90606700	-5.48243100	C	-10.35399900	7.29775500	-0.10788100
H	-11.93863600	1.25261800	-2.25357000	C	-8.83495500	7.26600500	-0.40473300
H	-8.67563000	-1.41498100	0.55951700	C	-8.41417400	7.92232800	-1.72940400
H	-4.72423900	2.63063300	3.58582800	C	-10.88873200	8.73380800	0.05638000
H	-3.03575600	-2.23472600	2.29705600	H	-10.18991400	6.87158600	2.03065900
H	1.06461500	3.63561200	5.02297800	H	-10.86730200	6.83982600	-0.96896200
H	1.10660700	0.89294500	6.05038400	H	-8.30417600	7.75199400	0.43132700
H	0.95962300	-4.89472400	1.52985600	H	-8.50685600	6.21594700	-0.41284600
H	2.78515800	8.50648200	3.29095100	H	-8.94043900	7.46723400	-2.57812400
H	5.29576600	10.88327000	0.55564100	H	-8.63580300	8.99622300	-1.74233000
H	-3.97182000	10.87785600	-1.25048600	H	-7.33787100	7.79996400	-1.89598900
H	-4.44195700	7.43444300	1.55803600	H	-11.96594700	8.72895100	0.26157200
H	-2.31032500	6.27864900	-8.96560200	H	-10.72540100	9.33713200	-0.84304000
H	-0.73419100	5.58189000	-8.56144600	H	-10.39104500	9.23734400	0.89680700
H	-11.57559600	11.66675300	-1.47756100	C	7.10928300	3.05639600	-8.02240700
H	-9.98053500	12.01588900	-0.78480400	C	6.51742700	1.88505600	-7.26723000
H	5.59734200	-3.67533100	-6.14674100	C	5.13081400	1.65641500	-7.26545000
H	1.24935600	-12.50809600	1.91236800	C	4.58416000	0.55599400	-6.59589800
H	5.14780400	-11.00841900	0.26725600	C	5.41416500	-0.34129400	-5.91020500
H	7.98042600	3.79670700	-5.34099000	C	6.79773000	-0.12005100	-5.90279100
H	-2.85925000	-2.25749200	-5.12628100	C	7.34185800	0.98235000	-6.57220800
H	-4.07133800	-0.23076000	-6.47196300	H	8.04621300	3.39520900	-7.56693300
H	-5.39792100	4.72814500	-5.19562000	H	6.41847700	3.90634000	-8.05001400
H	-5.27659000	6.17169500	-2.88287100	H	4.47670300	2.34500200	-7.79420900
H	-5.00461100	4.93383600	2.19556300	H	3.50952900	0.39790000	-6.61033100
H	-2.28906300	-3.42299200	-0.01663000	H	4.98371400	-1.19748500	-5.39802400
				H	7.45342500	-0.80672700	-5.37506700
				H	8.41660200	1.14497700	-6.55931200
				C	-3.70060500	9.45236200	-2.09068100
				C	-2.29717700	9.16224200	-2.68857600
				C	-2.27044800	7.93402500	-3.61737500
				C	-0.85760700	7.52700700	-4.08111300
				N	-0.05814200	6.92053400	-3.00523700
				C	0.83313700	7.53639500	-2.22081900
				N	1.20736800	8.82404900	-2.40481800
				N	1.38334400	6.86065900	-1.18424600
				C	-4.12855900	8.41126900	-1.06761800
				O	-4.77785300	7.38268000	-1.41912000
				H	-4.44830800	9.43694200	-2.88955200
				H	-1.57690000	9.02688900	-1.87077400
				H	-1.97294700	10.05020900	-3.25046300
				H	-2.72895500	7.07478500	-3.11524300
				H	-2.88058200	8.13950500	-4.50760300
				H	-0.93594400	6.77158900	-4.86890200
				H	-0.32653700	8.37962500	-4.52456800
				H	-0.19730500	5.89352000	-2.86659100
				H	0.85673800	9.36686400	-3.17386700
				H	1.93521200	9.20658800	-1.80076600
				H	1.17673000	5.85213300	-1.04868900
				H	2.16749100	7.28979500	-0.70248200
				N	-3.76696400	8.59778800	0.23034000
				C	-4.15532700	7.61675100	1.27479700
				C	-3.77232600	8.31567400	2.59180900
				C	-2.58972400	9.22479900	2.18878300
				C	-2.99192600	9.73287200	0.79038300
				H	-3.60202600	6.68094800	1.12727400
				H	-4.61085600	8.91882600	2.96060300
				H	-3.50582700	7.59928100	3.37391700
				H	-2.41949600	10.04607500	2.89095400
				H	-1.67486900	8.62462200	2.11989000
				H	-2.12514200	9.96607900	0.16621100
				H	-3.61962400	10.63227200	0.85733800
				C	-0.43333400	3.28752300	-7.65836400
				C	-1.52524200	3.62053500	-6.63065400
				H	0.43380100	3.95190400	-7.55560700
				H	-1.14191700	3.54615100	-5.60448900
				H	-1.89808900	4.64477000	-6.77322000
				H	-2.37824200	2.93819800	-6.73114600
				C	3.25977000	-3.48766600	-7.15701000
				C	1.99868800	-3.59004800	-8.03830100

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C	5.31520300	10.08109600	-0.83617700
C	6.28770800	9.02811700	-1.43929700
C	5.66100800	7.99873800	-2.40973400
C	5.05773200	8.66584300	-3.66176100
C	6.72217600	6.95425000	-2.81068900
C	4.26039000	9.46589800	0.05941100
O	3.14321200	9.06582400	-0.39234400
H	4.80092300	10.62055200	-1.63579300
H	7.07872200	9.57777600	-1.96896700
H	6.77755800	8.48795700	-0.61701900
H	4.85465600	7.47047200	-1.87995600
H	4.67286400	7.90694000	-4.35232400
H	4.22626900	9.33436500	-3.41281800
H	5.81735100	9.24936900	-4.19852000
H	6.29129800	6.19481600	-3.47255400
H	7.12730900	6.44129600	-1.93074100
H	7.55701100	7.42777100	-3.34389400
N	4.58009300	9.33805800	1.37164400
C	3.70663600	8.72482200	2.37797000
C	4.32360200	7.46353000	3.02395800
C	4.60927800	6.33969100	2.04495800
C	3.55538600	5.64295500	1.42468800
C	3.81638700	4.61766300	0.50808200
C	5.13961400	4.26918100	0.20437100
C	6.19549000	4.94999100	0.81997500
C	5.92964600	5.98060000	1.73104100
H	5.48766100	9.66484500	1.67423000
H	2.77057000	8.48104600	1.87200100
H	5.24729600	7.74068700	3.54954700
H	3.62063900	7.12324400	3.79811100
H	2.52416800	5.89899200	1.66091800
H	2.98856700	4.09981200	0.03370300
H	5.34300100	3.47065800	-0.50166800
H	7.22254600	4.67813100	0.59745000
H	6.75490200	6.49912800	2.21245500
C	1.03053800	3.63554600	7.57423000
C	0.71967500	3.98983400	6.15923400
N	0.70835000	5.31132300	5.68504700
C	0.39469700	5.33030600	4.36535700
N	0.20255500	4.06274600	3.98465200
C	0.39738800	3.21594300	5.07073700
H	2.03908800	3.95556800	7.86183400

C	0.86145100	-2.62575400	-7.72452400	H	-7.02994900	-2.07281700	-1.47779200
C	-0.29890400	-2.67580600	-8.52218200	H	-6.43956000	-1.65179000	-3.10472700
C	-1.36229100	-1.79819600	-8.30403800	N	-9.63114300	-0.11184400	-4.25026700
C	-1.29512700	-0.84285900	-7.27823000	C	-9.93558400	0.67041000	-5.44594200
C	-0.14860100	-0.78925900	-6.47926800	C	-8.73392400	1.31663400	-6.14462200
C	0.92104800	-1.67153800	-6.69650500	O	-8.86072700	1.73176800	-7.31763800
C	3.10650400	-3.85601000	-5.68574200	H	-9.92395900	0.23374200	-3.34735200
O	3.55802200	-3.11450800	-4.76892100	H	-10.40778900	0.03496700	-6.20065400
H	3.66470400	-2.47321100	-7.18779100	N	-7.56666600	1.39224600	-5.43933100
H	1.60821600	-4.61886500	-8.02305100	C	-6.32682700	1.81538700	-6.07368200
H	2.31730500	-3.42575600	-9.07732500	C	-5.36133300	0.67198100	-6.39971400
H	-0.36090200	-3.40653000	-9.32525600	O	-4.13950900	0.93024700	-6.61535000
H	-2.24346900	-1.85040800	-8.93614300	H	-7.53531400	1.11609600	-4.46003800
H	-2.12683200	-0.16416100	-7.11093900	H	-5.79413100	2.52792000	-5.44036300
H	-0.08157300	-0.05482900	-5.68227700	H	-6.59075100	2.31749700	-7.01089400
H	1.79270000	-1.61055800	-6.05394000	N	-5.88004200	-0.57040000	-6.46452500
N	2.49710200	-5.04532200	-5.41523200	C	-5.07857200	-1.73572100	-6.83046200
C	2.34539800	-5.59232700	-4.05586900	H	-6.85932600	-0.73589000	-6.23826600
C	0.87454000	-5.98688300	-3.75876800	H	-4.17430000	-1.79551800	-6.21821700
C	0.74178500	-6.57143700	-2.33969300	C	-6.97058900	0.54295300	2.31393900
C	-0.06600300	-4.78288800	-3.94838600	C	-6.26362200	-0.57811200	1.90801200
C	3.27725300	-6.81480000	-3.99328100	C	-6.27401700	-1.85105500	2.58866300
O	3.00803000	-7.82117900	-4.69848000	C	-5.36119300	-2.65413900	1.96203500
H	2.22537500	-5.65998000	-6.17153400	C	-4.80388700	-1.89606100	0.86634400
H	2.65489200	-4.79982300	-3.37352800	N	-5.35805600	-0.61980900	0.85007400
H	0.60409900	-6.77253800	-4.47853500	C	-3.92245500	-2.39412200	-0.08194400
H	1.32623500	-7.48525600	-2.20303000	C	-3.53550900	-1.70729100	-1.22253200
H	-0.30372800	-6.82506700	-2.13076000	C	-2.76399000	-2.26583700	-2.31011600
H	1.06381000	-5.84528400	-1.58098800	C	-2.71399700	-1.32424100	-3.30026400
H	-1.10723900	-5.08976400	-3.78830700	C	-3.42186400	-0.16099900	-2.81846000
H	0.00996000	-4.35542500	-4.95250400	N	-3.92411100	-0.40998900	-1.54089900
H	0.17057200	-3.98836600	-3.22821900	C	-3.49956700	1.04735700	-3.49537200
N	4.40878300	-6.74880100	-3.22600000	C	-3.99030000	2.22531600	-2.95296300
C	5.46213400	-7.78372700	-3.36995600	C	-3.95626900	3.51148500	-3.60092500
C	6.76725200	-6.98143100	-3.18049400	C	-4.45817300	4.43057500	-2.71793600
C	6.36979100	-5.90881100	-2.14301900	C	-4.83747600	3.71539100	-1.52617400
C	4.91928900	-5.53265700	-2.51981000	N	-4.51801200	2.36099800	-1.66090700
C	5.37626500	-8.93591200	-2.36068300	C	-5.52231400	4.27243800	-0.45824200
O	6.29046600	-9.79504900	-2.31201000	C	-6.09433300	3.52903200	0.56397900
H	5.37549800	-8.23437300	-4.36278500	C	-6.96082000	4.06459200	1.58862200
H	7.58234900	-7.62882700	-2.85195600	C	-7.42588000	3.00779800	2.32084200
H	7.05356300	-6.51358000	-4.12921200	C	-6.82680600	1.81255900	1.77524400
H	6.40451300	-6.33383400	-1.13313400	N	-6.01320700	2.14549100	0.69526300
H	7.02845400	-5.03594600	-2.15881800	Fe	-5.06507200	0.83727000	-0.48355100
H	4.88442800	-4.66687600	-3.18917100	H	-7.63732700	0.43294700	3.16206700
H	4.30917100	-5.31058900	-1.63810900	H	-3.56763500	-3.41124500	0.04098800
N	4.29449200	-8.97537300	-1.54591700	H	-3.13705600	1.08101700	-4.51646300
C	4.10343000	-10.05512800	-0.59898400	H	-5.66916300	5.34690200	-0.48278300
C	2.81877500	-9.80276400	0.18446600	O	0.62434400	4.23340700	-0.70575500
O	2.12120400	-8.77678200	-0.02234700	C	-0.13043200	3.66868500	-1.62036800
H	3.56686500	-8.27232300	-1.58134200	O	-0.45475800	4.23381900	-2.70857400
H	4.04801200	-11.02092200	-1.12108800	C	-0.69273200	2.27050600	-1.31745600
N	2.49945200	-10.75300000	1.10288200	C	0.34806000	1.28015000	-0.80068800
C	1.30226400	-10.68688000	1.95421300	C	1.51084800	1.05501800	-1.78533800
C	0.27864700	-11.79789300	1.65730700	C	2.50184900	-0.02185000	-1.30541600
C	-0.33520300	-11.78740100	0.23775000	C	3.71066100	-0.18538100	-2.24618100
C	-1.25349300	-13.01283400	0.05525600	C	4.71151100	-1.27861100	-1.82342000
C	-1.09665700	-10.48023100	-0.06216500	C	5.42889700	-1.01476100	-0.48561100
H	3.10439200	-11.55754400	1.20120700	C	6.48696400	-2.08091800	-0.15639100
H	0.86886300	-9.69752500	1.79653400	H	-1.16639400	1.90226100	-2.22911200
H	0.75082800	-12.77629900	1.83525500	H	-2.64698200	2.43298600	-0.67555400
H	-0.53065500	-11.71010800	2.39826200	H	0.73671400	1.64539800	0.15838600
H	0.48959000	-11.87256800	-0.48651500	H	-0.16472800	0.33062200	-0.60111800
H	-1.65887400	-13.05117900	-0.96226300	H	2.05341600	2.00024900	-1.92989500
H	-2.10140000	-12.97076300	0.75191600	H	1.10873100	0.77487700	-2.76931100
H	-0.71415100	-13.95022900	0.23906000	H	2.84591300	0.24025000	-0.29402300
H	-1.56780100	-10.53073600	-1.05095500	H	1.97838300	-0.98587600	-1.21481000
H	-0.43063900	-9.61126200	-0.05683200	H	3.34879800	-0.42185300	-3.25570600
H	-1.89280700	-10.31651700	0.67738900	H	4.23879300	0.77827100	-2.32446400
C	-8.59367200	-1.93315200	-2.97477800	H	4.19026300	-2.24646700	-1.78056800
C	-7.23889900	-1.49012000	-2.37773800	H	5.46620200	-1.37920000	-2.61590200
S	-7.27534600	0.35322400	-1.89165700	H	5.90807200	-0.02419700	-0.52397000
C	-8.87350100	-1.24641200	-4.29896600	H	4.69605300	-0.97029700	0.33241200
O	-8.37842600	-1.66319000	-5.38007100	H	7.25641100	-2.12473800	-0.93756800
H	-9.39512600	-1.74425800	-2.25215000	H	6.03131000	-3.07689500	-0.08253600

O	-0.11287700	6.55015900	1.73850600
H	-0.50777600	5.65418300	1.57397200
H	0.22329500	6.91059600	0.89276800
O	-0.49011400	3.82272900	1.54079200
H	-1.21455600	3.26953400	1.12638900
H	0.16768600	3.93720500	0.76334000
O	-1.74618400	2.42486400	-0.27773600
H	-4.77170900	-1.69154100	-7.88169500
H	-5.68597600	-2.62779800	-6.67084700
H	-10.64949100	1.45334600	-5.17456000
H	-8.55533500	-3.01040700	-3.17189700
H	-8.10498300	3.02289700	3.16066300
H	-6.89064900	-2.08225900	3.44482200
H	0.90033600	6.12830500	6.24464800
H	0.31934200	4.09134400	8.27334600
H	6.98843000	-1.87289700	0.79616100
H	3.48633900	9.46705800	3.15601700
H	5.89794900	10.81872300	-0.27012400
H	-3.71013200	10.45497900	-1.64951700
H	-5.22162700	7.38966000	1.19349600
H	-0.81067300	3.38689600	-8.68283300
H	-0.08072400	2.25662400	-7.53857500
H	-11.75894300	6.43294300	1.33512900
H	-10.33779600	5.41801500	1.02049500
H	4.03043900	-4.14612400	-7.58313500
H	1.61710300	-10.74961700	3.00374800
H	4.96069900	-10.12307400	0.08522800
H	7.33342200	2.78730200	-9.06381900
H	-2.33679800	-3.25767400	-2.31628600
H	-2.22749100	-1.38781100	-4.26287000
H	-3.57185100	3.67315800	-4.59627300
H	-4.59517100	5.49519100	-2.83490700
H	-7.19949100	5.11189200	1.69926400
H	-5.09380200	-3.67336500	2.19989200

⁴P_{OH,B,β}

C	5.20464900	10.51455800	-1.19513200
C	6.04962700	9.68200300	-2.20148200
C	5.25536100	8.83227600	-3.22201500
C	4.34948300	6.92272000	-4.12453100
C	6.23731900	8.00039000	-4.07218100
C	4.35599200	9.65265500	-0.28418500
O	3.17342600	9.30791800	-0.59283500
H	4.53552900	11.19055000	-1.73375000
H	6.69081600	10.38582800	-2.75084500
H	6.72098800	9.02006900	-1.63695300
H	4.61752500	8.13013600	-2.66575800
H	3.85654900	9.06865600	-4.87867100
H	3.56329300	10.19947200	-3.55439600
H	4.93542700	10.45482900	-4.65532300
H	5.69515700	7.36453400	-4.78149000
H	6.85472200	7.34977400	-3.44214800
H	6.90570300	8.65224800	-4.64995300
N	4.93246200	9.23832600	0.87109300
C	4.28431900	8.34682200	1.83912900
C	5.05640400	7.02413300	2.04406700
C	5.22018800	6.19717500	0.78205600
C	4.10417300	5.61879200	0.14850200
C	4.25534400	4.86460100	-1.02146800
C	5.53072200	4.67312900	-1.57125600
C	6.64789700	5.23877000	-0.94751300
C	6.49097300	5.99811600	0.21944700
H	5.88042300	9.53226000	1.06356300
H	3.27884500	8.15409300	1.46023700
H	6.04404000	7.24398800	2.47153100
H	4.51325500	6.45030900	2.80928300
H	3.11067100	5.75409800	0.57194100
H	3.38283900	4.43419900	-1.50418300
H	5.64402500	4.08108500	-2.47348600
H	7.63992800	5.08671900	-1.36175800
H	7.36464300	6.42706800	0.70391100
C	2.84165000	2.06130000	5.76522300
C	2.27776600	2.74573600	4.56608900
N	2.10102700	4.13686000	4.49042800
C	1.57323500	4.47387600	3.28676900

N	1.40894300	3.34173900	2.59439400
C	1.83448700	2.26099600	3.35945300
H	3.86284900	2.39652700	5.98268700
H	2.87756700	0.98275500	5.59581600
H	1.31309800	5.45517700	2.90222000
H	1.78809200	1.24886100	2.99728600
H	0.98234700	3.34117200	1.59283000
C	-9.62796500	10.68164400	-2.53131400
C	-9.69389500	9.38658200	-1.69735200
C	-8.27794100	8.78922500	-1.50867000
C	-8.19992100	7.59490700	-0.54304100
C	-10.67097800	8.38083300	-2.33762700
H	-9.24300300	10.47470800	-3.53900400
H	-10.07949000	9.64616000	-0.69744700
H	-7.88764900	8.49203100	-2.49492100
H	-7.61407600	9.58801500	-1.14228000
H	-8.60542800	7.86186300	0.44199100
H	-8.77012100	6.73625500	-0.91472700
H	-7.16221200	7.27003700	-0.40628400
H	-11.66487600	8.82715700	-2.46163400
H	-10.78637500	7.47761800	-1.72907200
H	-10.31590000	8.07530500	-3.33114300
C	5.29603500	4.10068900	-6.76121100
C	4.91196300	2.87333900	-5.96320700
C	3.74293400	2.15375000	-6.26136500
C	3.40751500	0.99663400	-5.54652600
C	4.23162900	0.53951400	-4.50911000
C	5.39873700	1.25232700	-4.20181600
C	5.73477700	2.40392600	-4.92256100
H	5.73777800	4.87444000	-6.12232300
H	4.42839100	4.53519300	-7.26814100
H	3.09677000	2.49684900	-7.06484400
H	2.51136000	0.44306700	-5.81110800
H	3.97367800	-0.36309600	-3.96196200
H	6.05020900	0.90584300	-3.40480400
H	6.65161100	2.93955500	-4.68704300
C	-3.98058000	9.31373900	-0.61751200
C	-2.76478900	9.44602500	-1.57510100
C	-2.83452500	8.49188100	-2.78198500
C	-1.53506200	8.43513600	-3.60926400
N	-0.47390100	7.65587100	-2.95345200
C	0.54638700	8.12073000	-2.23038300
N	0.79036400	9.44078700	-2.05511100
N	1.37692900	7.23754800	-1.61579800
C	-3.93923100	8.02338200	0.18557100
O	-4.50008000	6.97025800	-0.23889400
H	-4.90720800	9.30109100	-1.19932600
H	-1.84039100	9.26411400	-1.01045800
H	-2.71666600	10.48376900	-1.93553800
H	-3.07457600	7.47680800	-2.44520900
H	-3.65384100	8.80640100	-3.44279000
H	-1.73243900	7.93769200	-4.56373500
H	-1.18029200	9.44533900	-3.85424500
H	-0.49334100	6.61956200	-3.13260500
H	0.21884300	10.14067600	-2.49436900
H	1.63061800	9.71455700	-1.54596200
H	1.29825900	6.21933000	-1.81119400
H	2.24038700	7.60271600	-1.22432300
N	-3.24322100	8.02216400	1.35437500
C	-3.12443300	6.78759300	2.17011700
C	-2.50575500	7.28264500	3.48921500
C	-1.66038900	8.49955400	3.05280400
C	-2.53060500	9.16903300	1.97166600
H	-2.47045800	6.07187900	1.65844000
H	-3.29178200	7.59220100	4.18883800
H	-1.90765100	6.50730600	3.97630400
H	-1.42775100	9.18246800	3.87498700
H	-0.72390800	8.14588600	2.60736900
H	-1.93171100	9.70870800	1.23329200
H	-3.24734400	9.87410800	2.41484300
C	-1.44959500	5.88904900	-7.80822500
C	-2.38867700	5.50709500	-6.65433400
H	-0.83763400	6.76335700	-7.55326900
H	-1.82751000	5.26437500	-5.74429600
H	-3.08151400	6.32718000	-6.42162400

H	-2.99749000	4.63368000	-6.91970800	C	-8.80201900	-1.76272900	-2.95244800
C	4.25939100	-3.35167200	-5.46430100	O	-8.73828800	-2.14897600	-4.14915300
C	3.59923500	-4.01783700	-6.69142300	H	-8.45352100	-2.26913200	-0.87057800
C	2.25039800	-3.46309100	-7.13348000	H	-5.96229300	-2.52368900	-1.10259300
C	1.72252900	-3.89077400	-8.36693900	H	-6.08018400	-2.07234600	-2.82012600
C	0.49473700	-3.41398900	-8.83149500	N	-9.54962200	-0.67947800	-2.58773900
C	-0.23474400	-2.49270700	-8.06835400	C	-10.35201300	0.06810000	-3.55231500
C	0.27636100	-2.06112400	-6.84132400	C	-9.56759100	0.81543900	-4.63671000
C	1.50928900	-2.54186300	-6.37502600	O	-10.17387800	1.24454600	-5.64281600
C	3.60125600	-3.61071300	-4.11244500	H	-9.48885400	-0.34879800	-1.63541700
O	3.28799000	-2.66802500	-3.33398100	H	-11.02042100	-0.61184200	-4.08852300
H	4.30333300	-2.26812600	-5.59670300	N	-8.22307400	0.95754000	-4.44607200
H	3.50203500	-5.10076400	-6.51959100	C	-7.35859500	1.48039400	-5.49381000
H	4.30076500	-3.92480000	-7.53144700	C	-6.52657400	0.41782400	-6.22066000
H	2.28451900	-4.60044800	-8.96910000	O	-5.49099900	0.76425800	-6.85721900
H	0.10976900	-3.75487500	-9.78752800	H	-7.79469900	0.65933000	-3.57399700
H	-1.18608100	-2.11568800	-8.43036400	H	-6.66732400	2.22219200	-5.08789400
H	-0.28211600	-1.35085200	-6.23934000	H	-8.00024500	1.97497700	-6.23127400
H	1.88154700	-2.19484000	-5.41747500	N	-6.97745400	-0.85564500	-6.17292400
N	3.40652800	-4.91883800	-3.78595400	C	-6.31760900	-1.93231100	-6.90803500
C	2.88309900	-5.37367900	-2.49075900	H	-7.76507800	-1.10725400	-5.57968200
C	1.43444700	-5.94464800	-2.60662900	H	-5.42083900	-2.28831600	-6.38645400
C	0.90402100	-6.40682000	-1.23524200	C	-4.06275300	-0.63988500	2.24191200
C	0.48611700	-4.91490500	-3.24608500	C	-3.63151200	-1.54564000	1.28736100
C	3.86165400	-6.45703600	-2.02249200	C	-3.23915100	-2.90597100	1.56481800
O	4.19277500	-7.36095100	-2.85343800	C	-2.82025500	-3.45577800	0.38360300
H	3.72548500	-5.65990200	-4.39825600	C	-2.97036000	-2.44451400	-0.63448100
H	2.87907300	-4.50223500	-1.83287600	N	-3.46454200	-1.27047800	-0.06889900
H	1.49768200	-6.82431500	-3.26302000	C	-2.70491700	-2.63763800	-1.98126200
H	1.49666700	-7.22217700	-0.81153900	C	-2.92002900	-1.68758400	-2.96567500
H	-0.11733200	-6.78925400	-1.34247900	C	-2.75063300	-1.91669500	-4.38119200
H	0.86960000	-5.56645700	-0.52731000	C	-3.12586400	-0.76938800	-5.02642900
H	-0.51747900	-5.34807400	-3.34008800	C	-3.49396800	0.18711500	-4.01143000
H	0.81621500	-4.61541800	-4.24465200	N	-3.37609400	-0.38781200	-2.74487700
H	0.41444500	-4.01032300	-2.62867600	C	-3.85053800	1.49960200	-4.27690900
N	4.37908000	-6.41712900	-0.77438700	C	-4.09472800	2.45155000	-3.30153700
C	5.46565700	-7.35889700	-0.36048300	C	-4.40362500	3.83449300	-3.55681900
C	6.12689400	-6.63035300	0.81884100	C	-4.56999000	4.44994200	-2.34428200
C	4.95989000	-5.85255300	1.46473500	C	-4.38539400	3.44537200	-1.32986300
C	4.10864300	-5.38696300	0.26745200	N	-4.06044700	2.21672900	-1.91908900
C	4.90622200	-8.73910500	0.05077900	C	-4.56519800	3.66485600	0.02498400
O	4.95963000	-9.14601900	1.23536300	C	-4.51426900	2.66882900	0.98768100
H	6.13574200	-7.49581900	-1.21571100	C	-4.77745700	2.87775100	2.39085500
H	6.58085200	-7.33865000	1.51281400	C	-4.67048900	1.66301900	3.00956600
H	6.89679200	-5.94422700	0.44759100	C	-4.32395100	0.69777300	1.99457700
H	4.38417300	-6.53297200	2.09965100	N	-4.23672300	1.32319800	0.75358200
H	5.29592900	-5.01038700	2.07632700	Fe	-4.02574300	0.40530100	-1.02377900
H	4.42738100	-4.40135900	-0.09478200	H	-4.16463700	-0.99315400	3.26213300
H	3.04291800	-5.34548100	0.50240800	H	-2.33241300	-3.60797500	-2.28924000
N	4.39996900	-9.47418600	-0.97790100	H	-3.96332500	1.78098100	-5.31769200
C	3.77212300	-10.75679100	-0.74461200	H	-4.78439600	4.68271400	0.32910700
C	2.23905200	-10.68909200	-0.79318900	O	1.07637100	4.45352800	-2.00455300
O	1.61489700	-9.60353000	-0.78779400	C	0.22484300	4.16017500	-2.95898100
H	4.31076800	-9.01569000	-1.88547400	O	-0.47508500	5.04612200	-3.54867700
H	4.13228400	-11.49067200	-1.47669300	C	0.06729200	2.72006300	-3.43747600
N	1.62377400	-11.90712400	-0.82300500	C	-0.18323400	1.64445700	-2.35595900
C	0.16394000	-12.07749800	-0.81803300	C	1.07580000	1.07420100	-1.69594300
C	-0.38951900	-12.67200700	-2.12634800	C	0.77198400	-0.06699600	-0.70821600
C	-0.15857600	-11.82696000	-3.40104800	C	2.02803500	-0.85072200	-0.28064600
C	-0.66568300	-12.59357500	-4.63931600	C	1.73282600	-1.99227000	0.71507400
C	-0.81536200	-10.43494400	-3.30854500	C	1.34386200	-1.53468500	2.13448200
H	2.19439400	-12.74160800	-0.84204700	C	0.99163200	-2.70503600	3.06780000
H	-0.25915600	-11.09009400	-0.62279600	H	0.97327700	2.44647500	-3.99635300
H	0.04653700	-13.67154300	-2.27739400	H	-0.76408800	2.72573900	-4.14686800
H	-1.47080000	-12.82760500	-1.99066300	H	-2.01992200	2.20148100	-1.57289700
H	0.92700600	-11.68208200	-3.51524400	H	-0.71697900	0.81123100	-2.83027000
H	-0.46534200	-12.03099300	-5.55855800	H	1.63981100	1.87427700	-1.20293300
H	-1.74959900	-12.75922900	-4.57879100	H	1.71874900	0.69690500	-2.50293100
H	-0.18163000	-13.57373200	-4.73091500	H	0.25030000	0.34547400	0.16481600
H	-0.68599500	-9.88780800	-4.25029000	H	0.06595800	-0.76870000	-1.17778100
H	-0.37236200	-9.83196800	-2.50935500	H	2.49843800	-1.27825900	-1.17640800
H	-1.89464000	-10.52607300	-3.12349700	H	2.76629300	-0.16182300	0.16190800
C	-7.99670000	-2.43199100	-1.85292500	H	0.92400600	-2.61977800	0.30992200
C	-6.53261100	-1.94729900	-1.83357200	H	2.61831600	-2.64043400	0.79212900
S	-6.42659100	-0.10477100	-1.34315800	H	2.18660500	-0.96583300	2.56180900

H	-1.84962600	4.13781600	-7.88929400	C	-9.24795000	-1.03833000	-2.52868700
H	-2.08079000	5.22932600	-5.60636700	C	-7.81003000	-0.88513800	-1.99265900
H	-2.20307400	6.45256900	-6.87965400	S	-7.47487000	0.90754100	-1.43186300
H	-3.67008900	5.87186500	-6.07951000	C	-9.46218800	-0.25630000	-3.81256600
C	0.40870100	-2.44285700	-4.66178500	O	-9.07843800	-0.69676100	-4.92835200
C	0.31551300	-3.09548600	-6.07554900	H	-9.96503100	-0.73877800	-1.75662600
C	-0.78471200	-4.13131600	-6.25167300	H	-7.66547600	-1.54032400	-1.13147200
C	-0.49462100	-5.50586200	-6.34109100	H	-7.08776200	-1.14906000	-2.76880700
C	-1.52506000	-6.44419200	-6.49856900	N	-10.03510600	0.97702000	-3.68675600
C	-2.85630100	-6.02481500	-6.57717600	C	-10.28742500	1.83818600	-4.83902600
C	-3.15631200	-4.65776900	-6.50019800	C	-9.04627800	2.35881600	-5.57144200
C	-2.12969300	-3.72221700	-6.33935500	O	-9.17615200	2.87238100	-6.70416400
C	1.17465800	-3.23792900	-3.61098100	H	-10.23058600	1.32583600	-2.75926400
O	2.04415100	-2.68016600	-2.88151400	H	-10.86633700	1.29463700	-5.59153200
H	-0.60167000	-2.22983600	-4.28609100	N	-7.84253900	2.21260700	-4.94257300
H	1.28569400	-3.53593900	-6.33338900	C	-6.59211800	2.50194400	-5.62774000
H	0.14575500	-2.28180300	-6.79208900	C	-5.82849800	1.26424600	-6.10880000
H	0.53360900	-5.85246100	-6.28067200	O	-4.59723300	1.35954800	-6.38822100
H	-1.27902400	-7.49903100	-6.56426600	H	-7.80137800	1.86588300	-3.98805700
H	-3.65212600	-6.75113000	-6.70650400	H	-5.92418600	3.07501200	-4.98146400
H	-4.18580800	-4.32160500	-6.57883700	H	-6.83079300	3.11325300	-6.50501100
H	-2.36983500	-2.66219900	-6.30544800	N	-6.53441300	0.12099800	-6.24892600
N	0.87027300	-4.55788000	-3.49546000	C	-5.94160800	-1.09321500	-6.80352600
C	1.62994700	-5.49944200	-2.65382600	H	-7.49985800	0.06541500	-5.92998300
C	0.68119900	-6.52468200	-1.97944300	H	-5.47771800	-1.70974500	-6.02291900
C	1.47183400	-7.52571100	-1.11667000	C	-6.42060300	0.03307600	2.76022100
C	-0.39263000	-5.81130900	-1.13655100	C	-5.95250200	-0.98283800	1.94478200
C	2.63586000	-6.18841200	-3.59851700	C	-5.97113000	-2.38264300	2.29138300
O	2.19647400	-6.86197000	-4.56848900	C	-5.38927700	-0.06328700	1.25784500
H	0.22343100	-4.97409800	-4.15545600	C	-5.01681700	-2.08929100	0.26124700
H	2.13054800	-4.90498300	-1.88917500	N	-5.36496900	-0.80939400	0.69236200
H	0.18941500	-7.08278800	-2.78956900	C	-4.42788000	-2.39478600	-0.95473900
H	2.16958300	-8.13372400	-1.69877200	C	-4.10318000	-1.46060200	-1.92363800
H	0.78532400	-8.21962600	-0.61915100	C	-3.56529000	-1.77796900	-3.22530500
H	2.03958200	-7.00790000	-0.33156500	C	-3.42620600	-0.59782500	-3.90492300
H	-1.08592500	-6.54482700	-0.70948700	C	-3.85488800	0.45547600	-3.01801500
H	-0.97224100	-5.09764000	-1.73087800	N	-4.28098500	-0.08263100	-1.80387300
H	0.06699700	-5.26176600	-0.30378900	C	-3.81045700	1.80268400	-3.33907500
N	3.97435500	-5.99431900	-3.40458300	C	-4.16676600	2.82430600	-2.47644600
C	4.94026500	-6.36228800	-4.47187700	C	-4.10853900	4.22690300	-2.79480200
C	6.02808200	-5.27382200	-4.34393100	C	-4.56678900	4.91395700	-1.70205400
C	6.07088200	-4.99598500	-2.82627100	C	-4.91420400	3.94055200	-0.70115800
C	4.59348500	-5.08778300	-2.38694000	N	-4.64045400	2.64756900	-1.16710700
C	5.55011000	-7.76436700	-4.34706700	C	-5.46912900	4.25124100	0.52833800
O	6.44835800	-8.12614900	-5.14592200	C	-5.87781600	3.30712600	1.45602500
H	4.42251500	-6.33761300	-5.43479800	C	-6.48537200	3.62352000	2.72575500
H	6.97899000	-5.61755900	-4.75499100	C	-6.76821600	2.43891400	3.34605500
H	5.71756700	-4.37341300	-4.88557900	C	-6.33112800	1.38265000	2.46571000
H	6.67009100	-5.76086700	-2.31856300	N	-5.78476000	1.92400900	1.30398500
H	6.49815800	-4.01773300	-2.59094100	Fe	-5.24397500	0.90547500	-0.34801700
H	4.10386000	-4.10906100	-2.42068300	H	-6.86586000	-0.24722700	3.70832400
H	4.48416800	-5.50408800	-1.38040100	H	-4.22593700	-3.43802100	-1.17055900
N	5.08665700	-8.56573800	-3.35836700	H	-3.51054300	2.06031500	-4.34836600
C	5.55947700	-9.92707900	-3.20610500	H	-5.59900900	5.30403100	0.75477100
C	4.78188900	-10.59365500	-2.07442500	O	0.87964500	4.56421300	-1.74447600
O	3.91792800	-9.95778600	-1.41774900	C	0.04155300	4.24860800	-2.71079300
H	4.35183300	-8.27249200	-2.72696300	O	-0.68839900	5.12263200	-3.29249000
H	5.42752800	-10.48448000	-4.14385600	C	-0.11154300	2.84617900	-3.17943500
N	5.09613200	-11.89387200	-1.83576400	C	0.58778800	1.74066900	-2.84139200
C	4.45278900	-12.70378400	-0.78974800	C	1.71831400	1.54790900	-1.86856000
C	3.60949600	-13.86389000	-1.34988400	C	1.49361700	0.30057500	-0.97867000
C	2.41825200	-13.45737400	-2.24865100	C	2.69518300	-0.00908000	-0.06621100
C	1.74890100	-14.71682000	-2.83488800	C	2.61041400	-1.38826700	0.62110300
C	1.38903600	-12.58699100	-1.49922900	C	1.46619500	-1.53394400	1.64251400
H	5.79146600	-12.34151500	-2.41812200	C	1.43712300	-2.91600900	2.31506900
H	3.84091600	-12.01650200	-0.20269000	H	-0.88071900	2.75448200	-3.94039100
H	4.26631800	-14.54416000	-1.91355900	H	-2.74732100	2.41843100	-0.29030800
H	3.23186900	-14.44347000	-0.49390200	H	-1.43089200	1.96177100	-1.07402900
H	2.81638300	-12.86534700	-3.08732400	H	0.30510000	0.82350200	-3.36343300
H	0.93185500	-14.44682300	-3.51373400	H	1.87757600	2.44332500	-1.26495400
H	1.32734400	-15.34162800	-2.03623800	H	2.64106700	1.38431700	-2.44972100
H	2.46570000	-15.32846300	-3.39650200	H	0.58381900	0.44556000	-0.37802700
H	0.53235600	-12.36503900	-2.14667500	H	1.32163100	-0.57062500	-1.62511100
H	1.81842300	-11.63186800	-1.17970400	H	3.60980900	0.02152500	-0.67453700
H	1.00827400	-13.11321100	-0.61304800	H	2.80634200	0.78375400	0.69219500

H	2.49765500	-2.15541900	-0.15821700	H	2.07527400	4.89321100	3.10069200
H	3.56405500	-1.59484400	1.13084900	H	4.55522600	3.51485600	4.29069000
H	1.57034900	-0.75675800	2.41864800	H	2.97824500	2.79093100	3.99584800
H	0.50125600	-1.34859100	1.15213600	H	2.15362700	3.00363800	1.40001800
H	2.37824900	-3.12130700	2.84089700	H	2.91037700	2.36836000	-0.88010000
H	1.29609800	-3.70805300	1.56911200	H	5.32390000	2.12579800	-1.37408300
O	0.67535600	6.38706400	1.42521900	H	7.00295500	2.52228400	0.43254100
H	0.23752700	5.53657300	1.14494200	H	6.24940000	3.16073600	2.70471700
H	0.80157300	6.95065500	0.63318100	C	-1.60900700	-2.74237600	3.09115500
O	0.14023100	3.83831400	0.62480400	C	-1.21363600	-1.33573600	2.79568600
H	-0.69571800	3.29223600	0.45633000	N	-0.49600100	-0.53690400	3.70144200
H	0.54533500	4.05859800	-0.28353900	C	-0.29406700	0.69488000	3.17083400
O	-1.77205000	2.31976200	-0.23119900	N	-0.85037600	0.70080900	1.95751900
H	-5.17455400	-0.81916500	-7.53107900	C	-1.43245200	-0.53405400	1.70193800
H	-6.72308500	-1.67742000	-7.29401900	H	-0.73964200	-3.37339100	3.31053500
H	-10.88648500	2.69212900	-4.51076500	H	-2.12103900	-3.17115500	2.22698300
H	-9.42177400	-2.09479300	-2.76398600	H	0.18932700	1.55435000	3.61099400
H	-7.23010500	2.28023400	4.30951100	H	-1.98151100	-0.71305400	0.79581100
H	-6.37388200	-2.78013700	3.21144300	H	-0.80714700	1.55211200	1.28494300
H	2.92711900	4.87331100	5.18648600	C	-3.94484700	11.10669300	-8.04122300
H	2.87740000	2.32155600	6.64068000	C	-4.92638400	10.04487300	-7.50688300
H	0.62057700	-2.99405000	3.04216600	C	-4.69793000	9.80837200	-5.99394200
H	4.38530100	8.97463200	2.73764800	C	-5.73891400	8.90134600	-5.31705100
H	5.84803500	11.29804900	-0.71978900	C	-4.81548600	8.74319400	-8.32514100
H	-3.70619700	10.60761900	0.45426800	H	-2.90605900	10.76572600	-7.93335100
H	-4.47785200	6.81666100	2.66072000	H	-5.94937000	10.43633400	-7.62882000
H	-3.40928200	4.81076500	-8.38026600	H	-3.68972400	9.38544500	-5.85368500
H	-3.34110700	3.57234700	-7.11913200	H	-4.69456100	10.78756700	-5.48984500
H	-10.08382200	11.28793700	-4.34211500	H	-6.75316600	9.29592600	-5.45501600
H	-8.53285400	11.69974800	-3.58615500	H	-5.72136300	7.88566400	-5.72761100
H	0.93183300	-1.48533000	-4.73783300	H	-5.55521300	8.82527300	-4.23791800
H	5.23260800	-13.10242700	-0.12854900	H	-4.97502200	8.93982700	-9.39168100
H	6.63636600	-9.94223000	-2.98632700	H	-5.55395100	7.99691900	-8.01333500
H	9.63120500	-0.23458600	-4.63633900	H	-3.81623900	8.29933500	-8.21399000
H	-3.35011100	-2.77794100	-3.57387400	C	3.64523400	4.60924200	-5.45674700
H	-3.10897900	-0.42460300	-4.92230800	C	3.57341900	3.11645900	-5.21601000
H	-3.73898200	4.62165300	-3.72916400	C	2.42912200	2.38037800	-5.56416000
H	-4.67963200	5.97715900	-1.55197000	C	2.37775800	0.99388400	-5.36896200
H	-6.67601700	4.62689600	3.07729000	C	3.47089300	0.31340600	-4.81740300
H	-5.22490400	-4.12687400	1.16550600	C	4.61696000	1.04117900	-4.46510300
4P_{DC,B}				C	4.66656100	2.42565100	-4.66092100
C	4.66419700	7.77400500	1.76030200	H	4.06611900	5.13654800	-4.59164300
C	5.64300800	7.22799300	0.68223300	H	2.65427500	5.02883600	-5.66043800
C	5.04745900	7.01949200	-0.73116600	H	1.57743700	2.89611900	-6.00079800
C	4.62113900	8.35024300	-1.38301200	H	1.48645700	0.44306200	-5.65652400
C	6.06967900	6.28713300	-1.62353500	H	3.43302200	-0.76314500	-4.67448500
C	3.58868900	6.77447300	2.13930600	H	5.47602000	0.52485800	-4.04643600
O	2.52223300	6.65776300	1.45757700	H	5.56424800	2.97725900	-4.39229100
H	4.16967100	8.68106400	1.40062600	C	-2.46934100	10.40252500	-2.10869900
H	6.48437600	7.93165000	0.60979700	C	-1.36325200	9.33714300	-2.18078400
H	6.05836200	6.27503800	1.03721500	C	-1.69987200	8.18431100	-3.14385400
H	4.16052900	6.37682100	-0.63841600	C	-0.75551500	6.97210700	-3.05110100
H	4.20092300	8.17447300	-2.38045500	N	-0.79574100	6.27096600	-1.75331700
H	3.86646800	8.88264600	-0.79123500	C	0.13275300	6.36059500	-0.77309400
H	5.48374900	9.01918500	-1.49958000	N	1.08397800	7.31581400	-0.79728600
H	5.66609800	6.12697100	-2.63053000	N	0.12684900	5.48353700	0.23773000
H	6.32840300	5.30818700	-1.20493000	C	-3.68770500	9.90609300	-1.32793300
H	6.99337300	6.87216700	-1.72436200	O	-3.66820500	8.79292900	-0.72537500
N	3.84344500	6.00068100	3.21917900	H	-2.77363600	10.71203300	-3.11833300
C	2.99072500	4.90299600	3.69254900	H	-1.22448800	8.93586800	-1.17117200
C	3.69357700	3.52898400	3.60926800	H	-0.42509300	9.81944500	-2.49369200
C	4.14855800	3.13882700	2.21443700	H	-2.71877900	7.83832900	-2.94617700
C	3.21390700	2.90665100	1.18816300	H	-1.67959400	8.54573400	-4.18179100
C	3.63868300	2.54855400	-0.09514100				
C	5.00420200	2.41073500	-0.37723200				
C	5.94257500	2.63557600	0.63589700				
C	5.51485100	2.99888600	1.91988900				
H	4.71406800	6.15420700	3.70993300				

H	-1.02945200	6.24003000	-3.81858200	C	6.02584100	-4.78016900	-2.87976900
H	0.28303500	7.25817200	-3.25193200	C	8.22717300	-7.34911800	-3.56184600
H	-1.61249200	5.70339100	-1.56183400	O	9.44745200	-7.57280500	-3.75391300
H	1.00901500	8.11371500	-1.40389000	H	7.59248800	-6.35048000	-5.32074400
H	1.80837500	7.28977200	-0.07182300	H	9.32652200	-4.98926100	-3.68818000
H	-0.37071400	4.57827600	0.20572000	H	8.13621900	-4.09547900	-4.65642500
H	0.79136900	5.62317300	0.99502800	H	7.86442100	-4.93663200	-1.71451300
N	-4.78250500	10.70473700	-1.30092600	H	7.59184400	-3.32144400	-2.38145400
C	-6.01550500	10.29683400	-0.57705400	H	5.46887900	-3.95149000	-3.33059300
C	-7.06665800	11.31181000	-1.06036500	H	5.49679400	-5.10031900	-1.97667000
C	-6.23911800	12.57905200	-1.37452500	N	7.45983900	-8.12401600	-2.75890200
C	-4.92768600	12.02401000	-1.96537500	C	7.99488100	-9.30910400	-2.11866400
H	-5.84550800	10.35801300	0.50508600	C	6.88078500	-9.98118000	-1.32078100
H	-7.55776300	10.94433300	-1.96911400	O	5.73850700	-9.46136800	-1.23695600
H	-7.84313400	11.49071900	-0.31208300	H	6.47635600	-7.93714400	-2.60747500
H	-6.74504200	13.25932800	-2.06471400	H	8.40300200	-10.00004900	-2.86930100
H	-6.02883600	13.13231400	-0.45152500	N	7.21910600	-11.14993400	-0.71598600
H	-4.06826700	12.66832400	-1.75564700	C	6.28685900	-11.93912200	0.10393000
H	-5.00293700	11.89743600	-3.05427400	C	5.92159100	-13.29686700	-0.52334400
C	-1.23871300	4.86953700	-6.96453000	C	5.17326800	-13.23464700	-1.87563100
C	-2.18648700	4.20003200	-5.95855400	C	4.99546100	-14.65779100	-2.44249400
H	-0.49732700	5.50300200	-6.46042200	C	3.81349000	-12.51624300	-1.76213200
H	-1.63665200	3.56820200	-5.24961900	H	8.15248300	-11.51529100	-0.85107500
H	-2.74736700	4.94305100	-5.37792400	H	5.40077700	-11.31791900	0.24667700
H	-2.91922600	3.56408500	-6.46768500	H	6.84004200	-13.89033300	-0.64993700
C	2.94600600	-3.25397800	-7.06646800	H	5.30261500	-13.84376900	0.20408800
C	1.88774500	-3.94946300	-7.94841100	H	5.79900800	-12.66657400	-2.58136600
C	0.46334800	-3.97646300	-7.41000100	H	4.50940500	-14.63062300	-3.42444200
C	-0.45454600	-4.88966700	-7.96215400	H	4.36994200	-15.26741800	-1.77684600
C	-1.78702300	-4.91616900	-7.54209500	H	5.95961300	-15.16802700	-2.55777700
C	-2.22884900	-4.02731700	-6.55396200	H	3.28466200	-12.54699500	-2.72211200
C	-1.32611800	-3.12082200	-5.99026700	H	3.92986100	-11.46407200	-1.48310600
C	0.00939100	-3.09617100	-6.41367600	H	3.17517800	-13.00856300	-1.01549500
C	3.15986800	-3.84302000	-5.67694300	C	-9.65857200	1.84736800	2.06399000
O	3.20443200	-3.10803700	-4.65080900	C	-8.29908500	1.48538000	1.43086100
H	2.70320000	-2.19800700	-6.92648700	S	-7.25547200	3.03867300	1.07171300
H	2.20123500	-4.97904000	-8.17117800	C	-10.53221300	2.64844400	1.11700100
H	1.89074600	-3.43613400	-8.92147600	O	-11.18623900	2.10273600	0.18909100
H	-0.12036300	-5.58210900	-8.73074100	H	-9.49385700	2.39021500	3.00135800
H	-2.47740900	-5.62847700	-7.98301100	H	-7.73738700	0.84652400	2.11578700
H	-3.26379600	-4.04494900	-6.22724600	H	-8.45565200	0.94602200	0.49284100
H	-1.65477900	-2.42854900	-5.22113500	N	-10.52417100	4.00421000	1.28702300
H	0.69578500	-2.39650700	-5.94900800	C	-11.29805200	4.89816800	0.43260800
N	3.35017400	-5.18952700	-5.61758000	C	-10.84224800	5.00040100	-1.02745800
C	3.69355400	-5.92126300	-4.38564800	O	-11.57898000	5.58328600	-1.85494200
C	2.71168400	-7.09345400	-4.11708300	H	-9.88024000	4.39793100	1.95824300
C	3.09210500	-7.83527700	-2.82199700	H	-12.33767600	4.55974300	0.39155300
C	1.25621500	-6.59599100	-4.05461100	N	-9.65187300	4.41827700	-1.35190900
C	5.12903100	-6.42963900	-4.60639200	C	-9.23516900	4.26740400	-2.73771100
O	5.34092500	-7.26441200	-5.52346100	C	-9.34690500	2.83830200	-3.28063000
H	3.38653900	-5.73355200	-6.47002200	O	-8.69331100	2.50964400	-4.31093800
H	3.62811600	-5.19849900	-3.57216000	H	-9.04520200	4.04102800	-0.62616100
H	2.81739900	-7.79397200	-4.95787300	H	-8.19981500	4.58967800	-2.86764800
H	4.09345600	-8.27336300	-2.85838400	H	-9.87663400	4.91528700	-3.34518400
H	2.39039200	-8.65609200	-2.63707500	N	-10.18703100	1.99887600	-2.63484000
H	3.04439200	-7.16237500	-1.95473700	C	-10.43889500	0.64392200	-3.12012500
H	0.57655800	-7.44208900	-3.90122100	H	-10.63074200	2.27523600	-1.76162300
H	0.95647700	-6.08261900	-4.97287100	H	-9.59978500	-0.02691400	-2.89986900
H	1.11666600	-5.89871800	-3.21783400	C	-4.03344200	1.98833400	3.72611900
N	6.14623900	-5.90787200	-3.85427100	C	-4.54257600	0.86163800	3.09594000
C	7.55701200	-6.15036700	-4.24628900	C	-4.75608200	-0.41648800	3.73771900
C	8.25922700	-4.83215100	-3.85417200	C	-5.20169500	-1.28312900	2.77600400
C	7.49169200	-4.39064100	-2.58885800	C	-5.27953500	-0.54255100	1.53635500

N	-4.88005000	0.77082600	1.75182900	H	2.71122400	-4.99885300	1.16450000
C	-5.72071400	-1.06776800	0.32853200	H	2.70582200	5.10217000	4.73336300
C	-5.88681100	-0.33913900	-0.84139800	H	5.23989800	8.05550300	2.65059900
C	-6.45480400	-0.85982000	-2.06810600	H	-2.08475400	11.30768300	-1.61693600
C	-6.54208400	0.18280000	-2.94892800	H	-6.26194700	9.25941400	-0.81503700
C	-6.00495000	1.34830300	-2.28009100	H	-1.79010100	5.50275000	-7.66902100
N	-5.60552600	1.01118200	-0.99241700	H	-0.69076800	4.12373000	-7.55203100
C	-5.91138900	2.60522400	-2.85720100	H	-4.12002000	11.30814200	-9.10422000
C	-5.37918500	3.72500300	-2.23267400	H	-4.04646000	12.05417400	-7.49772400
C	-5.29226800	5.03673000	-2.83671600	H	3.90893800	-3.28294500	-7.59625600
C	-4.72266400	5.87059700	-1.91241100	H	6.74301800	-12.10057600	1.08884900
C	-4.45087000	5.07531600	-0.73363000	H	8.82996000	-9.04552500	-1.45439800
N	-4.86031200	3.76817200	-0.94529300	H	4.28356100	4.84448900	-6.31869200
C	-3.88616700	5.57531800	0.43456800	H	-6.76894200	-1.88361600	-2.21143700
C	-3.70098100	4.83603500	1.59506600	H	-6.96255900	0.20181700	-3.94298200
C	-3.18861900	5.37528700	2.83464900	H	-5.64708000	5.27495800	-3.82905900
C	-3.24544900	4.37179400	3.76711200	H	-4.53426700	6.93204800	-1.96548700
C	-3.78736300	3.20486600	3.10434800	H	-2.86820200	6.39845200	2.96884600
N	-4.04224000	3.49992500	1.77260600	H	-5.47880500	-2.32171000	2.88802800
Fe	-4.90868100	2.27727600	0.41589600	4P_{CO2}			
H	-3.81452400	1.91476200	4.78627200	C	-0.11828100	0.00000000	-1.25934500
H	-6.00188900	-2.11535100	0.31011600	O	0.44240400	-0.12886500	-0.22003800
H	-6.33970000	2.72605100	-3.84549400	O	-0.67896600	0.12886500	-2.29865200
H	-3.63031300	6.63022100	0.44532000	2ReB			
C	-2.32454300	0.25158900	-3.76566300	C	5.71912100	7.48874300	1.98175400
C	-1.70066500	-0.34015600	-2.73533200	C	6.24870100	6.35922200	1.05106200
C	-0.28541500	-0.06756300	-2.28742800	C	5.46206300	6.13772300	-0.26419300
C	0.53183900	-1.34541400	-1.99523000	C	5.55161100	7.35353100	-1.20704000
C	1.90331400	-1.03136200	-1.36864400	C	5.98034600	4.86740300	-0.96886200
C	2.76674600	-2.27300300	-1.06764500	C	4.38345700	7.15060300	2.60900800
C	2.18888900	-3.20284100	0.01748400	O	3.28452600	7.33685300	2.00284500
C	3.13971100	-4.35240900	0.38958000	H	5.60100500	8.41770600	1.41671500
H	-1.82367200	0.98626100	-4.39255200	H	7.29171600	6.59895200	0.80057900
H	-3.35229500	0.01657200	-4.02537400	H	6.26944500	5.41820000	1.61805900
H	-2.87520700	1.41675500	-1.31295100	H	4.40489900	5.97476700	-0.01082700
H	-2.24527000	-1.08320200	-2.14860400	H	5.00417500	7.16048200	-2.13656400
H	-0.32379900	0.53176000	-1.36165500	H	5.12733500	8.25931800	-0.75869200
H	0.23651100	0.54545300	-3.03476700	H	6.59575700	7.56451600	-1.47305200
H	-0.05004900	-1.99196000	-1.32165700	H	5.42480600	4.67909300	-1.89460000
H	0.67882000	-1.91305700	-2.92401900	H	5.87126400	3.98649100	-0.32571100
H	2.45823100	-0.37509100	-2.05321300	H	7.04154400	4.96953600	-1.23172200
H	1.75429600	-0.45829900	-0.43816000	N	4.41700300	6.60578700	3.85215300
H	2.91780600	-2.83456000	-2.00023300	C	3.22267800	6.16600200	4.57913900
H	3.76198800	-1.93442800	-0.74220300	C	3.20912900	4.64391900	4.84969100
H	1.96447200	-2.60831600	0.91764600	C	3.27815500	3.78977800	3.59695300
H	1.23210200	-3.62354600	-0.32206300	C	2.21918700	3.77156800	2.67001400
H	4.09619400	-3.96727500	0.76524600	C	2.30028000	3.00202600	1.50307200
H	3.35397500	-4.98244500	-0.48296100	C	3.44375500	2.23150400	1.25053400
O	0.06114900	3.64397100	2.83624400	C	4.49938000	2.23323300	2.16867300
H	-0.17508900	3.37185100	1.89341400	C	4.41553800	3.00993900	3.33157400
H	-0.68856600	4.14124900	3.21925200	H	5.31687300	6.47038100	4.29176000
O	-0.59154800	2.78551800	0.40710900	H	2.36723300	6.45922300	3.96750400
H	-1.46569369	2.44460600	0.06120681	H	4.04538300	4.38805400	5.51416000
H	0.14672800	2.55212900	-0.19408800	H	2.29068500	4.42517800	5.41418000
O	-2.82948100	1.65648200	-0.36755400	H	1.32123200	4.35849600	2.85243200
H	-10.58729300	0.65737800	-4.20323200	H	1.47615000	3.01311800	0.79576300
H	-11.33601600	0.26118000	-2.63044900	H	3.50935800	1.63500700	0.34634600
H	-11.29172100	5.89864900	0.87389900	H	5.38447400	1.63268500	1.98325400
H	-10.19823600	0.92123200	2.29504900	H	5.23787400	3.00496600	4.04262200
H	-2.99035700	4.41877900	4.81674100	C	0.02924100	1.62925700	7.42290200
H	-4.59720900	-0.60923200	4.78932800	C	-0.46914400	2.16743100	6.12055700
H	-0.18423300	-0.83247600	4.61377900	N	-0.73090500	3.53281800	5.91930400
H	-2.29758800	-2.79853700	3.94221600	C	-1.14537100	3.74747900	4.64606700
				N	-1.16318300	2.56164600	4.02678100
				C	-0.75010900	1.57016600	4.91464200
				H	0.99472100	2.06975400	7.69877900
				H	0.16765200	0.54784100	7.35334600
				H	-1.36066900	4.69069500	4.14765700
				H	-0.68212500	0.53677200	4.62460100
				H	-1.44886900	2.47481500	2.97768200

C	-3.45388500	13.42763200	-6.54570200	C	-0.17661300	0.26154300	-6.78227600
C	-3.55779800	12.02265000	-7.17111900	C	0.57363900	-0.88907100	-7.06680900
C	-3.40034400	10.93050700	-6.08536200	C	2.61304000	-3.33524600	-6.37480500
C	-3.65691300	9.49413100	-6.57308100	O	3.35879600	-2.50622600	-5.78447800
C	-2.53555300	11.86023800	-8.31332900	H	2.82325400	-2.33240300	-8.22856500
H	-2.46086500	13.58192100	-6.10110000	H	0.29001400	-4.04800800	-7.82437600
H	-4.56725500	11.91594500	-7.60093300	H	0.74518100	-3.29822500	-9.33388600
H	-2.38450300	11.00932300	-5.66277100	H	-1.70043600	-2.53417400	-8.98945800
H	-4.09627000	11.16088200	-5.26390900	H	-3.02137900	-0.50569900	-8.48676400
H	-4.62848000	9.42583400	-7.07998700	H	-2.03737600	1.31368000	-7.08854400
H	-2.88840200	9.16990100	-7.28473800	H	0.26049600	1.04640600	-6.17230100
H	-3.66948800	8.77974600	-5.74117300	H	1.57526400	-0.97631800	-6.66126100
H	-2.66310800	12.64601300	-9.06798700	N	2.05419600	-4.39523200	-5.72091500
H	-2.63816300	10.89373200	-8.81823400	C	2.27132300	-4.67564900	-4.29089500
H	-1.50939000	11.93259100	-7.92659200	C	0.92519800	-4.88311900	-3.54733300
C	6.41948700	3.26665000	-10.19460500	C	1.16249300	-5.25204100	-2.07040000
C	5.90952800	2.17515200	-9.27832600	C	0.03560600	-3.63224800	-3.66598800
C	4.53104400	1.98611700	-9.07923100	C	3.14046200	-5.94201000	-4.21721700
C	4.05680800	0.95705900	-8.25782800	O	2.64596900	-7.04108100	-4.57787900
C	4.95414400	0.09387500	-7.61421800	H	1.55222500	-5.10334300	-6.24115800
C	6.33029800	0.27691200	-7.80321800	H	2.78243200	-3.80214900	-3.88430900
C	6.80140500	1.30716600	-8.62437000	H	0.42254300	-5.73163300	-4.03259900
H	7.41057200	3.61785200	-9.88728700	H	1.70716400	-6.19376200	-1.96055200
H	5.74364700	4.12877100	-10.20683600	H	0.20411000	-5.37195900	-1.55139200
H	3.82606400	2.65007100	-9.57300200	H	1.72906400	-4.47042700	-1.54762800
H	2.98682300	0.82819800	-8.12164100	H	-0.94451500	-3.82435400	-3.21278700
H	4.58705800	-0.70576300	-6.97718800	H	-0.12543000	-3.34020500	-4.70814800
H	7.03751800	-0.38336700	-7.30938000	H	0.49438700	-2.77988300	-3.14581600
H	7.87133500	1.44094800	-8.76214700	N	4.43833000	-5.82707400	-3.79957300
C	-3.79350500	9.19927400	-2.25225100	C	5.36473300	-6.97732200	-3.93228900
C	-2.29102200	9.28382300	-1.87498400	C	6.69240000	-6.30661100	-4.34379900
C	-1.35258200	8.73598600	-2.96793800	C	6.66617500	-4.97462000	-3.56119500
C	0.09194700	8.56367800	-2.47157700	C	5.18047900	-4.54468600	-3.57856000
N	0.18682500	7.44123500	-1.52261300	C	5.54582800	-7.79897400	-2.64935600
C	1.02476900	7.36857300	-0.48429300	O	6.38699800	-8.72942900	-2.61295200
N	1.90635300	8.35099200	-0.19279700	H	4.97249700	-7.65825400	-4.69221500
N	0.99274600	6.28324800	0.33136200	H	7.54789300	-6.93967500	-4.10141000
C	-4.21949400	7.75316700	-2.44625600	H	6.68967100	-6.12074200	-5.42366900
O	-4.17379700	7.21667000	-3.58703200	H	7.00405800	-5.13918700	-2.53151300
H	-3.96768100	9.71817300	-3.19895100	H	7.31079600	-4.21009600	-4.00345600
H	-2.12027500	8.72798100	-0.94278100	H	4.96675400	-3.84373500	-4.39122900
H	-2.03790900	10.33335800	-1.66831600	H	4.87716700	-4.07878200	-2.63504900
H	-1.72282800	7.77648400	-3.34723500	N	4.78368600	-7.46523900	-1.57732400
H	-1.34226900	9.42369000	-3.82318700	C	4.88383600	-8.19710900	-0.33066500
H	0.76490900	8.38820300	-3.32155000	C	4.04466300	-7.49334700	0.73095300
H	0.41200800	9.49025300	-1.97718700	O	3.31244500	-6.51274400	0.44078300
H	-0.34640000	6.56990100	-1.75265300	H	4.11472400	-6.70611600	-1.60738200
H	2.00352500	9.15677800	-0.78460000	H	4.53394100	-9.23245000	-0.45669400
H	2.53967600	8.22330000	0.59783400	N	4.14832400	-8.00473200	1.98790700
H	0.44681200	5.43391600	0.08504900	C	3.40255000	-7.47845100	3.13987300
H	1.71716300	6.20996900	1.03731800	C	2.34868100	-8.45826400	3.68726900
N	-4.55563400	7.03124200	-1.34014500	C	1.20551900	-8.83247900	2.71465900
C	-4.78424500	5.56806500	-1.44202900	C	0.30854500	-9.91374200	3.35016900
C	-5.23507700	5.15930500	-0.02567500	C	0.37188500	-7.60665200	2.28958500
C	-4.65725800	6.25596900	0.89902800	H	4.75998500	-8.79521800	2.14238000
C	-4.72279600	7.53445200	0.04180700	H	2.94211500	-6.54650400	2.80633600
H	-3.84911900	5.08587600	-1.74934700	H	2.85441200	-9.37948700	4.01453900
H	-6.32960300	5.15871500	0.03354200	H	1.91549000	-8.00952400	4.59448500
H	-4.88846400	4.15607300	0.23807900	H	1.66130300	-9.26152300	1.80914200
H	-5.22056100	6.36133000	1.83172400	H	-0.48061700	-10.22683900	2.65706000
H	-3.61780200	6.03639800	1.16693000	H	-0.17582300	-9.53338400	4.25960500
H	-3.93942900	8.24994600	0.30482000	H	0.88721100	-10.80371000	3.62583300
H	-5.69426600	8.03832500	0.15346200	H	-0.46318700	-7.91600000	1.64975200
C	-2.77689000	5.55136000	-7.25180700	H	0.97041000	-6.88405600	1.72558100
C	-2.50739700	5.01409000	-5.83809400	H	-0.05212000	-7.10272400	3.16982000
H	-2.81065000	6.64683800	-7.26177700	C	-8.01171000	-3.90099900	0.15452500
H	-1.51405800	5.30733600	-5.47707500	C	-6.74033100	-3.09304400	-0.13640500
H	-3.23591000	5.39892600	-5.11784600	S	-7.14409100	-1.29396900	-0.57196900
H	-2.54979100	3.91573800	-5.81774000	C	-8.97385200	-3.87076900	-1.02434300
C	2.30390900	-3.22130400	-7.86227300	O	-8.59599300	-4.13063800	-2.19447900
C	0.80769000	-3.17231800	-8.24449700	H	-8.49396000	-3.52996700	1.06579500
C	0.03734700	-1.91164600	-7.86759500	H	-6.07180500	-3.08508900	0.72880100
C	-1.27145000	-1.75506000	-8.36413500	H	-6.20486500	-3.50954300	-0.99323300
C	-2.01978400	-0.60993700	-8.08117900	N	-10.26123800	-3.50225600	-0.74844700
C	-1.47116100	0.40930600	-7.28981900	C	-11.29891200	-3.46806300	-1.77934300

C	-11.18969600	-2.33014500	-2.80245000	H	-2.72960500	2.27794500	1.19598800
O	-11.95427000	-2.32379300	-3.79004700	H	-1.28099400	3.01038100	0.81834300
H	-10.51551300	-3.28397600	0.20349800	O	-4.13493000	1.55757300	0.35239200
H	-11.27295000	-4.39550100	-2.35950800	H	-7.15520700	-2.59061400	-6.06623400
N	-10.22527600	-1.38954000	-2.58078500	H	-6.47699100	-3.21646400	-4.54274600
C	-9.87977200	-0.38358200	-3.57612500	H	-12.27592600	-3.40603400	-1.29325400
C	-8.57299200	-0.65898700	-4.32962200	H	-7.72848100	-4.94805300	0.33266400
O	-8.01872000	0.27431700	-4.96846600	H	-5.89807900	-1.20623700	4.88413800
H	-9.66462200	-1.43537800	-1.73939200	H	-2.12618900	-3.36820300	1.89675000
H	-9.79228600	0.60369400	-3.11505400	H	-0.63598500	4.25140900	6.62057800
H	-10.69554400	-0.34875300	-4.30580300	H	-0.67609000	1.82183700	8.24012500
N	-8.09497900	-1.92631000	-4.28288400	H	6.91600900	-0.82857000	-1.41403200
C	-6.90727500	-2.33800300	-5.02805400	H	3.16118700	6.71063300	5.52996700
H	-8.55501500	-2.62907300	-3.71264800	H	6.46101500	7.68064000	2.76675700
H	-6.17771200	-1.52646400	-5.03779900	H	-4.39470800	9.69832900	-1.48434100
C	-4.36007700	-1.69148300	2.52096200	H	-5.53248500	5.35304400	-2.21014900
C	-3.64497500	-1.81520200	1.33504100	H	-3.74259900	5.19619400	-7.63311900
C	-2.51976700	-2.70192400	1.14294000	H	-2.00280600	5.23217400	-7.96112400
C	-2.08534100	-2.52595700	-0.14103400	H	-3.60695200	14.20978300	-7.29879500
C	-2.94747300	-1.53826200	-0.74897400	H	-4.20180200	13.56864700	-5.75525100
N	-3.89946100	-1.11241800	0.16831900	H	2.75646800	-4.08668700	-8.36685700
C	-2.85554500	-1.11456000	-2.06565600	H	4.11888700	-7.23119300	3.93368400
C	-3.71241600	-0.20750000	-2.67053300	H	5.93370200	-8.26392100	-0.01579600
C	-3.68237100	0.14154700	-4.07583200	H	6.50813300	2.90914900	-11.22981200
C	-4.73821700	0.97913800	-4.29873400	H	-2.95696800	-0.22500400	-4.78765300
C	-5.40324500	1.16776300	-3.02845600	H	-5.07112900	1.41816400	-5.22604300
N	-4.76331500	0.44006600	-2.04207500	H	-8.73503400	3.66118900	-2.22184600
C	-6.52294400	1.96818400	-2.84676100	H	-9.32479500	3.63639100	0.42184500
C	-7.13285600	2.21136400	-1.62595000	H	-7.68570500	0.79309800	4.54134700
C	-8.25336400	3.10454300	-1.43154300	H	-1.26567200	-3.01700800	-0.64432300
C	-8.54737600	3.09462400	-0.09664400				
C	-7.62581200	2.17605000	0.53429700				
N	-6.76186900	1.64750100	-0.41253500	²TS1 _{HA,B,α}			
C	-7.65964100	1.82020700	1.87518600	C	4.30489000	9.85266700	1.18045800
C	-6.88774900	0.82503300	2.44816900	C	5.33977400	9.14893400	0.25720000
C	-6.99663100	0.38100800	3.81861800	C	4.77155800	8.46830100	-1.01100200
C	-6.09466700	-0.63076400	3.99114000	C	4.06066300	9.46809000	-1.94417900
C	-5.40616900	-0.80989700	2.73353900	C	5.90849500	7.74166600	-1.75782500
N	-5.91687800	0.07583100	1.78520600	C	3.28898000	8.89648700	1.76945100
Fe	-5.22338800	0.38422600	-0.08711700	O	2.19885800	8.62513200	1.17897300
H	-4.05788100	-2.31879600	3.35311600	H	3.75739000	10.61458400	0.61920100
H	-2.07522100	-1.55183100	-2.67802700	H	6.07455800	9.90733500	-0.04807600
H	-6.95268400	2.42427500	-3.72950500	H	5.88801100	8.39991700	0.84564800
H	-8.38433000	2.32037400	2.50844500	H	4.03837700	7.71091000	-0.69787900
O	-0.52223600	3.96944500	-0.20719600	H	3.73199900	8.96833100	-2.86251700
C	-0.92267000	3.99813000	-1.46592600	H	3.17358700	9.90794900	-1.47557900
O	-0.94946500	5.06787000	-2.15008200	H	4.73708400	10.28352800	-2.23309500
C	-1.34280500	2.68526200	-2.10090800	H	5.52374100	7.22222600	-2.64251300
C	-0.19930400	1.64418700	-2.10878000	H	6.39331300	6.99736000	-1.11542900
C	1.03448000	2.07796300	-2.91958100	H	6.67423500	8.45296700	-2.09414200
C	2.15846400	1.02554700	-2.91664900	N	3.61252500	8.32204900	2.95535000
C	3.40728200	1.46438900	-3.70503700	C	2.77107300	7.34217600	3.65079400
C	4.55968900	0.43863900	-3.70530400	C	3.45532000	5.96588500	3.81516100
C	5.23219000	0.23703400	-2.33287600	C	3.83060900	5.29764700	2.50546100
C	6.45293900	-0.69559200	-2.39924500	C	2.83770600	4.83875500	1.61970400
H	-1.68065700	2.89510800	-3.11933600	C	3.18471400	4.24314200	0.40084300
H	-2.19526600	2.28000000	-1.53881800	C	4.53470900	4.08950600	0.05621300
H	0.09762900	1.43318300	-1.07195400	C	5.53085300	4.53299800	0.93269000
H	-0.59067000	0.70439000	-2.52051400	C	5.17847500	5.13631000	2.14693700
H	1.42620900	3.02400600	-2.51704800	H	4.49762700	8.56723500	3.37776000
H	0.73210800	2.29198500	-3.95570100	H	1.85350700	7.24954500	3.06663700
H	2.43256500	0.80525000	-1.87364600	H	4.35008100	6.07927500	4.44199000
H	1.78028800	0.08181600	-3.34022200	H	2.76134300	5.32978800	4.38395500
H	3.11697300	1.66646900	-4.74597000	H	1.78633000	4.94131800	1.88160000
H	3.77316400	2.42130100	-3.29877300	H	2.40265700	3.90971900	-0.27477500
H	4.18933900	-0.52612600	-4.08151800	H	4.80538400	3.62291300	-0.88539600
H	5.32218300	0.77046900	-4.42415600	H	6.57823900	4.40775000	0.67636500
H	5.54314000	1.21674000	-1.93710800	H	5.95756200	5.47332200	2.82609600
H	4.50554800	-0.17088300	-1.61507400	C	1.22808100	0.28457800	6.05806800
H	7.21554900	-0.29416100	-3.07799100	C	0.71677800	1.15167200	4.95743100
H	6.16800000	-1.68701600	-2.77340000	N	0.45411100	2.52117500	5.12087300
O	-1.40008700	5.42375200	2.37445300	C	0.00390100	3.04943300	3.95385100
H	-1.72921500	4.63403600	1.88636100	N	-0.02938700	2.06176300	3.05438500
H	-0.84680000	5.96277200	1.77538400	C	0.40514300	0.88126200	3.64675100
O	-1.89575400	2.67574100	1.56028800	H	2.20268300	0.62660900	6.42643100
				H	1.35267500	-0.73951200	5.69873900

H	-0.28055800	4.07350400	3.73517700	C	0.31695500	-3.78303400	-8.60801200
H	0.46007600	-0.04496200	3.10242300	C	-0.55338200	-2.68993200	-8.62314900
H	-0.38039600	2.23952300	2.02138700	C	-0.13501000	-1.45328200	-8.11315000
C	-9.52017200	11.74131200	-2.39092900	C	1.15408000	-1.32846300	-7.58604000
C	-9.80538600	10.24029000	-2.18513500	C	2.02685800	-2.42487000	-7.57505100
C	-8.56313400	9.52429400	-1.60086600	C	3.67722500	-4.62958500	-5.83445500
C	-8.79603800	8.06551300	-1.17290800	O	4.26522200	-3.70990300	-5.20249800
C	-10.28555600	9.59641800	-3.50083000	H	4.48084500	-3.98452500	-7.68243100
H	-8.70943700	11.88723600	-3.11778500	H	1.97187700	-5.77405900	-7.87780300
H	-10.61741800	10.14810900	-1.44513900	H	2.83259500	-5.04308500	-9.20827700
H	-7.75261500	9.56560700	-2.34662900	H	-0.01352600	-4.73721200	-9.01097400
H	-8.21185900	10.09944900	-0.73041300	H	-1.55131700	-2.79988400	-9.03629400
H	-9.61172500	7.99978500	-0.44093700	H	-0.80388300	-0.59859900	-8.13312000
H	-9.06443100	7.43132300	-2.02559000	H	1.48764400	-0.37633200	-7.18430100
H	-7.89465300	7.64337200	-0.71418300	H	3.01615900	-2.30588700	-7.14812000
H	-11.16475500	10.12081500	-3.89354800	N	2.87424100	-5.53809800	-5.20816600
H	-10.55900100	8.54438100	-3.36697800	C	2.64032100	-5.55285600	-3.75369300
H	-9.49817800	9.64642500	-4.26539900	C	1.13354500	-5.72441700	-3.42690700
C	9.54793100	-0.50177000	-10.11974300	C	0.90319900	-5.73723800	-1.90371500
C	8.62776700	-1.09999200	-9.07737800	C	0.28941600	-4.62422400	-4.09631400
C	7.24950900	-0.82539100	-9.08809800	C	3.46832000	-6.72846000	-3.20332600
C	6.40241000	-1.35797700	-8.10937800	O	3.14304400	-7.90150000	-3.52126800
C	6.91657200	-2.18173400	-7.09908000	H	2.51458300	-6.33108600	-5.72333500
C	8.28887900	-2.46442300	-7.08205600	H	2.99112400	-4.59016000	-3.37993000
C	9.13338200	-1.92951200	-8.06074100	H	0.83263400	-6.70367400	-3.82572600
H	10.38736700	-1.16903100	-10.34332900	H	1.41648600	-6.56240200	-1.40237600
H	9.97339800	0.45169400	-9.77732200	H	-0.16560200	-5.84837700	-1.68467000
H	6.83924100	-0.19232000	-9.87056500	H	1.24042800	-4.79635400	-1.44732500
H	5.33981700	-1.13324600	-8.13794000	H	-0.77575500	-4.79888100	-3.89960800
H	6.25528700	-2.60032500	-6.34632500	H	0.43174500	-4.59491400	-5.18028500
H	8.70035800	-3.10681800	-6.30890400	H	0.55448700	-3.63491000	-3.69899300
H	10.19554800	-2.15929600	-8.04113500	N	4.57488200	-6.46458700	-2.44294200
C	-4.60455200	9.33671600	0.05724100	C	5.56416000	-7.53943100	-2.18001800
C	-3.28227600	9.39864000	-0.75462900	C	6.90922700	-6.78250900	-2.17487200
C	-3.29996900	8.52932700	-2.02654800	C	6.53765400	-5.41037000	-1.57149600
C	-1.91863600	8.36864300	-2.69479600	C	5.13688200	-5.10888800	-2.14864600
N	-1.02947700	7.44535700	-1.97259700	C	5.35916200	-8.30603900	-0.86772700
C	-0.12281500	7.76077000	-1.04168800	O	6.21784600	-9.13924900	-0.48801200
N	0.17071400	9.04020600	-0.70608100	H	5.49468400	-8.28062500	-2.98162200
N	0.52845100	6.76967300	-0.38746300	H	7.66308500	-7.32471800	-1.60121300
C	-4.78923500	7.99287800	0.74407200	H	7.27023400	-6.66599400	-3.20289800
O	-5.43195000	7.05670000	0.18326200	H	6.49456300	-5.48091700	-0.47818200
H	-5.45811300	9.47605700	-0.61275100	H	7.25458200	-4.62506400	-1.82681700
H	-2.45212300	9.09018700	-0.10679900	H	5.19404200	-4.52043600	-3.07031400
H	-3.09352700	10.44559200	-1.03326200	H	4.50239100	-4.57424800	-1.43405400
H	-3.68934000	7.53110500	-1.79665000	N	4.23083900	-8.05238400	-0.16050200
H	-3.98866600	8.97451600	-2.75792200	C	3.91982800	-8.79549900	1.04376800
H	-2.04561400	7.94312800	-3.69461800	C	2.53416600	-8.39086900	1.53589900
H	-1.43288300	9.34447200	-2.83485200	O	1.90945300	-7.43206100	1.01351200
H	-1.07885400	6.44043300	-2.26833100	H	3.54150900	-7.37963600	-0.47040700
H	-0.25733000	9.81573100	-1.17991400	H	3.96285400	-9.87497500	0.84535300
H	0.91471800	9.20442500	-0.02803000	N	2.04865600	-9.12475900	2.57254200
H	0.41777600	5.77657800	-0.68703200	C	0.73939400	-8.88202100	3.19572500
H	1.30852100	7.03227300	0.20651100	C	-0.26766500	-10.02405800	2.96666700
N	-4.20460400	7.81121400	1.95925500	C	-0.65879300	-10.29326100	1.49454300
C	-4.31607400	6.51583400	2.67836500	C	-1.57806700	-11.52885800	1.41437400
C	-3.81504800	6.84551800	4.09471000	C	-1.32313300	-9.06982600	0.83150700
C	-2.78688300	7.97235300	3.85413400	H	2.59701800	-9.90203600	2.91617800
C	-3.43210300	8.81397100	2.73546000	H	0.37175300	-7.94187400	2.78001000
H	-3.67712000	5.76820700	2.19473400	H	0.13637400	-10.94987000	3.40408500
H	-4.64004700	7.20831900	4.71986400	H	-1.17628500	-9.78654300	3.54104600
H	-3.37506700	5.97307600	4.58500700	H	0.26232000	-10.52183700	0.93673100
H	-2.57791100	8.56697400	4.74803700	H	-1.82442400	-11.76730900	0.37352800
H	-1.84772300	7.53385100	3.49767500	H	-2.52057600	-11.34915800	1.94862300
H	-2.68809800	9.31387200	2.10952100	H	-1.10322000	-12.41204600	1.85905400
H	-4.10238300	9.57972100	3.14973800	H	-1.64179700	-9.31434800	-0.18867300
C	-0.85539700	5.81463800	-7.17753800	H	-0.63626000	-8.21955700	0.76832500
C	-2.07591600	5.80988900	-6.24542900	H	-2.21575300	-8.76114000	1.39346200
H	-0.04621900	6.43283400	-6.77007000	C	-8.33484300	-1.58033000	-1.26446700
H	-1.82028800	5.41739000	-5.25451600	C	-6.81638700	-1.36394300	-1.32994600
H	-2.47869400	6.82408700	-6.11928700	S	-6.40435200	0.40643200	-1.87213500
H	-2.88272300	5.19046700	-6.65726700	C	-9.00844700	-1.33547600	-2.60673000
C	3.84867700	-4.80582500	-7.33742800	O	-8.66003200	-1.94582800	-3.64856000
C	2.54393400	-4.87840800	-8.15984200	H	-8.76991400	-0.94552400	-0.48458000
C	1.62192300	-3.66723000	-8.09156300	H	-6.36467400	-1.53074300	-0.34868100

C	1.12779200	1.48727100	2.86132300	C	4.37033300	-3.49767000	-6.27311300
H	2.95164500	1.29683800	5.62694700	C	3.55838700	-3.84521100	-7.53701400
H	2.14335500	-0.09773000	4.90542800	C	2.23329600	-3.11636200	-7.72340400
H	0.31280700	4.64726900	2.95472600	C	1.50766500	-3.33716800	-8.90994300
H	1.21504500	0.56441000	2.31456900	C	0.29652000	-2.68380000	-9.14749000
H	0.26963400	2.80408800	1.24409700	C	-0.21677300	-1.79035100	-8.19774900
C	-9.88954100	10.89064300	-2.58697700	C	0.49086400	-1.56469000	-7.01409100
C	-9.34581600	9.44137700	-2.06197600	C	1.70674000	-2.22282900	-6.77632100
C	-8.40029000	9.00524200	-1.76427500	C	3.78025100	-3.91762200	-4.93073200
C	-8.25890200	7.64120900	-1.06819000	O	3.76572400	-3.13015800	-3.94394900
C	-10.55955800	8.49165100	-3.05124800	H	4.54834600	-2.42081200	-6.21658500
H	-9.34508100	10.97165100	-3.53753400	H	3.37964800	-4.53072300	-7.58533400
H	-10.41049400	9.41262000	-1.10957300	H	4.19758400	-3.62812900	-8.40405700
H	-7.83647700	8.99617600	-2.71080400	H	1.90107300	-4.02493500	-9.65439100
H	-7.93197600	9.77692900	-1.13381200	H	-0.24398200	-2.86708100	-10.07083600
H	-8.82820000	7.62184000	-0.12923100	H	-1.15485900	-1.27640800	-8.38244400
H	-8.62986300	6.82497600	-1.69848300	H	0.09781000	-0.87899400	-6.27007000
H	-7.20951500	7.42985200	-0.83429200	H	2.23156800	-2.03752900	-5.84542700
H	-11.58378800	8.82709700	-3.25308700	N	3.32169800	-5.19797000	-4.84230100
H	-10.61537100	7.46749800	-2.66702000	C	2.84376600	-5.80968700	-3.58967000
H	-10.02256300	8.46393800	-4.00915600	C	1.38883000	-6.33525600	-3.70993900
C	6.06865800	4.13704300	-5.73208700	C	0.92155300	-6.93435000	-2.36977100
C	5.64970800	2.76369400	-5.25319000	C	0.43324000	-5.21976400	-4.17159600
C	4.55503500	2.10144100	-5.83570200	C	3.83578600	-6.94929600	-3.30081600
C	4.19039200	0.81420300	-5.42392000	O	3.88316800	-7.92702800	-4.09161500
C	4.91134200	0.16026600	-4.41430800	H	3.41032700	-5.82719300	-5.62976300
C	6.00085600	0.81432400	-3.82407000	H	2.88095700	-5.02367100	-2.83506700
C	6.36439300	2.10145500	-4.23880300	H	1.39837700	-7.13548100	-4.46325800
H	6.55111200	4.71210300	-4.93395700	H	1.51593500	-7.79635900	-2.05379500
H	5.21046600	4.71336700	-6.09486000	H	-0.11710300	-7.27482500	-2.44723200
H	3.99049000	2.59584500	-6.62205700	H	0.96363100	-6.17867500	-1.57227900
H	3.34777500	0.31788100	-5.89671900	H	-0.58266300	-5.61796100	-4.28018000
H	4.62942900	-0.84176200	-4.10225400	H	0.73458700	-4.79222900	-5.13222900
H	6.57105200	0.31927900	-3.04344800	H	0.40349100	-4.40389300	-3.43607800
H	7.22001300	2.59371000	-3.78263100	N	4.69463300	-6.83144500	-2.24257500
C	-4.10827100	9.73884300	-0.99938100	C	5.86205000	-7.74137100	-2.12605100
C	-2.81972200	9.81394300	-1.86555800	C	6.95239600	-6.83263900	-1.52114000
C	-2.82954400	8.82012900	-3.04419500	C	6.14895800	-5.89836900	-0.58999800
C	-1.45560000	8.61609700	-3.71548600	C	4.83726900	-5.63206300	-1.36127700
N	-0.58458300	7.69315800	-2.97218700	C	5.63714300	-8.98101300	-1.24913400
C	0.33914900	8.00803800	-2.06058300	O	6.60785500	-9.71875200	-0.94953600
N	0.67085400	9.28685100	-1.75889600	H	6.11643200	-8.11032800	-3.12400500
N	0.97371600	7.01494800	-1.39089000	H	7.71062900	-7.42255500	-1.00326300
C	-4.10010200	8.51197300	-0.10170100	H	7.43923100	-6.25783700	-2.31716500
O	-4.57407400	7.40804100	-0.50338200	H	5.93706900	-6.40696000	0.35779500
H	-4.98637200	9.66216500	-1.64791700	H	6.67749400	-4.96914200	-0.35925100
H	-1.94972400	9.62473100	-1.22293400	H	4.90394500	-4.72326000	-1.96937900
H	-2.71188800	10.83674700	-2.25348500	H	3.97513200	-5.53662200	-0.69383200
H	-3.18978500	7.84304700	-2.70393700	N	4.37336300	-9.23255700	-0.83344200
H	-3.54091100	9.17407300	-3.80289400	C	4.05324600	-10.41549900	-0.06035200
H	-1.59590500	8.16466200	-4.70207100	C	2.55877500	-10.41104600	0.24967700
H	-0.95024500	9.57709900	-3.88550700	O	1.82265000	-9.45764900	-0.11228800
H	-0.66637500	6.67885900	-3.23522900	H	3.59691900	-8.63008900	-1.07556400
H	0.25654700	10.06116600	-2.24676200	H	4.32601000	-11.32428200	-0.61506700
H	1.43030700	9.44728600	-1.09687400	N	2.10269300	-11.49078400	0.93710300
H	0.83644100	6.02160200	-1.66806100	C	0.69503900	-11.67116100	1.32456500
H	1.77189600	7.26882600	-0.81764600	C	0.00813800	-12.84146700	0.59728300
N	-3.51931400	8.62402900	1.12297000	C	-0.10049800	-12.70831400	-0.93998700
C	-3.43701800	7.46271600	2.04790200	C	-0.68640300	-14.00333300	-1.53813800
C	-3.05328100	8.10302400	3.39390400	C	-0.93288300	-11.48187700	-1.36527000
C	-2.22873700	9.34322600	2.98262100	H	2.75412000	-12.22738000	1.17397400
C	-2.95111700	9.85801400	1.72236900	H	0.19379900	-10.72487200	1.11276300
H	-2.66731900	6.76141300	1.70257800	H	0.54127900	-13.77391400	0.83884400
H	-3.95120600	8.41112600	3.94316500	H	-1.00232100	-12.94963500	1.02018700
H	-2.48953400	7.41437900	4.02928700	H	0.91751900	-12.58205400	-1.34011100
H	-2.17622300	10.10451300	3.76599000	H	-0.72716600	-13.94669100	-2.63187700
H	-1.20423300	9.04462600	2.72947200	H	-1.70834000	-14.17289400	-1.17375000
H	-2.26934700	10.35889000	1.02913500	H	-0.08392900	-14.87929600	-1.26792200
H	-3.75225100	10.56249000	1.98424200	H	-1.03908400	-11.45222600	-2.45612200
C	-0.91877400	6.46219800	-7.97399300	H	-0.46331400	-10.54321800	-1.05392500
C	-2.05799200	6.01019600	-7.04796900	H	-1.94262700	-11.52902200	-0.93454200
H	-0.31425500	7.25023600	-7.50768500	C	-8.04505800	-0.81138700	-0.32286300
H	-1.67171900	5.61921300	-6.09925800	C	-6.53393600	-0.84987600	-0.58657300
H	-2.73822200	6.84365200	-6.82335100	S	-5.96716200	0.67889800	-1.55011200
H	-2.65763900	5.22187800	-7.52051600	C	-8.84252300	-0.72322100	-1.61535100

N	0.73440700	2.40130500	4.49940400	H	-2.00910100	5.42453400	-5.49723600
C	0.25218400	3.01637400	3.38819200	H	-3.46921300	6.28004700	-6.03201300
N	0.18271900	2.10008100	2.41875000	H	-3.03109400	4.73606000	-6.77220100
C	0.62635600	0.87705200	2.90923900	C	3.87092700	-4.51616900	-7.20225000
H	2.51179000	0.40669300	5.60089400	C	2.58661000	-4.52480300	-8.05757400
H	1.62768900	-0.89729200	4.80358000	C	1.67866600	-3.30536400	-7.94967700
H	-0.03128600	4.05493000	3.25672800	C	0.51678000	-3.26369300	-8.74466200
H	0.65583200	-0.00675300	2.29653900	C	-0.33892400	-2.16020100	-8.71590200
H	-0.19815700	2.36412800	1.39683500	C	-0.04929400	-1.06888200	-7.88494800
C	-9.74067600	11.71038900	-2.55559300	C	1.09630100	-1.10116100	-7.08479000
C	-9.77598500	10.16924400	-2.53871600	C	1.95516200	-2.20947900	-7.11498000
C	-8.55253700	9.60550800	-1.77500600	C	3.68089900	-4.56307100	-5.69075000
C	-8.58370500	8.08722000	-1.53169700	O	4.25654300	-3.74177400	-4.92533600
C	-9.87622100	9.61535700	-3.97368100	H	4.47129600	-3.62934400	-7.41901900
H	-8.85156100	12.07277500	-3.08955400	H	1.99708300	-5.42844500	-7.84110000
H	-10.67953100	9.85683700	-1.98976400	H	2.89615100	-4.63354900	-9.10642900
H	-7.63972700	9.87316200	-2.33239300	H	0.28840600	-4.10198900	-9.39818700
H	-8.48348800	10.12061800	-0.80498800	H	-1.22363800	-2.14662900	-9.34493000
H	-9.49107300	7.79852700	-0.98543900	H	-0.70580800	-0.20480300	-7.86741400
H	-8.57306900	7.52655000	-2.47363900	H	1.33144900	-0.26203300	-6.43671400
H	-7.71775500	7.76427800	-0.94235800	H	2.83308300	-2.21065300	-6.47882800
H	-10.74763200	10.03207800	-4.49255700	N	2.88320100	-5.56084300	-5.21181500
H	-9.97344300	8.52449400	-3.98708300	C	2.64821300	-5.80127800	-3.77674400
H	-8.98292200	9.88268400	-4.55492400	C	1.13306900	-5.86586300	-3.44830300
C	8.68990900	1.44736800	-8.86665700	C	0.91156400	-6.12000100	-1.94519800
C	7.90660200	0.47704200	-8.00872000	C	0.41167000	-4.58243200	-3.89852700
C	6.51171100	0.36360200	-8.13653000	C	3.34393500	-7.13670300	-3.46056300
C	5.79063300	-0.55561500	-7.36535100	O	2.87459400	-8.19652200	-3.95024800
C	6.45151400	-1.38171800	-6.44607000	H	2.51444700	-6.26106000	-5.84236700
C	7.84196000	-1.27333300	-6.30901000	H	3.10274000	-4.96114600	-3.25025000
C	8.55963500	-0.35303800	-7.08041200	H	0.72539200	-6.72217000	-4.00371700
H	9.57794600	1.81861100	-8.34354600	H	1.33462600	-7.07070600	-1.60958800
H	8.08061900	2.31103300	-9.15411400	H	-0.16118900	-6.15034900	-1.72036900
H	5.98898800	0.99984700	-8.84606400	H	1.35639800	-5.31852900	-1.33963300
H	4.71305800	-0.62781200	-7.48360400	H	-0.66604100	-4.67770500	-3.71497500
H	5.89192500	-2.09543600	-5.84830400	H	0.55733700	-4.38035700	-4.96366900
H	8.36704800	-1.90668000	-5.59980900	H	0.77913100	-3.71119100	-3.33925600
H	9.63771100	-0.27633300	-6.96469900	N	4.49317500	-7.12699200	-2.71893700
C	-4.49628200	9.39342500	-0.04539700	C	5.34240000	-8.34253600	-2.65257000
C	-3.20429200	9.46147100	-0.90299800	C	6.77331600	-7.76575900	-2.60751200
C	-3.24829500	8.57879500	-2.16506600	C	6.60001300	-6.46021200	-1.80154100
C	-1.89411300	8.47218400	-2.89865200	C	5.22994800	-5.90932800	-2.25673500
N	-0.93643600	7.57019700	-2.23959700	C	5.07705300	-9.25046200	-1.44460000
C	-0.02191700	7.89737100	-1.31998600	O	5.82415500	-10.23460800	-1.22455800
N	0.20990300	9.17587500	-0.93596100	H	5.15374100	-8.94968500	-3.54248300
N	0.70158700	6.91700100	-0.72798000	H	7.46853300	-8.47317700	-2.15186700
C	-4.65259900	8.05048600	0.65028600	H	7.11503600	-7.54817100	-3.62570700
O	-5.34027300	7.12328200	0.12916500	H	6.58490000	-6.68148200	-0.72799500
H	-5.37421500	9.52741200	-0.68411500	H	7.40297600	-5.73999900	-1.98106200
H	-2.34848300	9.17255300	-0.28091700	H	5.33046600	-5.19584800	-3.08124800
H	-3.04041100	10.50775800	-1.20041900	H	4.69187100	-5.41729300	-1.43976800
H	-3.58697700	7.56787800	-1.91056000	N	4.02330500	-8.94352400	-0.64950500
H	-3.98821400	8.99040200	-2.86545900	C	3.66128400	-9.78064300	0.47614200
H	-2.05411400	8.05653500	-3.89777900	C	2.43496500	-9.18498300	1.16101000
H	-1.45104200	9.46756600	-3.04692800	O	1.93169600	-8.10069800	0.76860500
H	-0.90593200	6.58638100	-2.60481100	H	3.42762800	-8.14508400	-0.82845600
H	-0.27142400	9.94519100	-1.36705800	H	3.45290700	-10.80672100	0.14179200
H	0.96086100	9.35295300	-0.26871500	N	1.94745000	-9.90070400	2.20898800
H	0.64416900	5.93306900	-1.07332400	C	0.77827200	-9.48750400	2.99896300
H	1.48235300	7.19702800	-0.14302300	C	-0.43202800	-10.42570600	2.83876900
N	-3.99620500	7.85960600	1.82672800	C	-1.02450600	-10.52589100	1.41353900
C	-4.07095600	6.55977400	2.54234700	C	-2.14122700	-11.58879800	1.38238800
C	-3.47667900	6.87376200	3.92583000	C	-1.54384100	-9.16873900	0.89718600
C	-2.46006900	7.99699800	3.62809200	H	2.39505300	-10.77483200	2.45094200
C	-3.17302300	8.85250100	2.56233500	H	0.53663700	-8.47192100	2.67994800
H	-3.47075300	5.81204900	2.01169800	H	-0.14970500	-11.43348400	3.17987600
H	-4.25663900	7.23462200	4.60747300	H	-1.21551500	-10.07810700	3.52948200
H	-3.01019300	5.99443100	4.37790400	H	-0.22232200	-10.86048400	0.73778900
H	-2.18839500	8.58194600	4.51150900	H	-2.54065500	-11.70780200	0.36876700
H	-1.55007400	7.55610200	3.20518000	H	-2.97370200	-11.30001500	2.03797600
H	-2.46885700	9.35759100	1.89631000	H	-1.77434600	-12.56686000	1.71685300
H	-3.81382500	9.61464200	3.02691200	H	-2.00571000	-9.28759900	-0.09009300
C	-1.80190600	6.41251600	-7.44051900	H	-0.73664800	-8.43556400	0.79907800
C	-2.62055400	5.67208300	-6.37262000	H	-2.30796100	-8.76269100	1.57471300
H	-1.39046800	7.35109500	-7.04849700	C	-8.11169600	-1.67677800	-0.74969400

H	6.47938200	5.87708800	1.98182500	C	-1.49819300	6.32594300	-7.96026500
C	2.07824500	0.96600300	5.24116100	C	-2.33833900	5.60433200	-6.89589900
C	1.50925600	1.80236200	4.14506800	H	-1.05227500	7.24654500	-7.56239300
N	1.17241000	3.15549100	4.31022100	H	-1.73293400	5.32671700	-6.02538300
C	0.68360300	3.65502300	3.14494700	H	-3.16488800	6.23840300	-6.54787200
N	0.69937000	2.66704800	2.24686900	H	-2.78208400	4.68737900	-7.30338900
C	1.20211500	1.51325900	2.83720200	C	4.30724100	-3.16090500	-6.25003800
H	3.04055100	1.35606400	5.59420500	C	3.48467500	-3.41551100	-7.52895300
H	2.24709000	-0.05202200	4.88255800	C	2.12814900	-2.72793400	-7.62234700
H	0.33665100	4.65848500	2.92651200	C	1.34111700	-2.94816300	-8.76907000
H	1.30216900	0.59073800	2.29221200	C	0.10056300	-2.32552200	-8.92331600
H	0.31615300	2.81577800	1.21029600	C	-0.38207400	-1.46618000	-7.92716800
C	-9.40546900	10.53279100	-3.90437600	C	0.38625800	-1.24227100	-6.78187600
C	-9.50892500	9.17774600	-3.17630800	C	1.63254700	-1.86746400	-6.62906000
C	-8.15420500	8.80672800	-2.52463000	C	3.73111300	-3.68615800	-4.93882400
C	-8.18676900	7.56779900	-1.61421500	O	3.72683500	-2.97862600	-3.89280000
C	-10.01278400	8.08400000	-4.13857600	H	4.48169300	-2.09108500	-6.11234600
H	-8.67286600	10.47957000	-4.72118800	H	3.34772000	-4.49654700	-7.68242000
H	-10.24780200	9.28423100	-2.36504400	H	4.09974500	-3.08859700	-8.37939800
H	-7.41076900	8.65684000	-3.32416600	H	1.70879000	-3.61197400	-9.54764400
H	-7.80650400	9.67120600	-1.93808200	H	-0.48792200	-2.50815100	-9.81698800
H	-8.92782700	7.69118900	-0.81343000	H	-1.34455400	-0.97871300	-8.04570700
H	-8.44915500	6.66222000	-2.17298600	H	0.01934600	-0.58381200	-6.00080500
H	-7.20869500	7.39866900	-1.14976500	H	2.20464700	-1.68542800	-5.72592700
H	-10.96929800	8.37211700	-4.59051600	N	3.27467500	-4.96952500	-4.95134100
H	-10.16209200	7.12603500	-3.62912900	C	2.80342600	-5.68966100	-3.75522300
H	-9.29326000	7.92473400	-4.95327300	C	1.35133700	-6.21032200	-3.92964900
C	6.47628300	4.22372700	-5.51629900	C	0.89754000	-6.99443200	-2.68422000
C	5.97049500	2.87224500	-5.05967300	C	0.38341600	-5.05089300	-4.22980600
C	4.86584500	2.26702700	-5.68385600	C	3.79934800	-6.84616100	-3.56613100
C	4.42197800	0.99886600	-5.28986100	O	3.86151200	-7.74172900	-4.44760200
C	5.07221700	0.30785300	-4.25746800	H	3.36131100	-5.53113200	-5.78873100
C	6.17101600	0.90507700	-3.62556100	H	2.83518900	-4.97335700	-2.93392100
C	6.61336400	2.17308800	-4.02194200	H	1.36236000	-6.90066600	-4.78492500
H	6.90320300	4.79614900	-4.68496600	H	1.50463300	-7.88463500	-2.49880400
H	5.67425000	4.82096200	-5.96321300	H	-0.13780000	-7.33213600	-2.80537700
H	4.35663300	2.79001000	-6.48920400	H	0.93520200	-6.36536100	-1.78411000
H	3.56937300	0.54939200	-5.79073600	H	-0.62802700	-5.44055400	-4.39628600
H	4.72952900	-0.67921500	-3.95899600	H	0.68057300	-4.48707500	-5.11892800
H	6.68698100	0.38051500	-2.82673400	H	0.34367300	-4.34980500	-3.38469700
H	7.47471500	2.62093800	-3.53212800	N	4.63969100	-6.83223200	-2.48643600
C	-4.15097000	9.65847200	-1.13900100	C	5.79550300	-7.76269400	-2.43563400
C	-2.86465300	9.70581200	-2.00960100	C	6.87969700	-6.93275400	-1.71435900
C	-2.85066700	8.64309400	-3.12679100	C	6.06314900	-6.07595300	-0.72238100
C	-1.47477500	8.44297800	-3.79647000	C	4.77972000	-5.71587700	-1.50202500
N	-0.57160700	7.57960300	-3.01969300	C	5.53470800	-9.08310300	-1.69883600
C	0.32802100	7.96176100	-2.10810700	O	6.47505800	-9.89667900	-1.52786700
N	0.59993600	9.26268800	-1.84353100	H	6.07383700	-8.03170000	-3.45836400
N	0.99839400	7.01987400	-1.40237100	H	7.61607400	-7.57939700	-1.23371000
C	-4.12345500	8.47911600	-0.18036500	H	7.39759500	-6.29379200	-2.43871500
O	-4.60162000	7.35519600	-0.51632600	H	5.81540500	-6.66599100	0.16771200
H	-5.02946900	9.53843500	-1.77998700	H	6.59869000	-5.18172200	-0.39136800
H	-1.99254800	9.57349200	-1.35613200	H	4.88250000	-4.76035200	-2.02820600
H	-2.77746000	10.70530700	-2.45893600	H	3.90235500	-5.65634900	-0.85070400
H	-3.17970600	7.67700600	-2.72811800	N	4.27757600	-9.31344800	-1.25025100
H	-3.57664600	8.93041100	-3.89973800	C	3.92603300	-10.55519200	-0.59113700
H	-1.60789500	7.94151400	-4.75951600	C	2.45865200	-10.49210700	-0.17583700
H	-0.99691000	9.40834300	-4.01574300	O	1.76657400	-9.46397400	-0.39181300
H	-0.59192900	6.56043700	-3.26756200	H	3.52744900	-8.64626200	-1.38106300
H	0.16130200	10.00268100	-2.36240300	H	4.09618600	-11.41018500	-1.26074000
H	1.33714900	9.47661300	-1.17142600	N	1.97604600	-11.60639800	0.43399900
H	0.91615900	6.01265700	-1.65271800	C	0.58888000	-11.73696200	0.90572700
H	1.77349100	7.32841700	-0.82422400	C	-0.22699600	-12.78438300	0.12604600
N	-3.51825800	8.65317500	1.02515500	C	-0.42749000	-12.49823000	-1.38077800
C	-3.40692900	7.53641200	2.00052800	C	-1.15601800	-13.68278700	-2.04725700
C	-3.00505600	8.24081500	3.30860600	C	-1.18367200	-11.17764700	-1.63029200
C	-2.20417900	9.47124300	2.82713100	H	2.59118900	-12.40013300	0.55488500
C	-2.95519100	9.91957400	1.55794700	H	0.14131000	-10.74482900	0.82238000
H	-2.63812100	6.82569500	1.67227100	H	0.25109900	-13.76912600	0.24276900
H	-3.89603500	8.56289000	3.86111100	H	-1.21277100	-12.86407400	0.60916000
H	-2.42096200	7.58781000	3.96294200	H	0.56787500	-12.41201200	-1.84349500
H	-2.14871700	10.26796300	3.57424500	H	-1.26463000	-13.51951700	-3.12554200
H	-1.17997200	9.17547700	2.56946400	H	-2.16195500	-13.80929300	-1.62529900
H	-2.29255900	10.39683700	0.83054900	H	-0.61033100	-14.62319500	-1.90187200
H	-3.76083500	10.62521400	1.80239000	H	-1.36012800	-11.03518800	-2.70309400

H	-0.61954900	-10.31135600	-1.26962800	H	3.69562000	-0.34587900	-1.28664300
H	-2.16267200	-11.19099200	-1.13161000	H	2.65454600	0.07189500	0.06948800
C	-8.04910900	-0.76594500	0.24766600	H	2.81837000	-2.69563400	-1.25412200
C	-6.54284800	-0.83545000	-0.03772100	H	3.67760000	-2.23960200	0.21401800
S	-6.00077400	0.60480400	-1.14400500	H	1.48514900	-1.80915400	1.37696600
C	-8.87395100	-0.77437900	-1.03090200	H	0.61806700	-2.33090900	-0.05930500
O	-8.72298600	-1.65185300	-1.91743900	H	2.53745600	-4.10770600	1.57659400
H	-8.27404000	0.11979900	0.85239900	H	1.64847200	-4.62942200	0.13611100
H	-5.97383700	-0.78533200	0.89405100	O	-0.35428100	5.63250000	1.22000300
H	-6.28935200	-1.76054300	-0.56075200	H	-0.59457500	4.78489500	0.74593500
N	-9.77034200	0.24942300	-1.17716400	H	-0.12012400	6.30743700	0.55115300
C	-10.67652200	0.33363500	-2.32051600	O	-0.33768300	3.21157000	0.01354900
C	-10.04736900	0.74606000	-3.65581600	H	-1.03883400	2.50683700	-0.33086600
O	-10.75802800	0.75818300	-4.68372500	H	0.17748300	3.56891700	-0.77655200
H	-9.83015600	0.95436200	-0.45759900	O	-1.77149100	1.46122200	-1.05143900
H	-11.13380000	-0.64547200	-2.49547400	H	-6.18712400	-2.20801400	-6.04887900
N	-8.71576300	1.04543300	-3.64964700	H	-7.37288300	-3.18422300	-5.13847000
C	-7.96808400	1.24694700	-4.88178800	H	-11.47847500	1.03812600	-2.08625800
C	-7.10342400	0.05501800	-5.30819700	H	-8.33554700	-1.64971100	0.83511600
O	-6.23643300	0.22058900	-6.20885500	H	-4.28833300	3.21202900	3.95610400
H	-8.20474700	1.06058800	-2.77559400	H	-2.76813700	-2.68582400	2.61569700
H	-7.31180100	2.11667500	-4.79461100	H	1.27100600	3.67662400	5.16774800
H	-8.69134800	1.44167600	-5.68023700	H	1.40226900	0.90631200	6.10273000
N	-7.35081600	-1.13068600	-4.70172400	H	0.76780500	-4.19891300	1.60959300
C	-6.65661700	-2.36002700	-5.07593800	H	2.94578500	3.57923000	3.55305800
H	-8.00292800	-1.17927400	-3.92466700	H	5.18515800	10.86036100	0.75617300
H	-5.88052000	-2.61963300	-4.34687900	H	-4.26561800	10.60201200	-0.59533300
C	-3.61890700	0.02341400	2.21365800	H	-4.36338800	7.01063000	2.06394200
C	-3.23935700	-0.94218100	1.28347000	H	-2.10272800	6.60158200	-8.83246500
C	-2.80360300	-2.27951000	1.61528600	H	-0.67704400	5.69099600	-8.31324300
C	-2.45442800	-2.88924500	0.44084100	H	-10.36846800	10.82443100	-4.33974300
C	-2.68956200	-1.93396400	-0.61869900	H	-9.08909000	11.32983800	-3.21996400
N	-3.18155900	-0.75056500	-0.08668400	H	5.29652500	-3.62268300	-6.38144700
C	-2.48286900	-2.18537000	-1.97012100	H	0.60833900	-12.00513000	1.96966600
C	-2.78302000	-1.31120100	-3.00720400	H	4.56565300	-10.71817000	0.28725600
C	-2.75046400	-1.65607200	-4.41402500	H	7.26406300	4.11853200	-6.27468300
C	-3.26909900	-0.59199400	-5.09852200	H	-2.40364400	-2.59966100	-4.80866500
C	-3.58163000	0.42569600	-4.11963500	H	-3.47135500	-0.49702400	-6.15371200
N	-3.27111900	-0.02356800	-2.84718100	H	-4.85859400	4.42299500	-4.82060600
C	-4.08696500	1.68611600	-4.42371800	H	-4.89412100	5.80874000	-2.47019500
C	-4.27711600	2.70666500	-3.50049100	H	-4.60359100	4.52460400	2.58706500
C	-4.65484200	4.06589600	-3.82191000	H	-2.08178800	-3.89224400	0.29261500
C	-4.66617200	4.76842300	-2.64870700				
C	-4.32752800	3.83592400	-1.59416100				
N	-4.08541400	2.58144600	-2.13210200				
C	-4.34084300	4.15461200	-0.24144800				
C	-4.19886100	3.23956100	0.79409700				
C	-4.37273300	3.54360300	2.19911200				
C	-4.21669100	2.37477100	2.89025400				
C	-3.92195600	1.34396400	1.91820100				
N	-3.92844300	1.88783600	0.63850000				
Fe	-3.56028100	0.93976500	-1.11142900				
H	-3.63511200	-0.27218100	3.25793000				
H	-2.10179800	-3.16465700	-2.24100100				
H	-4.33644100	1.87987400	-5.45990700				
H	-4.53155200	5.19490600	0.00553900				
O	0.79647100	4.32310300	-2.08702100				
O	0.29730500	4.14997100	-3.28487400				
C	-0.41729100	5.02260300	-3.87512600				
C	0.64624900	2.86659000	-4.05971200				
C	0.61565100	1.57979300	-3.29036900				
C	1.68461900	1.20908700	-2.30900500				
C	1.60524800	-0.24434000	-1.80646000				
C	2.73271000	-0.58459400	-0.81403000				
C	2.75619500	-2.05786000	-0.36059700				
C	1.55027200	-2.47704500	0.50162800				
C	1.62923500	-3.93395800	0.98522300				
H	1.66948600	3.03607500	-4.44450300				
H	-0.02129500	2.82924800	-4.92343700				
H	-1.38340300	1.41886200	-1.95172800				
H	-0.07643900	0.80556900	-3.62241200				
H	1.65653300	1.89623100	-1.44809800				
H	2.67303700	1.38153900	-2.77241900				
H	0.62253100	-0.40316000	-1.34125100				
H	1.67378400	-0.93165500	-2.66196900				

Cartesian Coordinates of model A

²Re_A:

6	5.229138000	5.117466000	1.740911000
6	5.507686000	3.627326000	1.464534000
6	4.388030000	2.841559000	0.750360000
6	4.124237000	3.350051000	-0.674936000
6	4.735646000	1.345545000	0.727562000
6	4.054474000	5.481191000	2.623694000
8	3.365880000	6.491952000	2.433373000
1	5.083913000	5.660391000	0.802540000
1	6.420715000	3.575109000	0.854767000
1	5.768775000	3.111641000	2.401574000
1	3.459325000	2.961575000	1.326460000
1	3.230555000	2.873399000	-1.091550000
1	3.956648000	4.432214000	-0.703221000
1	4.975749000	3.129664000	-1.332871000
1	3.957943000	0.772542000	0.212273000
1	4.834272000	0.939419000	1.740947000
1	5.682961000	1.174034000	0.198427000
7	3.872184000	4.657000000	3.674242000
6	2.795071000	4.784519000	4.631052000
6	2.892186000	3.613448000	5.599879000
6	2.805848000	2.246450000	4.946248000
6	1.728497000	1.902152000	4.116893000
6	1.648196000	0.642062000	3.526465000
6	2.647816000	-0.305268000	3.771226000
6	3.729296000	0.023664000	4.589705000
6	3.809792000	1.295204000	5.165074000
1	4.376420000	3.781159000	3.680754000
1	1.828426000	4.785608000	4.114378000
1	3.833838000	3.691969000	6.157997000
1	2.091472000	3.719752000	6.345443000
1	0.944021000	2.624986000	3.911034000
1	0.813498000	0.423344000	2.866734000
1	2.587289000	-1.289041000	3.315598000
1	4.513424000	-0.704945000	4.778900000
1	4.656144000	1.556474000	5.796931000
6	2.436703000	2.342950000	-4.832323000
6	1.263254000	3.227471000	-4.376765000
6	-0.032495000	3.032028000	-5.174029000
6	2.228730000	0.842874000	-4.587815000
1	2.629072000	2.514624000	-5.902386000
1	1.061771000	3.049564000	-3.311813000
1	1.568374000	4.280144000	-4.462059000
1	0.132055000	3.206557000	-6.246893000
1	-0.429885000	2.015501000	-5.059615000
1	-0.800232000	3.732678000	-4.829586000
1	3.105191000	0.262904000	-4.903908000
1	1.360664000	0.457411000	-5.135424000
1	2.059636000	0.640453000	-3.522796000
6	-2.103634000	7.315190000	-1.921812000
6	-0.924068000	7.297893000	-0.923929000
6	0.364318000	6.658755000	-1.466283000
6	1.351234000	6.264688000	-0.354431000
7	0.817246000	5.176844000	0.472128000
6	0.270471000	5.318248000	1.670997000
7	0.478496000	6.467534000	2.394883000
7	-0.529439000	4.353445000	2.150664000
6	-2.393357000	5.933190000	-2.507965000
8	-1.968543000	5.629752000	-3.626486000
1	-1.867201000	7.956677000	-2.775842000
1	-1.232712000	6.757886000	-0.023095000
1	-0.719895000	8.327463000	-0.600683000
1	0.129331000	5.763992000	-2.053019000
1	0.871678000	7.350157000	-2.152346000
1	2.284878000	5.909051000	-0.799756000
1	1.602990000	7.118798000	0.277229000
1	0.637312000	4.252492000	-0.018292000
1	1.459219000	6.763233000	2.424329000
1	0.041074000	6.478837000	3.307326000
1	-0.580000000	3.397293000	1.657762000
1	-0.731373000	4.362967000	3.140867000
7	-3.077023000	5.042224000	-1.739803000
6	-3.287919000	3.664019000	-2.223967000

optimized structures.

6	-4.305743000	3.081025000	-1.235066000
6	-3.995237000	3.836109000	0.067714000
6	-3.677838000	5.261474000	-0.415092000
1	-2.333183000	3.124293000	-2.201618000
1	-5.326766000	3.305972000	-1.570240000
1	-4.214408000	1.996679000	-1.129289000
1	-4.818050000	3.817950000	0.789897000
1	-3.111964000	3.397607000	0.546030000
1	-2.995024000	5.781281000	0.261702000
1	-4.595034000	5.864871000	-0.498845000
6	1.438156000	-4.406531000	-7.407088000
6	0.477205000	-3.304024000	-7.792674000
6	-0.662365000	-3.577708000	-8.561539000
6	-1.529250000	-2.554810000	-8.952232000
6	-1.271596000	-1.234767000	-8.575010000
6	-0.143833000	-0.948481000	-7.800889000
6	0.719119000	-1.975217000	-7.414476000
1	1.886430000	-4.223841000	-6.424160000
1	0.940404000	-5.381810000	-7.377899000
1	-0.871746000	-4.602983000	-8.859379000
1	-2.405443000	-2.790256000	-9.551225000
1	-1.941572000	-0.435827000	-8.882218000
1	0.063282000	0.073775000	-7.495521000
1	1.592475000	-1.740663000	-6.809902000
16	-6.524155000	-3.632434000	-1.560259000
1	-7.653919000	-2.915387000	-1.758147000
6	-5.043215000	-2.801468000	2.000626000
6	-4.083205000	-3.362400000	1.168287000
6	-3.129691000	-4.363427000	1.582295000
6	-2.404207000	-4.693474000	0.479955000
6	-2.902644000	-3.879139000	-0.602709000
7	-3.929577000	-3.080992000	-0.165100000
6	-2.393107000	-3.886339000	-1.893479000
6	-2.817382000	-3.066237000	-2.934341000
6	-2.230175000	-3.057195000	-4.253262000
6	-2.903154000	-2.120339000	-4.973847000
6	-3.906958000	-1.570121000	-4.093716000
7	-3.834822000	-2.155309000	-2.856887000
6	-4.837666000	-0.610929000	-4.470841000
6	-5.850508000	-0.110095000	-3.662213000
6	-6.829890000	0.859404000	-4.087922000
6	-7.648907000	1.079780000	-3.025658000
6	-7.162082000	0.248698000	-1.948443000
7	-6.073385000	-0.473672000	-2.359101000
6	-7.723446000	0.203227000	-0.675254000
6	-7.260607000	-0.562796000	0.382613000
6	-7.826908000	-0.560174000	1.709170000
6	-7.060121000	-1.390980000	2.465929000
6	-6.030198000	-1.913542000	1.601891000
7	-6.175901000	-1.410263000	0.329769000
26	-4.906510000	-1.668765000	-1.229742000
1	-5.043234000	-3.112082000	3.040960000
1	-1.578009000	-4.572221000	-2.102975000
1	-4.778065000	-0.232442000	-5.486669000
1	-8.588047000	0.834097000	-0.491741000
8	-0.604374000	1.947908000	1.022280000
6	-0.226346000	1.900990000	-0.192145000
8	0.357596000	2.840996000	-0.809927000
6	-0.551074000	0.626400000	-0.979504000
6	-0.168585000	-0.682748000	-0.273958000
6	1.346654000	-0.875764000	-0.125666000
6	1.767993000	-2.198787000	0.536895000
6	1.503560000	-3.447968000	-0.312924000
1	-1.637016000	0.617954000	-1.140064000
1	-0.071013000	0.692118000	-1.961814000
1	-0.643783000	-0.698112000	0.714930000
1	-0.599732000	-1.516002000	-0.842604000
1	1.749265000	-0.042058000	0.464711000
1	1.822411000	-0.806343000	-1.116367000
1	2.841037000	-2.153139000	0.770801000
1	1.246943000	-2.302677000	1.500307000
1	0.434360000	-3.580648000	-0.509725000
1	2.014833000	-3.378390000	-1.281672000

8	-3.927570000	-0.455900000	-0.766481000	8	-2.591856000	6.712080000	-2.075873000
1	1.864328000	-4.353868000	0.189564000	1	-2.073122000	8.719008000	-0.684592000
1	2.263206000	-4.484279000	-8.128015000	1	-1.447017000	6.652668000	1.500720000
1	3.347448000	2.661017000	-4.305142000	1	-0.747863000	8.259636000	1.399142000
1	-3.636899000	3.680916000	-3.259883000	1	-0.401445000	6.225130000	-0.868762000
1	-2.988990000	7.731702000	-1.424234000	1	0.536205000	7.678577000	-0.587504000
1	6.121100000	5.563108000	2.205609000	1	1.871190000	5.759333000	0.087989000
1	2.880171000	5.738710000	5.164828000	1	1.442218000	6.647299000	1.550688000
1	-7.169166000	-1.641990000	3.513259000	1	0.061381000	4.120135000	0.610313000
1	-3.049545000	-4.758789000	2.586763000	1	1.948414000	5.380179000	3.331157000
1	-8.503823000	1.740203000	-2.953107000	1	0.724981000	5.032930000	4.484176000
1	-8.693905000	0.015678000	2.006952000	1	-1.246496000	3.167319000	2.184218000
1	-1.600340000	-5.412672000	0.390677000	1	-0.614687000	3.238539000	3.836108000
1	-1.407642000	-3.684454000	-4.571016000	7	-3.738760000	5.874012000	-0.312201000
1	-6.871984000	1.300516000	-5.075466000	6	-4.189354000	4.702023000	-1.088501000
1	-2.745537000	-1.823652000	-6.002655000	6	-5.178522000	3.990372000	-0.154388000
				6	-4.705373000	4.399567000	1.249848000
				6	-4.258600000	5.857010000	1.062767000
²TS1_{HA,α}:				1	-3.325242000	4.070663000	-1.324900000
6	6.056645000	5.128999000	2.183577000	1	-6.198647000	4.352025000	-0.335914000
6	6.242827000	5.790724000	0.798044000	1	-5.165391000	2.908052000	-0.301879000
6	5.309267000	6.973905000	0.472790000	1	-5.479476000	4.299294000	2.017636000
6	5.407098000	8.104698000	1.507801000	1	-3.848823000	3.779873000	1.532192000
6	5.607927000	7.494484000	-0.941570000	1	-3.495488000	6.155209000	1.787105000
6	4.651879000	4.587908000	2.411541000	1	-5.107964000	6.550401000	1.165278000
8	3.774086000	5.279584000	2.949146000	6	0.633765000	-6.327093000	-2.051830000
1	6.251611000	5.851226000	2.980533000	6	1.183774000	-5.239308000	-2.946839000
1	7.285543000	6.133044000	0.735035000	6	1.007984000	-5.288507000	-4.336330000
6	6.126565000	5.024602000	0.018684000	6	1.545483000	-4.299771000	-5.166855000
1	4.274923000	6.601984000	0.483242000	6	2.266393000	-3.238943000	-4.612881000
1	4.791862000	8.959858000	1.204172000	6	2.442381000	-3.172004000	-3.227684000
1	5.057382000	7.779173000	2.492321000	6	1.905534000	-4.163829000	-2.406410000
1	6.441433000	8.461286000	1.606448000	1	0.214636000	-5.913119000	-1.127511000
1	4.917250000	8.298869000	-1.219533000	1	-0.151215000	-6.901744000	-2.554926000
1	5.515547000	6.699677000	-1.691578000	1	0.447177000	-6.111091000	-4.774742000
1	6.627806000	7.896338000	-1.004768000	1	1.399521000	-4.360261000	-6.240327000
7	4.430288000	3.320846000	1.986968000	1	2.687246000	-2.470060000	-5.255626000
6	3.124139000	2.670100000	2.045962000	1	2.992928000	-2.345083000	-2.786689000
6	3.234890000	1.164110000	1.766484000	1	2.047356000	-4.104705000	-1.329374000
6	3.769638000	0.850181000	0.382319000	16	-5.959384000	-1.687698000	-3.957162000
6	3.001651000	1.134765000	-0.759550000	1	-6.505856000	-0.638172000	-4.610060000
6	3.504235000	0.859553000	-2.031987000	6	-5.970837000	-2.634539000	-0.019040000
6	4.778751000	0.303165000	-2.186442000	6	-4.841329000	-3.031958000	-0.721279000
6	5.548875000	0.018906000	-1.058650000	6	-4.176947000	-4.297677000	-0.535004000
6	5.044469000	0.291738000	0.216406000	6	-3.131017000	-4.328874000	-1.408070000
1	5.153310000	2.854971000	1.452866000	6	-3.143791000	-3.074927000	-2.118767000
1	2.438160000	3.128636000	1.325259000	7	-4.197062000	-2.307385000	-1.693826000
1	3.870489000	0.697738000	2.529502000	6	-2.193672000	-2.689910000	-3.056137000
1	2.230156000	0.739849000	1.884455000	6	-2.178950000	-1.463788000	-3.703571000
1	2.008823000	1.571347000	-0.656834000	6	-1.181376000	-1.069187000	-4.666886000
1	2.896957000	1.079193000	-2.905546000	6	-1.526923000	0.172407000	-5.106049000
1	5.166732000	0.094128000	-3.179880000	6	-2.742356000	0.537553000	-4.420261000
1	6.537926000	-0.418637000	-1.166890000	7	-3.106638000	-0.460825000	-3.548644000
1	5.641163000	0.049464000	1.094149000	6	-3.460219000	1.696634000	-4.672253000
6	1.868469000	3.979161000	-4.301226000	6	-4.692458000	2.004709000	-4.111823000
6	0.683077000	4.555435000	-3.507785000	6	-5.462370000	3.182137000	-4.428801000
6	-0.507397000	5.001473000	-4.365360000	6	-6.602307000	3.117319000	-3.685753000
6	1.538951000	2.717827000	-5.109355000	6	-6.523907000	1.908913000	-2.901731000
1	2.259501000	4.749638000	-4.982285000	7	-5.361722000	1.238374000	-3.193500000
1	0.345680000	3.819163000	-2.764972000	6	-7.467257000	1.530650000	-1.955828000
1	1.044504000	5.420710000	-2.933157000	6	-7.373560000	0.413023000	-1.139416000
1	-0.195003000	5.724178000	-5.131534000	6	-8.345815000	0.047624000	-0.133880000
1	-0.970807000	4.151791000	-4.881786000	6	-7.911508000	-1.112299000	-0.427503000
1	-1.276123000	5.475405000	-3.746802000	6	-6.679895000	-1.463660000	-0.242983000
1	2.436748000	2.305452000	-5.586432000	7	-6.368048000	-0.513504000	-1.175729000
1	0.814095000	2.926287000	-5.904783000	26	-4.703624000	-0.475505000	-2.352665000
1	1.106575000	1.937485000	-4.469577000	1	-6.352102000	-3.314415000	-0.736492000
6	-2.358332000	7.908512000	-0.007232000	1	-1.399292000	-3.391244000	-3.290470000
6	-1.126603000	7.425902000	0.792278000	1	-3.045136000	2.398660000	-5.388207000
6	0.008088000	6.861902000	-0.077451000	1	-8.333205000	2.172891000	-1.830069000
6	1.033308000	6.051992000	0.731031000	8	-1.984876000	2.245852000	1.036442000
7	0.425666000	4.837759000	1.281953000	6	-1.257914000	2.021549000	0.029640000
6	0.237736000	4.574430000	2.573167000	8	-0.258743000	2.714398000	-0.337529000
7	0.948930000	5.245035000	3.521502000	6	-1.486048000	0.763359000	-0.799692000
7	-0.687744000	3.673902000	2.927384000	6	-0.895772000	-0.504899000	-0.190958000
6	-2.926465000	6.797225000	-0.889861000				

1	-1.845769000	2.839303000	-6.047263000	6	5.129183000	7.135536000	2.176810000
1	-0.556201000	1.055747000	-7.202115000	8	3.909110000	6.950688000	2.065718000
1	-1.624921000	-0.320200000	-8.965333000	1	5.215497000	8.749253000	0.807238000
16	-5.545847000	-4.649239000	-3.328075000	1	7.065819000	7.857412000	-0.627088000
1	-6.702363000	-3.958148000	-3.445311000	1	7.194888000	6.429283000	0.389403000
6	-4.991681000	-4.994541000	0.650026000	1	4.909506000	5.719557000	-0.271983000
6	-3.837513000	-5.297944000	-0.066496000	1	3.768790000	6.851912000	-2.209563000
6	-2.941288000	-6.385373000	0.252854000	1	3.822908000	7.890384000	-0.779503000
6	-1.961846000	-6.376797000	-0.692146000	1	4.945145000	8.168816000	-2.127697000
6	-2.255700000	-5.278692000	-1.582207000	1	5.496147000	5.070146000	-2.605332000
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6	-1.480781000	-4.914268000	-2.676344000	1	6.770554000	6.298045000	-2.643171000
6	-1.740245000	-3.842396000	-3.528825000	7	5.873854000	6.601891000	3.180446000
6	-0.908924000	-3.460569000	-4.646509000	6	5.367875000	5.749430000	4.248191000
6	-1.503396000	-2.375837000	-5.217704000	6	5.955340000	4.322721000	4.236270000
6	-2.696138000	-2.106240000	-4.448235000	6	5.562254000	3.496699000	3.029563000
7	-2.815344000	-3.004854000	-3.423675000	6	4.281822000	2.930497000	2.941232000
6	-3.601741000	-1.091125000	-4.746237000	6	3.901479000	2.182198000	1.826191000
6	-4.780777000	-0.819753000	-4.057919000	6	4.802108000	1.985622000	0.775263000
6	-5.708101000	0.228959000	-4.421279000	6	6.083478000	2.533517000	0.855678000
6	-6.728753000	0.171513000	-3.521337000	6	6.458332000	3.281259000	1.974989000
6	-6.416472000	-0.910282000	-2.614111000	1	6.861616000	6.818249000	3.189967000
7	-5.233941000	-1.498873000	-2.960306000	1	4.283062000	5.713812000	4.137358000
6	-7.214047000	-1.300327000	-1.539317000	1	7.049020000	4.386228000	4.307899000
6	-6.931069000	-2.337972000	-0.661563000	1	5.617273000	3.829132000	5.157044000
6	-7.758824000	-2.718115000	0.460175000	1	3.580790000	3.066033000	3.763049000
6	-7.126712000	-3.750912000	1.079588000	1	2.908387000	1.743246000	1.776581000
6	-5.915682000	-4.006747000	0.332788000	1	4.508600000	1.398112000	-0.089824000
7	-5.819041000	-3.140759000	-0.726353000	1	6.796368000	2.370035000	0.052057000
26	-4.294945000	-3.037507000	-2.043876000	1	7.466610000	3.685113000	2.038007000
1	-5.205693000	-5.607914000	1.520621000	6	2.783876000	-1.258042000	-1.520392000
1	-0.593698000	-5.507555000	-2.878023000	6	2.043779000	0.057476000	-1.820224000
1	-3.371185000	-0.460728000	-5.599964000	6	1.251965000	0.057921000	-3.133775000
1	-8.132067000	-0.743909000	-1.373019000	6	1.860768000	-2.444150000	-1.215185000
8	-0.370799000	2.503622000	1.833026000	1	3.429895000	-1.508868000	-2.374439000
6	0.280188000	1.977764000	0.883326000	1	1.366609000	0.290700000	-0.985093000
8	0.956767000	2.571708000	0.005437000	1	2.777414000	0.877570000	-1.853003000
6	0.265575000	0.407203000	0.818304000	1	1.921297000	-0.113266000	-3.987725000
6	-1.086460000	-0.163794000	1.006155000	1	0.489306000	-0.728282000	-3.154661000
6	-1.742906000	-0.312737000	2.332561000	1	0.745505000	1.017126000	-3.284438000
6	-2.618266000	-1.580504000	2.456067000	1	2.439231000	-3.347212000	-0.986960000
6	-1.797012000	-2.871650000	2.535215000	1	1.198081000	-2.678798000	-2.054735000
1	0.703480000	0.115611000	-0.140041000	1	1.225007000	-2.232607000	-0.344888000
1	0.940383000	0.080047000	1.624503000	6	-1.235525000	5.359778000	-2.277646000
1	-2.514623000	-2.247894000	-0.843664000	6	-0.478592000	5.538502000	-0.943770000
1	-1.702079000	-0.343886000	0.126122000	6	0.916750000	4.896244000	-0.936689000
1	-2.382359000	0.573442000	2.497329000	6	1.656564000	5.055624000	0.393626000
1	-0.992113000	-0.281097000	3.134923000	7	0.940005000	4.360401000	1.476801000
1	-3.245548000	-1.490539000	3.353116000	6	0.821657000	4.789519000	2.729196000
1	-3.292300000	-1.628848000	1.592072000	7	1.565119000	5.808668000	3.193192000
1	-1.163369000	-2.992157000	1.647948000	7	-0.082052000	4.223386000	3.558112000
1	-1.138902000	-2.874647000	3.414249000	6	-1.369005000	3.884250000	-2.654848000
8	-3.391895000	-1.852343000	-0.982272000	8	-0.459837000	3.335375000	-3.292055000
1	-2.447510000	-3.751182000	2.597226000	1	-0.668801000	5.830819000	-3.086882000
1	-3.985174000	0.294414000	-10.924402000	1	-1.080684000	5.115231000	-0.128475000
1	4.008814000	0.069941000	-2.647333000	1	-0.386882000	6.613185000	-0.732352000
1	-2.640626000	1.870772000	-3.466125000	1	0.848062000	3.835446000	-1.201163000
1	-2.576581000	6.303485000	-2.763280000	1	1.539784000	5.352980000	-1.715686000
1	6.932463000	6.085169000	1.080387000	1	2.671193000	4.648641000	0.321701000
1	4.495104000	7.607807000	4.446583000	1	1.743327000	6.110700000	0.666339000
1	-7.437241000	-4.301938000	1.958324000	1	0.512323000	3.460241000	1.240799000
1	-3.066339000	-7.062643000	1.088265000	1	2.406039000	6.160403000	2.719203000
1	-7.615574000	0.790313000	-3.464030000	1	1.262462000	6.293500000	4.024873000
1	-8.695122000	-2.243464000	0.725377000	1	-0.691043000	3.462628000	3.244443000
1	-1.114078000	-7.042733000	-0.792104000	1	0.070847000	4.285161000	4.554230000
1	0.000907000	-3.966794000	-4.943094000	7	-2.457432000	3.208093000	-2.220216000
1	-5.572898000	0.901154000	-5.258962000	6	-2.610753000	1.761725000	-2.496535000
1	-1.187105000	-1.802686000	-6.079256000	6	-4.035061000	1.444683000	-2.027609000
				6	-4.279010000	2.474485000	-0.912377000
				6	-3.586783000	3.741597000	-1.439086000
				1	-1.852808000	1.205149000	-1.930627000
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				1	-5.338800000	2.641884000	-0.697370000
				1	-3.795038000	2.156333000	0.020548000
² TS _{DC,A} :							
6	5.902668000	7.982238000	1.173280000				
6	6.480678000	7.164526000	-0.006441000				
6	5.459335000	6.434052000	-0.900258000				
6	4.441454000	7.393939000	-1.534469000				
6	6.199956000	5.632922000	-1.981962000				

1	3.644694000	1.344855000	3.038882000	1	-5.235784000	-0.806451000	-9.800911000
1	4.568744000	0.632775000	1.700313000	1	-5.136297000	1.439898000	-8.820596000
7	4.542005000	5.837067000	3.646243000	1	-3.963326000	3.075853000	-7.378809000
6	3.597327000	6.615754000	4.433828000	1	-1.584142000	2.704147000	-6.734117000
6	3.124024000	5.888367000	5.698966000	1	-0.396530000	0.688169000	-7.571767000
6	2.397914000	4.564531000	5.512427000	1	-1.571755000	-0.946643000	-9.018087000
6	1.687383000	4.241665000	4.347865000	16	-5.137167000	-4.431539000	-2.859695000
6	0.991041000	3.033323000	4.237100000	1	-6.389752000	-3.9271805000	-2.889903000
6	0.994622000	2.128064000	5.300114000	6	-4.686593000	-3.929299000	1.178098000
6	1.701258000	2.433393000	6.464878000	6	-3.515591000	-4.319229000	0.539341000
6	2.397776000	3.638099000	6.564975000	6	-2.574520000	-5.270323000	1.082242000
1	5.255009000	5.320534000	4.143418000	6	-1.571561000	-5.397159000	0.169348000
1	2.762860000	6.856835000	3.773035000	6	-1.897346000	-4.521566000	-0.929952000
1	3.986293000	5.730063000	6.362218000	7	-3.080115000	-3.867833000	-0.683243000
1	2.473778000	6.590106000	6.242475000	6	-1.120746000	-4.367046000	-2.071456000
1	1.690287000	4.925590000	3.504185000	6	-1.445769000	-3.548496000	-3.145186000
1	0.455701000	2.792167000	3.321386000	6	-0.640970000	-3.400529000	-4.334899000
1	0.455424000	1.188552000	5.216837000	6	-1.306855000	-2.539771000	-5.152673000
1	1.715862000	1.731828000	7.294903000	6	-2.521062000	-2.166160000	-4.465107000
1	2.948310000	3.865650000	7.475853000	7	-2.580019000	-2.780686000	-3.293482000
6	3.378485000	0.035153000	-3.557211000	6	-3.479719000	-1.311893000	-4.994040000
6	2.361486000	1.177718000	-3.723518000	6	-4.664930000	-0.948439000	-4.367809000
6	1.304199000	0.935572000	-4.808264000	6	-5.640972000	-0.054244000	-4.947507000
6	2.784012000	-1.266540000	-3.005140000	6	-6.646553000	0.070470000	-4.038434000
1	3.856675000	-0.166538000	-4.527540000	6	-6.282923000	-0.743930000	-2.902209000
1	1.858389000	1.370742000	-2.766231000	7	-5.075640000	-1.358084000	-3.124796000
1	2.910639000	2.097846000	-3.969434000	6	-7.047774000	-0.874448000	-1.749694000
1	1.777745000	0.763747000	-5.785330000	6	-6.701182000	-1.650967000	0.651236000
1	0.681233000	0.061235000	-4.584270000	6	-7.512445000	-1.813524000	-0.582790000
1	0.641241000	1.802404000	-4.898532000	6	-6.847666000	-2.675107000	1.349034000
1	3.550868000	-2.045363000	-2.909809000	6	-5.628294000	-3.041798000	0.672289000
1	1.990125000	-1.659372000	-3.650232000	7	-5.547064000	-2.394246000	-0.540195000
1	2.349889000	-1.106070000	-2.009804000	26	-4.110623000	-2.666151000	-1.939121000
6	-1.134421000	6.161613000	-3.916692000	1	-4.892272000	-4.369567000	2.149260000
6	-0.264293000	6.468817000	-2.677185000	1	-0.199977000	-4.938682000	-2.135285000
6	1.064621000	5.699181000	-2.617517000	1	-3.287095000	-0.895453000	-5.977745000
6	1.714628000	5.765343000	-1.227481000	1	-7.989884000	-0.336340000	-1.707315000
7	0.899817000	5.042839000	-0.246032000	8	-0.978907000	2.285015000	1.048564000
6	0.392094000	5.553485000	0.864752000	6	-0.248424000	1.768915000	0.146415000
7	0.829300000	6.766708000	1.329140000	8	0.407875000	2.403466000	-0.733622000
7	-0.603843000	4.913646000	1.501907000	6	-0.100176000	0.269435000	0.122247000
6	-1.384404000	4.663642000	-4.086417000	6	-0.519005000	-0.521393000	1.122781000
8	-0.691428000	4.007244000	-4.873790000	6	-0.285910000	-2.003759000	1.220534000
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1	2.714960000	5.321749000	-1.249524000	1	-1.041335000	-0.033753000	1.945977000
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1	0.362857000	7.103215000	2.161131000	1	1.643414000	-1.919531000	2.205600000
1	-0.832733000	3.915521000	1.225887000	1	0.034257000	-1.001536000	3.915662000
1	-0.720022000	5.115565000	2.486343000	1	-0.820419000	-2.552360000	3.950283000
7	-2.326204000	4.077650000	-3.304637000	8	-3.188307000	-0.898529000	-1.029712000
6	-2.480402000	2.608331000	-3.303473000	1	0.847160000	-2.443367000	4.537169000
6	-3.730710000	2.369824000	-2.447462000	1	-3.927374000	-0.664483000	-10.979602000
6	-3.730628000	3.564805000	-1.480421000	1	4.182552000	0.368321000	-2.885622000
6	-3.255110000	4.726794000	-2.366542000	1	-2.573267000	2.231079000	-4.324501000
1	-1.585154000	2.159561000	-2.856368000	1	-2.075601000	6.721087000	-3.845400000
1	-4.629277000	2.387011000	-3.075968000	1	6.542116000	5.082538000	2.081666000
1	-3.694022000	1.402016000	-1.942673000	1	4.051096000	7.572062000	4.729131000
1	-4.708874000	3.763804000	-1.030656000	1	-7.145513000	-3.042582000	2.323128000
1	-3.010479000	3.392316000	-0.671761000	1	-2.686006000	-5.771677000	2.035566000
1	-2.766935000	5.516784000	-1.790500000	1	-7.554081000	0.656928000	-4.110380000
1	-4.099159000	5.178609000	-2.909895000	1	-8.466859000	-1.328817000	0.692178000
6	-4.148672000	-0.860805000	-9.921623000	1	-0.689669000	-6.023480000	0.218398000
6	-3.441370000	0.125604000	-9.020276000	1	0.304414000	-3.899915000	-4.505362000
6	-4.096826000	1.270069000	-8.545806000	1	-5.540154000	0.409447000	-5.920489000
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6	-1.435040000	0.856154000	-7.845071000	6	5.229138000	5.117466000	1.740911000
6	-2.099598000	-0.065837000	-8.656763000	6	5.506253000	3.627353000	1.463118000
1	-3.837894000	-1.890587000	-9.712892000	6	4.386324000	2.843677000	0.746816000

6	4.126930000	3.351951000	-0.679411000	1	-4.818597000	3.817548000	0.788863000
6	4.730290000	1.346847000	0.725534000	1	-3.112509000	3.397030000	0.545263000
6	4.054625000	5.481859000	2.623798000	1	-2.995175000	5.780943000	0.262101000
8	3.369612000	6.495601000	2.436272000	1	-4.594940000	5.865033000	-0.498798000
1	5.084759000	5.661398000	0.803012000	6	1.438156000	-4.406531000	-7.407088000
1	6.419774000	3.574682000	0.854138000	6	0.473633000	-3.303767000	-7.782758000
1	5.766024000	3.110466000	2.399861000	6	-0.672479000	-3.576929000	-8.542073000
1	3.456526000	2.966053000	1.320656000	6	-1.542877000	-2.553839000	-8.924160000
1	3.232638000	2.877698000	-1.097441000	6	-1.282174000	-1.234154000	-8.547717000
1	3.962744000	4.434600000	-0.708898000	6	-0.147955000	-0.948430000	-7.782890000
1	4.979115000	3.128500000	-1.335431000	6	0.718430000	-1.975462000	-7.404962000
1	3.952533000	0.775585000	0.208362000	1	1.900440000	-4.221424000	-6.431142000
1	4.825177000	0.940779000	1.739305000	1	0.939241000	-5.380882000	-7.367655000
1	5.678585000	1.172765000	0.199000000	1	-0.884049000	-4.601950000	-8.839233000
7	3.868831000	4.654601000	3.671380000	1	-2.424125000	-2.788694000	-9.515913000
6	2.793467000	4.783561000	4.630024000	1	-1.954354000	-0.434808000	-8.848910000
6	2.892186000	3.613448000	5.599879000	1	0.061591000	0.073653000	-7.478507000
6	2.805327000	2.246104000	4.947068000	1	1.596996000	-1.741795000	-6.807647000
6	1.727855000	1.901652000	4.117884000	16	-6.524155000	-3.632434000	-1.560259000
6	1.647613000	0.641426000	3.527789000	1	-7.661239000	-2.921096000	-1.7351142000
6	2.647092000	-0.305979000	3.772793000	6	-5.064135000	-2.835643000	2.027524000
6	3.728698000	0.023147000	4.590983000	6	-4.101386000	-3.386954000	1.191998000
6	3.809366000	1.294916000	5.165787000	6	-3.148129000	-4.391918000	1.596574000
1	4.370190000	3.777064000	3.675275000	6	-2.421985000	-4.710455000	0.491297000
1	1.825719000	4.784096000	4.115427000	6	-2.919301000	-3.885135000	-0.583499000
1	3.834674000	3.692580000	6.156567000	7	-3.946432000	-3.090711000	-0.137930000
1	2.092454000	3.720079000	6.346427000	6	-2.407680000	-3.880459000	-1.873392000
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1	0.813297000	0.422687000	2.867636000	6	-2.240392000	-3.028275000	-4.225988000
1	2.586479000	-1.289810000	3.317351000	6	-2.916170000	-2.087920000	-4.939226000
1	4.512942000	-0.705342000	4.780149000	6	-3.924219000	-1.550220000	-4.055589000
1	4.656144000	1.556474000	5.796931000	7	-3.851767000	-2.146659000	-2.824654000
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6	-0.034962000	3.025203000	-5.170124000	6	-6.850649000	0.875488000	-4.031102000
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1	2.626888000	2.512651000	-5.902777000	6	-7.183637000	0.248998000	-1.896691000
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1	1.564308000	4.279818000	-4.466338000	6	-7.746528000	0.189523000	-0.624754000
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1	3.112110000	0.265788000	-4.897521000	6	-6.053103000	-1.947582000	1.634010000
1	1.366825000	0.453053000	-5.127804000	7	-6.192715000	-1.426987000	0.368049000
1	2.066760000	0.644053000	-3.516560000	26	-4.928777000	-1.675154000	-1.188695000
6	-2.102694000	7.315800000	-1.921337000	1	-5.067838000	-3.157929000	3.064297000
6	-0.923112000	7.298954000	-0.923412000	1	-1.591599000	-4.563912000	-2.086999000
6	0.365686000	6.660936000	-1.465984000	1	-4.800334000	-0.204904000	-5.437881000
6	1.353461000	6.268703000	-0.354255000	1	-8.614063000	0.814805000	-0.436067000
7	0.820884000	5.180670000	0.472874000	8	-0.606464000	1.953102000	1.021493000
6	0.273657000	5.322401000	1.671592000	6	-0.226090000	1.905605000	-0.192163000
7	0.481733000	6.471682000	2.395332000	8	0.360644000	2.844545000	-0.808888000
7	-0.526212000	4.357738000	2.151323000	6	-0.551707000	0.631592000	-0.980057000
6	-2.391900000	5.933665000	-2.507307000	6	-0.175899000	-0.678490000	-0.272913000
8	-1.965934000	5.629671000	-3.625199000	6	1.338338000	-0.877477000	-0.121994000
1	-1.866479000	7.957406000	-2.775340000	6	1.753026000	-2.200075000	0.545720000
1	-1.231471000	6.758291000	-0.022881000	6	1.482009000	-3.451419000	-0.298821000
1	-0.719638000	8.328499000	-0.599658000	1	-1.637150000	0.626389000	-1.144168000
1	0.131181000	5.765510000	-2.051887000	1	-0.068153000	0.695745000	-1.960733000
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1	2.287420000	5.913975000	-0.799650000	1	-0.609306000	-1.510399000	-0.841755000
1	1.604285000	7.123453000	0.276935000	1	1.743838000	-0.043524000	0.466074000
1	0.641147000	4.256201000	-0.017281000	1	1.815665000	-0.813348000	-1.112306000
1	1.462409000	6.767497000	2.424661000	1	2.826370000	-2.158945000	0.779030000
1	0.044336000	6.483228000	3.307776000	1	1.231796000	-2.297347000	1.509735000
1	-0.578142000	3.401779000	1.658113000	1	0.411949000	-3.580537000	-0.493216000
1	-0.728933000	4.367686000	3.141339000	1	1.992003000	-3.387875000	-1.368671000
7	-3.076727000	5.042932000	-1.739770000	8	-3.934102000	-0.461904000	-0.752903000
6	-3.287617000	3.664998000	-2.224566000	1	1.839923000	-4.356702000	0.206812000
6	-4.305819000	3.081656000	-1.236296000	1	2.252799000	-4.488079000	-8.139338000
6	-3.995570000	3.835950000	0.066939000	1	3.347701000	2.665775000	-4.307292000
6	-3.677838000	5.261474000	-0.415092000	1	-3.636132000	3.682300000	-3.260637000
1	-2.332985000	3.125076000	-2.202106000	1	-2.988233000	7.731943000	-1.423793000
1	-5.326721000	3.306899000	-1.571518000	1	6.121213000	5.562127000	2.206303000
1	-4.214548000	1.997336000	-1.131062000	1	2.880074000	5.738443000	5.162253000

1	-7.204915000	-1.707794000	3.541636000	1	0.342886000	2.686929000	0.903395000
1	-3.068694000	-4.797702000	2.596926000	1	2.812622000	4.445664000	2.883748000
1	-8.525242000	1.747963000	-2.890752000	1	1.881889000	4.245011000	4.322346000
1	-8.729879000	-0.038807000	2.048045000	1	-0.573029000	2.113772000	2.862278000
1	-1.617653000	-5.428151000	0.394757000	1	0.400863000	2.446603000	4.309730000
1	-1.414361000	-3.648774000	-4.547927000	7	-3.464106000	4.914014000	0.389013000
1	-6.892516000	1.323564000	-5.015513000	6	-4.280635000	3.800120000	-0.138301000
1	-2.757453000	-1.781179000	-5.964956000	6	-5.075863000	3.310091000	1.079645000
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6	6.532634000	5.002306000	-0.469295000	1	-5.274881000	2.237280000	1.016978000
6	5.220760000	5.534838000	-1.079292000	1	-4.709805000	3.740350000	3.222347000
6	4.957408000	7.004660000	-0.719335000	1	-3.365322000	2.953544000	2.363196000
6	5.240895000	5.335513000	-2.602573000	1	-2.641182000	5.258894000	2.326099000
6	5.568835000	4.214261000	1.767668000	1	-4.292175000	5.864808000	2.099505000
8	4.493609000	4.710947000	2.124708000	6	0.602127000	-6.469530000	-0.324947000
1	6.530106000	6.073317000	1.436591000	6	1.288607000	-5.327106000	-1.039388000
1	7.375129000	5.579676000	-0.875904000	6	1.829627000	-5.492555000	-2.320910000
1	6.678777000	3.965618000	-0.801609000	6	2.474863000	-4.436976000	-2.972270000
1	4.392652000	4.937479000	-3.053990000	6	2.589183000	-3.194040000	-2.348067000
1	4.052587000	7.367998000	-1.220395000	6	2.048772000	-3.012865000	-1.070748000
1	4.812255000	7.138454000	0.357560000	6	1.405673000	-4.069414000	-0.426905000
1	5.790622000	7.645937000	-1.037488000	1	-0.391910000	-6.176648000	0.033978000
1	4.304165000	5.680239000	-3.056006000	1	0.480641000	-7.337332000	-0.981348000
1	5.369115000	4.278494000	-2.864282000	1	1.747495000	-6.458943000	-2.813803000
1	6.061039000	5.901128000	-3.064626000	1	2.887909000	-4.589853000	-3.966224000
7	5.876489000	2.901864000	1.937439000	1	3.094704000	-2.369886000	-2.844442000
6	4.980418000	1.895905000	2.493675000	1	2.126833000	-2.045141000	-0.583293000
6	4.978065000	0.590494000	1.673880000	1	0.983374000	-3.917264000	0.564251000
6	4.434208000	0.745752000	0.269094000	16	-4.398181000	-0.839994000	-5.058247000
6	3.051924000	0.835175000	0.048386000	1	-5.254289000	-1.857685000	-4.813008000
6	2.536158000	1.015287000	-1.236986000	6	-5.588042000	-2.952896000	-1.647079000
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6	4.787036000	1.005256000	-2.124671000	6	-3.410347000	-4.189208000	-1.853134000
6	5.293516000	0.827092000	-0.834287000	6	-2.173468000	-3.848546000	-2.310792000
1	6.784653000	2.590256000	1.620741000	6	-2.239902000	-2.456494000	-2.686815000
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1	5.999221000	0.185379000	1.641434000	6	-1.168907000	-1.721168000	-3.177203000
1	4.378689000	-0.139274000	2.232872000	6	-1.207165000	-0.370412000	-3.500897000
1	2.355091000	0.765846000	0.880067000	6	-0.066184000	0.392486000	-3.945322000
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6	-0.787971000	6.821577000	-4.431011000	6	-6.189162000	3.600145000	-3.595127000
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1	1.468318000	8.046192000	-5.582841000	7	-4.833117000	1.764697000	-3.234489000
1	0.820193000	5.394670000	-4.180670000	6	-7.230879000	1.431745000	-2.879551000
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1	1.954579000	6.618173000	-7.594068000	7	-6.033293000	-0.640005000	-2.350972000
1	0.250136000	6.483477000	-7.147159000	26	-4.169158000	-0.057465000	-2.778726000
1	1.377065000	5.185302000	-6.728911000	1	-6.043703000	-3.856589000	-1.253509000
6	-1.773147000	6.708889000	0.168010000	1	-0.220642000	-2.237308000	-3.290474000
6	-0.471294000	6.108028000	0.742992000	1	-2.226685000	3.772875000	-4.055828000
6	0.332439000	5.256049000	-0.249305000	1	-8.207012000	1.906363000	-2.912202000
6	1.466197000	4.470501000	0.428683000	8	-1.611734000	1.123579000	2.092887000
7	0.931890000	3.454835000	1.336747000	6	-1.269870000	0.790716000	0.914941000
6	1.008014000	3.461209000	2.662549000	8	-0.392546000	1.385587000	0.212758000
7	1.904983000	4.250680000	3.313304000	6	-1.915829000	-0.430679000	0.300514000
7	0.149793000	2.708134000	3.367089000	6	-2.550603000	-1.462460000	1.217070000
6	-2.688655000	5.649846000	-0.446465000	6	-3.865706000	-1.034929000	1.895562000
8	-2.676526000	5.444854000	-1.667605000	6	-4.402992000	-2.056914000	2.910749000
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1	2.069204000	3.957164000	-0.328491000	1	-4.620888000	-0.851607000	1.119962000
1	2.134166000	5.140909000	0.974358000				

1	-3.687637000	-0.082729000	2.403325000	7	1.299343000	3.345258000	1.596412000
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1	-5.592978000	-3.254279000	1.531256000	7	0.730639000	2.672972000	3.721089000
1	-3.988748000	-3.927848000	1.844192000	6	-2.528365000	5.290766000	-0.449778000
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1	1.176546000	-6.795582000	0.551882000	1	-0.635142000	5.183878000	1.704379000
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1	-2.288422000	7.271852000	0.956286000	1	0.861517000	5.571147000	-0.941246000
1	7.634916000	4.699520000	1.371206000	1	2.351553000	3.828766000	-0.135479000
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1	-9.332447000	-0.280956000	-1.973045000	1	-0.012407000	2.030612000	3.309226000
1	-1.284405000	-4.460928000	-2.388209000	1	1.074493000	2.469957000	4.648772000
1	0.919039000	-0.023275000	-4.112450000	7	-3.339765000	4.562074000	0.358929000
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⁴ IM1 _{A,c} :				1	-3.440383000	2.671666000	-0.575534000
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6	5.204104000	5.487605000	-2.820895000	1	-2.600700000	4.947773000	2.321212000
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1	0.556562000	6.886184000	-6.932390000	26	-4.474699000	-0.394431000	-3.099380000
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6	-1.653877000	6.366259000	0.192867000	1	-0.522546000	-2.594963000	-3.123555000
6	-0.369583000	5.795696000	0.834264000	1	-2.323838000	3.479511000	-3.934589000
6	0.497082000	4.952714000	-0.109905000	1	-8.428636000	1.736536000	-3.378689000
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6	-0.792135000	-3.597957000	-4.141834000	6	4.505581000	6.142878000	4.124114000
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6	-3.409136000	-1.233795000	-4.807224000	6	3.556021000	2.200558000	2.141394000
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6	-6.647195000	0.147149000	-4.123801000	6	6.013622000	3.055550000	3.155657000
6	-6.480113000	-0.862469000	-3.102717000	1	6.419376000	6.595054000	3.330743000
7	-5.272468000	-1.483365000	-3.233405000	1	3.518786000	6.118175000	3.659009000
6	-7.423887000	-1.163322000	-2.120394000	1	5.880680000	4.798280000	5.120976000
6	-7.277985000	-2.120476000	-1.126964000	1	4.186373000	4.528741000	5.490220000
6	-8.250523000	-2.393049000	-0.094964000	1	2.682181000	3.635213000	3.478066000
6	-7.712864000	-3.351373000	0.706242000	1	2.595285000	1.882971000	1.742699000
6	-6.414708000	-3.627654000	0.159944000	1	4.703372000	0.836991000	0.928026000
7	-6.171112000	-2.921164000	-0.963630000	1	6.893382000	1.592755000	1.840765000
26	-4.476895000	-2.919819000	-2.053215000	1	6.973812000	3.377073000	3.554070000
1	-5.874925000	-5.131121000	1.593868000	6	3.289000000	0.194405000	-2.077116000
1	-0.741226000	-5.469748000	-2.166747000	6	2.265502000	1.211825000	-2.610064000
1	-3.055415000	-0.681034000	-5.672664000	6	1.232866000	0.627989000	-3.582003000
1	-8.347855000	-0.592165000	-2.127532000	6	2.677396000	-0.867852000	-1.154366000
8	-0.410417000	2.747260000	1.566666000	1	3.800815000	-0.292896000	-2.920842000
6	0.305307000	2.151107000	0.702776000	1	1.739700000	1.655831000	-1.754905000
8	1.009375000	2.705642000	-0.186666000	1	2.803592000	2.027208000	-3.114614000
6	0.341274000	0.599347000	0.774837000	1	1.723960000	0.192551000	-4.464151000
6	-0.988152000	-0.039520000	1.001423000	1	0.638074000	-0.161787000	-3.108169000
6	-1.645790000	-0.091472000	2.343590000	1	0.539283000	1.405095000	-3.920541000
6	-2.643802000	-1.255194000	2.502680000	1	3.449147000	-1.526321000	-0.736056000
6	-1.965599000	-2.629292000	2.543950000	1	1.957778000	-1.501966000	-1.684841000
1	0.807570000	0.239429000	-0.148159000	1	2.143301000	-0.389329000	-0.324793000
1	1.024671000	0.356343000	1.604910000	6	-1.426005000	5.573765000	-2.905104000
1	-2.875143000	-1.976834000	-0.708842000	6	-0.502997000	5.749363000	-1.678387000
1	-1.622542000	-0.201706000	0.129720000	6	0.859052000	5.055147000	-1.809192000
1	-2.169810000	0.862918000	2.527035000	6	1.736321000	5.212561000	-0.556471000
1	-0.877940000	-0.150953000	3.131545000	7	1.106497000	4.598252000	0.612136000
1	-3.225308000	-1.108191000	3.423416000	6	0.682952000	5.235304000	1.698229000
1	-3.360691000	-1.126999000	1.671093000	7	1.153597000	6.471243000	2.013936000
1	-1.367248000	-2.798777000	1.640529000	7	-0.252604000	4.657003000	2.462750000
1	-1.288540000	-2.711303000	3.404602000	6	-1.717068000	4.107935000	-3.222951000
8	-3.732257000	-1.634330000	-1.015601000	8	-1.003490000	3.492582000	-4.025702000
1	-2.700216000	-3.439682000	2.615503000	1	-0.937936000	5.982913000	-3.795247000
1	-3.420877000	-0.445081000	-11.064557000	1	-1.010614000	5.368472000	-0.783820000
1	4.163874000	0.211077000	-2.582633000	1	-0.351468000	6.825553000	-1.513595000
1	-2.575662000	1.845818000	-3.697570000	1	0.718916000	3.989205000	-2.018208000
1	-2.480438000	6.305191000	-3.241446000	1	1.410736000	5.465173000	-2.665818000
1	6.773381000	6.388502000	0.940116000	1	2.708064000	4.733443000	-0.719361000
1	4.114005000	7.906132000	4.141010000	1	1.928495000	6.267878000	-0.348152000
1	-8.140524000	-3.810530000	1.588402000	1	0.855661000	3.576143000	0.550320000
1	-3.718839000	-6.629408000	1.580141000	1	2.121886000	6.721389000	1.796065000
1	-7.522169000	0.774865000	-4.236111000	1	0.727044000	6.950947000	2.792673000
1	-9.210045000	-1.899729000	-0.006048000	1	-0.737245000	3.774576000	2.127021000
1	-1.545767000	-6.797821000	-0.029877000	1	-0.372657000	4.961905000	3.417227000
1	0.142006000	-4.130453000	-4.266181000	7	-2.744922000	3.504583000	-2.574876000
1	-5.252259000	0.731108000	-5.736311000	6	-3.027891000	2.072402000	-2.791175000
1	-0.852842000	-2.075818000	-5.741357000	6	-4.312147000	1.822583000	-1.985518000
				6	-4.246689000	2.879526000	-0.869283000
				6	-3.655026000	4.102723000	-1.584873000
				1	-2.184600000	1.474591000	-2.424116000
				1	-5.190248000	1.998197000	-2.619657000
				1	-4.376102000	0.796651000	-1.611615000
				1	-5.221883000	3.095053000	-0.421238000
				1	-3.565446000	2.563052000	-0.070918000
				1	-3.120341000	4.765091000	-0.899586000
				1	-4.439252000	4.690452000	-2.086360000
				6	-2.795336000	-0.826121000	-10.136220000
				6	-2.420481000	0.076821000	-8.983380000
				6	-3.165260000	1.228445000	-8.694869000
				6	-2.800867000	2.077345000	-7.645913000
				6	-1.682766000	1.791096000	-6.858576000
				6	-0.933261000	0.643903000	-7.139070000
4IM1A,B:							
6	6.247363000	7.434044000	0.962105000				
6	6.878293000	6.218520000	0.243466000				
6	5.943151000	5.415940000	-0.682685000				
6	5.342726000	6.281519000	-1.800930000				
6	6.699553000	4.213315000	-1.266585000				
6	5.082177000	7.057154000	1.868855000				
8	3.910150000	7.133160000	1.482729000				
1	5.865387000	8.155811000	0.236247000				
1	7.731441000	6.587493000	-0.343392000				
1	7.294490000	5.536912000	0.997870000				
1	5.116509000	5.025475000	-0.072970000				
1	4.740633000	5.669322000	-2.482480000				
1	4.693015000	7.066859000	-1.401379000				

6	-1.300140000	-0.202797000	-8.187176000	6	6.080058000	5.872329000	0.929001000
1	-2.598961000	-1.878572000	-9.902808000	6	6.334578000	4.348187000	1.005133000
1	-3.855703000	-0.730146000	-10.393066000	6	5.263330000	3.466256000	0.338307000
1	-4.039266000	1.462260000	-9.299876000	6	5.258941000	3.634546000	-1.187677000
1	-3.394763000	2.964954000	-7.441016000	6	5.472303000	1.994077000	0.723374000
1	-1.403603000	2.440744000	-6.033482000	6	4.903220000	6.324884000	1.778298000
1	-0.058144000	0.413222000	-6.536482000	8	3.790299000	6.571455000	1.291012000
1	-0.709349000	-1.093265000	-8.393778000	1	5.877901000	6.185245000	-0.098068000
16	-5.031598000	-5.093916000	-3.341253000	1	7.306793000	4.142539000	0.536968000
1	-5.038958000	-4.460505000	-4.535066000	1	6.434658000	4.058049000	2.060148000
6	-6.785668000	-4.675997000	0.334447000	1	4.281597000	3.775654000	0.725392000
6	-5.445035000	-5.035344000	0.342661000	1	4.453789000	3.051146000	-1.643115000
6	-4.854977000	-5.951790000	1.284800000	1	5.118058000	4.677586000	-1.493438000
6	-3.527990000	-6.026682000	0.986352000	1	6.205559000	3.285942000	-1.620241000
6	-3.301324000	-5.152860000	-0.136601000	1	4.722718000	1.352367000	0.246775000
7	-4.485263000	-4.570671000	-0.519950000	1	5.396283000	1.852327000	1.807908000
6	-2.058025000	-4.919145000	-0.706344000	1	6.461232000	1.640436000	0.403787000
6	-1.814420000	-4.041719000	-1.752552000	7	5.167555000	6.422176000	3.105779000
6	-0.522674000	-3.828223000	-2.355509000	6	4.200100000	6.781143000	4.131061000
6	-0.701072000	-2.933840000	-3.366867000	6	4.205505000	5.806908000	5.320295000
6	-2.103501000	-2.597940000	-3.386337000	6	3.765100000	4.388489000	5.013067000
7	-2.757887000	-3.267303000	-2.382777000	6	2.477844000	4.124348000	4.522938000
6	-2.696647000	-1.762162000	-4.322511000	6	2.058365000	2.820233000	4.260845000
6	-4.056773000	-1.503042000	-4.403733000	6	2.926515000	1.748881000	4.487697000
6	-4.653380000	-0.625659000	-5.380515000	6	4.205820000	1.993904000	4.987422000
6	-5.991196000	-0.607105000	-5.124431000	6	4.617211000	3.303398000	5.250025000
6	-6.217291000	-1.468129000	-3.990922000	1	6.110108000	6.216147000	3.409320000
7	-5.029651000	-2.020851000	-3.579924000	1	3.222643000	6.801961000	3.647241000
6	-7.453851000	-1.665149000	-3.390694000	1	5.209942000	5.790450000	5.764025000
6	-7.672418000	-2.441675000	-2.266615000	1	3.551709000	6.240495000	6.090341000
6	-8.963073000	-2.640330000	-1.652073000	1	1.791737000	4.952110000	4.355476000
6	-8.772139000	-3.478349000	-0.597579000	1	1.052875000	2.635398000	3.891366000
6	-7.365402000	-3.798582000	-0.567381000	1	2.603151000	0.731676000	4.286666000
7	-6.715062000	-3.143830000	-1.582434000	1	4.882417000	1.166561000	5.182891000
26	-4.750230000	-3.221864000	-1.995007000	1	5.604411000	3.480452000	5.670137000
1	-7.429478000	-5.125900000	1.083260000	6	2.827095000	-0.380679000	-2.252004000
1	-1.210541000	-5.460480000	-0.298480000	6	1.965825000	0.848050000	-2.594454000
1	-2.055012000	-1.285586000	-5.056437000	6	1.157859000	0.717854000	-3.889361000
1	-8.309522000	-1.163010000	-3.833522000	6	2.020433000	-1.616632000	-1.837447000
8	-1.432198000	2.411711000	1.542158000	1	3.459649000	-0.627155000	-3.117297000
6	-0.641117000	1.637208000	0.932058000	1	1.285078000	1.049350000	-1.755007000
8	0.527478000	1.930461000	0.537563000	1	2.624950000	1.725710000	-2.678671000
6	-1.134137000	0.194605000	0.614316000	1	1.827118000	0.587745000	-4.749425000
6	-2.403845000	-0.198726000	1.295349000	1	0.483603000	-0.144884000	-3.868284000
6	-2.391614000	-0.551249000	2.750942000	1	0.544659000	1.609520000	-4.065392000
6	-3.761366000	-0.910779000	3.348647000	1	2.680686000	-2.460437000	-1.603735000
6	-4.377843000	-2.190445000	2.773817000	1	1.331456000	-1.941922000	-2.623226000
1	-1.226269000	0.137835000	-0.479408000	1	1.417803000	-1.409505000	-0.943465000
1	-0.309672000	-0.481181000	0.880042000	6	-1.455354000	5.768388000	-3.009922000
1	-3.565121000	-1.795570000	-0.586985000	6	-0.501386000	5.889790000	-1.801609000
1	-3.344577000	0.139427000	0.864831000	6	0.721333000	4.964392000	-1.879814000
1	-1.977499000	0.309875000	3.306889000	6	1.597199000	5.001127000	-0.623658000
1	-1.682511000	-1.378214000	2.930613000	7	0.846803000	4.560970000	0.570736000
1	-3.654214000	-1.013395000	4.437570000	6	0.448551000	5.338366000	1.573685000
1	-4.448975000	-0.068481000	3.187329000	7	1.026355000	6.536874000	1.783445000
1	-4.564382000	-2.099294000	1.698706000	7	-0.577323000	4.961178000	2.367409000
1	-3.714069000	-3.051540000	2.926121000	6	-1.768230000	4.308509000	-3.339553000
8	-4.494854000	-1.835133000	-0.882555000	8	-1.103590000	3.723213000	-4.203191000
1	-5.334581000	-2.419689000	3.259132000	1	-0.976915000	6.178405000	-3.903677000
1	-2.218184000	-0.582304000	-11.038596000	1	-1.060117000	5.668669000	-0.883456000
1	4.067356000	0.739080000	-1.523212000	1	-0.171180000	6.933926000	-1.713759000
1	-3.134613000	1.861541000	-3.858790000	1	0.406048000	3.931683000	-2.065381000
1	-2.352338000	6.137768000	-2.743640000	1	1.351246000	5.237805000	-2.735502000
1	7.023869000	7.941526000	1.549570000	1	2.453801000	4.332058000	-0.736451000
1	4.463677000	6.859929000	4.956021000	1	1.993414000	5.998428000	-0.436527000
1	-9.503781000	-3.863205000	0.101390000	1	0.439873000	3.626984000	0.509342000
1	-5.399843000	-6.457955000	2.071391000	1	2.025788000	6.663971000	1.573440000
1	-6.768392000	-0.056925000	-5.639762000	1	0.615811000	7.150995000	2.471394000
1	-9.884265000	-2.190783000	-2.000414000	1	-1.008114000	4.039026000	2.268869000
1	-2.757004000	-6.606638000	1.477401000	1	-0.637468000	5.359452000	3.294002000
1	0.390817000	-4.314744000	-2.038339000	7	-2.716888000	3.675241000	-2.607709000
1	-4.102656000	-0.097253000	-6.148211000	6	-2.990595000	2.235266000	-2.820376000
1	0.033957000	-2.533082000	-4.052708000	6	-4.236440000	1.956810000	-1.970147000
				6	-4.156658000	3.019540000	-0.859060000
				6	-3.588255000	4.258363000	-1.574622000

4TS2_{DC,A}:

1	3.179500000	3.473490000	1.628077000	6	-3.434350000	2.172321000	-7.702729000
1	3.061501000	2.480362000	-0.607141000	6	-2.098727000	1.968273000	-7.347895000
1	4.248885000	3.789924000	-0.653544000	6	-1.436189000	0.833490000	-7.825732000
1	4.799592000	2.108660000	-0.590783000	6	-2.101232000	-0.081191000	-8.645167000
1	2.839301000	1.005152000	1.459446000	1	-3.835719000	-1.892773000	-9.727153000
1	3.666020000	1.441039000	2.964392000	1	-5.235893000	-0.810055000	-9.799772000
1	4.585788000	0.748429000	1.612525000	1	-5.137076000	1.427902000	-8.796391000
7	4.524212000	5.895073000	3.635638000	1	-3.963484000	3.050220000	-7.339811000
6	3.576949000	6.647376000	4.445299000	1	-1.582741000	2.673575000	-6.701799000
6	3.124024000	5.888367000	5.698966000	1	-0.397504000	0.663224000	-7.554510000
6	2.396173000	4.568469000	5.492638000	1	-1.573861000	-0.959097000	-9.014088000
6	1.681927000	4.265199000	4.325227000	16	-5.285503000	-4.655676000	-2.819879000
6	0.982641000	3.060178000	4.197442000	1	-6.055103000	-4.021290000	-3.733220000
6	0.988624000	2.138021000	5.245744000	6	-4.805087000	-3.970317000	1.240370000
6	1.698690000	2.423890000	6.413440000	6	-3.643144000	-4.383543000	0.581855000
6	2.396736000	3.626062000	6.531045000	6	-2.686211000	-5.325000000	1.120235000
1	5.239115000	5.367524000	4.118240000	6	-1.685869000	-5.451825000	0.202297000
1	2.733749000	6.892020000	3.796791000	6	-2.013802000	-4.586744000	-0.909026000
1	3.996522000	5.716441000	6.345415000	7	-3.206834000	-3.954043000	-0.650551000
1	2.480882000	6.575481000	6.268955000	6	-1.205839000	-4.398647000	-2.819879000
1	1.682940000	4.962538000	3.492555000	6	-1.462507000	-3.555011000	-3.117891000
1	0.441595000	2.835857000	3.280761000	6	-0.629011000	-3.387935000	-4.291586000
1	0.448082000	1.200558000	5.148777000	6	-1.279698000	-2.515854000	-5.116260000
1	1.714149000	1.709406000	7.232384000	6	-2.515420000	-2.155102000	-4.451415000
1	2.948129000	3.839370000	7.444995000	7	-2.580019000	-2.780686000	-3.239428000
6	3.365958000	0.029017000	-3.526457000	6	-3.522917000	-1.341948000	-4.975670000
6	2.361486000	1.177718000	-3.723518000	6	-4.751755000	-1.045518000	-4.379083000
6	1.303167000	0.919668000	-4.803381000	6	-5.745260000	-0.164133000	-4.954170000
6	2.756693000	-1.249907000	-2.938492000	6	-6.771999000	-0.081051000	-4.061665000
1	3.841299000	-0.204298000	-4.491072000	6	-6.418661000	-0.905409000	-2.925462000
1	1.858669000	1.399098000	-2.771968000	7	-5.197388000	-1.490867000	-3.157995000
1	2.919927000	2.086151000	-3.990673000	6	-7.183873000	-1.020729000	-1.761148000
1	1.776077000	0.725676000	-5.776626000	6	-6.853128000	-1.732309000	-0.604931000
1	0.675501000	0.053368000	-4.562022000	6	-7.691381000	-1.908574000	0.561428000
1	0.645171000	1.788232000	-4.909840000	6	-7.017445000	-2.738347000	1.411778000
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6	-0.288847000	6.493374000	-2.730126000	1	-0.285338000	-4.974654000	-2.067624000
6	1.051846000	5.747933000	-2.634143000	1	-3.338076000	-0.895790000	-5.948504000
6	1.682880000	5.862706000	-1.238669000	1	-8.137415000	-0.499880000	-1.759899000
7	0.872305000	5.144892000	-0.250473000	8	-1.003406000	2.400393000	1.057037000
6	0.372845000	5.661169000	0.861749000	6	-0.287941000	1.875319000	0.147744000
7	0.814676000	6.876544000	1.316841000	8	0.381720000	2.502461000	-0.727686000
7	-0.618454000	5.024719000	1.508516000	6	-0.183394000	0.372976000	0.106366000
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1	-0.600684000	6.454194000	-4.885969000	6	0.455880000	-2.371175000	2.314633000
1	-0.875012000	6.272260000	-1.830535000	6	-0.086425000	-2.063756000	3.714651000
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