

Electronic Supporting Information

Properties and reactivities of nonheme iron(IV)-oxo versus iron(V)-oxo: Long-range electron transfer versus hydrogen atom abstraction

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Full reference for Gaussian-09:

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Table S1: Group spin densities and charges of UB3LYP/B1 optimized geometries in the gas-phase.

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
³ 1	1.05	1.03	-0.08	-	0.61	-0.27	1.65	-
⁵ 1	2.95	0.84	0.21	-	0.75	-0.28	1.53	-
³ RC ₁	1.04	1.02	-0.07	0.00	0.62	-0.28	1.61	0.06
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
³ TS _{HA}	0.85	0.78	-0.07	0.43	0.64	-0.17	1.47	0.06

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
² 2	0.99	1.07	-1.06	-	0.63	-0.24	2.60	-
⁴ 2	1.02	1.08	0.90	-	0.64	-0.23	2.60	-
² RC ₂	1.10	0.98	-0.08	-1.00	0.62	-0.32	1.70	1.00
⁴ RC ₂	2.98	0.82	0.20	-1.00	0.75	-0.33	1.58	1.00
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
² TS _{HA}	1.21	0.60	-0.11	-0.70	0.70	-0.12	1.80	0.62
⁴ TS _{HA}	1.80	0.66	-0.13	0.67	0.75	-0.17	1.83	0.59
² I	0.98	0.11	-0.09	0.00	0.65	-0.28	1.65	0.98
⁴ I	2.85	0.06	0.09	0.00	0.77	-0.29	1.53	0.99
² P	1.13	0.03	-0.14	-0.01	0.76	-0.22	1.85	0.60
⁴ P	3.05	0.02	0.02	-0.09	0.82	-0.22	1.74	0.66

Table S2: Group spin densities and charges of UB3LYP/B2//UB3LYP/B1 calculations in the gas-phase.

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
³ 1	1.11	0.97	-0.08	-	0.55	-0.25	1.79	-
⁵ 1	3.09	0.76	0.15	-	0.61	-0.24	1.63	-
³ RC ₁	1.10	0.96	-0.07	0.01	0.40	-0.21	1.85	-0.04
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
³ TS _{HA}	0.89	0.75	-0.07	0.43	0.47	-0.02	1.68	-0.14

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
² 2	1.05	1.01	-1.06	-	0.44	-0.19	2.76	-
⁴ 2	1.08	1.02	0.90	-	0.43	-0.19	2.76	-
² RC ₂	1.16	0.93	-0.09	-1.00	0.32	-0.26	1.93	1.01
⁴ RC ₂	3.12	0.74	0.14	-1.00	0.47	-0.27	1.79	1.01
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
² TS _{HA}	1.26	0.57	-0.12	-0.71	0.50	0.00	2.03	0.48
⁴ TS _{HA}	1.82	0.65	-0.16	0.68	0.59	-0.10	2.06	0.45
² I	1.00	0.10	-0.10	0.00	0.48	-0.29	1.82	0.99
⁴ I	2.93	0.04	0.03	0.00	0.61	-0.24	1.64	0.99
² P	1.14	0.02	-0.15	-0.01	0.60	-0.13	2.02	0.50
⁴ P	3.12	0.00	-0.04	-0.08	0.67	-0.01	1.84	0.50

Table S3: Group spin densities and charges of UB3LYP/B1 single point calculations in solvent on gas-phase optimized geometries.

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
² RC ₂	1.09	0.99	-0.08	-1.00	0.63	-0.32	1.68	1.00
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
² TS _{HA}	1.18	0.62	-0.10	-0.70	0.71	-0.12	1.78	0.62

Table S4: Group spin densities and charges of UB3LYP/B2 optimized geometries in solvent.

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
³ RC ₁	1.11	0.96	-0.07	0.01	0.39	-0.21	1.85	-0.04
⁵ RC ₁	3.15	0.68	0.13	0.00	0.61	-0.33	1.28	0.21
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
³ TS _{HA}	0.89	0.75	-0.07	0.43	0.47	-0.02	1.68	-0.14
⁵ TS _{HA}	4.08	0.31	0.28	-0.69	0.69	-0.55	1.18	0.44

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
² RC ₂	1.17	0.92	-0.09	-1.00	0.32	-0.26	1.93	1.01
⁴ RC ₂	3.16	0.69	0.12	-1.00	0.61	-0.32	1.27	1.20
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
² TS _{HA}	1.29	0.55	-0.13	-0.71	0.50	0.00	2.03	0.47
⁴ TS _{HA}	1.84	0.64	-0.16	0.68	0.59	-0.11	2.06	0.45

Table S5: Group spin densities and charges of UB3LYP*/B2// UB3LYP/B2 calculations in solvent.

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
³ RC ₁	1.26	0.90	-0.16	0.00	1.83	0.38	-0.20	-0.01
⁵ RC ₁	2.95	0.72	0.11	0.00	3.16	0.41	-0.75	0.01
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
³ TS _{HA}	1.14	0.84	-0.13	0.16	-2.66	1.21	3.80	-0.35
⁵ TS _{HA}	3.80	0.27	0.47	-0.63	-1.72	1.36	2.67	-0.30

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
² RC ₂	1.25	0.91	-0.16	-1.00	-2.35	0.36	3.98	1.01
⁴ RC ₂	3.18	0.75	0.08	-1.00	-1.97	0.63	0.02	1.02
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
² TS _{HA}	1.36	0.52	-0.19	-0.69	-2.44	1.40	3.73	0.31
⁴ TS _{HA}	1.57	0.82	-0.18	0.78	-2.91	2.11	3.55	0.26

Table S6: Group spin densities and charges of UB3LYP-D3/B2//UB3LYP/B2 calculations in solvent.

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
³ RC ₁	1.22	0.93	-0.14	0.00	1.87	0.38	-0.24	-0.01
⁵ RC ₁	2.96	0.71	0.11	0.00	3.18	0.41	-0.75	0.01
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
³ TS _{HA}	1.08	0.86	-0.11	0.17	-2.61	1.21	3.73	-0.34
⁵ TS _{HA}	3.84	0.25	0.47	-0.64	-1.67	1.35	2.61	-0.29

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
² RC ₂	1.20	0.93	-0.14	-1.00	-2.30	0.37	3.92	1.01
⁴ RC ₂	3.19	0.75	0.08	-1.00	-1.93	0.63	3.25	1.02
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
² TS _{HA}	1.34	0.55	-0.18	-0.71	-2.37	1.40	3.65	0.32
⁴ TS _{HA}	1.57	0.81	-0.17	0.79	-2.87	2.11	3.51	0.26

Table S7: Group spin densities and charges of OPBE/B2//UB3LYP/B2 calculations in solvent.

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
³ RC ₁	1.36	0.91	-0.27	0.00	0.92	0.64	0.45	0.00
⁵ RC ₁	2.91	0.73	0.22	0.00	2.26	0.61	-0.17	0.01
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
³ TS _{HA}	1.27	0.84	-0.23	0.13	-4.08	1.72	4.90	-0.54
⁵ TS _{HA}	3.64	0.34	0.46	-0.53	-2.80	1.79	3.50	-0.50

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
² RC ₂	1.27	0.83	-0.28	-0.82	-3.53	0.70	5.00	0.83
⁴ RC ₂	3.19	0.79	-0.26	-0.81	-2.97	0.96	4.07	0.82
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
² TS _{HA}	1.36	0.48	-0.28	-0.55	-3.36	1.87	4.47	0.03
⁴ TS _{HA}	1.64	0.86	-0.25	0.75	-4.23	2.60	4.59	0.04

Table S8: Group spin densities and charges of MO6/B2//UB3LYP/B2 calculations in solvent.

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
³ RC ₁	1.32	0.81	-0.12	0.00	1.63	0.35	0.03	-0.01
⁵ RC ₁	3.03	0.62	0.22	0.00	2.74	0.41	-0.42	0.01
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
³ TS _{HA}	1.35	0.72	-0.17	0.10	-2.58	1.07	3.79	-0.28
⁵ TS _{HA}	3.67	0.33	0.59	-0.69	-1.69	1.22	2.56	-0.09

	Spin				Charge			
	Fe	O	BQEN	EB	Fe	O	BQEN	EB
² RC ₂	1.40	0.80	-0.21	-1.00	-2.32	0.32	3.99	1.01
⁴ RC ₂	3.40	0.64	-0.14	-1.00	-1.94	0.58	3.40	1.03
	Fe	OH	BQEN	EB-H	Fe	OH	BQEN	EB-H
² TS _{HA}	1.58	0.44	-0.26	-0.76	-2.44	1.29	3.71	0.44
⁴ TS _{HA}	1.91	0.62	-0.25	0.72	-2.81	1.87	3.56	0.37

Table S9: Absolute energies (in au) of solvent optimized geometries at UB3LYP/B2 level of theory in Jaguar. Also given are absolute energies obtained at UB3LYP-D3/B2// UB3LYP/B2 and UB3LYP/B2 single points with counter-ions and/or solvent models included.

	E _{B2} (au)	E _{solv} (kcal/mol)	E _{B1} (au)	ZPE (au)	G (au)	E(B3LYP-D3)	E(counterions)
² RC	-1712.74651	-216.5617	-1711.65619	0.62045	-1711.09320	-1712.863521	-1711.904542
² TS _{HA}	-1712.73652	-226.2400	-1711.63556	0.61687	-1711.07854	-1712.865673	-1711.895622
² I	-1712.81313	-219.1558	-1711.71574	0.62094	-1711.15372		
² P	-1712.82206	-233.8217	-1711.70324	0.62513	-1711.13774		
⁴ TS _{HA}	-1712.72814	-225.4092	-1711.63093	0.61585	-1711.07653	-1712.855127	-1711.869671
⁴ I	-1712.80531	-216.8435	-1711.71212	0.61853	-1711.15367		
⁴ P	-1712.80766	-230.6535	-1711.69278	0.62205	-1711.13279		
³ RC	-1713.01226	-112.4750	-1712.08207	0.62259	-1711.51579	-1713.139412	-1712.239256
³ TS _{HA}	-1712.99183	-112.1291	-1712.06820	0.62009	-1711.50518	-1713.129724	-1712.223723
³ TS _{reb}	-1713.01969	-104.1334	-1712.10465	0.61805	-1711.54721		
⁵ RC	-1713.00582	-120.2618	-1712.06849	0.62011	-1711.50593	-1713.125068	-1712.222864
⁵ TS _{HA}	-1712.99448	-103.7208	-1712.83526	0.61547	-1712.30187	-1713.123225	-1712.229450

Table S10: Relative energies (in kcal/mol) of solvent optimized geometries in Jaguar followed by single points with dispersion and/or counter-ions included.

gas/solvent	ΔE	ΔE	$\Delta E+ZPE$	$\Delta E+ZPE$	ΔG	ΔG	$\Delta G+E_{disp}$	$\Delta E+ZPE+E_{disp}$	$\Delta E+ZPE$
	gas	solv	gas	solv	gas	solv	solv	solv	counterions
² RC	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
² TS _{HA}	15.95	6.27	13.70	4.02	9.20	2.52	-5.10	-3.60	3.35
² I	-39.21	-41.80	-38.90	-41.50	-37.98	-42.41			
² P	0.00	-47.41	-27.21	-44.47	-27.95	-45.84			
⁴ TS _{HA}	20.38	11.53	17.49	8.64	10.46	6.14	-0.12	2.38	18.99
⁴ I	-36.62	-36.90	-37.82	-38.11	-37.94	-39.75			
⁴ P	-24.28	-38.37	-23.27	-37.36	-24.84	-40.25			
³ RC	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
³ TS _{HA}	12.48	12.82	10.91	11.25	6.65	10.77	4.03	4.51	8.18
³ TS _{reb}	-13.00	-4.66	-15.85	-7.51	-19.72	-10.21			
³ RC	11.83	4.04	10.27	2.49	6.19	1.71	6.67	7.44	8.73
⁵ TS _{HA}	14.69	11.16	10.22	6.69	3.66	-9.48	-10.48	5.69	1.68

Table S11: Absolute (in au) and relative (in kcal/mol) energies of UB3LYP-D3/BS2 optimized geometries in solvent using Jaguar.

	E (au)	ZPE (au)	G (au)	ΔE	$\Delta E+ZPE$	ΔG
² RC ₂	-1711.857781	0.616669	-1711.315668	0.00	0.00	0.00
² TS _{HA}	-1711.790995	0.616889	-1711.243077	41.91	42.05	45.55
⁴ RC ₂	-1711.842463	0.614722	-1711.307660	9.61	8.39	5.03
⁴ TS _{HA}	-1711.769837	0.610991	-1711.227567	55.19	51.62	55.28
³ RC ₁	-1712.232231	0.619824	-1711.679293	0.00	0.00	0.00
³ TS _{HA}	-1712.225490	0.618635	-1711.672314	4.23	3.48	4.38
⁵ RC ₁	-1712.216906	0.617624	-1711.667722	9.62	8.24	7.26
⁵ TS _{HA}	-1712.212018	0.608498	-1711.668939	12.68	5.58	6.50

Table S12: Absolute energies for the individual components of the thermodynamic cycles displayed in Fig 6. Data obtained after a UB3LYP/B1 geometry optimization in Jaguar followed by single points with solvent at UB3LYP/B2 and UB3LYP-D3.

	E	ZPE	G	E	Esolv
	[in au, BS1]	[in au, BS1]	[in au, BS1]	[in au, BS2]	[in au, BS2]
H	-0.500273	0.000000	-0.512911	-0.502257	-0.502313
$^3[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{2+}$	-1401.266720	0.461886	-1400.861516	-1401.882792	-1401.438646
$^2[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^+$	-1401.550421	0.459390	-1401.147290	-1402.169877	-1401.610266
$^4[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^+$	-1401.575277	0.458005	-1401.177038	-1402.200044	-1401.632442
$^2[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{3+}$	-1400.762866	0.459175	-1400.358975	-1401.375046	-1401.133819
$^4[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{3+}$	-1400.763880	0.459204	-1400.360585	-1401.375849	-1401.135186
$^2[\text{Fe}(\text{OH})(\text{BQEN})(\text{NCCH}_3)]^{2+}$	-1401.913891	0.472648	-1401.496957	-1402.534099	-1402.086966
$^4[\text{Fe}(\text{OH})(\text{BQEN})(\text{NCCH}_3)]^{2+}$	-1401.906223	0.468655	-1401.496106	-1402.528603	-1402.078055
$^3[\text{Fe}(\text{OH})(\text{BQEN})(\text{NCCH}_3)]^{3+}$	-1401.417264	0.470718	-1401.003078	-1402.034687	-1401.796828

Table S13: Relative energies (in kcal/mol) for the electron and hydrogen atom transfer reactions of the thermodynamic cycles in Fig 6.

	ΔE	$\Delta E + \text{ZPE}$	$\Delta E_{\text{solv}} + \text{ZPE}$	ΔG	ΔG_{solv}
	B2	B2	B2	B2	B2
$^3[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{2+} + e^- \rightarrow$ $^2[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^+ + \text{EA}$	-180.15	-181.71	-111.38	-181.45	-108.99
$^3[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{2+} + e^- \rightarrow$ $^4[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^+ + \text{EA}$	-199.08	-201.51	-129.50	-203.45	-125.98
$^3[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{2+} + \text{H} \rightarrow$ $^2[\text{Fe}(\text{OH})(\text{BQEN})(\text{NCCH}_3)]^{2+} + \text{BDE}_{\text{OH}}$		93.53	91.62	78.24	76.33
$^2[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{3+} + e^- \rightarrow$ $^3[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{2+} + \text{EA}$	-318.62	-316.92	-192.02	-317.79	-190.46
$^4[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{3+} + e^- \rightarrow$ $^3[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{2+} + \text{EA}$	-318.11	-316.43	-191.32	-316.91	-189.23
$^2[\text{Fe}(\text{O})(\text{BQEN})(\text{NCCH}_3)]^{3+} + \text{H} \rightarrow$ $^3[\text{Fe}(\text{OH})(\text{BQEN})(\text{NCCH}_3)]^{3+} + \text{BDE}_{\text{OH}}$		91.52	96.89	84.37	86.45

Table S14: Absolute energies for the individual components of the thermodynamic cycles displayed in Fig 7. Data obtained after a UB3LYP/B1 geometry optimization in Jaguar followed by single points with solvent at UB3LYP/B2 and UB3LYP-D3.

	E	ZPE	G	E	Esolv
	[in au, B1]	[in au, B1]	[in au, B1]	[in au, B2]	[in au, B2]
³ [Fe(O)(BQEN)(OH)] ⁺	-1344.640154	0.426784	-1344.263911	-1345.236049	-1344.701872
² [Fe(O)(BQEN)(OH)] ²⁺	-1344.262697	0.426691	-1343.886110	-1344.850734	-1344.448874
⁴ [Fe(O)(BQEN)(OH)] ²⁺	-1344.276599	0.427571	-1343.899539	-1344.866957	-1344.462715
² [Fe(O)(BQEN)(OH)] ⁰	-1344.783244	0.422066	-1344.412137	-1345.387793	-1344.814723
⁴ [Fe(O)(BQEN)(OH)] ⁰	-1344.793373	0.421041	-1344.426164	-1345.403078	-1344.824752
³ [Fe(OH)(BQEN)(OH)] ²⁺	-1344.934494	0.438374	-1344.546587	-1345.529067	-1345.122397
² [Fe(OH)(BQEN)(OH)] ⁺	-1345.288254	0.437570	-1344.901024	-1345.887425	-1345.347652
⁴ [Fe(OH)(BQEN)(OH)] ⁺	-1345.273599	0.435068	-1344.891585	-1345.877056	-1345.333367

Cartesian coordinates:

Gas-phase optimized geometries:

³ 1:				6	2.635251000	0.662788000	4.610927000
26	0.000000000	0.000000000	0.000000000	6	3.753262000	0.677373000	3.800536000
7	0.000000000	0.000000000	1.987721000	6	3.633151000	0.458576000	2.405234000
7	2.048457000	0.000000000	0.190792000	6	2.396134000	0.230067000	1.826050000
7	0.010434000	-0.145226000	-1.984366000	6	1.235328000	0.215123000	2.640852000
6	-1.063272000	-0.002981000	2.801967000	1	-2.047668000	-0.135894000	2.299475000
6	-0.942827000	0.182394000	4.194980000	1	-1.985884000	0.184253000	4.777570000
6	0.307477000	0.389048000	4.750736000	1	0.215957000	0.575108000	5.896259000
6	1.457002000	0.408121000	3.914832000	1	2.724295000	0.829656000	5.678789000
6	2.780068000	0.623541000	4.388653000	1	4.733847000	0.857602000	4.224811000
6	3.841560000	0.634941000	3.504035000	1	4.530024000	0.477804000	1.795740000
6	3.631987000	0.433838000	2.114977000	6	-0.024196000	0.885206000	-2.848574000
6	2.353981000	0.225833000	1.628005000	6	-0.066634000	0.701903000	-4.245274000
6	1.258793000	0.206580000	2.514598000	6	-0.006812000	-0.580684000	-4.767057000
1	-2.031037000	-0.146170000	2.344022000	6	0.102807000	-1.701548000	-3.897874000
1	-1.834553000	0.169075000	4.808734000	6	0.169589000	-3.050335000	-4.343320000
1	0.420699000	0.543137000	5.818506000	6	0.279704000	-4.079790000	-3.427446000
1	2.943711000	0.781851000	5.448923000	6	0.326469000	-3.810896000	-2.035080000
1	4.849728000	0.801899000	3.864100000	6	0.257486000	-2.508186000	-1.570960000
1	4.489718000	0.453442000	1.452221000	6	0.145855000	-1.445567000	-2.493028000
6	-0.071521000	0.903163000	-2.815153000	1	-0.080951000	1.866788000	-2.393751000
6	-0.176006000	0.738882000	-4.213095000	1	-0.148319000	1.567291000	-4.890796000
6	-0.208471000	-0.535973000	-4.750442000	1	-0.042553000	-0.741474000	-5.839272000
6	-0.137623000	-1.668767000	-3.892693000	1	0.133060000	-3.259857000	-5.406491000
6	-0.175767000	-3.014401000	-4.350954000	1	0.330350000	-5.107812000	-3.766487000
6	-0.105082000	-4.058708000	-3.448586000	1	0.411936000	-4.644225000	-1.346140000
6	0.010682000	-3.808572000	-2.056450000	7	0.293581000	-2.148107000	-0.133354000
6	0.047084000	-2.509751000	-1.579545000	6	1.669172000	-2.415549000	0.460851000
6	-0.025918000	-1.429980000	-2.487834000	6	2.671939000	-1.383899000	-0.027537000
1	-0.059342000	1.882799000	-2.353656000	1	1.564431000	-2.372628000	1.547702000
1	-0.231457000	1.616945000	-4.844216000	1	1.996329000	-3.427402000	0.194970000
1	-0.290530000	-0.683410000	-5.822125000	1	3.669129000	-1.603520000	0.373841000
1	-0.261038000	-3.209048000	-5.414466000	1	2.743967000	-1.394724000	-1.118855000
1	-0.134757000	-5.083869000	-3.798313000	6	-0.752338000	-2.916761000	0.638443000
1	0.068860000	-4.653359000	-1.378932000	1	-1.725742000	-2.751784000	0.179843000
7	0.189332000	-2.163759000	-0.147578000	1	-0.764359000	-2.556206000	1.666602000
6	1.605858000	-2.434597000	0.327252000	1	-0.524586000	-3.987412000	0.641232000
6	2.529887000	-1.377728000	-0.244087000	8	-0.069483000	1.651262000	-0.053635000
1	1.598415000	-2.401593000	1.419760000	7	-2.282215000	-0.189458000	-0.170502000
1	1.924856000	-3.437734000	0.021547000	6	-3.394517000	0.082626000	-0.408834000
1	3.560731000	-1.529901000	0.092851000	6	-4.774065000	0.431769000	-0.699683000
1	2.525110000	-1.394938000	-1.336330000	1	-4.897379000	1.522486000	-0.673816000
6	-0.792260000	-2.928438000	0.701153000	1	-5.446987000	-0.013646000	0.040460000
1	-1.798131000	-2.770233000	0.314555000	1	-5.059530000	0.067029000	-1.692079000
1	-0.730263000	-2.565248000	1.726474000	6	2.900818000	1.063797000	-0.441030000
1	-0.568558000	-4.000094000	0.694674000	1	2.544724000	2.039801000	-0.113528000
8	-0.043663000	1.654364000	-0.045087000	1	2.634969000	0.915406000	-1.488249000
7	-2.024503000	-0.066565000	-0.150335000	1	3.990754000	1.014722000	-0.343772000
6	-3.153422000	0.155311000	-0.343003000	1	-1.343867000	3.259608000	2.055953000
6	-4.559901000	0.442761000	-0.580229000	6	-2.248843000	3.759911000	2.429242000
1	-4.730933000	1.524735000	-0.555937000	6	-3.277125000	3.839300000	1.314868000
1	-5.185755000	-0.025441000	0.186961000	6	-2.872444000	4.000696000	-0.024825000
1	-4.869219000	0.062822000	-1.559657000	6	-3.816788000	4.156972000	-1.047647000
6	2.699759000	1.066790000	-0.660947000	6	-5.187358000	4.149165000	-0.748327000
1	2.356938000	2.043026000	-0.322324000	6	-5.603576000	3.979722000	0.580920000
1	2.409806000	0.912869000	-1.698428000	6	-4.655119000	3.824549000	1.600336000
1	3.788416000	1.001691000	-0.582868000	6	-1.864019000	5.151181000	2.983591000
⁵ 1:				1	-1.810958000	4.026606000	-0.258001000
26	0.000000000	0.000000000	0.000000000	1	-3.487127000	4.312053000	-2.070996000
7	0.000000000	0.000000000	2.060394000	1	-5.920213000	4.298387000	-1.534974000
7	2.230084000	0.000000000	0.383529000	1	-6.661716000	3.987183000	0.824125000
7	0.079758000	-0.153870000	-2.005284000	1	-4.986826000	3.713362000	2.629541000
6	-1.107639000	0.004947000	2.814807000	1	-2.643473000	3.146298000	3.251625000
6	-1.063765000	0.197232000	4.210513000	1	-2.741933000	5.667532000	3.386275000
6	0.156451000	0.412526000	4.825262000	1	-1.439401000	5.782044000	2.194919000
6	1.348920000	0.432167000	4.051564000	1	-1.123112000	5.062792000	3.786600000

³RC₁:

6	-5.061825000	3.778697000	1.126283000	1	3.998764000	1.053708000	-0.279173000
6	-3.774498000	3.499646000	1.597331000	1	-0.760879000	2.659519000	0.728840000
6	-0.242335000	4.628039000	1.201226000	6	-1.154850000	3.593859000	1.399871000
1	-1.978893000	4.449492000	-1.146342000	6	-2.591023000	3.794723000	1.072880000
1	-4.256542000	4.923851000	-1.984059000	6	-3.006216000	4.440134000	-0.116277000
1	-6.235817000	4.524173000	-0.529120000	6	-4.361605000	4.633358000	-0.388068000
1	-5.920364000	3.620002000	1.770742000	6	-5.336466000	4.178678000	0.514930000
1	-3.640677000	3.123169000	2.607898000	6	-4.944043000	3.518371000	1.690227000
1	-1.310630000	3.116481000	2.361696000	6	-3.587865000	3.320253000	1.958689000
1	-0.548105000	5.491199000	1.806064000	6	-0.171451000	4.721379000	1.085021000
1	-0.138520000	4.969180000	0.166424000	1	-2.264640000	4.807594000	-0.817500000
1	0.742297000	4.302057000	1.551653000	1	-4.662692000	5.151966000	-1.292122000

⁵TS_{HA}:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	2.073632000
7	2.242388000	0.000000000	0.408033000
7	0.124377000	-0.113653000	-2.017761000
6	-1.103784000	-0.028333000	2.831893000
6	-1.062431000	0.134205000	4.232550000
6	0.155859000	0.348748000	4.851277000
6	1.347771000	0.391356000	4.077676000
6	2.633181000	0.606279000	4.645573000
6	3.753655000	0.626000000	3.839161000
6	3.635860000	0.426978000	2.440617000
6	2.399956000	0.219341000	1.850926000
6	1.234519000	0.203569000	2.661841000
1	-2.042794000	-0.174040000	2.314486000
1	-1.982760000	0.092181000	4.801477000
1	0.215747000	0.485477000	5.925920000
1	2.719720000	0.751508000	5.716904000
1	4.734657000	0.789772000	4.269365000
1	4.535537000	0.441191000	1.835015000
6	0.033073000	0.936971000	-2.844254000
6	0.049225000	0.780724000	-4.246236000
6	0.156089000	-0.488876000	-4.788745000
6	0.252424000	-1.624259000	-3.936489000
6	0.366371000	-2.960930000	-4.407594000
6	0.461025000	-4.007600000	-3.510175000
6	0.447870000	-3.766695000	-2.112142000
6	0.334422000	-2.476722000	-1.622161000
6	0.234401000	-1.394355000	-2.525821000
1	-0.056671000	1.903728000	-2.364026000
1	-0.022514000	1.656390000	-4.878910000
1	0.168242000	-0.630545000	-5.864273000
1	0.379314000	-3.147131000	-5.475997000
1	0.548874000	-5.026614000	-3.868130000
1	0.526819000	-4.612146000	-1.437296000
7	0.321462000	-2.153739000	-0.176666000
6	1.683002000	-2.416392000	0.448688000
6	2.694399000	-1.377446000	-0.007534000
1	1.551041000	-2.381181000	1.533163000
1	2.022921000	-3.425258000	0.185905000
1	3.684414000	-1.604183000	0.408664000
1	2.786479000	-1.377853000	-1.097266000
6	-0.731503000	-2.952082000	0.548194000
1	-1.692121000	-2.803357000	0.057742000
1	-0.788163000	-2.601267000	1.578734000
1	-0.484691000	-4.019041000	0.550704000
8	-0.097333000	1.730480000	-0.095915000
7	-2.310895000	-0.200524000	-0.195135000
6	-3.427110000	0.045698000	-0.440245000
6	-4.815756000	0.365147000	-0.733447000
1	-5.060686000	1.358001000	-0.339484000
1	-5.484610000	-0.371073000	-0.275221000
1	-4.988323000	0.363741000	-1.814694000
6	2.910392000	1.071828000	-0.404601000
1	2.514296000	2.039006000	-0.098969000
1	2.675290000	0.909037000	-1.457024000

1	3.998764000	1.053708000	-0.279173000
1	-0.760879000	2.659519000	0.728840000
6	-1.154850000	3.593859000	1.399871000
6	-2.591023000	3.794723000	1.072880000
6	-3.006216000	4.440134000	-0.116277000
6	-4.361605000	4.633358000	-0.388068000
6	-5.336466000	4.178678000	0.514930000
6	-4.944043000	3.518371000	1.690227000
6	-3.587865000	3.320253000	1.958689000
6	-0.171451000	4.721379000	1.085021000
1	-2.264640000	4.807594000	-0.817500000
1	-4.662692000	5.151966000	-1.292122000
1	-6.388139000	4.353115000	0.313405000
1	-5.692980000	3.185119000	2.401374000
1	-3.285997000	2.832953000	2.882039000
1	-1.028612000	3.225874000	2.425694000
1	-0.401734000	5.605531000	1.692996000
1	-0.206574000	5.023410000	0.033924000
1	0.854377000	4.415166000	1.312085000

³I:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.981731000
7	2.273563000	0.000000000	0.359931000
7	0.059444000	-0.119456000	-1.997379000
6	-1.115164000	-0.046403000	2.728021000
6	-1.089768000	0.081216000	4.130988000
6	0.120713000	0.283680000	4.770337000
6	1.322134000	0.349403000	4.013797000
6	2.597207000	0.563640000	4.605368000
6	3.729704000	0.608295000	3.816808000
6	3.634775000	0.427844000	2.414279000
6	2.410115000	0.218204000	1.800286000
6	1.232592000	0.188195000	2.592652000
1	-2.045263000	-0.182804000	2.192883000
1	-2.017234000	0.022450000	4.686468000
1	0.166895000	0.393124000	5.848860000
1	2.665715000	0.689000000	5.680516000
1	4.702184000	0.773832000	4.265431000
1	4.542408000	0.454383000	1.820923000
6	-0.067098000	0.933410000	-2.810350000
6	-0.062144000	0.790373000	-4.216693000
6	0.071340000	-0.467465000	-4.776101000
6	0.207248000	-1.606818000	-3.933912000
6	0.352748000	-2.937732000	-4.412470000
6	0.486025000	-3.986693000	-3.522283000
6	0.482954000	-3.755261000	-2.122303000
6	0.340171000	-2.470684000	-1.627546000
6	0.199174000	-1.387980000	-2.522218000
1	-0.175154000	1.889373000	-2.312661000
1	-0.162651000	1.671763000	-4.837602000
1	0.075945000	-0.598616000	-5.853088000
1	0.359513000	-3.118246000	-5.481979000
1	0.597657000	-5.000719000	-3.887906000
1	0.594208000	-4.601885000	-1.453520000
7	0.343873000	-2.145219000	-0.181494000
6	1.712920000	-2.410772000	0.423531000
6	2.722607000	-1.374388000	-0.047628000
1	1.597667000	-2.376329000	1.509983000
1	2.045319000	-3.420322000	0.155193000
1	3.715485000	-1.607151000	0.360780000
1	2.804520000	-1.383212000	-1.138250000
6	-0.702167000	-2.947753000	0.551511000
1	-1.673604000	-2.764214000	0.095761000
1	-0.721584000	-2.632357000	1.594854000
1	-0.473226000	-4.017547000	0.510112000
8	-0.205957000	1.772320000	-0.134762000
7	-2.411068000	-0.284299000	-0.250460000
6	-3.499474000	-0.014525000	-0.583948000

6 -4.855863000 0.330052000 -0.987105000
 1 -5.116507000 1.325268000 -0.611962000
 1 -5.572207000 -0.393798000 -0.584867000
 1 -4.943881000 0.332222000 -2.078391000
 6 2.925626000 1.073120000 -0.455553000
 1 2.511345000 2.036195000 -0.159874000
 1 2.691514000 0.900297000 -1.507126000
 1 4.015447000 1.080400000 -0.333054000
 1 -0.664827000 2.359679000 0.518786000
 6 -1.217460000 4.294050000 1.324553000
 6 -2.592490000 4.063533000 1.601423000
 6 -3.628856000 4.312221000 0.647168000
 6 -4.964606000 4.108847000 0.979725000
 6 -5.319145000 3.650157000 2.262037000
 6 -4.318500000 3.395605000 3.218032000
 6 -2.981888000 3.595126000 2.897635000
 6 -0.667179000 4.955360000 0.101881000
 1 -3.374633000 4.691382000 -0.335973000
 1 -5.740688000 4.334222000 0.255438000
 1 -6.363669000 3.512722000 2.520114000
 1 -4.595944000 3.065924000 4.213550000
 1 -2.211301000 3.425047000 3.644396000
 1 -0.522712000 4.149486000 2.152083000
 1 -0.655174000 6.049994000 0.235704000
 1 -1.252055000 4.750436000 -0.799661000
 1 0.366585000 4.649620000 -0.083694496

³P:

26 0.000000000 0.000000000 0.000000000
 7 0.000000000 0.000000000 1.989435000
 7 2.225277000 0.000000000 0.361378000
 7 -0.055560000 -0.049066000 -1.978104000
 6 -1.116109000 -0.033663000 2.733226000
 6 -1.089941000 0.039323000 4.142857000
 6 0.125902000 0.169273000 4.792946000
 6 1.330853000 0.217873000 4.039132000
 6 2.617568000 0.363907000 4.627882000
 6 3.744839000 0.401714000 3.831145000
 6 3.637691000 0.287229000 2.420996000
 6 2.401174000 0.147864000 1.814149000
 6 1.231066000 0.117422000 2.614641000
 1 -2.056426000 -0.097298000 2.197178000
 1 -2.021033000 -0.000750000 4.694339000
 1 0.172639000 0.238038000 5.875128000
 1 2.699862000 0.445879000 5.706483000
 1 4.725133000 0.515113000 4.278759000
 1 4.543539000 0.311924000 1.824961000
 6 -0.208496000 1.016247000 -2.779539000
 6 -0.226425000 0.906162000 -4.187144000
 6 -0.093477000 -0.339714000 -4.775384000
 6 0.059980000 -1.495040000 -3.958853000
 6 0.196552000 -2.813017000 -4.476768000
 6 0.345773000 -3.886128000 -3.619023000
 6 0.371036000 -3.689696000 -2.214034000
 6 0.241513000 -2.418346000 -1.679039000
 6 0.079733000 -1.308427000 -2.541400000
 1 -0.330347000 1.972695000 -2.287969000
 1 -0.345339000 1.800815000 -4.786318000
 1 -0.105438000 -0.449156000 -5.855046000
 1 0.182326000 -2.963422000 -5.551102000
 1 0.447716000 -4.890577000 -4.014343000
 1 0.492375000 -4.553204000 -1.568083000
 7 0.271005000 -2.141003000 -0.227030000
 6 1.638285000 -2.429400000 0.356885000
 6 2.641491000 -1.378722000 -0.101510000
 1 1.537283000 -2.423662000 1.445089000
 1 1.977171000 -3.429644000 0.059258000
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 1 2.696954000 -1.352151000 -1.193672000

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⁵P:

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1	-0.822518000	-2.657546000	1.551125000	6	2.523050000	-1.380896000	-0.273044000
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²RC₂:

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6	3.853537000	0.503651000	3.526354000
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6	2.358877000	0.196559000	1.635354000
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6	-0.011896000	-3.853794000	-1.988213000
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⁴RC₂:

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6	-1.104574000	0.001508000	2.813010000
6	-1.050690000	0.135034000	4.214571000
6	0.178557000	0.286535000	4.832729000
6	1.367794000	0.308813000	4.054564000
6	2.663050000	0.468113000	4.619496000
6	3.779741000	0.482520000	3.806834000
6	3.648733000	0.335640000	2.402755000
6	2.402827000	0.177655000	1.818219000
6	1.243789000	0.161111000	2.634822000
1	-2.049853000	-0.105278000	2.297875000
1	-1.969888000	0.115846000	4.786424000
1	0.246778000	0.391025000	5.910540000
1	2.760773000	0.574080000	5.694289000
1	4.767463000	0.600917000	4.236370000
1	4.545646000	0.346157000	1.792746000
6	-0.004729000	0.852549000	-2.857409000
6	-0.047342000	0.658620000	-4.250626000
6	-0.018042000	-0.631153000	-4.760847000
6	0.063862000	-1.744659000	-3.881062000
6	0.095447000	-3.098271000	-4.316836000

6	0.182153000	-4.122805000	-3.392622000
6	0.247603000	-3.842730000	-2.003013000
6	0.214430000	-2.534228000	-1.549122000
6	0.117540000	-1.477244000	-2.477028000
1	-0.041048000	1.838669000	-2.411665000
1	-0.105140000	1.517996000	-4.906653000
1	-0.056059000	-0.800737000	-5.831777000
1	0.051920000	-3.315103000	-5.378560000
1	0.205754000	-5.154599000	-3.722737000
1	0.323402000	-4.672913000	-1.309317000
7	0.299338000	-2.161180000	-0.115684000
6	1.702217000	-2.419825000	0.422382000
6	2.672586000	-1.370807000	-0.087843000
1	1.638999000	-2.396187000	1.513032000
1	2.027561000	-3.423833000	0.127896000
1	3.686493000	-1.582677000	0.273391000
1	2.705264000	-1.360380000	-1.180775000
6	-0.698157000	-2.943666000	0.706626000
1	-1.689286000	-2.819726000	0.273005000
1	-0.693357000	-2.560087000	1.726100000
1	-0.432256000	-4.004968000	0.729872000
8	-0.128338000	1.657709000	-0.056115000
7	-2.300598000	-0.332521000	-0.195076000
6	-3.427882000	-0.329733000	-0.506111000
6	-4.835796000	-0.338685000	-0.877205000
1	-5.186500000	0.678435000	-1.080854000
1	-5.442451000	-0.758961000	-0.067437000
1	-4.993391000	-0.946704000	-1.774564000
6	2.897188000	1.086386000	-0.425223000
1	2.537823000	2.052234000	-0.072170000
1	2.637271000	0.964972000	-1.477552000
1	3.986594000	1.037212000	-0.324335000
1	-0.695367000	4.550794000	0.499351000
6	-1.577395000	5.150948000	0.238052000
6	-1.480493000	6.554407000	0.727589000
6	-2.682611000	7.294868000	1.037561000
6	-2.614293000	8.612437000	1.429404000
6	-1.339457000	9.255285000	1.524281000
6	-0.135452000	8.540094000	1.224256000
6	-0.204623000	7.222420000	0.831742000
6	-1.719934000	5.138482000	-1.330409000
1	-3.640732000	6.792960000	0.957255000
1	-3.512424000	9.171865000	1.664497000
1	-1.284575000	10.297507000	1.822991000
1	0.818208000	9.048420000	1.306671000
1	0.697500000	6.668612000	0.596315000
1	-2.461743000	4.662218000	0.661960000
1	-0.859616000	5.613172000	-1.810118000
1	-2.629000000	5.652471000	-1.653647000
1	-1.772252000	4.094111000	-1.651533000

²TS_{HA}:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.978362000
7	2.058824000	0.000000000	0.185594000
7	0.030222000	-0.174524000	-1.990210000
6	-1.064548000	-0.034450000	2.795931000
6	-0.937674000	0.070613000	4.195905000
6	0.318860000	0.228518000	4.759162000
6	1.467263000	0.282605000	3.922942000
6	2.793978000	0.456427000	4.406352000
6	3.855947000	0.502122000	3.521974000
6	3.644100000	0.367182000	2.124725000
6	2.362554000	0.196286000	1.628824000
6	1.265506000	0.157060000	2.512634000
1	-2.034301000	-0.149278000	2.332708000
1	-1.826139000	0.024967000	4.813285000
1	0.435748000	0.311967000	5.834411000
1	2.961878000	0.551165000	5.473437000

1	4.866628000	0.634809000	3.889589000
1	4.504577000	0.396347000	1.465528000
6	-0.033143000	0.858634000	-2.843543000
6	-0.124917000	0.671183000	-4.237818000
6	-0.167212000	-0.613450000	-4.713327000
6	-0.118182000	-1.730361000	-3.874735000
6	-0.165406000	-3.083088000	-4.311579000
6	-0.112743000	-4.113901000	-3.392071000
6	-0.002817000	-3.841950000	-2.003579000
6	0.045249000	-2.534408000	-1.549582000
6	-0.015336000	-1.468677000	-2.472018000
1	-0.016758000	1.845021000	-2.399351000
1	-0.162977000	1.537085000	-4.886857000
1	-0.239102000	-0.778245000	-5.823111000
1	-0.241233000	-3.294590000	-5.372387000
1	-0.147543000	-5.144368000	-3.725251000
1	0.048717000	-4.677875000	-1.314621000
7	0.212549000	-2.165479000	-0.122232000
6	1.644044000	-2.433885000	0.321059000
6	2.544055000	-1.374077000	-0.270131000
1	1.663170000	-2.410522000	1.413459000
1	1.952584000	-3.434928000	0.000721000
1	3.583657000	-1.513469000	0.043926000
1	2.515987000	-1.385146000	-1.361612000
6	-0.732281000	-2.944477000	0.760562000
1	-1.748407000	-2.838287000	0.386091000
1	-0.667363000	-2.562250000	1.778179000
1	-0.465008000	-4.005499000	0.770343000
8	-0.042016000	1.685562000	-0.135093000
7	-2.016681000	-0.225756000	-0.174618000
6	-3.145257000	-0.323081000	-0.457339000
6	-4.552384000	-0.456663000	-0.803289000
1	-5.117764000	0.419884000	-0.468870000
1	-4.983096000	-1.346025000	-3.329457000
1	-4.671113000	-0.551595000	-1.888376000
6	2.723851000	1.065321000	-0.656884000
1	2.408382000	2.043727000	-0.303774000
1	2.424743000	0.931546000	-1.694289000
1	3.811120000	0.973136000	-0.586925000
1	-0.337714000	2.841247000	0.654854000
6	-0.378589000	3.848427000	1.397188000
6	-1.097693000	4.873510000	0.655660000
6	-0.425347000	5.803806000	-0.214396000
6	-1.122811000	6.833253000	-0.815046000
6	-2.521886000	6.963538000	-0.601280000
6	-3.215673000	6.038723000	0.223427000
6	-2.524689000	5.005319000	0.823636000
6	1.086764000	4.077588000	1.773658000
1	0.642043000	5.713835000	-0.373544000
1	-0.609629000	7.550374000	-1.445355000
1	-3.064514000	7.774619000	-1.075801000
1	-4.280160000	6.160403000	0.386569000
1	-3.040863000	4.306648000	1.474013000
1	-0.972449000	3.455426000	2.231606000
1	1.166625000	4.911267000	2.482741000
1	1.716709000	4.316330000	0.911426000
1	1.499786000	3.190107000	2.259009000

⁴TS_{HA}:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.982555000
7	2.067282000	0.000000000	0.199508000
7	0.043731000	-0.244611000	-1.984012000
6	-1.070398000	-0.025987000	2.791564000
6	-0.954095000	0.118480000	4.188626000
6	0.296636000	0.307070000	4.755731000
6	1.450118000	0.351430000	3.926299000
6	2.772142000	0.546987000	4.414120000
6	3.840191000	0.575547000	3.536497000

6	3.638610000	0.408367000	2.141379000	7	0.037565000	-0.123545000	-1.987816000
6	2.361011000	0.218183000	1.642120000	6	-1.052914000	-0.043727000	2.815283000
6	1.259463000	0.188291000	2.518530000	6	-0.916242000	0.079389000	4.212215000
1	-2.035836000	-0.159213000	2.325240000	6	0.343256000	0.259316000	4.760245000
1	-1.846682000	0.800576000	4.800524000	6	1.482343000	0.314213000	3.911871000
1	0.405110000	0.422575000	5.829169000	6	2.811157000	0.491025000	4.387184000
1	2.931533000	0.671309000	5.479699000	6	3.867731000	0.521624000	3.497053000
1	4.847673000	0.722523000	3.907405000	6	3.646052000	0.372950000	2.102919000
1	4.503121000	0.430967000	1.487144000	6	2.362954000	0.205295000	1.610786000
6	-0.001483000	0.767225000	-2.864151000	6	1.270028000	0.175891000	2.503668000
6	-0.084155000	0.547294000	-4.253556000	1	-2.026181000	-0.180311000	2.366179000
6	-0.140946000	-0.749517000	-4.736831000	1	-1.798649000	0.029492000	4.837879000
6	-0.108334000	-1.844387000	-3.830803000	1	0.470934000	0.355656000	5.833387000
6	-0.171151000	-3.205737000	-4.238710000	1	2.983521000	0.594331000	5.452964000
6	-0.129440000	-4.216789000	-3.297395000	1	4.881362000	0.650957000	3.857608000
6	-0.010877000	-3.915312000	-1.915866000	1	4.502871000	0.387894000	1.438550000
6	0.051048000	-2.599121000	-1.488140000	6	0.005385000	0.924123000	-2.821065000
6	-0.006311000	-1.551736000	-2.433145000	6	-0.082447000	0.761930000	-4.219966000
1	0.021113000	1.764638000	-2.447859000	6	-0.152857000	-0.512171000	-4.757826000
1	-0.105841000	1.397057000	-4.924323000	6	-0.132416000	-1.645116000	-3.898154000
1	-0.210973000	-0.940542000	-5.802579000	6	-0.208324000	-2.990457000	-4.353208000
1	-0.250025000	-3.438514000	-5.295037000	6	-0.179823000	-4.033269000	-3.446068000
1	-0.177432000	-5.253914000	-3.607610000	6	-0.066922000	-3.783143000	-2.052983000
1	0.037448000	-4.736590000	-1.209362000	6	0.006038000	-2.483373000	-1.581799000
7	0.231632000	-2.208379000	-0.070171000	6	-0.029443000	-1.406285000	-2.492535000
6	1.668990000	-2.442822000	0.367802000	1	0.050504000	1.895227000	-2.347178000
6	2.555734000	-1.378894000	-0.238700000	1	-0.093332000	1.637726000	-4.856719000
1	1.692276000	-2.403753000	1.459695000	1	-0.223645000	-0.657201000	-5.830537000
1	1.995376000	-3.442767000	0.060452000	1	-0.287306000	-3.187049000	-5.416880000
1	3.596585000	-1.506731000	0.077143000	1	-0.237652000	-5.058294000	-3.792601000
1	2.527930000	-1.403860000	-1.329969000	1	-0.036573000	-4.629309000	-1.375562000
6	-0.698823000	-2.973138000	0.837361000	7	0.165980000	-2.130975000	-0.148015000
1	-1.719427000	-2.878723000	0.471242000	6	1.590427000	-2.425028000	0.306907000
1	-0.625443000	-2.569429000	1.846079000	6	2.523648000	-1.381179000	-0.270574000
1	-0.427257000	-4.032989000	0.867988000	1	1.596560000	-2.402321000	1.399589000
8	-0.095118000	1.695072000	-0.071908000	1	1.882418000	-3.431686000	-0.011273000
7	-2.027374000	-0.257074000	-0.178665000	1	3.554648000	-1.551755000	0.057046000
6	-3.167424000	-0.349413000	-0.412631000	1	2.510433000	-1.396504000	-1.362440000
6	-4.589402000	-0.472583000	-0.697426000	6	-0.802599000	-2.902984000	0.712128000
1	-5.158300000	0.287749000	-0.151146000	1	-1.812491000	-2.766708000	0.329178000
1	-4.957816000	-1.460388000	-0.397792000	1	-0.739400000	-2.537252000	1.735781000
1	-4.777198000	-0.344937000	-1.769204000	1	-0.561304000	-3.970193000	0.708229000
6	2.731527000	1.057775000	-0.649344000	8	0.004410000	1.845410000	-0.067997000
1	2.419537000	2.037805000	-0.297707000	7	-2.011720000	-0.085222000	-0.114714000
1	2.433434000	0.918624000	-1.686576000	6	-3.160701000	-0.129754000	-0.315886000
1	3.818934000	0.965819000	-0.579508000	6	-4.592804000	-0.192359000	-0.571675000
1	-0.269370000	3.000492000	-0.002271000	1	-5.054026000	0.790466000	-0.426225000
6	-0.087544000	4.308689000	0.073936000	1	-5.076528000	-0.904163000	0.106207000
6	-1.361313000	4.896254000	0.420964000	1	-4.781791000	-0.514090000	-1.601841000
6	-2.293274000	5.368363000	-0.567345000	6	2.716773000	1.061684000	-0.674641000
6	-3.461726000	6.000843000	-0.184867000	1	2.314044000	2.027515000	-0.380358000
6	-3.758272000	6.176329000	1.191023000	1	2.483375000	0.871027000	-1.720496000
6	-2.871200000	5.696322000	2.185376000	1	3.802311000	1.038614000	-0.545994000
6	-1.706898000	5.052689000	1.811608000	1	-0.752439000	2.292848000	0.367077000
6	0.592808000	4.635902000	-1.249951000	6	-0.160234000	5.221148000	0.094404000
1	-2.064331000	5.255333000	-1.620026000	6	-0.777231000	6.431953000	-0.210921000
1	-4.149361000	6.379603000	-0.932242000	6	-1.485822000	6.555739000	-1.463702000
1	-4.671157000	6.684632000	1.483441000	6	-2.064831000	7.755646000	-1.830502000
1	-3.102893000	5.852764000	3.232511000	6	-1.963805000	8.868520000	-0.966109000
1	-1.008359000	4.703557000	2.565337000	6	-1.283956000	8.780454000	0.270899000
1	0.608743000	4.284433000	0.921295000	6	-0.701500000	7.586695000	0.652250000
1	0.940703000	5.678076000	-1.238489000	6	0.686406000	4.914500000	1.267405000
1	-0.066498000	4.522125000	-2.115723000	1	-1.545814000	5.694545000	-2.121806000
1	1.474102000	4.007199000	-1.403425000	1	-2.589106000	7.852448000	-2.773560000
				1	-2.417309000	9.811116000	-1.256611000
				1	-1.223393000	9.650855000	0.913321000
				1	-0.181894000	7.522977000	1.600479000
				1	-0.257670000	4.415512000	-0.634555000
				1	0.526989000	5.567005000	2.126678000
Σ:							
26	0.000000000	0.000000000	0.000000000				
7	0.000000000	0.000000000	1.983149000				
7	2.058529000	0.000000000	0.170417000				

1	1.744464000	5.022968000	0.965579000	1	-2.672205000	7.239123000	0.503119000
1	0.579967000	3.865062000	1.558105933	1	-2.158550000	9.649139000	0.419855000
⁴I:				1	0.193516000	10.417710000	0.229929000
26	0.000000000	0.000000000	0.000000000	1	2.069877000	8.793536000	0.124570000
7	0.000000000	0.000000000	2.025129000	1	1.595150000	6.357191000	0.211441000
7	2.243332000	0.000000000	0.368398000	1	0.083889000	4.583367000	0.372760000
7	0.067815000	-0.030064000	-1.974286000	1	-2.965186000	5.149521000	0.371292000
6	-1.109401000	-0.039909000	2.782605000	1	-2.187028000	4.139783000	1.595530000
6	-1.064673000	0.035510000	4.188834000	1	-2.109431000	3.645314000	-0.088536000
6	0.160018000	0.162911000	4.821974000	²P:			
6	1.355245000	0.209809000	4.054116000	26	0.000000000	0.000000000	0.000000000
6	2.647062000	0.334056000	4.636318000	7	0.000000000	0.000000000	1.977165000
6	3.771824000	0.359246000	3.834839000	7	2.053914000	0.000000000	0.208792000
6	3.652860000	0.255238000	2.425615000	7	0.042388000	-0.070805000	-2.003571000
6	2.410651000	0.137270000	1.823304000	6	-1.072807000	-0.038294000	2.788546000
6	1.242994000	0.118634000	2.627920000	6	-0.960035000	0.072122000	4.188245000
1	-2.051021000	-0.135812000	2.258195000	6	0.290608000	0.244040000	4.763567000
1	-1.987591000	-0.010613000	4.753312000	6	1.446225000	0.301098000	3.937571000
1	0.220062000	0.223716000	5.903651000	6	2.768561000	0.482932000	4.430863000
1	2.735757000	0.401887000	5.715156000	6	3.838423000	0.522094000	3.554793000
1	4.756750000	0.449490000	4.277583000	6	3.639685000	0.376644000	2.155980000
1	4.556047000	0.264062000	1.824630000	6	2.361196000	0.203729000	1.650740000
6	-0.036972000	1.054854000	-2.755501000	6	1.258659000	0.166148000	2.525801000
6	-0.074192000	0.950653000	-4.160194000	1	-2.039653000	-0.157805000	2.320888000
6	-0.011151000	-0.300632000	-4.755487000	1	-1.854666000	0.026141000	4.796854000
6	0.095214000	-1.469542000	-3.951868000	1	0.395235000	0.336757000	5.839789000
6	0.159075000	-2.791551000	-4.472759000	1	2.926982000	0.588798000	5.498829000
6	0.263331000	-3.871516000	-3.615308000	1	4.845611000	0.659217000	3.930750000
6	0.313379000	-3.681405000	-2.209700000	1	4.506711000	0.400754000	1.504915000
6	0.250989000	-2.405180000	-1.675185000	6	0.065325000	0.966496000	-2.859866000
6	0.138236000	-1.293292000	-2.534442000	6	-0.024355000	0.790665000	-4.255168000
1	-0.103381000	1.999942000	-2.231220000	6	-0.145879000	-0.487519000	-4.777362000
1	-0.155917000	1.849169000	-4.758676000	6	-0.162856000	-1.608697000	-3.903343000
1	-0.043585000	-0.399105000	-5.835673000	6	-0.267586000	-2.956549000	-4.347699000
1	0.125361000	-2.941672000	-5.546327000	6	-0.256084000	-3.993779000	-3.433561000
1	0.311064000	-4.878971000	-4.011313000	6	-0.130611000	-3.734812000	-2.043257000
1	0.399401000	-4.553144000	-1.570123000	6	-0.033613000	-2.431548000	-1.584203000
7	0.312956000	-2.117974000	-0.218722000	6	-0.057134000	-1.358190000	-2.498318000
6	1.705394000	-2.412143000	0.328276000	1	0.174031000	1.957075000	-2.437194000
6	2.693951000	-1.353720000	-0.125647000	1	0.004379000	1.660354000	-4.900130000
1	1.625727000	-2.432393000	1.418111000	1	-0.221574000	-0.642265000	-5.848892000
1	2.023120000	-3.406978000	-0.002601000	1	-0.350649000	-3.159604000	-5.410063000
1	3.699000000	-1.588324000	0.245959000	1	-0.333450000	-5.020623000	-3.771764000
1	2.746730000	-1.305955000	-1.216816000	1	-0.108949000	-4.577687000	-1.361261000
6	-0.695268000	-2.947806000	0.542780000	7	0.144076000	-2.079457000	-0.146380000
1	-1.678053000	-2.818481000	0.095868000	6	1.555852000	-2.419646000	0.323033000
1	-0.713308000	-2.616979000	1.580917000	6	2.509594000	-1.390778000	-0.235901000
1	-0.420057000	-4.006564000	0.515702000	1	1.550045000	-2.412206000	1.415474000
8	-0.211088000	1.836355000	-0.040154000	1	1.819442000	-3.429144000	-0.008787000
7	-2.354965000	-0.357065000	-0.203121000	1	3.533201000	-1.566733000	0.109747000
6	-3.481697000	-0.419725000	-0.512775000	1	2.514724000	-1.400656000	-1.328218000
6	-4.886670000	-0.514366000	-0.884381000	6	-0.853441000	-2.828529000	0.713797000
1	-5.440416000	0.360867000	-0.528445000	1	-1.857425000	-2.669779000	0.327408000
1	-5.339855000	-1.409999000	-0.445241000	1	-0.780191000	-2.477736000	1.740837000
1	-4.993688000	-0.572404000	-1.972740000	1	-0.629101000	-3.898488000	0.695624000
6	2.907706000	1.112033000	-0.391739000	8	-0.186605000	1.964845000	-0.002199000
1	2.515582000	2.063222000	-0.034959000	7	-2.022489000	-0.076407000	-0.212507000
1	2.670738000	1.003814000	-1.450781000	6	-3.174569000	-0.089499000	-0.405986000
1	3.995799000	1.087359000	-0.267958000	6	-4.609664000	-0.112425000	-0.644379000
1	-0.377159000	2.280898000	0.818212000	1	-5.114750000	0.645685000	-0.034677000
6	-0.796302000	5.225792000	0.428446000	1	-5.025548000	-1.094184000	-0.388498000
6	-0.574211000	6.597922000	0.367404000	1	-4.827187000	0.089121000	-1.699886000
6	-1.643265000	7.567562000	0.422973000	6	2.748605000	1.034494000	-0.650596000
6	-1.359613000	8.918614000	0.376510000	1	2.444952000	2.032927000	-0.349832000
6	-0.017727000	9.353561000	0.268448000	1	2.481269000	0.867910000	-1.691801000
6	1.051849000	8.432613000	0.207704000	1	3.832788000	0.935892000	-0.550239000
6	0.784701000	7.077824000	0.255547000	1	-0.917801000	2.248953000	-0.588389000
6	-2.092851000	4.525997000	0.565194000	6	0.209625000	3.272892000	0.867149000

6	0.565983000	4.351314000	-0.108868000	1	-4.976497000	-1.334517000	-1.571766000
6	-0.425773000	4.989086000	-0.886862000	6	2.942161000	1.074029000	-0.407462000
6	-0.077271000	6.016362000	-1.768583000	1	2.615984000	2.049384000	-0.049745000
6	1.259109000	6.429830000	-1.873134000	1	2.697589000	0.968090000	-1.464662000
6	2.249314000	5.811011000	-1.097796000	1	4.027723000	0.991357000	-0.293363000
6	1.906687000	4.770715000	-0.228860000	1	-0.136472000	2.209172000	1.191934000
6	-0.947315000	3.557066000	1.808714000	6	-0.755621000	3.384891000	-0.426267000
1	-1.475763000	4.722861000	-0.779568000	6	-1.596473000	4.054226000	0.614148000
1	-0.844167000	6.514156000	-2.351214000	6	-2.986516000	3.795743000	0.651169000
1	1.523112000	7.241627000	-2.540265000	6	-3.804911000	4.441893000	1.575721000
1	3.277017000	6.148334000	-1.160662000	6	-3.245301000	5.356398000	2.486280000
1	2.674446000	4.318220000	0.394306000	6	-1.865074000	5.615256000	2.468247000
1	1.087573000	2.906042000	1.395295000	6	-1.043381000	4.968357000	1.544040000
1	-0.685432000	4.427085000	2.421950000	6	0.446420000	4.157337000	-0.940601000
1	-1.147351000	2.717363000	2.477273000	1	-3.423298000	3.116250000	-0.074814000
1	-1.865557000	3.817231000	1.274363000	1	-4.874375000	4.261989000	1.580814000

4P:

26	0.000000000	0.000000000	0.000000000	1	-1.439783000	6.335532000	3.157390000
7	0.000000000	0.000000000	2.030177000	1	0.014104000	5.210680000	1.524316000
7	2.229557000	0.000000000	0.369510000	1	-1.376843000	2.986488000	-1.230557000
7	0.142369000	-0.101738000	-1.980727000	1	1.136987000	4.430065000	-0.139549000
6	-1.112864000	-0.047790000	2.787168000	1	0.098928000	5.086713000	-1.404948000
6	-1.066389000	0.032895000	4.191249000	1	1.010122000	3.601060000	-1.693219000
6	0.158810000	0.176064000	4.824274000				
6	1.354013000	0.231276000	4.057995000				
6	2.645322000	0.380972000	4.636450000				
6	3.768466000	0.419641000	3.832455000				
6	3.650848000	0.301420000	2.423788000				
6	2.408107000	0.157975000	1.826732000				
6	1.244647000	0.128729000	2.631837000				
1	-2.055714000	-0.142140000	2.264926000				
1	-1.989349000	-0.012603000	4.755757000				
1	0.215958000	0.247254000	5.905619000				
1	2.735085000	0.462400000	5.714283000				
1	4.752044000	0.534325000	4.272460000				
1	4.554565000	0.323192000	1.824210000				
6	0.137386000	0.939704000	-2.834195000				
6	0.109187000	0.771546000	-4.229427000				
6	0.082818000	-0.510047000	-4.760935000				
6	0.097126000	-1.636367000	-3.895849000				
6	0.078743000	-2.981550000	-4.358800000				
6	0.107370000	-4.028635000	-3.456650000				
6	0.160869000	-3.779009000	-2.061440000				
6	0.174099000	-2.477904000	-1.583563000				
6	0.135344000	-1.396233000	-2.484546000				
1	0.161514000	1.926092000	-2.400229000				
1	0.107497000	1.644884000	-4.869753000				
1	0.055899000	-0.660909000	-5.835422000				
1	0.044125000	-3.173347000	-5.425765000				
1	0.096077000	-5.053568000	-3.808118000				
1	0.195114000	-4.625387000	-1.384198000				
7	0.267836000	-2.142415000	-0.141208000				
6	1.669151000	-2.418731000	0.394984000				
6	2.657097000	-1.375532000	-0.096812000				
1	1.604276000	-2.416850000	1.485444000				
1	1.980552000	-3.420439000	0.079101000				
1	3.662430000	-1.606887000	0.274848000				
1	2.704272000	-1.354726000	-1.188703000				
6	-0.740882000	-2.918576000	0.672167000				
1	-1.732206000	-2.777592000	0.247227000				
1	-0.719209000	-2.563601000	1.701363000				
1	-0.493848000	-3.984587000	0.667397000				
8	-0.212694000	2.013619000	0.234856000				
7	-2.287452000	-0.245172000	-0.262993000				
6	-3.414367000	-0.339112000	-0.565597000				
6	-4.819142000	-0.463574000	-0.924817000				
1	-5.163586000	0.429266000	-1.458215000				
1	-5.434807000	-0.587098000	-0.026023000				

Solvent optimized geometries at UB3LYP/BS2:

³RC₁:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.994904000
7	2.052683000	0.000000000	0.199156000
7	0.009767000	-0.185165000	-1.991318000
6	-1.046620000	-0.037150000	2.810696000
6	-0.932248000	0.148085000	4.198704000
6	0.305499000	0.401503000	4.744065000
6	1.444381000	0.451200000	3.904858000
6	2.757082000	0.704879000	4.373820000
6	3.811042000	0.728397000	3.490867000
6	3.606716000	0.498871000	2.110173000
6	2.340196000	0.257942000	1.624662000
6	1.246257000	0.232640000	2.512546000
1	-2.014295000	-0.215601000	2.361626000
1	-1.825553000	0.102074000	4.810580000
1	0.418760000	0.564693000	5.811240000
1	2.916206000	0.878898000	5.433186000
1	4.817233000	0.923672000	3.845266000
1	4.466269000	0.520406000	1.450122000
6	-0.070225000	0.831905000	-2.840461000
6	-0.179837000	0.645362000	-4.230628000
6	-0.224170000	-0.632698000	-4.737845000
6	-0.151879000	-1.740956000	-3.857458000
6	-0.194524000	-3.092108000	-4.283832000
6	-0.123174000	-4.110962000	-3.361525000
6	-0.007070000	-3.832763000	-1.979235000
6	0.047510000	-2.529582000	-1.536200000
6	-0.028542000	-1.469935000	-2.465430000
1	-0.050655000	1.823034000	-2.404223000
1	-0.230578000	1.514363000	-4.876404000
1	-0.315109000	-0.802686000	-5.806354000
1	-0.284049000	-3.309504000	-5.343483000
1	-0.158646000	-5.144813000	-3.687247000
1	0.051829000	-4.664204000	-1.286310000
7	0.197485000	-2.169282000	-0.118041000
6	1.603689000	-2.427897000	0.353929000
6	2.534063000	-1.374000000	-0.199075000
1	1.592400000	-2.404280000	1.444492000
1	1.933820000	-3.425630000	0.052666000
1	3.554226000	-1.528789000	0.160084000
1	2.563059000	-1.404178000	-1.288221000
6	-0.754948000	-2.944627000	0.731067000
1	-1.765501000	-2.827004000	0.347446000
1	-0.707251000	-2.572522000	1.751997000
1	-0.498481000	-4.005960000	0.743913000
8	-0.029182000	1.630945000	-0.068406000
7	-2.002793000	-0.144540000	-0.121685000
6	-3.138805000	-0.087233000	-0.288125000
6	-4.571317000	-0.016158000	-0.488138000
1	-4.842046000	0.936334000	-0.952769000
1	-5.086796000	-0.104476000	0.471468000
1	-4.896520000	-0.835635000	-1.132243000
6	2.723269000	1.031658000	-0.657803000
1	2.407800000	2.020894000	-0.337525000
1	2.437521000	0.873589000	-1.693951000
1	3.808038000	0.941131000	-0.582362000
1	-2.859814000	5.733405000	-0.405981000
6	-3.930699000	5.893336000	-0.243667000
6	-4.721584000	4.832053000	-0.977270000
6	-4.271969000	4.309004000	-2.197829000
6	-5.037041000	3.382298000	-2.907800000
6	-6.266726000	2.953958000	-2.404555000
6	-6.718402000	3.453642000	-1.182075000
6	-5.953190000	4.385452000	-0.480502000
6	-4.299293000	7.321330000	-0.680444000
1	-3.318408000	4.637462000	-2.604425000
1	-4.679768000	3.006424000	-3.862527000

1	-6.871100000	2.243545000	-2.960648000
1	-7.677710000	3.134098000	-0.785034000
1	-6.322866000	4.778372000	0.463505000
1	-4.098806000	5.794440000	0.833861000
1	-5.356989000	7.530388000	-0.497737000
1	-4.111266000	7.471198000	-1.747211000
1	-3.711694000	8.060702000	-0.128674000

³TS_{HA}:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.997814000
7	2.063826000	0.000000000	0.206522000
7	0.061871000	-0.178306000	-2.000151000
6	-1.037614000	-0.062727000	2.820804000
6	-0.917940000	0.096865000	4.211098000
6	0.318772000	0.348250000	4.755620000
6	1.451515000	0.417372000	3.912247000
6	2.763828000	0.662403000	4.384117000
6	3.815950000	0.698994000	3.501577000
6	3.608701000	0.489545000	2.119534000
6	2.342764000	0.259732000	1.629920000
6	1.247660000	0.224912000	2.516801000
1	-2.006601000	-0.246885000	2.374865000
1	-1.803040000	0.024182000	4.830564000
1	0.435873000	0.490704000	5.825727000
1	2.922824000	0.819956000	5.446134000
1	4.823548000	0.885297000	3.857319000
1	4.468758000	0.510818000	1.460346000
6	0.009770000	0.836305000	-2.851054000
6	-0.069605000	0.654791000	-4.242739000
6	-0.112785000	-0.621062000	-4.751451000
6	-0.062397000	-1.728619000	-3.871283000
6	-0.104969000	-3.075894000	-4.305215000
6	-0.050913000	-4.096990000	-3.857073000
6	0.051708000	-3.822710000	-2.004522000
6	0.089886000	-2.523759000	-1.548549000
6	0.031678000	-1.460555000	-2.476181000
1	0.032806000	1.825608000	-2.411135000
1	-0.100379000	1.524828000	-4.888313000
1	-0.184237000	-0.790737000	-5.821563000
1	-0.180591000	-3.287392000	-5.367210000
1	-0.084657000	-5.130043000	-3.716137000
1	0.100342000	-4.657252000	-1.314311000
7	0.207069000	-2.168244000	-0.128004000
6	1.602590000	-2.427519000	0.364302000
6	2.544365000	-1.377124000	-0.174102000
1	1.574188000	-2.409273000	1.454468000
1	1.936424000	-3.425554000	0.069367000
1	3.556064000	-1.537781000	0.204273000
1	2.595439000	-1.414281000	-1.262261000
6	-0.755405000	-2.952016000	0.696262000
1	-1.759576000	-2.840501000	0.294891000
1	-0.729054000	-2.589607000	1.721424000
1	-0.493622000	-4.011676000	0.707353000
8	-0.019320000	1.664294000	-0.101609000
7	-1.980440000	-0.160731000	-0.137880000
6	-3.114723000	-0.143341000	-0.319158000
6	-4.545335000	-0.108027000	-0.533147000
1	-4.920129000	0.885578000	-0.275878000
1	-5.037704000	-0.849251000	0.100986000
1	-4.778152000	-0.324743000	-1.578079000
6	2.748112000	1.014674000	-0.652266000
1	2.435452000	2.009213000	-0.347807000
1	2.474782000	0.846074000	-1.689744000
1	3.831652000	0.921625000	-0.566843000
1	-0.876250000	2.660765000	0.563505000
6	-1.445351000	3.541925000	1.027596000
6	-2.825148000	3.632474000	0.432229000
6	-3.019661000	3.939656000	-0.923898000

6	-4.299234000	4.023576000	-1.468488000
6	-5.421777000	3.804574000	-0.667631000
6	-5.247935000	3.499076000	0.681440000
6	-3.962990000	3.414059000	1.219845000
6	-0.575038000	4.787347000	0.836366000
1	-2.161824000	4.124189000	-1.563904000
1	-4.422343000	4.269366000	-2.519435000
1	-6.419791000	3.877946000	-1.089258000
1	-6.112543000	3.339541000	1.319557000
1	-3.841792000	3.195557000	2.277062000
1	-1.528095000	3.314587000	2.095713000
1	-1.037959000	5.669656000	1.290438000
1	-0.408367000	5.013199000	-0.219800000
1	0.405559000	4.649956000	1.300376000

⁵RC₁:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	2.085952000
7	2.210495000	0.000000000	0.399120000
7	0.077794000	-0.186253000	-2.020602000
6	-1.082083000	-0.025898000	2.854429000
6	-1.039667000	0.211548000	4.238421000
6	0.167467000	0.508377000	4.826315000
6	1.342675000	0.548620000	4.039372000
6	2.618634000	0.850907000	4.575591000
6	3.721518000	0.876007000	3.756290000
6	3.598407000	0.596068000	2.377281000
6	2.372698000	0.300702000	1.819770000
6	1.220590000	0.277111000	2.644414000
1	-2.024748000	-0.232794000	2.363918000
1	-1.958056000	0.171421000	4.812182000
1	0.230811000	0.716118000	5.889944000
1	2.708782000	1.062230000	5.636283000
1	4.700308000	1.109727000	4.160669000
1	4.491267000	0.619193000	1.762791000
6	-0.032032000	0.826479000	-2.875005000
6	-0.043130000	0.634294000	-4.265085000
6	0.066331000	-0.643893000	-4.766703000
6	0.194904000	-1.743221000	-3.883284000
6	0.323891000	-3.086081000	-4.314866000
6	0.457796000	-4.094536000	-3.390111000
6	0.466546000	-3.810764000	-2.005621000
6	0.323708000	-2.518046000	-1.549564000
6	0.193321000	-1.470311000	-2.485806000
1	-0.115943000	1.813673000	-2.437292000
1	-0.134765000	1.493494000	-4.918657000
1	0.058080000	-0.1818691000	-5.838160000
1	0.319935000	-3.303381000	-5.378034000
1	0.559904000	-5.124249000	-3.714443000
1	0.577577000	-4.634852000	-1.309152000
7	0.299023000	-2.156324000	-0.121302000
6	1.639283000	-2.409460000	0.524756000
6	2.662030000	-1.391280000	0.066749000
1	1.492089000	-2.359659000	1.604206000
1	1.982119000	-3.420834000	0.292049000
1	3.632988000	-1.601109000	0.524811000
1	2.798664000	-1.441169000	-1.014927000
6	-0.747344000	-2.944955000	0.603365000
1	-1.706521000	-2.816678000	0.108178000
1	-0.814540000	-2.591842000	1.630888000
1	-0.490135000	-4.005994000	0.620641000
8	-0.057767000	1.624929000	-0.064855000
7	-2.222458000	-0.195000000	-0.185342000
6	-3.344344000	0.037821000	-0.303570000
6	-4.764844000	0.302516000	-0.394652000
1	-4.965679000	1.296467000	-0.809154000
1	-5.199260000	0.238406000	0.602964000
1	-5.241040000	-0.447564000	-1.031206000
6	2.905016000	1.001069000	-0.460261000

1	2.582401000	2.000218000	-0.177513000
1	2.638965000	0.820605000	-1.500294000
1	3.991123000	0.924017000	-0.366712000
1	-5.076541000	7.275163000	-1.498722000
6	-6.081182000	7.044783000	-1.130006000
6	-6.437712000	5.615839000	-1.478852000
6	-5.962448000	5.003134000	-2.646387000
6	-6.354427000	3.707225000	-2.991857000
6	-7.232641000	2.998957000	-2.170036000
6	-7.700948000	3.597264000	-1.000008000
6	-7.307410000	4.888822000	-0.658536000
6	-7.080785000	8.065322000	-1.699731000
1	-5.288942000	5.550862000	-3.300748000
1	-5.985973000	3.259501000	-3.910549000
1	-7.565973000	2.000492000	-2.437467000
1	-8.389895000	3.063456000	-0.355415000
1	-7.691355000	5.342614000	0.252176000
1	-6.043658000	7.155709000	-0.041099000
1	-8.089876000	7.886481000	-1.317545000
1	-7.125855000	8.009982000	-2.790707000
1	-6.795475000	9.085005000	-1.425637000

⁵TS_{HA}:

26	0.115735000	-0.063531000	0.109478000
7	2.241229000	0.047894000	-0.183755000
7	0.471541000	2.195934000	0.016976000
7	-1.993537000	0.141619000	-0.113606000
6	3.047808000	-1.007624000	-0.325944000
6	4.452527000	-0.905023000	-0.258727000
6	5.025363000	0.332462000	-0.033172000
6	4.200991000	1.481665000	0.108762000
6	4.719696000	2.786748000	0.326109000
6	3.863554000	3.864054000	0.427927000
6	2.462397000	3.680576000	0.322032000
6	1.921149000	2.420688000	0.133557000
6	2.783557000	1.301110000	0.015534000
1	2.566913000	-1.962842000	-0.498535000
1	5.059639000	-1.793555000	-0.380435000
1	6.102887000	0.440195000	0.036667000
1	5.793358000	2.924423000	0.396809000
1	4.255276000	4.863032000	0.581531000
1	1.817979000	4.549901000	0.397663000
6	-2.825240000	0.049640000	0.930591000
6	-4.227604000	0.107766000	0.784428000
6	-4.771751000	0.259555000	-0.477524000
6	-3.920579000	0.354401000	-1.611512000
6	-4.407496000	0.508513000	-2.938440000
6	-3.523406000	0.600069000	-3.994337000
6	-2.125964000	0.545361000	-3.765527000
6	-1.616868000	0.389499000	-2.486479000
6	-2.507144000	0.290982000	-1.388271000
1	-2.351812000	-0.079817000	1.895760000
1	-4.859542000	0.031553000	1.660499000
1	-5.847242000	0.306997000	-0.616378000
1	-5.478142000	0.556635000	-3.108306000
1	-3.890066000	0.721014000	-5.007583000
1	-1.457894000	0.628115000	-4.616608000
7	-0.174391000	0.354142000	-2.210570000
6	0.437537000	1.713851000	-2.430152000
6	-0.003106000	2.673576000	-1.338090000
1	1.523335000	1.589436000	-2.430023000
1	0.151278000	2.109862000	-3.413869000
1	0.383991000	3.679602000	-1.542286000
1	-1.093674000	2.741591000	-1.297841000
6	0.526487000	-0.675961000	-3.047047000
1	0.038055000	-1.640014000	-2.910858000
1	1.564707000	-0.745971000	-2.720681000
1	0.512729000	-0.414391000	-4.112023000
8	0.103129000	-0.301338000	1.887029000

7	-0.095862000	-2.269841000	-0.384699000	1	3.564491000	-1.515400000	0.091681000
6	-0.351607000	-3.396183000	-0.292233000	1	2.531466000	-1.372971000	-1.325387000
6	-0.695976000	-4.805606000	-0.191153000	6	-0.711734000	-2.962618000	0.784174000
1	-0.399308000	-5.194410000	0.788260000	1	-1.735419000	-2.857043000	0.433033000
1	-0.191478000	-5.382690000	-0.973388000	1	-0.634192000	-2.587853000	1.802428000
1	-1.777059000	-4.937392000	-0.308668000	1	-0.447566000	-4.021786000	0.794269000
6	-0.294739000	2.855575000	1.128190000	8	-0.044531000	1.635472000	-0.079423000
1	0.074337000	2.479389000	2.080554000	7	-1.996086000	-0.228465000	-0.124931000
1	-1.347778000	2.593158000	1.022401000	6	-3.133684000	-0.307429000	-0.274690000
1	-0.200503000	3.946461000	1.091070000	6	-4.565656000	-0.437234000	-0.456446000
1	0.599319000	-0.807920000	2.872028000	1	-5.098334000	0.228416000	0.226766000
6	1.176145000	-1.199796000	4.046765000	1	-4.873520000	-1.466683000	-0.255293000
6	0.954141000	-2.636707000	4.069505000	1	-4.838946000	-0.183074000	-1.482875000
6	-0.234011000	-3.220570000	4.585680000	6	2.724421000	1.046026000	-0.629283000
6	-0.399263000	-4.603211000	4.586390000	1	2.408689000	2.027637000	-0.286575000
6	0.599785000	-5.437908000	4.055216000	1	2.437936000	0.911287000	-1.668596000
6	1.766037000	-4.876917000	3.506506000	1	3.809259000	0.954908000	-0.556223000
6	1.936102000	-3.496297000	3.504875000	1	0.093822000	4.632056000	-0.116079000
6	0.531088000	-0.265672000	5.047320000	6	-0.539937000	5.528211000	0.027799000
1	-1.010380000	-2.589133000	5.003312000	6	0.343107000	6.689669000	0.307905000
1	-1.296420000	-5.039367000	5.012453000	6	0.290413000	7.907480000	-0.435405000
1	0.475393000	-6.515318000	4.080747000	6	1.096446000	8.960398000	-0.088015000
1	2.544778000	-5.520552000	3.111142000	6	1.996284000	8.840463000	1.014278000
1	2.843871000	-3.059843000	3.097547000	6	2.073526000	7.639192000	1.760474000
1	2.198536000	-0.918783000	3.772905000	6	1.269540000	6.587142000	1.414543000
1	0.977277000	-0.423213000	6.039268000	6	-1.567525000	5.658570000	-1.090528000
1	-0.547358000	-0.423633000	5.144154000	1	-0.393744000	8.001654000	-1.269457000
1	0.696722000	0.779509000	4.771386000	1	1.058542000	9.893276000	-0.639296000
				1	2.626073000	9.682747000	1.281505000
				1	2.759311000	7.570620000	2.597181000
				1	1.300810000	5.657690000	1.974650000
				1	-1.040166000	5.297706000	0.982213000
				1	-2.253879000	6.491017000	-0.917680000
				1	-2.166470000	4.747927000	-1.138912000
				1	-1.098959000	5.802247000	-2.067533000

²RC₂:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.992671000
7	2.053110000	0.000000000	0.205467000
7	0.031067000	-0.216877000	-1.991615000
6	-1.047357000	-0.046478000	2.805865000
6	-0.929611000	0.063108000	4.201866000
6	0.314184000	0.246437000	4.760825000
6	1.453855000	0.314814000	3.923289000
6	2.772345000	0.513698000	4.402259000
6	3.825602000	0.565456000	3.519447000
6	3.616431000	0.408678000	2.129434000
6	2.345273000	0.214901000	1.636003000
6	1.250964000	0.174413000	2.521369000
1	-2.019637000	-0.174990000	2.349608000
1	-1.823883000	0.008415000	4.811315000
1	0.430198000	0.343945000	5.836016000
1	2.936105000	0.625052000	5.469288000
1	4.835863000	0.718971000	3.882403000
1	4.476876000	0.437465000	1.470868000
6	-0.022977000	0.788539000	-2.856800000
6	-0.136314000	0.588732000	-4.243336000
6	-0.217528000	-0.693985000	-4.734012000
6	-0.170278000	-1.790298000	-3.839756000
6	-0.252605000	-3.142501000	-4.254237000
6	-0.198493000	-4.152757000	-3.323160000
6	-0.052619000	-3.862266000	-1.947314000
6	0.026302000	-2.557480000	-1.510245000
6	-0.035232000	-1.506459000	-2.450071000
1	0.021722000	1.784480000	-2.434154000
1	-0.167956000	1.449446000	-4.901270000
1	-0.316925000	-0.875218000	-5.799700000
1	-0.358570000	-3.365677000	-5.310968000
1	-0.263221000	-5.188981000	-3.636234000
1	-0.002551000	-4.688512000	-1.247699000
7	0.207862000	-2.185282000	-0.099454000
6	1.630014000	-2.434090000	0.329417000
6	2.533477000	-1.363628000	-0.235670000
1	1.651018000	-2.428804000	1.420051000
1	1.960199000	-3.423533000	0.003387000

²TS_{HA}:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.981006000
7	2.056016000	0.000000000	0.187016000
7	0.030149000	-0.209359000	-1.998073000
6	-1.049198000	-0.037697000	2.800152000
6	-0.920577000	0.076057000	4.193462000
6	0.328564000	0.248812000	4.747995000
6	1.465850000	0.302915000	3.908575000
6	2.787655000	0.490986000	4.384408000
6	3.839240000	0.534567000	3.499499000
6	3.625003000	0.384845000	2.109953000
6	2.350282000	0.203384000	1.619710000
6	1.257246000	0.164765000	2.506372000
1	-2.027648000	-0.160436000	2.352211000
1	-1.810435000	0.028143000	4.809489000
1	0.448997000	0.344717000	5.822626000
1	2.955414000	0.600113000	5.450790000
1	4.851618000	0.680689000	3.859245000
1	4.483307000	0.412596000	1.448529000
6	-0.024612000	0.796208000	-2.863764000
6	-0.127581000	0.591889000	-4.250251000
6	-0.192681000	-0.692320000	-4.739697000
6	-0.141278000	-1.787796000	-3.844856000
6	-0.198891000	-3.142001000	-4.257809000
6	-0.136306000	-4.150624000	-3.325231000
6	-0.007703000	-3.856844000	-1.948392000
6	0.048135000	-2.549426000	-1.516064000
6	-0.021974000	-1.500786000	-2.454818000
1	0.007608000	1.793864000	-2.442897000
1	-0.159897000	1.451086000	-4.909501000
1	-0.281193000	-0.875648000	-5.805926000
1	-0.290062000	-3.368671000	-5.315147000

1	-0.178323000	-5.188046000	-3.638112000	6	-0.029316000	-3.887983000	-1.924692000
1	0.054006000	-4.681647000	-1.247856000	6	0.040824000	-2.579553000	-1.494552000
7	0.221899000	-2.168242000	-0.104588000	6	-0.040446000	-1.532639000	-2.435705000
6	1.645252000	-2.426367000	0.324920000	1	0.004168000	1.761899000	-2.437381000
6	2.542532000	-1.363285000	-0.252554000	1	-0.173793000	1.418763000	-4.901985000
1	1.670383000	-2.416698000	1.415187000	1	-0.318537000	-0.913638000	-5.789392000
1	1.964862000	-3.419257000	0.000471000	1	-0.356217000	-3.405623000	-5.289256000
1	3.575970000	-1.504689000	0.071020000	1	-0.234598000	-5.221480000	-3.609298000
1	2.536879000	-1.377368000	-1.342287000	1	0.042206000	-4.711352000	-1.223209000
6	-0.694825000	-2.953398000	0.778635000	7	0.232782000	-2.201664000	-0.083426000
1	-1.716420000	-2.867347000	0.418033000	6	1.662563000	-2.435824000	0.347896000
1	-0.626791000	-2.574952000	-1.795700000	6	2.548894000	-1.366379000	-0.240594000
1	-0.409622000	-4.006782000	0.791857000	1	1.686047000	-2.409305000	1.438158000
8	-0.059442000	1.654873000	-0.147778000	1	1.994216000	-3.428406000	0.031576000
7	-1.998492000	-0.209680000	-0.136619000	1	3.585612000	-1.501513000	0.077744000
6	-3.128203000	-0.257751000	-0.347456000	1	2.530820000	-1.376810000	-1.330078000
6	-4.552647000	-0.317330000	-0.600061000	6	-0.676398000	-2.982846000	0.816486000
1	-5.038701000	0.581562000	-0.211802000	1	-1.700329000	-2.899924000	0.460849000
1	-4.985109000	-1.194327000	-0.111292000	1	-0.601246000	-2.593037000	1.829210000
1	-4.739592000	-0.381618000	-1.675263000	1	-0.387981000	-4.036096000	0.836362000
6	2.730669000	1.045197000	-0.648897000	8	-0.097953000	1.670388000	-0.076335000
1	2.431703000	2.030677000	-0.306521000	7	-2.019999000	-0.260345000	-0.166780000
1	2.441698000	0.912986000	-1.687643000	6	-3.139774000	-0.331723000	-0.419267000
1	3.813836000	0.938366000	-0.576958000	6	-4.548051000	-0.419949000	-0.753803000
1	-0.272370000	2.772438000	0.733561000	1	-5.116995000	0.328993000	-0.195664000
6	-0.282752000	3.735958000	1.518175000	1	-4.935323000	-1.413155000	-0.509451000
6	-1.162824000	4.688327000	0.872472000	1	-4.686929000	-0.239591000	-1.824342000
6	-0.678414000	5.682650000	-0.035002000	6	2.737271000	1.053021000	-0.623298000
6	-1.531232000	6.634380000	-0.545220000	1	2.432962000	2.032962000	-0.267481000
6	-2.899509000	6.613549000	-0.200643000	1	2.449289000	0.925828000	-1.663665000
6	-3.410589000	5.616240000	0.655675000	1	3.821206000	0.948887000	-0.548616000
6	-2.565819000	4.657383000	1.163273000	1	-0.336565000	3.025677000	-0.056555000
6	1.177743000	4.085215000	1.762366000	6	-0.261045000	4.315391000	-0.032919000
1	0.370306000	5.704095000	-0.304754000	6	-1.596361000	4.748239000	0.294728000
1	-1.157623000	7.404461000	-1.210874000	6	-2.569138000	5.072791000	-0.704879000
1	-3.566368000	7.368576000	-0.603825000	6	-3.810194000	5.546212000	-0.342132000
1	-4.463936000	5.617453000	0.911735000	6	-4.139162000	5.695862000	1.023032000
1	-2.946198000	3.887644000	1.826880000	6	-3.210729000	5.354111000	2.027339000
1	-0.757296000	3.272273000	2.387700000	6	-1.970551000	4.871919000	1.674403000
1	1.244418000	4.901230000	2.489808000	6	0.392202000	4.672942000	-1.359297000
1	1.705070000	4.404293000	0.861629000	1	-2.321022000	4.968265000	-1.754198000
1	1.711708000	3.231234000	2.180707000	1	-4.536010000	5.816067000	-1.101143000
				1	-5.115318000	6.078927000	1.301196000
				1	-3.474300000	5.486739000	3.070696000
				1	-1.243288000	4.618237000	2.439114000
				1	0.425788000	4.388866000	0.816223000
				1	0.646702000	5.739801000	-1.366253000
				1	-0.243344000	4.486820000	-2.229110000
				1	1.324887000	4.121321000	-1.492188000

⁴TS_{HA}:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.984341000
7	2.062006000	0.000000000	0.207790000
7	0.021475000	-0.237571000	-1.985058000
6	-1.059396000	-0.028418000	2.789501000
6	-0.949940000	0.113144000	4.182664000
6	0.292349000	0.302271000	4.748548000
6	1.440478000	0.347366000	3.921494000
6	2.757957000	0.540959000	4.408210000
6	3.820120000	0.567663000	3.533530000
6	3.621003000	0.401384000	2.142674000
6	2.349985000	0.213990000	1.643598000
6	1.249660000	0.185408000	2.519136000
1	-2.029063000	-0.165530000	2.329344000
1	-1.847251000	0.070795000	4.788135000
1	0.399218000	0.415686000	5.822796000
1	2.915463000	0.663941000	5.474603000
1	4.829047000	0.713667000	3.902588000
1	4.486560000	0.421465000	1.490268000
6	-0.032555000	0.765718000	-2.855916000
6	-0.146173000	0.559767000	-4.240395000
6	-0.225609000	-0.727622000	-4.724332000
6	-0.181701000	-1.820649000	-3.825166000
6	-0.255090000	-3.176393000	-4.233574000
6	-0.183243000	-4.183785000	-3.299324000

UB3LYP-D3 optimized geometries in solvent:

³RC₁:

26	-0.206978000	-0.228835000	0.247973000
7	1.752286000	-0.251618000	0.479682000
7	-0.026444000	1.805549000	0.396538000
7	-2.150458000	-0.194834000	-0.126372000
6	2.546439000	-1.327699000	0.524002000
6	3.909213000	-1.234725000	0.876714000
6	4.448402000	-0.001343000	1.199751000
6	3.626193000	1.158707000	1.174881000
6	4.080568000	2.465415000	1.502576000
6	3.205819000	3.535318000	1.464582000
6	1.845280000	3.350338000	1.104086000
6	1.378208000	2.088721000	0.785202000
6	2.257287000	0.987811000	0.808305000
1	2.091174000	-2.277456000	0.287137000
1	4.511892000	-2.133746000	0.897808000
1	5.492223000	0.090811000	1.480038000
1	5.117391000	2.609762000	1.785592000
1	3.551747000	4.530737000	1.716153000
1	1.185631000	4.210428000	1.090485000
6	-3.099404000	-0.335631000	0.807219000
6	-4.463027000	-0.460869000	0.465901000
6	-4.836354000	-0.455282000	-0.867022000
6	-3.846924000	-0.322028000	-1.880644000
6	-4.130134000	-0.319131000	-3.274091000
6	-3.104564000	-0.192299000	-4.192343000
6	-1.757767000	-0.060299000	-3.763878000
6	-1.451824000	-0.063441000	-2.414940000
6	-2.487510000	-0.191625000	-1.463363000
1	-2.757454000	-0.354516000	1.833392000
1	-5.197180000	-0.564302000	1.254851000
1	-5.878424000	-0.524355000	-1.150660000
1	-5.157858000	-0.418719000	-3.604918000
1	-3.321324000	-0.190754000	-5.253954000
1	-0.978304000	0.043465000	-4.510378000
7	-0.080723000	0.085552000	-1.884419000
6	0.393228000	1.519726000	-2.018341000
6	-0.322053000	2.365999000	-0.985401000
1	1.472395000	1.524355000	-1.845706000
1	0.206465000	1.889365000	-3.032695000
1	-0.004282000	3.412475000	-1.035772000
1	-1.404503000	2.328939000	-1.125457000
6	0.881882000	-0.842262000	-2.573836000
1	0.490849000	-1.856734000	-2.525155000
1	1.840522000	-0.794354000	-2.059718000
1	1.025294000	-0.555720000	-3.620218000
8	-0.436591000	-0.370973000	1.882828000
7	-0.346284000	-2.193335000	-0.050796000
6	-0.588956000	-3.332905000	-0.014100000
6	-0.887757000	-4.752458000	0.012923000
1	-1.699763000	-4.941215000	0.725483000
1	-0.016107000	-5.317484000	0.356240000
1	-1.181670000	-5.106203000	-0.980606000
6	-0.988017000	2.381802000	1.408914000
1	-0.744138000	1.973986000	2.387907000
1	-1.998459000	2.089852000	1.130854000
1	-0.919451000	3.472826000	1.421740000
1	0.961086000	-2.265706000	2.735282000
6	0.989817000	-3.131429000	3.410783000
6	-0.309601000	-3.906369000	3.288977000
6	-1.533091000	-3.225164000	3.130883000
6	-2.742557000	-3.926675000	3.052654000
6	-2.751912000	-5.327059000	3.140316000
6	-1.542024000	-6.015272000	3.314354000
6	-0.333411000	-5.309640000	3.384761000
6	1.243109000	-2.627446000	4.849178000
1	-1.523487000	-2.140541000	3.086694000

1	-3.678645000	-3.386182000	2.945340000
1	-3.688312000	-5.873002000	3.097895000
1	-1.542132000	-7.096635000	3.404262000
1	0.597786000	-5.850384000	3.531078000
1	1.829688000	-3.767390000	3.097685000
1	1.296109000	-3.465218000	5.552097000
1	0.431061000	-1.967723000	5.174215000
1	2.184774000	-2.069825000	4.909697000

³TS_{HA}:

26	-0.200769000	0.098745000	0.050065000
7	1.757493000	-0.097578000	0.219871000
7	0.181403000	2.109319000	-0.084970000
7	-2.149216000	0.280012000	-0.256055000
6	2.456311000	-1.230449000	0.353276000
6	3.839639000	-1.228190000	0.632315000
6	4.500590000	-0.024199000	0.799195000
6	3.782598000	1.197855000	0.680500000
6	4.368197000	2.482100000	0.848736000
6	3.595058000	3.620248000	0.716544000
6	2.212105000	3.527888000	0.410514000
6	1.616379000	2.290599000	0.249068000
6	2.388908000	1.118219000	0.380097000
1	1.908766000	-2.156244000	0.263537000
1	4.360992000	-2.172499000	0.725138000
1	5.560968000	0.000015000	1.026620000
1	5.424380000	2.555374000	1.083571000
1	4.040186000	4.599417000	0.846479000
1	1.636754000	4.441102000	0.311199000
6	-3.064704000	0.358064000	0.716945000
6	-4.448422000	0.338222000	0.437619000
6	-4.878268000	0.226000000	-0.873126000
6	-3.926236000	0.130033000	-1.926524000
6	-4.270430000	0.001204000	-3.300012000
6	-3.279432000	-0.092638000	-4.259312000
6	-1.908384000	-0.061832000	-3.893008000
6	-1.543331000	0.054564000	-2.563904000
6	-2.543223000	0.160090000	-1.571440000
1	-2.677874000	0.425985000	1.725600000
1	-5.153313000	0.407974000	1.256452000
1	-5.936704000	0.206270000	-1.109222000
1	-5.317091000	-0.023250000	-3.582987000
1	-3.542314000	-0.189175000	-5.306012000
1	-1.156766000	-0.134634000	-4.671097000
7	-0.139458000	0.107933000	-2.100874000
6	0.487368000	1.445562000	-2.443994000
6	-0.085323000	2.505848000	-1.526477000
1	1.566270000	1.345216000	-2.300598000
1	0.305264000	1.691928000	-3.495941000
1	0.352437000	3.488625000	-1.729464000
1	-1.168651000	2.582077000	-1.644173000
6	0.677045000	-1.007639000	-2.691779000
1	0.177275000	-1.954039000	-2.495019000
1	1.659609000	-1.007236000	-2.224950000
1	0.799385000	-0.878780000	-3.771653000
8	-0.400307000	0.243532000	1.717369000
7	-0.514829000	-1.864609000	0.064797000
6	-0.794492000	-2.987819000	0.196056000
6	-1.136359000	-4.388791000	0.356354000
1	-0.936604000	-4.700664000	1.387994000
1	-0.536763000	-5.010788000	-0.316459000
1	-2.196421000	-4.550803000	0.134596000
6	-0.691147000	2.914346000	0.846953000
1	-0.462567000	2.623025000	1.870076000
1	-1.732070000	2.688151000	0.626201000
1	-0.518491000	3.984668000	0.705321000
1	0.440392000	-0.752213000	2.779553000
6	1.086841000	-1.307518000	3.520084000
6	0.829826000	-2.793473000	3.423919000

6	-0.352923000	-3.368628000	3.933694000
6	-0.556000000	-4.753777000	3.896167000
6	0.413072000	-5.597170000	3.329442000
6	1.583163000	-5.039400000	2.795197000
6	1.785246000	-3.654418000	2.844032000
6	0.826122000	-0.686778000	4.903682000
1	-1.101572000	-2.735023000	4.398203000
1	-1.456816000	-5.178248000	4.328002000
1	0.265928000	-6.672053000	3.322421000
1	2.347136000	-5.684494000	2.372589000
1	2.720877000	-3.237193000	2.480705000
1	2.120678000	-1.096393000	3.214333000
1	1.457650000	-1.157175000	5.665926000
1	-0.216748000	-0.806080000	5.215035000
1	1.048260000	0.385570000	4.890520000

⁵RC₁:

26	-0.591313000	0.292347000	-0.325337000
7	-0.639867000	0.722471000	1.675802000
7	1.586208000	0.693538000	0.010516000
7	-0.443862000	-0.281643000	-2.240182000
6	-1.744197000	0.694304000	2.432384000
6	-1.772553000	1.234958000	3.733784000
6	-0.634255000	1.836878000	4.240143000
6	0.552214000	1.889705000	3.457632000
6	1.757820000	2.494331000	3.905885000
6	2.873458000	2.508809000	3.091142000
6	2.833053000	1.918203000	1.802884000
6	1.674134000	1.324497000	1.333726000
6	0.517541000	1.304969000	2.153026000
1	-2.623609000	0.253937000	1.983446000
1	-2.687903000	1.185753000	4.309291000
1	-0.635239000	2.276526000	5.231839000
1	1.788079000	2.942672000	4.892636000
1	3.791978000	2.971778000	3.431424000
1	3.725377000	1.940801000	1.187455000
6	-0.684243000	0.517457000	-3.290306000
6	-0.621579000	0.034286000	-4.612467000
6	-0.305823000	-1.297048000	-4.838357000
6	-0.052472000	-2.167845000	-3.742437000
6	0.275532000	-3.545108000	-3.876281000
6	0.505200000	-4.317138000	-2.752147000
6	0.417314000	-3.753318000	-1.452617000
6	0.098048000	-2.416650000	-1.293078000
6	-0.136335000	-1.614484000	-2.428901000
1	-0.928181000	1.546311000	-3.057081000
1	-0.818687000	0.711024000	-5.434083000
1	-0.249822000	-1.686124000	-5.849341000
1	0.342530000	-3.979687000	-4.867517000
1	0.755201000	-5.366402000	-2.854098000
1	0.601589000	-4.386146000	-0.591508000
7	-0.008519000	-1.751029000	0.025088000
6	1.347905000	-1.669182000	0.707024000
6	2.232714000	-0.669530000	-0.018766000
1	1.169065000	-1.354610000	1.737450000
1	1.813916000	-2.660439000	0.728960000
1	3.229260000	-0.630768000	0.436700000
1	2.351300000	-0.952041000	-1.068419000
6	-0.996225000	-2.465119000	0.912402000
1	-1.948422000	-2.535815000	0.390647000
1	-1.121806000	-1.885279000	1.825738000
1	-0.635823000	-3.466084000	1.168445000
8	-0.874058000	1.868669000	-0.736163000
7	-2.818217000	-0.237628000	-0.445132000
6	-3.916085000	-0.087454000	-0.820105000
6	-5.278210000	0.094622000	-1.286999000
1	-5.318099000	0.939307000	-1.984459000
1	-5.937536000	0.334443000	-0.447625000
1	-5.641934000	-0.810754000	-1.783653000

6	2.094784000	1.581140000	-1.087396000
1	1.581600000	2.539453000	-1.020748000
1	1.858865000	1.114177000	-2.043905000
1	3.177668000	1.725567000	-1.016986000
1	-2.540206000	2.659288000	0.782784000
6	-3.453352000	3.223035000	1.007514000
6	-4.311703000	3.287283000	-0.240557000
6	-3.716478000	3.317363000	-1.516888000
6	-4.502621000	3.431131000	-2.671314000
6	-5.898784000	3.518584000	-2.567313000
6	-6.500983000	3.494726000	-1.301327000
6	-5.712708000	3.378085000	-0.149943000
6	-3.055932000	4.620022000	1.532162000
1	-2.633944000	3.269487000	-1.596080000
1	-4.030162000	3.473569000	-3.648330000
1	-6.507894000	3.624257000	-3.458799000
1	-7.579159000	3.578592000	-1.212657000
1	-6.185493000	3.376043000	0.828697000
1	-3.991030000	2.680878000	1.798954000
1	-3.942634000	5.210181000	1.785621000
1	-2.493530000	5.171493000	0.770806000
1	-2.431132000	4.538202000	2.429967000

⁵TS_{HA}:

26	0.002172000	-0.003544000	0.012880000
7	2.150766000	0.003302000	-0.000789000
7	0.479463000	2.235736000	0.005032000
7	-2.043307000	0.319169000	-0.493380000
6	2.915995000	-1.090179000	-0.059481000
6	4.303716000	-1.060394000	0.188564000
6	4.902883000	0.143304000	0.508945000
6	4.124627000	1.331408000	0.565921000
6	4.674516000	2.605853000	0.870890000
6	3.866447000	3.724367000	0.880491000
6	2.483581000	3.613968000	0.591385000
6	1.910277000	2.385414000	0.312994000
6	2.724115000	1.224707000	0.288054000
1	2.415185000	-2.016750000	-0.312810000
1	4.877120000	-1.977126000	0.127838000
1	5.966483000	0.194904000	0.717731000
1	5.735809000	2.687993000	1.079628000
1	4.283684000	4.700331000	1.100440000
1	1.878352000	4.514182000	0.598482000
6	-3.015338000	0.262710000	0.424415000
6	-4.378923000	0.399607000	0.087233000
6	-4.734553000	0.594148000	-1.234643000
6	-3.731262000	0.653590000	-2.239017000
6	-4.021979000	0.848359000	-3.617379000
6	-2.997762000	0.902277000	-4.540851000
6	-1.650204000	0.768146000	-4.123912000
6	-1.331397000	0.570647000	-2.790146000
6	-2.367429000	0.509761000	-1.824802000
1	-2.687744000	0.097897000	1.443151000
1	-5.129538000	0.349583000	0.866102000
1	-5.776416000	0.702230000	-1.519432000
1	-5.054875000	0.957440000	-3.931592000
1	-3.214878000	1.053990000	-5.592383000
1	-0.867948000	0.822980000	-4.874022000
7	0.055788000	0.454479000	-2.322263000
6	0.759071000	1.782502000	-2.432828000
6	0.220532000	2.751347000	-1.394023000
1	1.827201000	1.601752000	-2.288493000
1	0.629087000	2.203664000	-3.438969000
1	0.682023000	3.737878000	-1.526056000
1	-0.860366000	2.875722000	-1.502660000
6	0.809084000	-0.601680000	-3.076840000
1	0.257169000	-1.539440000	-3.026953000
1	1.788380000	-0.732098000	-2.615082000
1	0.953644000	-0.326402000	-4.128620000

8	-0.265498000	-0.259818000	1.770849000	1	-0.222253000	3.294009000	-4.188041000
7	-0.251604000	-2.185135000	-0.564576000	1	-1.024908000	2.555576000	-1.916062000
6	-0.570993000	-3.298652000	-0.539460000	1	-2.033392000	1.830725000	-3.182261000
6	-0.992893000	-4.690462000	-0.528598000	6	1.176627000	1.409646000	-5.807926000
1	-0.848668000	-5.117007000	0.469169000	1	1.097491000	0.729111000	-6.655852000
1	-0.416533000	-5.273522000	-1.254806000	1	2.041029000	1.142130000	-5.201319000
1	-2.053540000	-4.763370000	-0.792574000	1	1.304147000	2.434333000	-6.174393000
6	-0.391950000	2.923346000	1.017234000	8	-0.549822000	-2.061201000	-3.194845000
1	-0.170354000	2.519316000	2.003270000	7	0.204621000	-1.575840000	-5.675019000
1	-1.433777000	2.716892000	0.770320000	6	0.334278000	-2.286289000	-6.584945000
1	-0.239146000	4.008194000	1.010404000	6	0.496402000	-3.188818000	-7.713588000
1	0.062107000	-0.802176000	2.809653000	1	0.480596000	-4.228717000	-7.367674000
6	0.448793000	-1.240869000	4.043068000	1	1.449865000	-3.006031000	-8.220800000
6	0.144877000	-2.662466000	4.000756000	1	-0.315092000	-3.049444000	-8.436537000
6	-1.134588000	-3.183538000	4.333275000	6	-1.846796000	-0.129117000	-1.527535000
6	-1.375767000	-4.553918000	4.277238000	1	-1.580318000	-1.138387000	-1.220663000
6	-0.360946000	-5.437485000	3.869186000	1	-2.709354000	-0.165779000	-2.188886000
6	0.899558000	-4.937313000	3.499166000	1	-2.087067000	0.486296000	-0.655987000
6	1.145551000	-3.569239000	3.555014000	1	1.318578000	3.490314000	19.667900000
6	-0.276607000	-0.285464000	4.965226000	6	1.656678000	2.444040000	19.814251000
1	-1.925135000	-2.514222000	4.654059000	6	1.593519000	2.161787000	21.275092000
1	-2.346692000	-4.943325000	4.564135000	6	0.879348000	1.042186000	21.822565000
1	-0.548196000	-6.505917000	3.850666000	6	0.858722000	0.834523000	23.184489000
1	1.688373000	-5.619248000	3.199537000	6	1.554471000	1.734728000	24.061176000
1	2.123813000	-3.180517000	3.286021000	6	2.268305000	2.851275000	23.542111000
1	1.513614000	-1.016730000	3.919968000	6	2.290783000	3.062076000	22.181705000
1	0.019401000	-0.481248000	6.005310000	6	0.910403000	1.499075000	18.866559000
1	-1.365048000	-0.383694000	4.909876000	1	0.356045000	0.366538000	21.157170000
1	-0.018360000	0.752289000	4.736395000	1	0.319129000	-0.005824000	23.607794000

²RC₂:

26	-0.255121000	-0.626909000	-3.969302000
7	1.604910000	-0.595773000	-3.299738000
7	-0.684188000	0.461882000	-2.289987000
7	-2.089961000	-0.526593000	-4.707464000
6	2.676629000	-1.162071000	-3.866025000
6	3.925909000	-1.216378000	-3.212992000
6	4.056156000	-0.681043000	-1.942211000
6	2.931492000	-0.087663000	-1.306712000
6	2.960657000	0.484093000	-0.005531000
6	1.814641000	1.029889000	0.542087000
6	0.592667000	1.027025000	-0.180207000
6	0.539996000	0.480538000	-1.450357000
6	1.700021000	-0.071143000	-2.027967000
1	2.540628000	-1.584391000	-4.851155000
1	4.764123000	-1.683342000	-3.714052000
1	5.006978000	-0.715650000	-1.420743000
1	3.892571000	0.487472000	0.549578000
1	1.851670000	1.479915000	1.528171000
1	-0.287793000	1.464389000	0.276825000
6	-3.024765000	-1.468228000	-4.527468000
6	-4.265631000	-1.420183000	-5.198028000
6	-4.525975000	-0.385325000	-6.078999000
6	-3.544188000	0.619672000	-6.302608000
6	-3.712093000	1.709137000	-7.200044000
6	-2.700865000	2.637679000	-7.363316000
6	-1.483883000	2.521631000	-6.641380000
6	-1.289624000	1.469380000	-5.765537000
6	-2.314386000	0.514307000	-5.583496000
1	-2.767742000	-2.269992000	-3.847308000
1	-4.994640000	-2.199382000	-5.015239000
1	-5.472247000	-0.332334000	-6.606781000
1	-4.640782000	1.800132000	-7.753069000
1	-2.829990000	3.468009000	-8.046940000
1	-0.713334000	3.270043000	-6.789862000
7	-0.061515000	1.284232000	-4.961998000
6	-0.014539000	2.283086000	-3.818873000
6	-1.024071000	1.865705000	-2.767515000
1	0.999618000	2.270150000	-3.411907000

²TS_{HA}:

26	-0.120035000	-0.110440000	-0.215900000
7	1.853272000	-0.163175000	-0.149183000
7	0.099864000	1.908083000	0.039939000
7	-2.083955000	-0.027610000	-0.462500000
6	2.641933000	-1.238665000	-0.270016000
6	4.037613000	-1.166137000	-0.077904000
6	4.618614000	0.044985000	0.261652000
6	3.804863000	1.201834000	0.415077000
6	4.302233000	2.484923000	0.775756000
6	3.435648000	3.555978000	0.902842000
6	2.043085000	3.397123000	0.672878000
6	1.534912000	2.158488000	0.325234000
6	2.401545000	1.055301000	0.192497000
1	2.158650000	-2.170569000	-0.524066000
1	4.636287000	-2.059752000	-0.202833000
1	5.690347000	0.121922000	0.412093000
1	5.365931000	2.612947000	0.944380000
1	3.814981000	4.534175000	1.173718000
1	1.395219000	4.260670000	0.772322000
6	-2.975209000	-0.203748000	0.523313000
6	-4.359996000	-0.279875000	0.269330000
6	-4.821176000	-0.189346000	-1.033805000
6	-3.897846000	-0.020499000	-2.102233000
6	-4.275017000	0.065474000	-3.470859000
6	-3.310910000	0.222897000	-4.449020000
6	-1.935539000	0.307422000	-4.106954000
6	-1.538872000	0.223237000	-2.783357000
6	-2.509227000	0.059492000	-1.772178000
1	-2.567243000	-0.293375000	1.521364000
1	-5.043915000	-0.413463000	1.098052000
1	-5.882292000	-0.250296000	-1.250422000

1	-5.324842000	0.006084000	-3.735335000	6	1.072381000	-3.181229000	-3.916055000
1	-3.598792000	0.288342000	-5.491493000	6	0.766529000	-4.049725000	-2.834394000
1	-1.208859000	0.440944000	-4.900333000	6	0.962628000	-3.633188000	-1.528502000
7	-0.130559000	0.336363000	-2.335257000	6	1.477140000	-2.344647000	-1.275982000
6	0.335162000	1.781501000	-2.412278000	1	2.254574000	-0.508097000	1.378145000
6	-0.299450000	2.557588000	-1.278890000	1	2.786134000	1.187053000	-0.417423000
1	1.424604000	1.780928000	-2.326876000	1	2.498258000	0.538233000	-2.815079000
1	0.069832000	2.212325000	-3.383503000	1	1.796044000	-1.247451000	-4.513138000
1	0.017457000	3.605299000	-1.281317000	1	0.910821000	-3.526738000	-4.930606000
1	-1.389329000	2.528345000	-1.335877000	1	0.374583000	-5.038496000	-3.049177000
6	0.783228000	-0.534759000	-3.158662000	7	0.664124000	-4.474217000	-0.347388000
1	0.390740000	-1.549462000	-3.172431000	6	1.611667000	-5.661348000	-0.273783000
1	1.775483000	-0.527454000	-2.711178000	6	2.999202000	-5.186432000	0.121681000
1	0.858971000	-0.164444000	-4.185208000	1	1.208073000	-6.348271000	0.473660000
8	-0.242209000	-0.362041000	1.422172000	1	1.633431000	-6.181208000	-1.238629000
7	-0.314067000	-2.057401000	-0.655578000	1	3.707799000	-6.023436000	0.133316000
6	-0.576116000	-3.174793000	-0.859093000	1	3.368631000	-4.439280000	-0.586682000
6	-0.907766000	-4.569445000	-1.109915000	6	-0.766668000	-4.950490000	-0.370452000
1	-0.470131000	-5.212849000	-0.338598000	1	-1.422455000	-4.086054000	-0.463564000
1	-0.526269000	-4.888656000	-2.086268000	1	-0.973720000	-5.470181000	0.564426000
1	-1.994769000	-4.708444000	-1.100818000	1	-0.934969000	-5.635455000	-1.207795000
6	-0.771286000	2.434771000	1.154388000	8	1.553686000	-2.336825000	2.667734000
1	-0.449833000	1.978304000	2.087795000	7	-0.966895000	-2.238035000	1.319035000
1	-1.803353000	2.161561000	0.947284000	6	-1.749768000	-1.385694000	1.482081000
1	-0.693312000	3.523416000	1.215823000	6	-2.730301000	-0.331866000	1.694026000
1	0.824772000	-0.524697000	3.229404000	1	-2.519269000	0.198848000	2.629010000
6	1.604455000	-0.320256000	4.005666000	1	-3.738969000	-0.754098000	1.753067000
6	1.217135000	-1.004725000	5.271513000	1	-2.703655000	0.387939000	0.868589000
6	0.344092000	-0.382682000	6.238673000	6	4.108012000	-3.627782000	1.728690000
6	0.038129000	-1.022583000	7.419794000	1	3.992941000	-3.176530000	2.714150000
6	0.576531000	-2.321213000	7.687777000	1	4.104737000	-2.842125000	0.971417000
6	1.425737000	-2.966019000	6.735977000	1	5.052908000	-4.178582000	1.672448000
6	1.729637000	-2.327219000	5.555002000	1	-2.748340000	19.419068000	-3.900108000
6	1.784785000	1.1211936000	4.084703000	6	-3.505420000	19.413116000	-3.109297000
1	-0.057357000	0.602275000	6.036630000	6	-4.567460000	20.411203000	-3.377594000
1	-0.605149000	-0.553235000	8.155166000	6	-5.340017000	20.966410000	-2.287505000
1	0.335201000	-2.821593000	8.620375000	6	-6.341592000	21.878343000	-2.535141000
1	1.828146000	-3.947447000	6.958748000	6	-6.626578000	22.264492000	-3.881412000
1	2.381933000	-2.798965000	4.828376000	6	-5.884937000	21.716590000	-4.975623000
1	2.513158000	-0.790364000	3.607198000	6	-4.883009000	20.804241000	-4.730943000
1	2.522916000	1.485689000	4.844604000	6	-4.138989000	17.965023000	-3.038655000
1	0.848973000	1.731496000	4.314215000	1	-5.105577000	20.658797000	-1.273988000
1	2.139325000	1.581924000	3.118698000	1	-6.916644000	22.308589000	-1.723021000

⁴RC₂:

26	1.082666000	-3.298449000	1.407812000
7	0.435833000	-4.765390000	2.673745000
7	2.933474000	-4.529267000	1.479145000
7	1.674839000	-1.960961000	0.036268000
6	-0.789869000	-4.827351000	3.209571000
6	-1.115002000	-5.746082000	4.227730000
6	-0.135347000	-6.597986000	4.708436000
6	1.178849000	-6.546253000	4.169988000
6	2.239631000	-7.379967000	4.617014000
6	3.494436000	-7.271996000	4.050592000
6	3.740287000	-6.334383000	3.014846000
6	2.730548000	-5.506494000	2.557401000
6	1.437165000	-5.599457000	3.128523000
1	-1.518734000	-4.127073000	2.825642000
1	-2.121423000	-5.765428000	4.625507000
1	-0.357351000	-7.305831000	5.500291000
1	2.049279000	-8.097942000	5.407199000
1	4.303849000	-7.904998000	4.393294000
1	4.734433000	-6.273281000	2.586261000
6	2.137363000	-0.734654000	0.325041000
6	2.438907000	0.197133000	-0.689900000
6	2.268378000	-0.162821000	-2.019333000
6	1.781135000	-1.457121000	-2.353418000
6	1.567352000	-1.910020000	-3.685127000

⁴TS_{HA}:

26	-0.051309000	-0.038438000	-0.001092000
7	1.969656000	0.022509000	0.039402000
7	0.188828000	2.155062000	0.031026000
7	-2.029831000	-0.009727000	-0.220904000
6	2.776605000	-1.049231000	0.002661000
6	4.173463000	-0.934409000	0.139799000
6	4.734722000	0.318426000	0.334700000
6	3.903481000	1.470237000	0.392430000
6	4.403654000	2.785926000	0.595995000
6	3.536105000	3.861324000	0.632279000
6	2.141222000	3.670567000	0.456732000
6	1.620599000	2.403171000	0.256480000
6	2.492447000	1.286847000	0.228865000
1	2.299171000	-2.008622000	-0.142589000
1	4.789233000	-1.823126000	0.081561000
1	5.808799000	0.431721000	0.438137000
1	5.472073000	2.932971000	0.709492000

1	3.916888000	4.864882000	0.779180000
1	1.488639000	4.536544000	0.468816000
6	-2.909400000	-0.088881000	0.792906000
6	-4.291271000	-0.196766000	0.560767000
6	-4.765722000	-0.238933000	-0.745144000
6	-3.859994000	-0.163962000	-1.836634000
6	-4.252268000	-0.209239000	-3.203503000
6	-3.298952000	-0.125991000	-4.202962000
6	-1.922499000	0.013905000	-3.884438000
6	-1.515502000	0.056369000	-2.560278000
6	-2.468572000	-0.037425000	-1.531618000
1	-2.485334000	-0.073474000	1.788656000
1	-4.969056000	-0.251029000	1.403111000
1	-5.828662000	-0.329378000	-0.942081000
1	-5.302902000	-0.310517000	-3.452219000
1	-3.596082000	-0.161634000	-5.244331000
1	-1.206520000	0.090197000	-4.695123000
7	-0.104311000	0.239868000	-2.137257000
6	0.349396000	1.677094000	-2.382511000
6	-0.253661000	2.601145000	-1.346730000
1	1.440692000	1.682817000	-2.329838000
1	0.059196000	1.978134000	-3.394504000
1	0.049595000	3.638466000	-1.528624000
1	-1.345580000	2.560332000	-1.367800000
6	0.814599000	-0.695296000	-2.888672000
1	0.425498000	-1.708003000	-2.825778000
1	1.808407000	-0.644775000	-2.448910000
1	0.882694000	-0.397926000	-3.939016000
8	-0.202930000	-0.131962000	1.685000000
7	-0.151600000	-2.222376000	-0.373579000
6	-0.432062000	-3.344408000	-0.541435000
6	-0.786880000	-4.737766000	-0.765766000
1	-0.441974000	-5.359903000	0.067229000
1	-0.330054000	-5.108421000	-1.690612000
1	-1.873869000	-4.845741000	-0.854762000
6	-0.675039000	2.762911000	1.099808000
1	-0.325045000	2.416141000	2.069979000
1	-1.701418000	2.431349000	0.946009000
1	-0.644279000	3.856123000	1.056053000
1	0.719223000	-0.310540000	2.755635000
6	1.550026000	-0.283251000	3.674024000
6	0.956548000	-1.103307000	4.717192000
6	0.096770000	-0.548814000	5.726856000
6	-0.384470000	-1.342708000	6.750992000
6	-0.057483000	-2.722693000	6.793069000
6	0.755091000	-3.302124000	5.786537000
6	1.237432000	-2.514940000	4.758116000
6	1.786392000	1.207480000	3.908715000
1	-0.154581000	0.503945000	5.698332000
1	-1.009832000	-0.917145000	7.527246000
1	-0.438741000	-3.340702000	7.599228000
1	0.998708000	-4.357010000	5.834829000
1	1.868597000	-2.945799000	3.987699000
1	2.399666000	-0.777597000	3.187411000
1	2.541209000	1.349260000	4.692165000
1	0.879792000	1.736188000	4.217582000
1	2.157066000	1.680843000	2.996993000