

Electronic Supporting Information

Dramatic rate-enhancement of oxygen atom transfer by an iron(IV)-oxo species by equatorial ligand field perturbations

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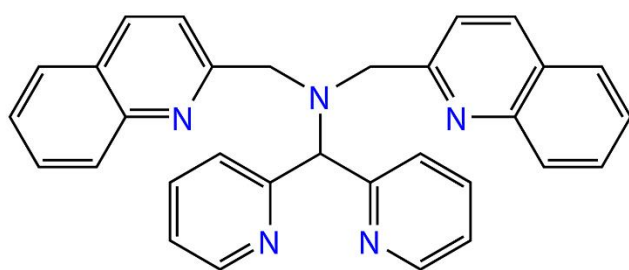
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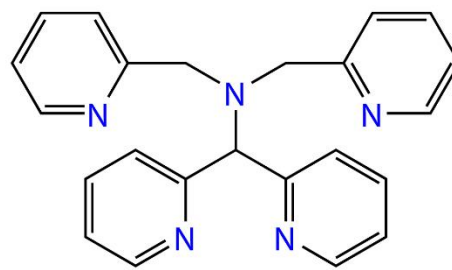
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Part I: Ligands and complexes studied.



2PyN2Q



N4Py

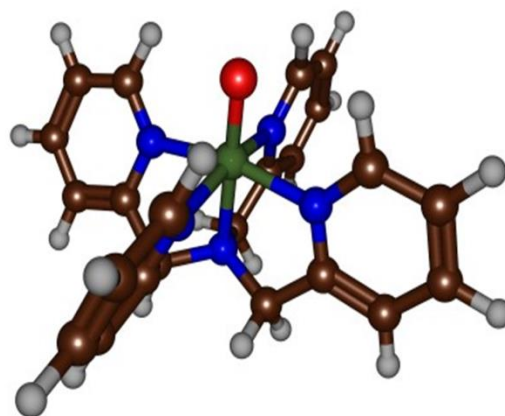
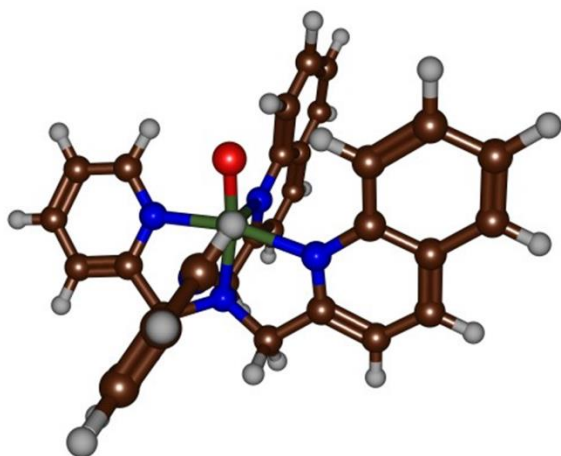


Fig. S1. Ligand frameworks under study and DFT optimised structures of the corresponding iron(IV)-oxo complexes.

Part II: Experimental data.

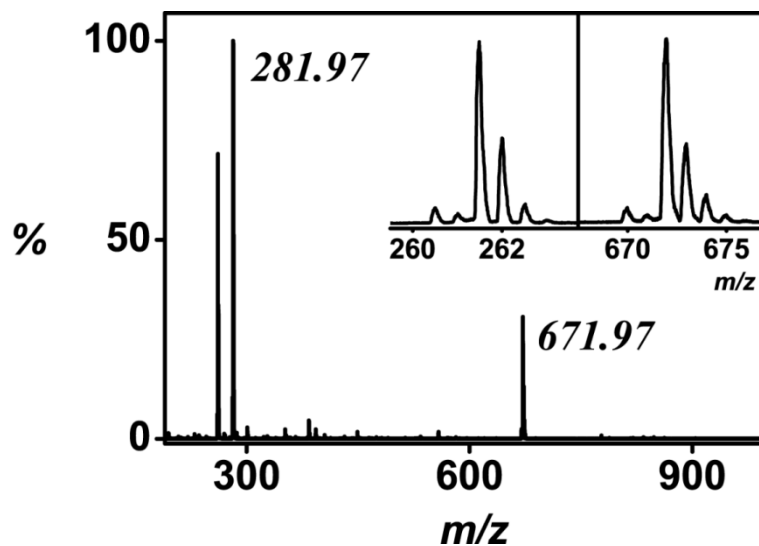


Fig. S2. Electrospray Ionization mass spectra of **1a**, in CH₃CN at 298 K. The peaks at m/z 261.49, 281.97 and 671.97 are assigned to $[\text{Fe}^{\text{II}}(2\text{PyN2Q})]^{2+}$, $[\text{Fe}^{\text{II}}(2\text{PyN2Q})(\text{CH}_3\text{CN})]^{2+}$ and $[\text{Fe}^{\text{II}}(2\text{PyN2Q})(\text{OTf})]^+$ respectively. Inset shows the observed isotopic distribution pattern of m/z 261.49 and 671.97.

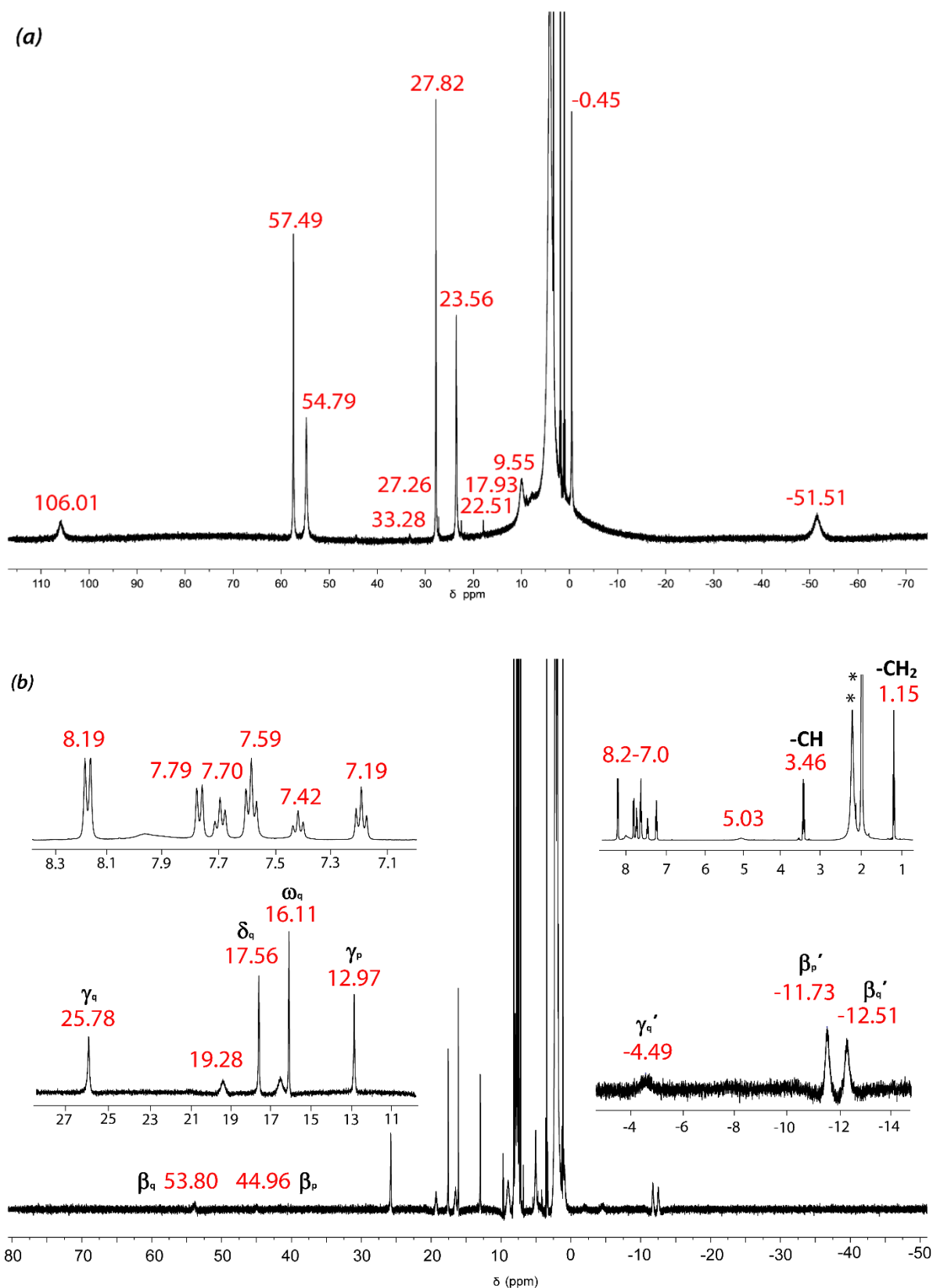


Fig. S3. ^1H -NMR spectrum of complex (a) **1a** and (b) **1b** in CD_3CN at 298 K with a spectral width of ~ 200 ppm (no. of scans = 82 and 64 respectively). Inset shows the individual expanded portions of the spectrum. Solvent peaks are denoted by (*). The peaks have been assigned based on previous reported literature (see Ref. 10a, 13b, 20 in main text).

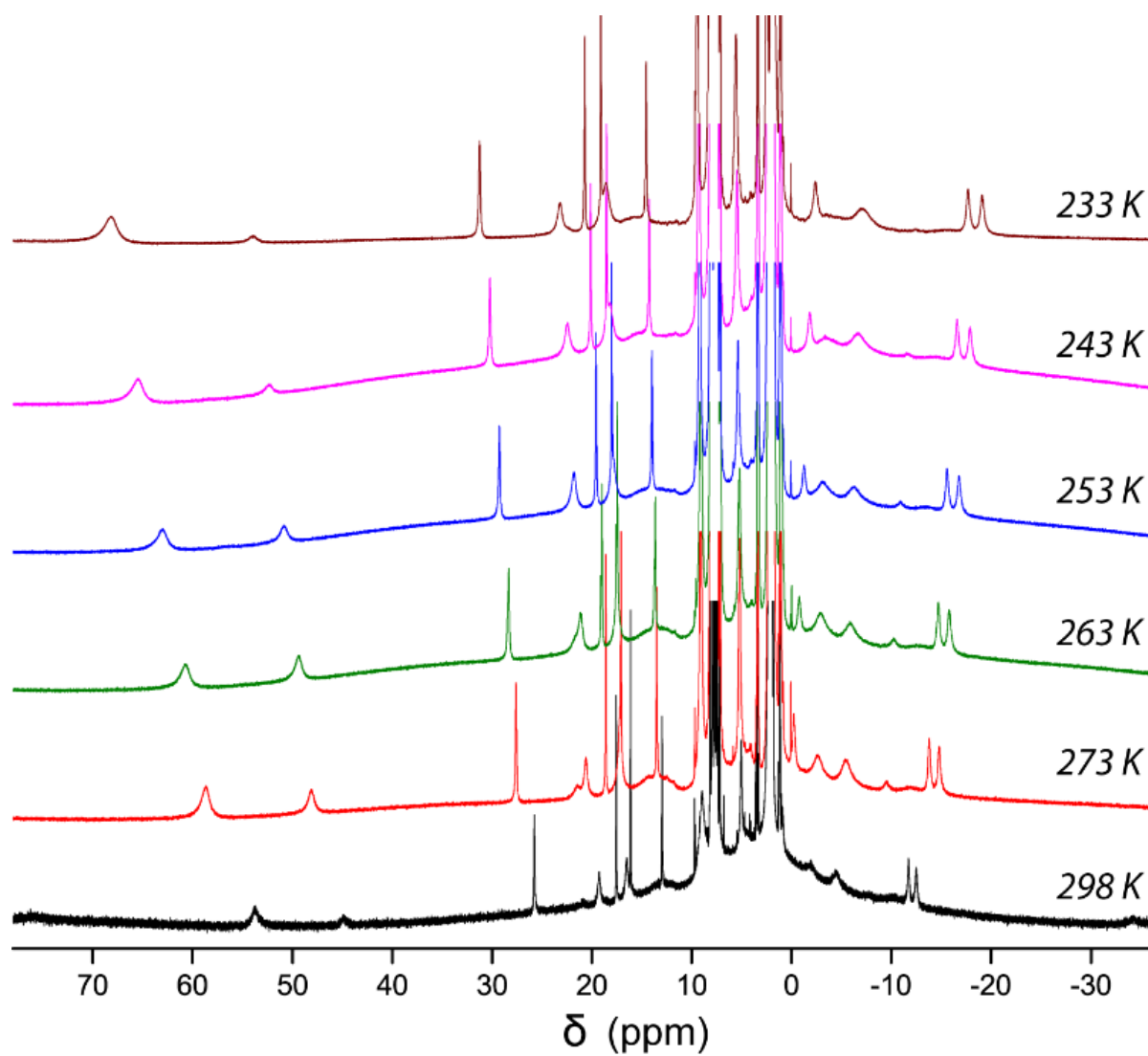


Fig. S4. VT-NMR spectrum of complex **1b** in CD₃CN recorded within the temperature range of 25 °C and -40 °C.

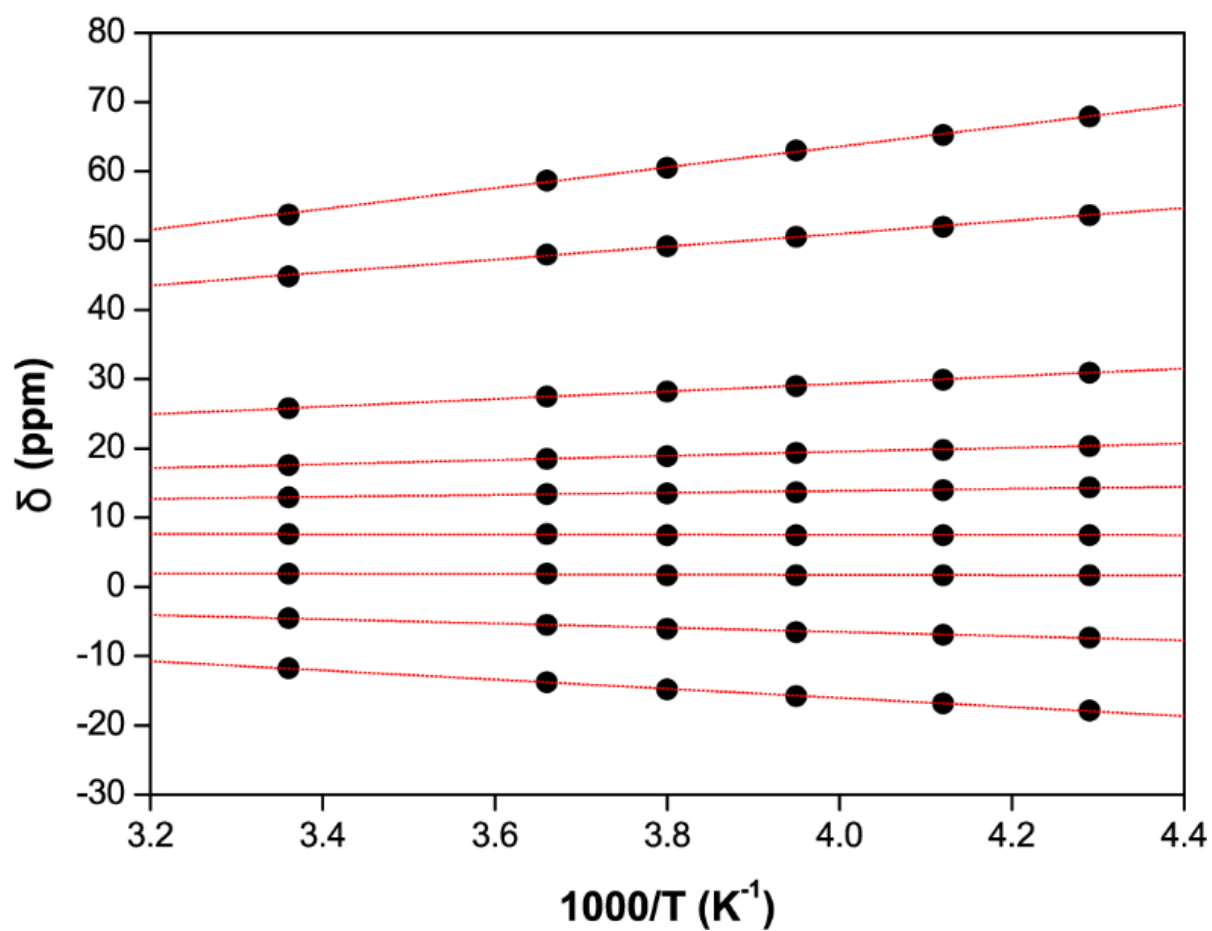


Fig. S5. Curie plot showing the linear dependence of chemical shift of the ^1H -NMR signals of **1b** as a function of temperature.

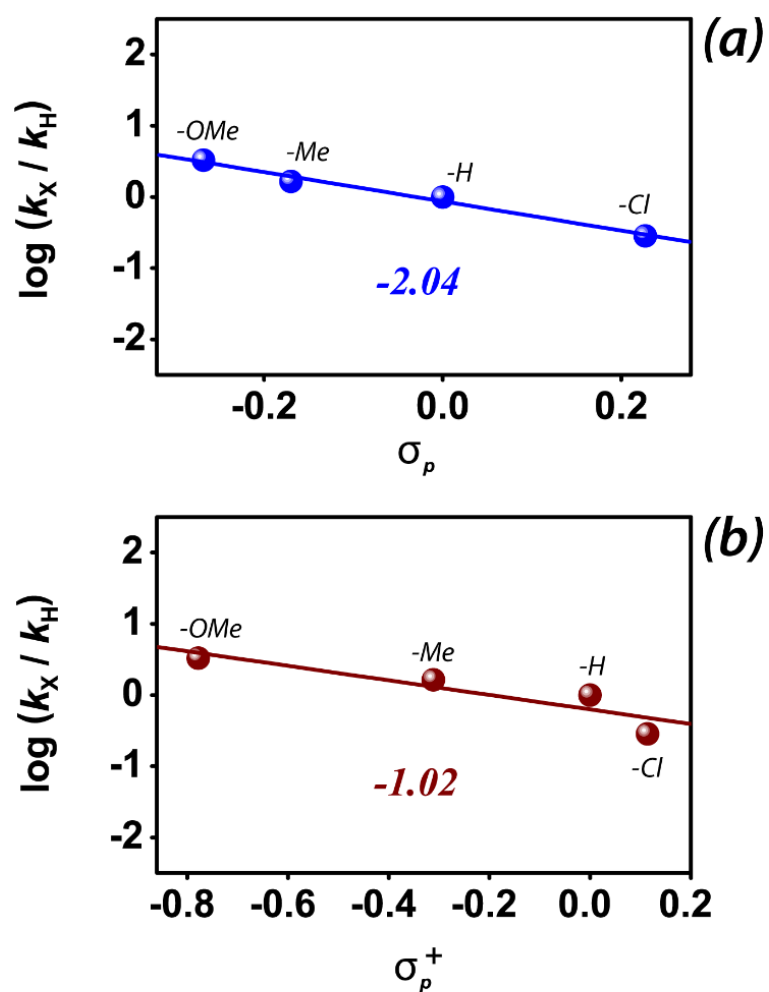


Fig. S6: Plot of $\log(k_X/k_H)$ against (a) σ_p values^[a] and (b) σ_p^+ values^[a] in the reaction of **1b** with *p*-X-thioanisole at -40 °C, where k_X and k_H are the pseudo first-order rate constants of *p*-X-thioanisole and thioanisole respectively.

^[a] Values taken from Brown et al, *J. Am. Chem. Soc.*, 1958, **80**, 49797.

Table S1: Pseudo first-order rate constant (k_{obs}) determined in the reaction of **1b** (1 mM solution in CH₃CN) with benzyl alcohol and benzyl alcohol-D₇ at 25 °C in CH₃CN.^[a]

Benzyl alcohol concentration (mM)	$10^{-3} \times k_{\text{obs}} \text{ (s}^{-1}\text{)}$	Benzyl alcohol-D ₇ concentration (mM)	$10^{-3} \times k_{\text{obs}} \text{ (s}^{-1}\text{)}$
20	9.83(2)	60	3.9(2)
40	20.29(1)	80	5.08(3)
60	30.76(2)	100	6.63(2)
80	40.89(2)	120	7.97(3)

^[a] The reactions were followed by monitoring the UV-vis spectral changes of the reaction solution.

Table S2: Second-order rate constant (k_2) determined in the reaction of **1b** (1 mM solution in CH₃CN) with various *para*-substituted benzyl alcohols at 25 °C in CH₃CN.^[a]

<i>para</i> -substituents on Benzyl alcohol	σ_p ^[b]	σ_p^+ ^[b]	$k_2 \text{ (M}^{-1} \text{ s}^{-1}\text{)}$	k_X/k_H ^[c]	$\log (k_X/k_H)$
–OCH ₃	–0.268	–0.778	0.648(3)	1.270	0.104
–CH ₃	–0.170	–0.311	0.484(2)	0.948	–0.023
–H	0.000	0.000	0.510(1)	1.000	0.000
–Cl	0.227	0.114	0.434(2)	0.851	–0.069

^[a] All the reactions were followed by monitoring UV-vis spectral changes of the reaction solution.

^[b] Values taken from Brown et al, *J. Am. Chem. Soc.*, 1958, **80**, 4979.

^[c] Relative rate constant obtained by dividing the k_2 of *p*-X-benzyl alcohol by k_2 of *p*-H-benzyl alcohol.

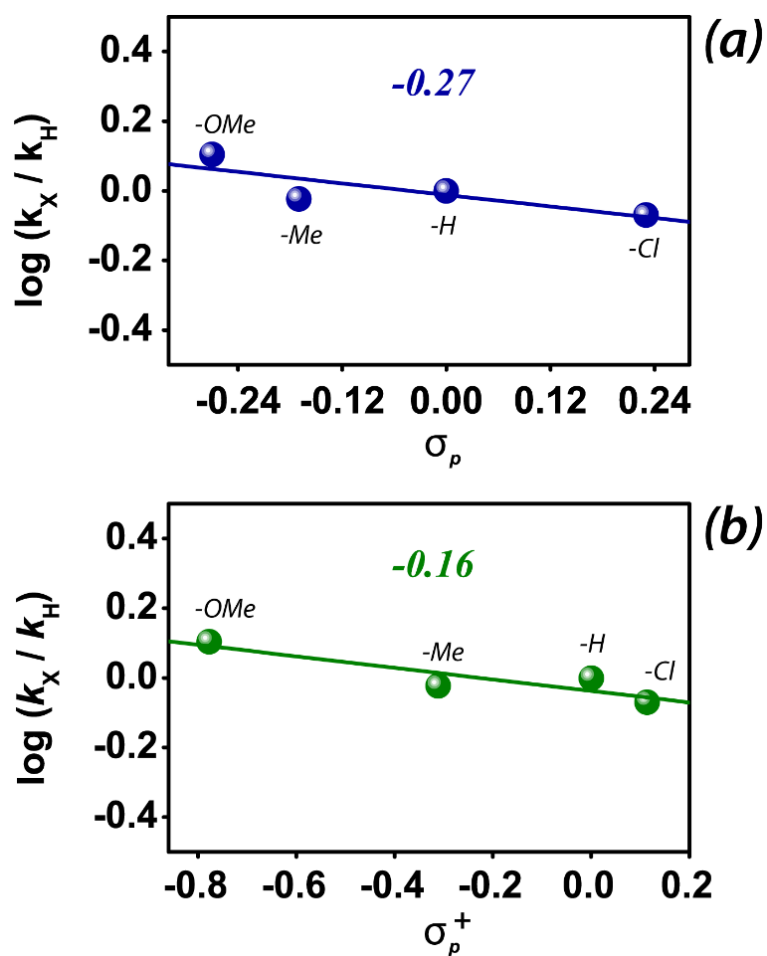


Fig. S7: Plot of $\log(k_X/k_H)$ against (a) σ_p values and (b) σ_p^+ values in the reaction of **1b** with *p*-X-benzyl alcohol at 25 °C, where k_X and k_H are the second-order rate constants of *p*-X-benzyl alcohol and benzyl alcohol respectively.

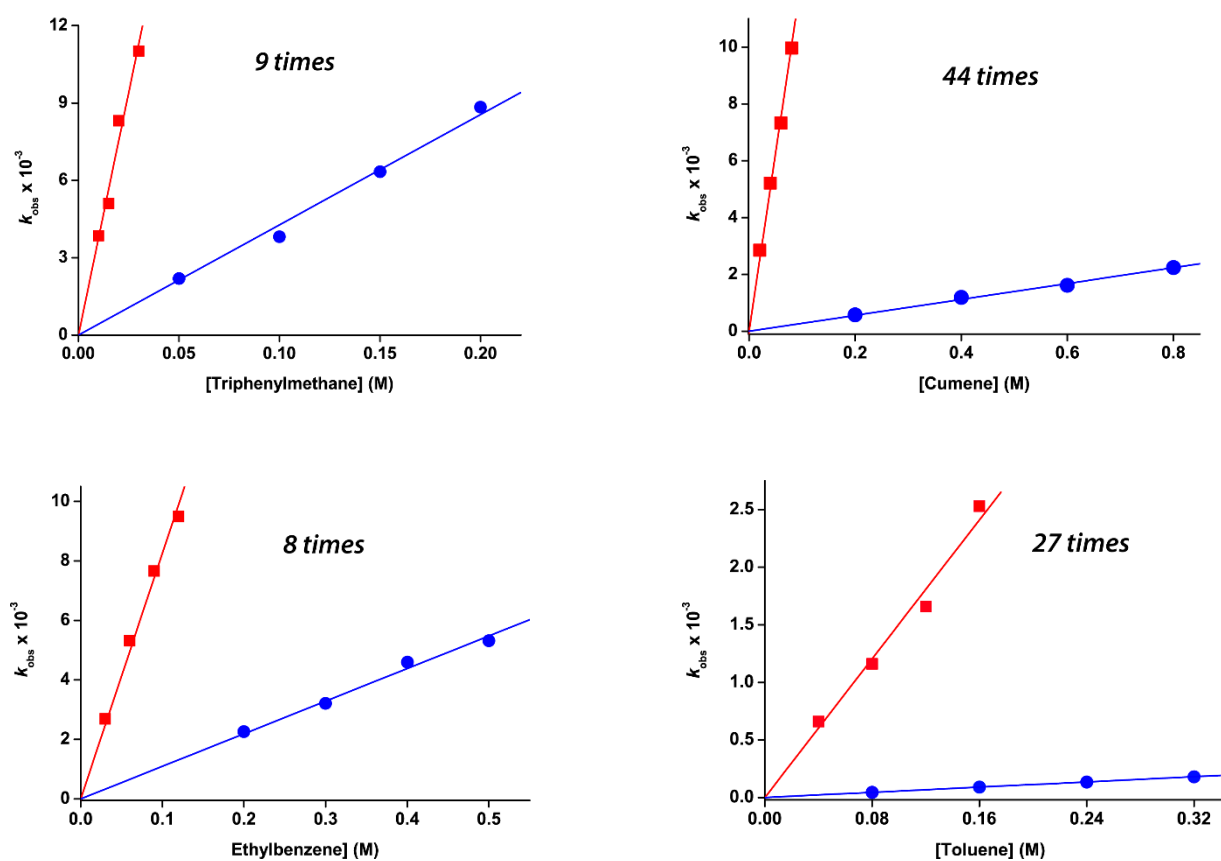


Fig. S8: Comparison of second-order rate constants of 1 mM **1b** (■) and 1 mM **2b** (●) against various hydrocarbon substrates at different concentration at 25 °C.

Part III: Computational data.

Table S3: DFT calculated absolute energies, zero-point energies and free energies (in au) of optimized structures at UB3LYP/BS1 in Gaussian-09 for the reaction mechanisms of substrate activation by $^{3,5}[\text{Fe}^{\text{IV}}(\text{O})(2\text{PyN2Q})]^{2+}$.

	E [BS1, au]	ZPE [BS1, au]	G [BS1, au]	E [BS2, au]
$^3[\text{Fe}^{\text{IV}}(\text{O})(2\text{PyN2Q})]^{2+}$	-1668.187589	0.509549	-1667.735641	-1668.917417
$^5[\text{Fe}^{\text{IV}}(\text{O})(2\text{PyN2Q})]^{2+}$	-1668.172719	0.507525	-1667.725382	-1668.910970
1,3-CHD	-233.367365	0.123550	-233.272069	-233.473820
DMS	-477.972788	0.076513	-477.923654	-478.059674
Toluene	-271.509659	0.129359	-271.411604	-271.629021
Reaction with DMS:				
$^3\text{Re}(\text{DMS})$	-2146.161801	0.586674	-2145.648192	-2147.003153
$^3\text{TS}_{\text{SO}}(\text{DMS})$	-2146.126280	0.583829	-2145.611197	-2146.975471
$^3\text{Prod}(\text{DMS})$	-2146.138683	0.585593	-2145.620298	-2147.000816
$^5\text{Re}(\text{DMS})$	-2146.147198	0.584573	-2145.636710	-2146.997234
$^5\text{TS}_{\text{SO}}(\text{DMS})$	-2146.142972	0.583732	-2145.630271	-2146.993774
$^5\text{Prod}(\text{DMS})$	-2146.165307	0.584029	-2145.651145	-2147.034318
Reaction with 1,3-CHD:				
$^3\text{Re}(\text{CHD})$	-1901.557005	0.633551	-1900.995932	-1902.391174
$^3\text{TS}_{\text{HA}}(\text{CHD})$	-1901.539281	0.627662	-1900.978990	-1902.367667
$^3\text{Int}(\text{CHD})$	-1901.576476	0.630967	-1901.016373	-1902.412280
$^3\text{TS}_{\text{reb}}(\text{CHD})$	-1901.564866	0.628031	-1901.006682	-1902.400146
$^3\text{Prod}(\text{CHD})$	-1901.639389	0.631491	-1901.080659	-1902.474219
$^5\text{Re}(\text{CHD})$	-1901.542204	0.631585	-1900.985394	-1902.385015
$^5\text{Prod}(\text{CHD})$	-1901.662494	0.630981	-1901.106993	-1902.501419
Reaction with toluene:				
$^3\text{Re}(\text{Tol})$	-1939.699088	0.639225	-1939.133793	-1940.575621
$^3\text{TS}_{\text{HA}}(\text{Tol})$	-1939.671270	0.633676	-1939.106775	-1940.538540
$^5\text{Re}(\text{Tol})$	-1939.684273	0.637370	-1939.122784	-1940.569647
$^5\text{TS}_{\text{HA}}(\text{Tol})$	-1939.671696	0.632493	-1939.111477	-1940.549566

Table S4: DFT calculated relative energies, zero-point energies and free energies (in kcal mol⁻¹) of optimized structures at UB3LYP/BS1 in Gaussian-09 for the reaction mechanisms of substrate activation by ^{3,5}[Fe^{IV}(O)(2PyN2Q)]²⁺..

	ΔE [BS1]	$\Delta E+ZPE$ [BS1]	ΔG [BS1]	ΔE [BS2]	$\Delta E+ZPE$ [BS2]	ΔG [BS2]
³ [Fe ^{IV} (O)(2PyN2Q)] ²⁺	0.00	0.00	0.00	0.00	0.00	0.00
⁵ [Fe ^{IV} (O)(2PyN2Q)] ²⁺	9.33	8.06	6.44	4.05	2.78	1.15
Reaction with DMS:						
³ Re(DMS)	-0.89	-0.51	6.97	-16.35	-15.97	-8.49
³ TS _{SO} (DMS)	21.40	19.99	30.18	1.02	-0.38	9.80
³ Prod(DMS)	13.61	13.32	24.47	-14.89	-15.18	-4.03
⁵ Re(DMS)	-1.06	-0.73	7.73	-12.64	-13.57	-6.74
⁵ TS _{SO} (DMS)	1.59	1.40	11.78	-10.47	-11.93	-3.18
⁵ Prod(DMS)	-12.43	-12.43	-1.32	-35.91	-37.19	-27.70
Reaction with 1,3-CHD:						
³ Re(Chd)	-1.29	-1.00	7.39	0.04	0.32	8.72
³ TS _{HA} (Chd)	9.83	6.42	18.02	14.79	11.38	22.98
³ Int(Chd)	-13.51	-14.84	-5.44	-13.20	-14.54	-5.14
³ TS _{reb} (Chd)	-6.22	-9.40	0.65	-5.59	-8.77	1.27
³ Prod(Chd)	-52.98	-53.99	-45.78	-52.07	-53.08	-44.86
⁵ Re(Chd)	-1.33	-1.01	7.57	3.90	2.95	9.91
⁵ Prod(Chd)	-76.81	-76.87	-68.74	-69.14	-70.47	-63.96
Reaction with toluene:						
³ Re(Tol)	-1.15	-0.96	8.44	-18.31	-18.11	-8.72
³ TS _{HA} (Tol)	16.30	13.02	25.40	4.96	1.67	14.05
⁵ Re(Tol)	8.14	7.18	15.35	-14.56	-15.53	-7.36
⁵ TS _{HA} (Tol)	16.03	12.01	22.44	-1.96	-5.99	4.45

Table S5: Group spin densities and charges of UB3LYP/BS1 optimized structures at UB3LYP/BS1 in Gaussian-09, L stands for 2PyN2Q.

	Spin densities				Charges			
	Fe	O	L	SubH	Fe	O	L	SubH
$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{L})]^{2+}$	1.08	0.95	-0.03		0.69	-0.38	1.69	
$^5[\text{Fe}^{\text{IV}}(\text{O})(\text{L})]^{2+}$	2.93	0.76	0.31		0.83	-0.38	1.55	
$^3\text{Re}(\text{CHD})$	1.08	0.95	-0.03	0.00	0.68	-0.38	1.67	0.03
$^3\text{TS}_{\text{HA}}(\text{CHD})$	0.83	0.69	-0.04	0.51	0.73	-0.54	1.44	0.36
$^3\text{Int}(\text{CHD})$	0.92	0.16	-0.07	0.99	0.71	-0.68	1.55	0.43
$^3\text{TS}_{\text{reb}}(\text{CHD})$	1.47	-0.01	-0.07	0.61	0.69	-0.70	1.32	0.69
$^3\text{Prod}(\text{CHD})$	1.98	0.02	0.00	0.00	0.68	-0.74	1.13	0.94
$^5\text{Re}(\text{CHD})$	2.93	0.76	0.31	0.00	0.82	-0.38	1.53	0.03
$^5\text{Prod}(\text{CHD})$	3.76	0.03	0.21	0.00	0.78	-0.76	1.01	0.96
$^3\text{Re}(\text{DMS})$	1.09	0.94	-0.03	0.00	0.70	-0.39	1.69	0.00
$^3\text{TS}_{\text{SO}}(\text{DMS})$	2.25	0.07	0.02	-0.34	0.73	-0.58	1.17	0.68
$^3\text{Prod}(\text{DMS})$	1.96	0.04	0.00	0.01	0.67	-0.70	1.06	0.98
$^5\text{Re}(\text{DMS})$	2.94	0.75	0.31	0.00	0.83	-0.38	1.54	0.02
$^5\text{TS}_{\text{SO}}(\text{DMS})$	3.32	0.49	0.34	-0.16	0.85	-0.42	1.39	0.18
$^5\text{Prod}(\text{DMS})$	3.74	0.06	0.18	0.02	0.74	-0.74	0.95	1.05

Table S6: Group spin densities and charges of UB3LYP/BS2//UB3LYP/BS1 calculated structures in Gaussian-09. L stands for 2PyN2Q.

	Spin densities				Charges			
	Fe	O	L	SubH	Fe	O	L	SubH
$^3[\text{Fe}^{\text{IV}}(\text{O})(\text{L})]^{2+}$	1.30	0.91	-0.21		-1.26	-0.32	3.58	
$^5[\text{Fe}^{\text{IV}}(\text{O})(\text{L})]^{2+}$	3.19	0.72	0.08		-1.35	-0.28	3.63	
$^3\text{Re}(\text{CHD})$	1.15	0.94	-0.09	0.00	-2.10	-0.10	4.20	0.00
$^3\text{TS}_{\text{HA}}(\text{CHD})$	0.90	0.70	-0.09	0.49	-2.38	-0.19	4.28	0.29
$^3\text{Int}(\text{CHD})$	1.00	0.14	-0.14	1.00	-2.02	-0.39	4.11	0.30
$^3\text{TS}_{\text{reb}}(\text{CHD})$	1.20	0.04	-0.17	0.93	-2.31	-0.54	4.44	0.41
$^3\text{Prod}(\text{CHD})$	2.07	0.02	-0.09	0.01	-1.26	-0.63	3.11	0.78
$^5\text{Re}(\text{CHD})$	3.21	0.74	0.06	0.00	-2.23	-0.01	4.22	0.01
$^5\text{Prod}(\text{CHD})$	3.89	0.02	0.09	0.01	-1.19	-0.61	3.02	0.78
$^3\text{Re}(\text{DMS})$	1.19	0.89	-0.08	0.00	-2.45	0.01	4.42	0.02
$^3\text{TS}_{\text{SO}}(\text{DMS})$	2.36	0.04	0.06	-0.46	-1.20	-0.10	2.57	0.73
$^3\text{Prod}(\text{DMS})$	1.92	0.04	0.03	0.01	-0.93	-0.19	2.29	0.84
$^5\text{Re}(\text{DMS})$	3.08	0.69	0.23	0.00	-1.93	0.08	3.82	0.03
$^5\text{TS}_{\text{SO}}(\text{DMS})$	3.39	0.49	0.27	-0.15	-1.29	0.21	2.91	0.16
$^5\text{Prod}(\text{DMS})$	3.29	0.06	0.63	0.02	3.90	-0.32	-2.62	1.03

Table S7: DFT calculated absolute (in au) and relative (in kcal mol⁻¹) energies of optimized structures at UB3LYP/BS2 in Gaussian-09 for the reaction mechanisms of toluene activation by ^{3,5}[Fe^{IV}(O)(2PyN2Q)]²⁺.

	B3LYP/BS2 geometry optimization	
	E [au]	ΔE [kcal mol ⁻¹]
³ Re(Tol)	-1940.575621	0.00
³ TS _{HA} (Tol)	-1940.541611	21.34
⁵ Re(Tol)	-1940.569647	3.75
⁵ TS _{HA} (Tol)	-1940.553012	14.19

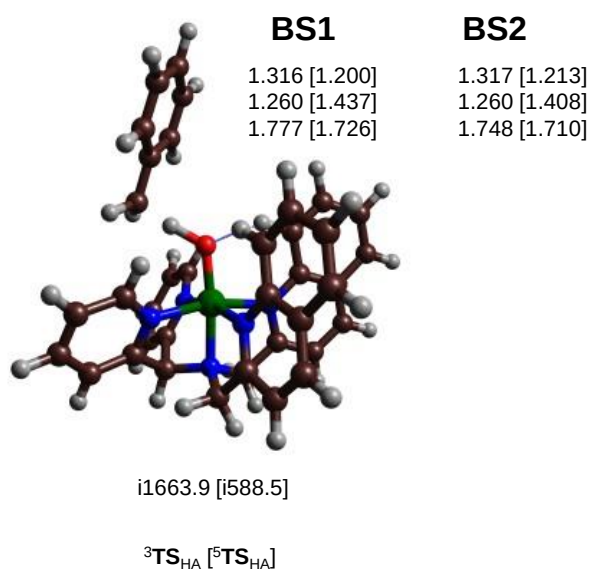


Fig. S9: Comparison of the optimized transition state geometries calculated at UB3LYP/BS1 versus UB3LYP/BS2 for hydrogen atom abstraction from toluene by ^{3,5}[Fe^{IV}(O)(2PyN2Q)]²⁺.

Part IV: Cartesian coordinates.

Cartesian coordinates of optimized geometries:

$^3[\text{Fe}^{\text{IV}}(\text{O})(2\text{PyN}2\text{Q})]^{2+}$:

26	-0.096077000	0.258708000	0.370126000
7	-0.095824000	-0.451989000	2.229905000
7	0.418352000	0.834933000	-1.527148000
7	0.749255000	1.902009000	1.112010000
7	-0.461217000	-1.619365000	-0.360158000
6	1.146674000	-0.459238000	2.787141000
6	1.361086000	-0.927990000	4.077471000
1	2.357811000	-0.931081000	4.499644000
6	0.257976000	-1.394368000	4.807675000
1	0.394135000	-1.766533000	5.815656000
6	-1.014034000	-1.375429000	4.226901000
1	-1.882344000	-1.724630000	4.770024000
6	-1.164333000	-0.896016000	2.923794000
1	-2.122111000	-0.852238000	2.425090000
6	1.722650000	0.622223000	-1.787252000
6	2.285688000	0.790558000	-3.070898000
1	3.338942000	0.586694000	-3.216412000
6	1.484063000	1.202873000	-4.110130000
1	1.888722000	1.325534000	-5.108618000
6	1.898667000	1.637574000	1.792702000
6	2.646698000	2.652457000	2.376924000
1	3.560531000	2.421848000	2.909398000
6	2.187171000	3.972053000	2.254347000
1	2.749955000	4.784555000	2.697295000
6	1.001957000	4.230224000	1.558387000
1	0.623177000	5.238369000	1.453408000
6	0.296193000	3.167135000	0.990922000
1	-0.627388000	3.304477000	0.446763000
6	0.642625000	-2.391238000	-0.355404000
6	0.683699000	-3.672009000	-0.948088000
1	1.607514000	-4.235719000	-0.924565000
6	-0.447706000	-4.174588000	-1.548195000
1	-0.437441000	-5.149825000	-2.022186000
6	-1.644551000	-3.415980000	-1.540035000
6	-1.641238000	-2.117893000	-0.920044000
6	2.181983000	0.148149000	1.858753000
1	3.206875000	-0.077473000	2.158616000
6	2.622671000	0.254646000	-0.638273000
1	3.100081000	1.164312000	-0.260652000
1	3.427471000	-0.407287000	-0.966992000
6	1.857668000	-1.885574000	0.375571000
1	1.861954000	-2.309160000	1.384842000
1	2.776671000	-2.223817000	-0.109487000
7	1.843278000	-0.387773000	0.471509000
8	-1.628764000	0.879701000	0.516559000
6	-4.008581000	-1.910909000	-1.430518000
6	-4.008763000	-3.176413000	-2.067101000
6	-2.855386000	-1.389050000	-0.872217000
1	-4.923223000	-3.561845000	-2.503122000
1	-2.873001000	-0.430781000	-0.375560000
6	-2.845136000	-3.915223000	-2.116338000
1	-2.825207000	-4.893121000	-2.585462000
1	-4.929244000	-1.340456000	-1.375863000
6	-2.058972000	2.248116000	-4.656001000
6	-2.568722000	2.098789000	-3.342727000
6	-0.737922000	1.946743000	-4.913181000
1	-3.602324000	2.356021000	-3.138905000

1	-0.321668000	2.068022000	-5.907583000
6	-1.771177000	1.634467000	-2.311947000
6	0.114786000	1.481449000	-3.874395000
1	-2.167988000	1.541034000	-1.312313000
6	-0.414212000	1.301841000	-2.548687000
1	-2.704895000	2.607282000	-5.448886000

$^5[\text{Fe}^{\text{IV}}(\text{O})(2\text{PyN}2\text{Q})]^{2+}$:

26	-0.223088000	0.308081000	0.384657000
7	-0.129993000	-0.438256000	2.370822000
7	0.367211000	0.897347000	-1.604427000
7	0.746857000	2.009420000	1.201711000
7	-0.558336000	-1.679603000	-0.377368000
6	1.146078000	-0.438404000	2.842720000
6	1.448444000	-0.895427000	4.120638000
1	2.470445000	-0.893321000	4.477955000
6	0.397353000	-1.358254000	4.926790000
1	0.602611000	-1.722027000	5.926233000
6	-0.911712000	-1.348565000	4.433985000
1	-1.739325000	-1.697990000	5.037321000
6	-1.147705000	-0.879843000	3.139473000
1	-2.137019000	-0.849983000	2.703140000
6	1.667892000	0.634556000	-1.825039000
6	2.262034000	0.749940000	-3.100934000
1	3.310876000	0.511124000	-3.223520000
6	1.492069000	1.161784000	-4.166917000
1	1.922666000	1.248921000	-5.158424000
6	1.900899000	1.667855000	1.836241000
6	2.709723000	2.624925000	2.438932000
1	3.626427000	2.335785000	2.937071000
6	2.305974000	3.967553000	2.382024000
1	2.917065000	4.735501000	2.840444000
6	1.114932000	4.307141000	1.731752000
1	0.781125000	5.335053000	1.676709000
6	0.348724000	3.297635000	1.144373000
1	-0.579808000	3.498750000	0.627289000
6	0.579090000	-2.398041000	-0.384347000
6	0.677103000	-3.660373000	-1.009703000
1	1.622202000	-4.188176000	-0.998781000
6	-0.434406000	-4.194890000	-1.624866000
1	-0.381868000	-5.158604000	-2.119531000
6	-1.662862000	-3.486982000	-1.608771000
6	-1.708705000	-2.204697000	-0.961793000
6	2.131261000	0.166153000	1.856500000
1	3.165799000	-0.091519000	2.092850000
6	2.526993000	0.284944000	-0.639320000
1	2.983617000	1.203684000	-0.258769000
1	3.346165000	-0.376740000	-0.930907000
6	1.756264000	-1.857231000	0.382952000
1	1.725221000	-2.267922000	1.396676000
1	2.699380000	-2.184121000	-0.061642000
7	1.728988000	-0.350680000	0.472567000
8	-1.757084000	0.915177000	0.499219000
6	-4.070925000	-2.047343000	-1.494594000
6	-4.027459000	-3.303714000	-2.150239000
6	-2.938951000	-1.503833000	-0.914172000
1	-4.927027000	-3.706582000	-2.601333000
1	-2.980299000	-0.550328000	-0.406730000

6	-2.843568000	-4.010494000	-2.204226000
1	-2.793545000	-4.977316000	-2.693682000
1	-5.008126000	-1.504004000	-1.445032000
6	-2.022804000	2.264416000	-4.804780000
6	-2.561467000	2.148016000	-3.498487000
6	-0.702050000	1.938321000	-5.035167000
1	-3.596678000	2.419080000	-3.322799000
1	-0.270104000	2.029938000	-6.026068000
6	-1.788705000	1.697202000	-2.443196000
6	0.124710000	1.482415000	-3.971613000
1	-2.203272000	1.619297000	-1.448022000
6	-0.431878000	1.347624000	-2.653473000
1	-2.649900000	2.615408000	-5.616281000

³Re_{DMS}:

26	0.112787000	-0.154519000	0.008336000
7	0.051812000	-0.841397000	1.875673000
7	0.706274000	0.468191000	-1.851095000
7	0.671235000	1.592884000	0.778794000
7	0.058666000	-2.070872000	-0.714005000
6	1.232187000	-0.675314000	2.534727000
6	1.396187000	-1.099586000	3.847538000
1	2.344038000	-0.963658000	4.352425000
6	0.307547000	-1.706319000	4.491428000
1	0.405966000	-2.048566000	5.514301000
6	-0.900670000	-1.865990000	3.805893000
1	-1.756791000	-2.326663000	4.280920000
6	-1.002430000	-1.420872000	2.485999000
1	-1.910665000	-1.511430000	1.907716000
6	2.044536000	0.427754000	-1.997609000
6	2.687437000	0.663618000	-3.232205000
1	3.766777000	0.600149000	-3.286322000
6	1.930076000	0.962222000	-4.341139000
1	2.399448000	1.133526000	-5.303494000
6	1.783353000	1.490909000	1.558099000
6	2.337686000	2.603067000	2.180068000
1	3.225292000	2.502779000	2.791370000
6	1.720098000	3.848154000	1.991113000
1	2.130770000	4.732954000	2.461811000
6	0.575618000	3.938775000	1.192460000
1	0.078178000	4.886330000	1.032787000
6	0.067247000	2.784795000	0.592174000
1	-0.816202000	2.790957000	-0.030212000
6	1.249472000	-2.690112000	-0.600060000
6	1.511471000	-3.957338000	-1.164199000
1	2.495832000	-4.393004000	-1.049433000
6	0.514043000	-4.608383000	-1.852580000
1	0.694071000	-5.576241000	-2.307195000
6	-0.768017000	-4.014961000	-1.962073000
6	-0.991346000	-2.725060000	-1.365296000
6	2.253393000	0.052982000	1.680604000
1	3.270898000	-0.031272000	2.066120000
6	2.885286000	0.186539000	-0.772846000
1	3.213343000	1.152604000	-0.376073000
1	3.790308000	-0.372600000	-1.023011000
6	2.317935000	-2.022946000	0.223437000
1	2.283985000	-2.430042000	1.238893000
1	3.312662000	-2.245609000	-0.170079000
7	2.103381000	-0.538544000	0.283182000
8	-1.496533000	0.257768000	0.015443000
6	-3.310687000	-2.838097000	-2.083795000
6	-3.086435000	-4.094268000	-2.699019000
6	-2.291067000	-2.165206000	-1.434410000

1	-3.899164000	-4.599403000	-3.208113000
1	-2.480125000	-1.216930000	-0.954747000
6	-1.835669000	-4.671694000	-2.633956000
1	-1.644474000	-5.639786000	-3.084498000
1	-4.300172000	-2.395645000	-2.118341000
6	-1.660839000	1.522750000	-5.199049000
6	-2.256283000	1.313093000	-3.930905000
6	-0.294346000	1.399905000	-5.339546000
1	-3.328562000	1.430056000	-3.818693000
1	0.184773000	1.570216000	-6.297790000
6	-1.494638000	0.965566000	-2.829402000
6	0.521025000	1.058097000	-4.225603000
1	-1.958885000	0.825309000	-1.864994000
6	-0.090441000	0.815866000	-2.946154000
1	-2.278910000	1.787758000	-6.049123000
6	-4.609007000	0.985935000	1.799991000
1	-3.704392000	0.943703000	1.191213000
1	-5.037958000	-0.012215000	1.900552000
1	-5.344180000	1.662541000	1.360555000
6	-3.600391000	3.321321000	3.167873000
1	-3.339263000	3.777992000	4.123388000
1	-2.724413000	3.291478000	2.518079000
1	-4.408466000	3.882356000	2.695411000
16	-4.182404000	1.563443000	3.550558000

³TS_{SO}:

26	-0.103974000	0.031457000	0.275133000
7	0.128475000	-0.958062000	2.387939000
7	0.670824000	0.710485000	-1.800777000
7	0.660267000	1.685772000	1.096975000
7	-0.273889000	-1.882930000	-0.609972000
6	1.403571000	-0.759098000	2.798077000
6	1.868923000	-1.207065000	4.033590000
1	2.896779000	-1.037707000	4.331003000
6	0.975884000	-1.888803000	4.871640000
1	1.305352000	-2.249907000	5.838705000
6	-0.336857000	-2.109646000	4.441378000
1	-1.046055000	-2.644363000	5.060696000
6	-0.725700000	-1.633331000	3.185371000
1	-1.722930000	-1.795017000	2.797759000
6	1.983025000	0.495340000	-1.914260000
6	2.675435000	0.618380000	-3.145853000
1	3.739586000	0.418730000	-3.184113000
6	1.978232000	0.990780000	-4.274556000
1	2.482782000	1.089018000	-5.230022000
6	1.810611000	1.462805000	1.795161000
6	2.491660000	2.499064000	2.428150000
1	3.404813000	2.294642000	2.973126000
6	1.982930000	3.800305000	2.329203000
1	2.495845000	4.623424000	2.811701000
6	0.823006000	4.026977000	1.581589000
1	0.417652000	5.023414000	1.463169000
6	0.187186000	2.946651000	0.969556000
1	-0.692764000	3.076101000	0.357667000
6	0.884880000	-2.565562000	-0.548647000
6	1.069967000	-3.828138000	-1.161947000
1	2.033191000	-4.316753000	-1.081289000
6	0.031511000	-4.408846000	-1.849928000
1	0.151764000	-5.373142000	-2.331648000
6	-1.213239000	-3.735590000	-1.933864000
6	-1.349860000	-2.454035000	-1.297143000
6	2.245364000	0.009798000	1.794663000
1	3.310655000	-0.085398000	2.023930000

6	2.754994000	0.194365000	-0.650504000
1	3.104462000	1.143339000	-0.231343000
1	3.648763000	-0.395557000	-0.876234000
6	2.025525000	-1.999531000	0.256286000
1	2.008034000	-2.454644000	1.250645000
1	2.982887000	-2.277270000	-0.195027000
7	1.931203000	-0.510404000	0.393709000
8	-1.832904000	0.393591000	0.355353000
6	-3.657716000	-2.364150000	-2.056220000
6	-3.523297000	-3.623269000	-2.692781000
6	-2.599043000	-1.789403000	-1.375733000
1	-4.365492000	-4.053720000	-3.222966000
1	-2.705276000	-0.837178000	-0.875143000
6	-2.320199000	-4.295506000	-2.629643000
1	-2.196572000	-5.262450000	-3.106470000
1	-4.607801000	-1.842381000	-2.102236000
6	-1.545385000	1.904064000	-5.169048000
6	-2.169909000	1.757535000	-3.902422000
6	-0.194442000	1.654839000	-5.310499000
1	-3.231058000	1.961000000	-3.805778000
1	0.293034000	1.766242000	-6.273695000
6	-1.443542000	1.359742000	-2.795263000
6	0.584048000	1.251000000	-4.190550000
1	-1.906149000	1.240325000	-1.823764000
6	-0.054958000	1.097403000	-2.915002000
1	-2.135162000	2.214686000	-6.024419000
6	-3.939125000	0.328614000	2.356187000
1	-4.116880000	-0.409225000	1.574632000
1	-3.405319000	-0.105642000	3.199003000
1	-4.866604000	0.794925000	2.689863000
6	-3.976398000	2.374935000	0.326072000
1	-3.410880000	3.130815000	-0.216310000
1	-4.277160000	1.561576000	-0.333397000
1	-4.834268000	2.822269000	0.828967000
16	-2.831044000	1.669110000	1.643428000

³P_{DMS}:

26	-0.047982000	-0.019825000	0.215621000
7	0.090389000	-0.914133000	2.243905000
7	0.699354000	0.642469000	-1.756198000
7	0.680002000	1.669765000	1.029240000
7	-0.202723000	-1.932948000	-0.610672000
6	1.342689000	-0.747720000	2.734792000
6	1.712517000	-1.214511000	3.995251000
1	2.722373000	-1.070581000	4.360023000
6	0.751371000	-1.881334000	4.767167000
1	1.008196000	-2.256504000	5.750737000
6	-0.534971000	-2.070292000	4.249625000
1	-1.294565000	-2.594323000	4.816038000
6	-0.830566000	-1.575578000	2.976325000
1	-1.801929000	-1.708470000	2.518851000
6	2.020520000	0.491688000	-1.890064000
6	2.690331000	0.713727000	-3.120626000
1	3.761879000	0.563436000	-3.177076000
6	1.968258000	1.115234000	-4.222127000
1	2.458371000	1.286736000	-5.174671000
6	1.828972000	1.455187000	1.735535000
6	2.519476000	2.498751000	2.347707000
1	3.429194000	2.295478000	2.899307000
6	2.026636000	3.803492000	2.221988000
1	2.547581000	4.631115000	2.688133000
6	0.868886000	4.024328000	1.469811000
1	0.470895000	5.021437000	1.331645000

6	0.224259000	2.935814000	0.881218000
1	-0.655459000	3.066704000	0.268023000
6	0.967929000	-2.598669000	-0.555432000
6	1.170195000	-3.848933000	-1.190258000
1	2.141250000	-4.323520000	-1.117805000
6	0.143346000	-4.435107000	-1.891661000
1	0.281867000	-5.386733000	-2.393545000
6	-1.115161000	-3.785547000	-1.957012000
6	-1.270773000	-2.521350000	-1.292400000
6	2.264523000	-0.001399000	1.783714000
1	3.306766000	-0.085793000	2.107828000
6	2.837392000	0.144358000	-0.661759000
1	3.234689000	1.076908000	-0.246300000
1	3.705726000	-0.458739000	-0.949658000
6	2.109827000	-2.037338000	0.264903000
1	2.067528000	-2.487457000	1.261712000
1	3.066270000	-2.346146000	-0.170885000
7	2.048879000	-0.555867000	0.391791000
8	-2.064338000	0.393268000	0.445000000
6	-3.593033000	-2.468653000	-2.005667000
6	-3.437523000	-3.705592000	-2.680772000
6	-2.537254000	-1.885565000	-1.327473000
1	-4.277699000	-4.141714000	-3.209802000
1	-2.665157000	-0.955236000	-0.787967000
6	-2.218903000	-4.352244000	-2.652652000
1	-2.081867000	-5.304770000	-3.154417000
1	-4.558123000	-1.972857000	-2.018273000
6	-1.597992000	1.925077000	-5.041280000
6	-2.203085000	1.686817000	-3.779947000
6	-0.239157000	1.739961000	-5.204147000
1	-3.270492000	1.841321000	-3.663726000
1	0.235487000	1.922421000	-6.162897000
6	-1.450403000	1.261779000	-2.700176000
6	0.565236000	1.310084000	-4.112840000
1	-1.905445000	1.079192000	-1.734076000
6	-0.054059000	1.061438000	-2.843400000
1	-2.207668000	2.255372000	-5.874998000
6	-4.001521000	0.454719000	2.486942000
1	-4.454229000	-0.232707000	1.773255000
1	-3.425386000	-0.071340000	3.244803000
1	-4.739513000	1.111182000	2.948181000
6	-4.000728000	2.429695000	0.389838000
1	-3.402823000	3.014263000	-0.306740000
1	-4.588999000	1.672895000	-0.127739000
1	-4.619873000	3.076607000	1.011305000
16	-2.788392000	1.546578000	1.538790000

⁵Re_{DMS}:

26	0.084110000	0.108306000	0.008856000
7	0.100304000	-0.488994000	2.042724000
7	0.750557000	0.596294000	-1.980396000
7	0.916197000	1.918978000	0.758408000
7	-0.090224000	-1.952165000	-0.621916000
6	1.347426000	-0.394378000	2.579755000
6	1.601920000	-0.757716000	3.897367000
1	2.601948000	-0.680932000	4.304918000
6	0.532332000	-1.224231000	4.676822000
1	0.700631000	-1.517398000	5.705960000
6	-0.747349000	-1.305518000	4.118920000
1	-1.590776000	-1.653969000	4.700623000
6	-0.936827000	-0.928583000	2.786759000
1	-1.909539000	-0.964105000	2.312098000
6	2.075869000	0.404743000	-2.111444000

6	2.735530000	0.477185000	-3.357894000
1	3.802563000	0.300914000	-3.406330000
6	2.005870000	0.767889000	-4.489986000
1	2.488703000	0.819415000	-5.459721000
6	2.046448000	1.684219000	1.477959000
6	2.768556000	2.721681000	2.057493000
1	3.669045000	2.516185000	2.622364000
6	2.300119000	4.033243000	1.886968000
1	2.842976000	4.862147000	2.324685000
6	1.133200000	4.263406000	1.150611000
1	0.750688000	5.265582000	1.007633000
6	0.456301000	3.176798000	0.591430000
1	-0.448943000	3.292179000	0.010657000
6	1.081126000	-2.601623000	-0.502143000
6	1.281806000	-3.908172000	-0.999944000
1	2.250690000	-4.377905000	-0.886924000
6	0.239089000	-4.558656000	-1.622684000
1	0.370454000	-5.559226000	-2.019799000
6	-1.021831000	-3.921544000	-1.744693000
6	-1.173022000	-2.591367000	-1.222708000
6	2.354515000	0.202679000	1.611976000
1	3.385565000	0.021086000	1.923003000
6	2.885010000	0.185770000	-0.861196000
1	3.266848000	1.152821000	-0.519922000
1	3.755951000	-0.442490000	-1.063886000
6	2.187409000	-1.929297000	0.265873000
1	2.145848000	-2.269234000	1.305122000
1	3.165699000	-2.222850000	-0.122386000
7	2.063633000	-0.425399000	0.247173000
8	-1.485919000	0.629428000	-0.007199000
6	-3.499591000	-2.612224000	-1.913402000
6	-3.351336000	-3.917914000	-2.445539000
6	-2.436778000	-1.958237000	-1.316145000
1	-4.197862000	-4.408209000	-2.912438000
1	-2.558404000	-0.967202000	-0.903069000
6	-2.133284000	-4.560604000	-2.359986000
1	-2.003059000	-5.562910000	-2.754081000
1	-4.463197000	-2.118249000	-1.973255000
6	-1.528200000	1.585204000	-5.394691000
6	-2.134583000	1.519326000	-4.114931000
6	-0.177789000	1.335759000	-5.528744000
1	-3.193690000	1.730134000	-4.015434000
1	0.305070000	1.390763000	-6.498599000
6	-1.398121000	1.193615000	-2.989952000
6	0.611971000	1.008237000	-4.392324000
1	-1.864819000	1.155410000	-2.015970000
6	-0.011836000	0.923173000	-3.100354000
1	-2.127469000	1.837863000	-6.261873000
6	-4.929096000	0.621126000	0.988519000
1	-3.933979000	0.896825000	0.634805000
1	-5.355639000	-0.148743000	0.343891000
1	-5.588343000	1.490364000	1.016061000
6	-4.127963000	1.359800000	3.658875000
1	-4.014581000	1.049235000	4.698208000
1	-3.159507000	1.651182000	3.248637000
1	-4.836835000	2.186613000	3.591697000
16	-4.800317000	-0.135732000	2.716974000

⁵TS_{so}:

26	-0.008269000	-0.063155000	0.204509000
7	0.036763000	-0.969314000	2.148506000
7	0.732229000	0.678915000	-1.704001000
7	0.918956000	1.595730000	1.203234000

7	-0.193617000	-2.024839000	-0.723282000
6	1.288097000	-0.968641000	2.680040000
6	1.546494000	-1.512914000	3.934207000
1	2.551021000	-1.506148000	4.338411000
6	0.478017000	-2.069572000	4.652239000
1	0.650192000	-2.502568000	5.630196000
6	-0.806199000	-2.064176000	4.097670000
1	-1.647886000	-2.486711000	4.630884000
6	-0.996979000	-1.502852000	2.832916000
1	-1.965583000	-1.470752000	2.352594000
6	2.050846000	0.468397000	-1.853184000
6	2.725947000	0.715308000	-3.070993000
1	3.787810000	0.515136000	-3.140335000
6	2.019809000	1.204348000	-4.147662000
1	2.515444000	1.394992000	-5.093458000
6	2.044154000	1.223196000	1.869259000
6	2.808938000	2.144354000	2.578486000
1	3.704312000	1.829424000	3.099605000
6	2.392151000	3.483497000	2.596491000
1	2.969452000	4.222699000	3.138562000
6	1.231853000	3.856605000	1.909993000
1	0.888196000	4.882857000	1.908181000
6	0.510745000	2.882216000	1.215939000
1	-0.392376000	3.110607000	0.666398000
6	0.963609000	-2.707962000	-0.698809000
6	1.140062000	-3.927702000	-1.391784000
1	2.099229000	-4.428474000	-1.351082000
6	0.088468000	-4.455600000	-2.108001000
1	0.202606000	-5.386342000	-2.653043000
6	-1.159645000	-3.782357000	-2.133413000
6	-1.284359000	-2.543152000	-1.417649000
6	2.309886000	-0.272154000	1.796060000
1	3.332610000	-0.516596000	2.093392000
6	2.850947000	0.030822000	-0.651331000
1	3.277721000	0.922612000	-0.181004000
1	3.695692000	-0.591246000	-0.960557000
6	2.083456000	-2.190267000	0.169733000
1	2.009514000	-2.676848000	1.147604000
1	3.055072000	-2.472055000	-0.245700000
7	2.019315000	-0.701414000	0.364244000
8	-1.580419000	0.502275000	0.289992000
6	-3.606976000	-2.406367000	-2.105893000
6	-3.485995000	-3.622093000	-2.825577000
6	-2.532587000	-1.871647000	-1.417434000
1	-4.341714000	-4.018385000	-3.360366000
1	-2.631554000	-0.947374000	-0.864374000
6	-2.282615000	-4.297492000	-2.837814000
1	-2.173679000	-5.232105000	-3.378050000
1	-4.559067000	-1.886957000	-2.093962000
6	-1.484119000	2.248691000	-4.934577000
6	-2.106094000	1.991349000	-3.686637000
6	-0.138210000	1.991344000	-5.098255000
1	-3.162005000	2.206251000	-3.563237000
1	0.355723000	2.188222000	-6.043934000
6	-1.389750000	1.473194000	-2.622308000
6	0.631287000	1.466619000	-4.023630000
1	-1.868202000	1.287109000	-1.670065000
6	-0.007507000	1.194385000	-2.766098000
1	-2.068143000	2.651451000	-5.754323000
6	-3.710305000	2.980907000	1.158697000
1	-2.854825000	2.670491000	1.759227000
1	-3.409738000	3.739660000	0.435639000
1	-4.512206000	3.363106000	1.792196000

6	-4.794654000	0.347547000	1.583720000
1	-5.152203000	-0.577571000	1.131172000
1	-3.908626000	0.153807000	2.189140000
1	-5.582766000	0.801047000	2.186828000
16	-4.336488000	1.504430000	0.167725000

⁵P_{DMS}:

26	-0.199888000	0.024429000	0.250824000
7	0.053507000	-0.850958000	2.309745000
7	0.569521000	0.636423000	-1.784840000
7	0.831582000	1.834327000	1.143357000
7	-0.203574000	-2.067933000	-0.631320000
6	1.336446000	-0.727455000	2.736545000
6	1.743706000	-1.185823000	3.989693000
1	2.775647000	-1.079083000	4.301754000
6	0.796366000	-1.790036000	4.826188000
1	1.087073000	-2.154762000	5.804282000
6	-0.522074000	-1.927729000	4.379729000
1	-1.276732000	-2.399924000	4.995995000
6	-0.855820000	-1.450034000	3.110379000
1	-1.856567000	-1.549775000	2.711086000
6	1.889587000	0.476849000	-1.930777000
6	2.543894000	0.661927000	-3.176694000
1	3.614255000	0.507327000	-3.242878000
6	1.809547000	1.032947000	-4.280588000
1	2.288721000	1.176282000	-5.243363000
6	1.973351000	1.466323000	1.780923000
6	2.789669000	2.394771000	2.427858000
1	3.698941000	2.072446000	2.920984000
6	2.414049000	3.744068000	2.419370000
1	3.030529000	4.484527000	2.915173000
6	1.243945000	4.123421000	1.753812000
1	0.929590000	5.158843000	1.717330000
6	0.480590000	3.139895000	1.120572000
1	-0.419946000	3.390025000	0.575233000
6	0.999586000	-2.652581000	-0.604641000
6	1.266285000	-3.872025000	-1.279477000
1	2.262623000	-4.295625000	-1.238081000
6	0.256829000	-4.495780000	-1.978433000
1	0.439821000	-5.425435000	-2.506969000
6	-1.040926000	-3.919205000	-2.008508000
6	-1.245242000	-2.682442000	-1.311352000
6	2.268887000	-0.028536000	1.755190000
1	3.311487000	-0.206859000	2.042062000
6	2.728547000	0.163224000	-0.708991000
1	3.106439000	1.110284000	-0.310061000
1	3.608811000	-0.419420000	-1.003993000
6	2.091086000	-2.031368000	0.242848000
1	2.030651000	-2.475229000	1.241785000
1	3.074179000	-2.303510000	-0.157838000
7	1.976925000	-0.547477000	0.368072000
8	-2.146861000	0.591707000	0.420235000
6	-3.577770000	-2.704301000	-1.978856000
6	-3.378470000	-3.921071000	-2.681930000
6	-2.535310000	-2.092578000	-1.306424000
1	-4.209947000	-4.381020000	-3.204540000
1	-2.685857000	-1.168567000	-0.758896000
6	-2.133180000	-4.517663000	-2.695446000
1	-1.969471000	-5.450921000	-3.224772000
1	-4.563344000	-2.250958000	-1.968921000
6	-1.766796000	1.812265000	-5.083963000
6	-2.356918000	1.610737000	-3.809202000
6	-0.409245000	1.626171000	-5.256135000

1	-3.423506000	1.766123000	-3.685925000
1	0.054381000	1.780706000	-6.225183000
6	-1.591240000	1.222234000	-2.724693000
6	0.407839000	1.231243000	-4.161128000
1	-2.036678000	1.075042000	-1.747568000
6	-0.195637000	1.020852000	-2.877346000
1	-2.386756000	2.115532000	-5.920417000
6	-4.415794000	0.446752000	2.051731000
1	-4.859889000	0.112555000	1.115070000
1	-4.031835000	-0.387908000	2.634348000
1	-5.105789000	1.049540000	2.642280000
6	-3.797177000	2.848604000	0.572523000
1	-3.018491000	3.508619000	0.195569000
1	-4.313991000	2.335500000	-0.237264000
1	-4.486078000	3.387370000	1.223289000
16	-2.936826000	1.543897000	1.633443000

³Re_{CHD}:

26	-0.351269000	0.059229000	0.261121000
7	-0.301291000	-0.651875000	2.119977000
7	0.133553000	0.740688000	-1.609928000
7	0.130070000	1.828063000	1.037831000
7	-0.318431000	-1.851784000	-0.479197000
6	0.891698000	-0.423907000	2.735869000
6	1.131267000	-0.852124000	4.035901000
1	2.088622000	-0.665634000	4.505455000
6	0.106348000	-1.529985000	4.712302000
1	0.264022000	-1.877464000	5.725958000
6	-1.115778000	-1.754082000	4.070349000
1	-1.924043000	-2.270923000	4.570789000
6	-1.294775000	-1.300763000	2.761733000
1	-2.217997000	-1.438624000	2.217266000
6	1.465330000	0.797221000	-1.802080000
6	2.046997000	1.105020000	-3.051291000
1	3.125688000	1.119812000	-3.142529000
6	1.232874000	1.372671000	-4.127198000
1	1.655732000	1.598674000	-5.099771000
6	1.276309000	1.783251000	1.772657000
6	1.787260000	2.917899000	2.390957000
1	2.703572000	2.863285000	2.964568000
6	1.086535000	4.125157000	2.250313000
1	1.460400000	5.025992000	2.721417000
6	-0.094062000	4.155778000	1.502013000
1	-0.662773000	5.069132000	1.387139000
6	-0.553276000	2.982790000	0.898133000
1	-1.464803000	2.949612000	0.318046000
6	0.910884000	-2.398615000	-0.419043000
6	1.224880000	-3.645243000	-1.002629000
1	2.237628000	-4.021034000	-0.931526000
6	0.240929000	-4.351874000	-1.654362000
1	0.460030000	-5.304715000	-2.123279000
6	-1.077960000	-3.836329000	-1.706744000
6	-1.353404000	-2.565285000	-1.091599000
6	1.834858000	0.374520000	1.855176000
1	2.868998000	0.343967000	2.202298000
6	2.365013000	0.581769000	-0.614922000
1	2.656226000	1.556199000	-0.210402000
1	3.288318000	0.078458000	-0.911891000
6	1.972080000	-1.673164000	0.363769000
1	2.012742000	-2.094037000	1.373337000
1	2.959052000	-1.827294000	-0.079048000
7	1.667980000	-0.206240000	0.455451000
8	-1.981132000	0.370916000	0.331972000

6	-3.689832000	-2.815381000	-1.714087000
6	-3.416108000	-4.052369000	-2.347784000
6	-2.686477000	-2.085241000	-1.102261000
1	-4.217420000	-4.603318000	-2.826546000
1	-2.912716000	-1.152578000	-0.608141000
6	-2.131070000	-4.553112000	-2.339015000
1	-1.900761000	-5.505471000	-2.804607000
1	-4.704881000	-2.433786000	-1.703849000
6	-2.416868000	1.674820000	-4.858500000
6	-2.952233000	1.393143000	-3.577619000
6	-1.050301000	1.662027000	-5.043986000
1	-4.026253000	1.421034000	-3.429843000
1	-0.617543000	1.887867000	-6.012780000
6	-2.129903000	1.086007000	-2.508055000
6	-0.174773000	1.361390000	-3.964207000
1	-2.549998000	0.892433000	-1.532894000
6	-0.722965000	1.048549000	-2.671510000
1	-3.081216000	1.907243000	-5.682804000
6	-4.288181000	3.683938000	0.168723000
6	-4.813559000	2.838113000	1.312368000
6	-3.936797000	4.972775000	0.367596000
6	-4.261902000	3.297785000	2.682762000
6	-4.193291000	4.807620000	2.800188000
6	-4.019037000	5.577012000	1.705345000
1	-4.269086000	3.248393000	-0.827508000
1	-5.915919000	2.900621000	1.316848000
1	-4.569291000	1.782031000	1.151446000
1	-3.612154000	5.595452000	-0.461817000
1	-4.870780000	2.874433000	3.489929000
1	-3.245497000	2.889431000	2.825916000
1	-4.227783000	5.248879000	3.793269000
1	-3.923404000	6.656038000	1.791252000

³TS_{HA,CHD}:

26	-0.462659000	0.337648000	0.238851000
7	-0.579606000	-0.314412000	2.116170000
7	0.193594000	0.878486000	-1.667566000
7	0.186495000	2.070846000	0.971624000
7	-0.601268000	-1.611320000	-0.463447000
6	0.604508000	-0.192149000	2.778227000
6	0.754614000	-0.623100000	4.091554000
1	1.707038000	-0.519548000	4.595984000
6	-0.349975000	-1.201287000	4.733405000
1	-0.262949000	-1.547191000	5.756193000
6	-1.556391000	-1.339961000	4.039652000
1	-2.421430000	-1.792610000	4.506584000
6	-1.640990000	-0.888767000	2.720652000
1	-2.541264000	-0.980095000	2.130784000
6	1.528124000	0.748502000	-1.783163000
6	2.213013000	0.888508000	-3.011939000
1	3.287255000	0.754843000	-3.036369000
6	1.502779000	1.185682000	-4.151827000
1	2.003700000	1.286401000	-5.108526000
6	1.288888000	1.924416000	1.757393000
6	1.931383000	3.018690000	2.324463000
1	2.809820000	2.878985000	2.941730000
6	1.420841000	4.298689000	2.062749000
1	1.902940000	5.171398000	2.486199000
6	0.294398000	4.438895000	1.246145000
1	-0.118587000	5.414501000	1.025610000
6	-0.308122000	3.298466000	0.709226000
1	-1.182352000	3.341579000	0.076216000
6	0.556841000	-2.279953000	-0.314595000

6	0.770357000	-3.576351000	-0.835697000
1	1.732644000	-4.051588000	-0.691631000
6	-0.245018000	-4.206332000	-1.516766000
1	-0.103514000	-5.197310000	-1.934078000
6	-1.495325000	-3.556357000	-1.670017000
6	-1.663611000	-2.237896000	-1.120848000
6	1.668900000	0.465772000	1.919793000
1	2.675193000	0.334063000	2.322175000
6	2.332922000	0.512738000	-0.531012000
1	2.688302000	1.478091000	-0.156871000
1	3.222501000	-0.085415000	-0.746280000
6	1.647812000	-1.640681000	0.503814000
1	1.588363000	-2.023212000	1.527492000
1	2.633642000	-1.920266000	0.122977000
7	1.506393000	-0.148220000	0.529766000
8	-2.141824000	0.858867000	0.124959000
6	-3.966044000	-2.246381000	-1.895265000
6	-3.798549000	-3.537061000	-2.456226000
6	-2.926591000	-1.606492000	-1.243771000
1	-4.626675000	-4.016550000	-2.965907000
1	-3.053278000	-0.625735000	-0.805453000
6	-2.583050000	-4.179418000	-2.341916000
1	-2.436097000	-5.172053000	-2.754609000
1	-4.927885000	-1.751247000	-1.976144000
6	-2.032937000	1.920167000	-5.110367000
6	-2.664368000	1.796704000	-3.847336000
6	-0.673287000	1.713102000	-5.218251000
1	-3.731008000	1.977042000	-3.765536000
1	-0.168232000	1.814565000	-6.173183000
6	-1.945116000	1.454388000	-2.716142000
6	0.099903000	1.371984000	-4.074192000
1	-2.419168000	1.372236000	-1.747123000
6	-0.549363000	1.222527000	-2.799657000
1	-2.618513000	2.184554000	-5.983734000
6	-4.842818000	2.317453000	1.016781000
6	-3.809030000	1.815894000	1.918720000
6	-4.942939000	3.651639000	0.716044000
6	-3.198407000	2.845929000	2.875833000
6	-3.229437000	4.256145000	2.348825000
6	-4.067481000	4.621831000	1.343955000
1	-5.490410000	1.598689000	0.522462000
1	-4.079816000	0.880765000	2.417740000
1	-2.918422000	1.399664000	1.130801000
1	-5.681863000	3.998676000	0.000874000
1	-3.763555000	2.824657000	3.827939000
1	-2.176449000	2.562060000	3.156893000
1	-2.600448000	4.993137000	2.839995000
1	-4.110151000	5.653959000	1.010386000

³Int_{CHD}:

26	-0.257219000	0.206795000	0.222741000
7	-0.493138000	-0.334785000	2.120434000
7	0.484270000	0.664951000	-1.661504000
7	0.249011000	1.996478000	0.920240000
7	-0.295746000	-1.773699000	-0.390031000
6	0.645051000	-0.159241000	2.848609000
6	0.717999000	-0.527404000	4.186531000
1	1.633922000	-0.384233000	4.745682000
6	-0.418934000	-1.091992000	4.783681000
1	-0.391592000	-1.391396000	5.824263000
6	-1.581288000	-1.269487000	4.027109000
1	-2.472032000	-1.702074000	4.463489000
6	-1.590549000	-0.881256000	2.685453000

1	-2.459714000	-0.992873000	2.052849000
6	1.828310000	0.597354000	-1.690140000
6	2.580207000	0.707507000	-2.880799000
1	3.659009000	0.628155000	-2.834609000
6	1.926612000	0.909359000	-4.074737000
1	2.479442000	0.986752000	-5.004572000
6	1.302247000	1.933021000	1.781366000
6	1.840592000	3.076709000	2.358889000
1	2.681417000	3.004590000	3.036845000
6	1.271686000	4.316816000	2.033389000
1	1.670624000	5.225848000	2.466648000
6	0.194585000	4.371440000	1.142919000
1	-0.260595000	5.315342000	0.872980000
6	-0.298998000	3.186284000	0.593624000
1	-1.124451000	3.164709000	-0.103766000
6	0.878935000	-2.384950000	-0.150450000
6	1.177536000	-3.686152000	-0.612735000
1	2.149441000	-4.113174000	-0.399834000
6	0.229631000	-4.382029000	-1.327373000
1	0.437814000	-5.378142000	-1.702491000
6	-1.037973000	-3.795680000	-1.568770000
6	-1.293962000	-2.469054000	-1.075989000
6	1.737151000	0.500458000	2.027990000
1	2.723401000	0.426811000	2.489646000
6	2.554854000	0.469670000	-0.377767000
1	2.833647000	1.469266000	-0.029946000
1	3.483990000	-0.093625000	-0.493712000
6	1.887407000	-1.668184000	0.708562000
1	1.775323000	-2.007258000	1.743032000
1	2.907390000	-1.916477000	0.405413000
7	1.682160000	-0.180516000	0.657636000
8	-2.009083000	0.662524000	0.002825000
6	-3.551881000	-2.610943000	-1.955460000
6	-3.297467000	-3.908635000	-2.465329000
6	-2.576719000	-1.900655000	-1.277829000
1	-4.076863000	-4.442451000	-2.997407000
1	-2.769952000	-0.915136000	-0.875876000
6	-2.061200000	-4.489688000	-2.271935000
1	-1.849624000	-5.486965000	-2.643175000
1	-4.531385000	-2.166447000	-2.096254000
6	-1.574264000	1.404626000	-5.280348000
6	-2.276444000	1.309904000	-4.052781000
6	-0.201745000	1.266713000	-5.295637000
1	-3.354086000	1.434490000	-4.045435000
1	0.356887000	1.347019000	-6.222297000
6	-1.614538000	1.065354000	-2.862486000
6	0.514390000	1.026190000	-4.090556000
1	-2.143976000	1.006973000	-1.921301000
6	-0.205944000	0.908048000	-2.851138000
1	-2.116721000	1.592378000	-6.200132000
6	-4.185957000	1.969719000	2.609184000
6	-4.289638000	2.663793000	1.426819000
6	-4.918148000	0.768018000	2.832162000
6	-5.192603000	2.207494000	0.308641000
6	-5.912612000	0.918225000	0.609437000
6	-5.769597000	0.264556000	1.808386000
1	-3.540195000	2.346871000	3.397964000
1	-3.742243000	3.591621000	1.284092000
1	-2.400777000	1.166443000	0.751301000
1	-4.830879000	0.244467000	3.777690000
1	-5.926734000	3.002953000	0.071502000
1	-4.615147000	2.110286000	-0.629969000
1	-6.569075000	0.520388000	-0.159449000

1	-6.318182000	-0.656462000	1.986414000
³ TS _{reb,CHD} :			
26	-0.232158000	0.393220000	0.148564000
7	-0.438931000	0.005714000	2.175459000
7	0.630862000	0.716432000	-1.753356000
7	0.411653000	2.202555000	0.710304000
7	-0.374855000	-1.620574000	-0.343973000
6	0.726719000	0.200628000	2.845290000
6	0.823055000	0.001210000	4.218584000
1	1.763841000	0.157182000	4.731715000
6	-0.325024000	-0.409967000	4.911822000
1	-0.281729000	-0.576185000	5.981509000
6	-1.520710000	-0.605819000	4.213021000
1	-2.421759000	-0.920906000	4.723395000
6	-1.546981000	-0.388832000	2.832453000
1	-2.442738000	-0.516598000	2.238672000
6	1.951040000	0.479429000	-1.760728000
6	2.714574000	0.463569000	-2.952491000
1	3.774478000	0.246754000	-2.900433000
6	2.096562000	0.723311000	-4.154957000
1	2.658804000	0.707134000	-5.082336000
6	1.491062000	2.121286000	1.540721000
6	2.152333000	3.259231000	1.992377000
1	3.011214000	3.167200000	2.645433000
6	1.685892000	4.515094000	1.580009000
1	2.182755000	5.416752000	1.916946000
6	0.582028000	4.591052000	0.725144000
1	0.201148000	5.545328000	0.385005000
6	-0.032266000	3.411501000	0.300359000
1	-0.877148000	3.416663000	-0.374975000
6	0.715896000	-2.312092000	0.035068000
6	0.903087000	-3.681213000	-0.269199000
1	1.808623000	-4.175810000	0.059922000
6	-0.061319000	-4.357039000	-0.979467000
1	0.062412000	-5.405540000	-1.227902000
6	-1.229285000	-3.671695000	-1.399506000
6	-1.369170000	-2.281146000	-1.065807000
6	1.834312000	0.691755000	1.929462000
1	2.819430000	0.619400000	2.397033000
6	2.656872000	0.311889000	-0.434846000
1	3.092812000	1.277596000	-0.156752000
1	3.490881000	-0.389393000	-0.529919000
6	1.764732000	-1.612628000	0.865225000
1	1.579644000	-1.829235000	1.921531000
1	2.758865000	-2.008412000	0.635942000
7	1.732090000	-0.133156000	0.655516000
8	-2.068049000	0.919864000	0.030359000
6	-3.513314000	-2.253583000	-2.205507000
6	-3.377563000	-3.624224000	-2.541496000
6	-2.535292000	-1.592510000	-1.482996000
1	-4.157146000	-4.120547000	-3.108529000
1	-2.644041000	-0.554201000	-1.208799000
6	-2.254541000	-4.319481000	-2.142716000
1	-2.132968000	-5.369496000	-2.387988000
1	-4.400301000	-1.714184000	-2.520537000
6	-1.310449000	1.682384000	-5.370028000
6	-2.016055000	1.704770000	-4.139996000
6	0.029785000	1.352522000	-5.389780000
1	-3.064969000	1.981549000	-4.133400000
1	0.587179000	1.342997000	-6.320742000
6	-1.388860000	1.383020000	-2.949544000
6	0.711445000	1.030490000	-4.183720000

1	-1.919163000	1.402834000	-2.004506000
6	-0.015663000	1.029640000	-2.945584000
1	-1.825543000	1.932987000	-6.290656000
6	-5.992748000	1.773002000	2.393198000
6	-5.549834000	1.752047000	1.090140000
6	-6.005278000	0.586580000	3.170040000
6	-5.014140000	0.515260000	0.470643000
6	-5.133684000	-0.703742000	1.307844000
6	-5.583865000	-0.644322000	2.609383000
1	-6.352648000	2.698101000	2.831572000
1	-5.557177000	2.658463000	0.492201000
1	-2.194451000	1.755385000	0.529868000
1	-6.361418000	0.617657000	4.193956000
1	-5.416772000	0.359020000	-0.545206000
1	-3.903906000	0.666226000	0.234854000
1	-4.830856000	-1.650592000	0.871189000
1	-5.636257000	-1.547258000	3.209074000

³P_{CHD}:

26	-0.295881000	0.427699000	0.084216000
7	-0.468435000	-0.018169000	2.248762000
7	0.680421000	0.785650000	-1.824161000
7	0.328825000	2.236770000	0.679913000
7	-0.448563000	-1.564666000	-0.363928000
6	0.723808000	0.221926000	2.851158000
6	0.909823000	0.053529000	4.221582000
1	1.875389000	0.248311000	4.672374000
6	-0.177662000	-0.376515000	4.994237000
1	-0.064273000	-0.517459000	6.062573000
6	-1.404936000	-0.625671000	4.371659000
1	-2.263537000	-0.960069000	4.940141000
6	-1.515556000	-0.438710000	2.990832000
1	-2.444110000	-0.619184000	2.466395000
6	1.986982000	0.500547000	-1.789689000
6	2.781810000	0.450079000	-2.962657000
1	3.831380000	0.193953000	-2.882255000
6	2.206702000	0.723353000	-4.183751000
1	2.792418000	0.677276000	-5.095563000
6	1.416513000	2.150926000	1.501978000
6	2.074747000	3.288505000	1.962924000
1	2.940046000	3.190292000	2.606891000
6	1.601818000	4.549045000	1.576002000
1	2.098182000	5.447329000	1.922748000
6	0.489980000	4.631921000	0.732496000
1	0.100347000	5.588692000	0.409346000
6	-0.119431000	3.454977000	0.295262000
1	-0.967919000	3.473171000	-0.376170000
6	0.578960000	-2.284780000	0.122871000
6	0.639610000	-3.696597000	0.013239000
1	1.494058000	-4.219016000	0.426339000
6	-0.382040000	-4.379395000	-0.602504000
1	-0.361272000	-5.460849000	-0.681141000
6	-1.467840000	-3.657337000	-1.163233000
6	-1.466372000	-2.227068000	-1.050908000
6	1.791433000	0.727000000	1.891714000
1	2.781359000	0.696771000	2.357929000
6	2.656278000	0.317332000	-0.440468000
1	3.100322000	1.278971000	-0.158282000
1	3.486951000	-0.390550000	-0.528269000
6	1.709915000	-1.588651000	0.851508000
1	1.622090000	-1.802144000	1.921180000
1	2.663608000	-2.025378000	0.533922000
7	1.721852000	-0.114489000	0.636982000

8	-2.337078000	1.062009000	0.162852000
6	-3.528396000	-2.155266000	-2.340571000
6	-3.550185000	-3.569669000	-2.422212000
6	-2.511709000	-1.498468000	-1.669530000
1	-4.358303000	-4.066985000	-2.946269000
1	-2.491009000	-0.420306000	-1.647522000
6	-2.532676000	-4.304870000	-1.847885000
1	-2.522897000	-5.387675000	-1.916620000
1	-4.314158000	-1.578870000	-2.816429000
6	-1.134045000	1.815636000	-5.482654000
6	-1.863679000	1.880793000	-4.267890000
6	0.191453000	1.428661000	-5.473834000
1	-2.897907000	2.206926000	-4.283192000
1	0.764730000	1.390238000	-6.394356000
6	-1.271084000	1.539956000	-3.065448000
6	0.834965000	1.085951000	-4.252546000
1	-1.827993000	1.609718000	-2.138928000
6	0.083861000	1.122059000	-3.031572000
1	-1.619615000	2.081475000	-6.414851000
6	-5.710527000	1.465189000	2.514260000
6	-5.749519000	1.569590000	1.117478000
6	-5.509126000	0.216143000	3.119304000
6	-5.582824000	0.423053000	0.323129000
6	-5.376170000	-0.826769000	0.929546000
6	-5.341364000	-0.929052000	2.328634000
1	-5.842275000	2.350370000	3.128038000
1	-5.917038000	2.533905000	0.648462000
1	-2.504880000	1.863010000	0.693601000
1	-5.485686000	0.135848000	4.201360000
1	-5.637393000	0.499687000	-0.758801000
1	-3.150957000	0.516941000	0.138865000
1	-5.256380000	-1.713724000	0.316233000
1	-5.192872000	-1.896526000	2.797578000

⁵Re_{CHD}:

26	-0.470293000	0.086413000	0.265805000
7	-0.317728000	-0.670439000	2.248941000
7	0.082337000	0.805541000	-1.692823000
7	0.113221000	1.925132000	1.145548000
7	-0.391153000	-1.921852000	-0.506560000
6	0.913400000	-0.433246000	2.776126000
6	1.247477000	-0.847842000	4.060778000
1	2.234050000	-0.653408000	4.461924000
6	0.275742000	-1.524088000	4.813834000
1	0.507325000	-1.861705000	5.816699000
6	-0.988522000	-1.760298000	4.263397000
1	-1.755152000	-2.277950000	4.825026000
6	-1.259331000	-1.318599000	2.966140000
1	-2.216684000	-1.472579000	2.486770000
6	1.417979000	0.824041000	-1.849325000
6	2.034798000	1.097804000	-3.090150000
1	3.115028000	1.086950000	-3.162031000
6	1.247426000	1.370927000	-4.187483000
1	1.697779000	1.575813000	-5.152515000
6	1.281332000	1.799223000	1.832208000
6	1.857461000	2.879430000	2.491262000
1	2.790011000	2.761669000	3.028515000
6	1.199439000	4.117788000	2.439244000
1	1.624963000	4.977262000	2.942918000
6	-0.004167000	4.234456000	1.736777000
1	-0.536724000	5.175231000	1.688479000
6	-0.528278000	3.111605000	1.090944000
1	-1.457303000	3.146009000	0.536773000

6	0.859457000	-2.414392000	-0.459241000
6	1.214210000	-3.647335000	-1.050131000
1	2.239739000	-3.989381000	-0.992747000
6	0.246489000	-4.390200000	-1.690189000
1	0.496445000	-5.335947000	-2.158351000
6	-1.091525000	-3.922826000	-1.736026000
6	-1.400485000	-2.661383000	-1.120858000
6	1.800754000	0.371794000	1.842274000
1	2.854588000	0.315658000	2.123044000
6	2.274514000	0.621055000	-0.628021000
1	2.528212000	1.601497000	-0.213575000
1	3.218397000	0.136164000	-0.888490000
6	1.893222000	-1.653278000	0.327969000
1	1.940590000	-2.074793000	1.336747000
1	2.886223000	-1.778205000	-0.110560000
7	1.566365000	-0.183209000	0.435223000
8	-2.096991000	0.382366000	0.312563000
6	-3.727074000	-2.956240000	-1.746269000
6	-3.424477000	-4.192411000	-2.370646000
6	-2.740746000	-2.202380000	-1.135545000
1	-4.214091000	-4.762865000	-2.846103000
1	-2.981782000	-1.266479000	-0.651587000
6	-2.128739000	-4.666806000	-2.362957000
1	-1.879835000	-5.614861000	-2.827841000
1	-4.750030000	-2.596254000	-1.744449000
6	-2.387695000	1.715152000	-4.993238000
6	-2.951267000	1.448754000	-3.719891000
6	-1.017964000	1.688141000	-5.157918000
1	-4.028049000	1.483021000	-3.595588000
1	-0.568983000	1.897326000	-6.123101000
6	-2.150889000	1.148142000	-2.632110000
6	-0.164711000	1.390391000	-4.059729000
1	-2.585510000	0.958547000	-1.660917000
6	-0.742173000	1.104122000	-2.775580000
1	-3.035813000	1.944474000	-5.831291000
6	-4.292938000	3.688980000	0.128550000
6	-4.879642000	2.872666000	1.263763000
6	-3.904968000	4.967555000	0.326441000
6	-4.350836000	3.325871000	2.645223000
6	-4.234654000	4.833580000	2.752093000
6	-4.004831000	5.586692000	1.656122000
1	-4.259372000	3.243443000	-0.862795000
1	-5.978791000	2.974036000	1.236444000
1	-4.668795000	1.807085000	1.118613000
1	-3.536118000	5.571293000	-0.498478000
1	-4.995737000	2.930572000	3.438498000
1	-3.353281000	2.884820000	2.819945000
1	-4.282017000	5.284908000	3.740097000
1	-3.875924000	6.662741000	1.735582000

⁵P_{CHD}:

26	-0.508315000	0.207338000	0.146457000
7	-0.563137000	-0.675960000	2.225741000
7	0.435368000	0.769461000	-1.825789000
7	0.146307000	2.032796000	1.261523000
7	-0.315259000	-1.911987000	-0.508898000
6	0.661102000	-0.536335000	2.801260000
6	0.952006000	-1.080844000	4.052366000
1	1.937902000	-0.959081000	4.484868000
6	-0.049995000	-1.787484000	4.729948000
1	0.151608000	-2.219996000	5.702841000
6	-1.306490000	-1.933576000	4.134133000
1	-2.101537000	-2.477880000	4.627984000

6	-1.526118000	-1.367594000	2.875712000
1	-2.477162000	-1.466587000	2.368847000
6	1.764151000	0.901644000	-1.712047000
6	2.585092000	1.293392000	-2.801525000
1	3.655279000	1.377839000	-2.655419000
6	2.010588000	1.568700000	-4.021073000
1	2.618424000	1.883042000	-4.862809000
6	1.216961000	1.748362000	2.047922000
6	1.809475000	2.713395000	2.861040000
1	2.666011000	2.460412000	3.474077000
6	1.277264000	4.009581000	2.862823000
1	1.720164000	4.778750000	3.484402000
6	0.174340000	4.299142000	2.053109000
1	-0.259756000	5.290670000	2.030521000
6	-0.366713000	3.283485000	1.261051000
1	-1.221415000	3.455053000	0.620919000
6	0.924661000	-2.398572000	-0.397132000
6	1.291741000	-3.658493000	-0.937634000
1	2.313191000	-4.004147000	-0.833659000
6	0.345579000	-4.418889000	-1.587448000
1	0.607214000	-5.380283000	-2.016529000
6	-0.991634000	-3.948672000	-1.692458000
6	-1.301162000	-2.669278000	-1.125733000
6	1.664629000	0.293615000	2.002934000
1	2.662907000	0.194321000	2.443276000
6	2.427497000	0.692616000	-0.363872000
1	2.568683000	1.674318000	0.098272000
1	3.431425000	0.278067000	-0.514582000
6	1.954731000	-1.622390000	0.400120000
1	2.024103000	-2.086316000	1.390970000
1	2.940678000	-1.742921000	-0.061342000
7	1.643144000	-0.170358000	0.565834000
8	-2.441438000	1.077316000	-0.007940000
6	-3.618019000	-2.946703000	-1.794595000
6	-3.312540000	-4.204209000	-2.375729000
6	-2.635084000	-2.190237000	-1.181694000
1	-4.097785000	-4.778689000	-2.854129000
1	-2.878152000	-1.237034000	-0.726853000
6	-2.023263000	-4.696912000	-2.323146000
1	-1.779550000	-5.662283000	-2.754702000
1	-4.637021000	-2.576902000	-1.828539000
6	-1.406639000	1.495312000	-5.552318000
6	-2.165609000	1.045535000	-4.442385000
6	-0.043354000	1.675428000	-5.427453000
1	-3.232661000	0.886840000	-4.553430000
1	0.552899000	2.005119000	-6.272072000
6	-1.560888000	0.798668000	-3.222932000
6	0.607284000	1.425638000	-4.187972000
1	-2.146903000	0.422152000	-2.396028000
6	-0.166075000	0.996287000	-3.058946000
1	-1.900006000	1.686708000	-6.498492000
6	-5.443431000	3.363680000	1.130715000
6	-6.289534000	2.443046000	0.495813000
6	-4.552142000	2.929315000	2.121077000
6	-6.245637000	1.087410000	0.848199000
6	-5.355317000	0.649429000	1.839587000
6	-4.507013000	1.570636000	2.477527000
1	-5.480033000	4.412988000	0.856735000
1	-6.980148000	2.781322000	-0.269900000
1	-2.712745000	1.674447000	-0.728320000
1	-3.899542000	3.640645000	2.616693000
1	-6.902387000	0.376609000	0.357431000
1	-3.084472000	1.118159000	0.733367000

1	-5.328563000	-0.398233000	2.121700000
1	-3.832693000	1.236463000	3.260153000
³ Re _{Tot} :			
26	0.004538000	0.489560000	0.702143000
7	0.156783000	-0.303627000	2.522728000
7	0.326998000	1.068305000	-1.236629000
7	1.206541000	1.939798000	1.347938000
7	-0.764419000	-1.267758000	-0.015075000
6	1.448918000	-0.534556000	2.886349000
6	1.767881000	-1.098160000	4.115796000
1	2.801061000	-1.279447000	4.383324000
6	0.720357000	-1.424824000	4.989619000
1	0.937814000	-1.867316000	5.954004000
6	-0.601752000	-1.175974000	4.607929000
1	-1.427989000	-1.413567000	5.265013000
6	-0.858219000	-0.610405000	3.357028000
1	-1.858018000	-0.391001000	3.010365000
6	1.532008000	0.674800000	-1.691409000
6	1.931033000	0.828106000	-3.037035000
1	2.908431000	0.475947000	-3.341590000
6	1.068436000	1.414403000	-3.933913000
1	1.346157000	1.531230000	-4.975568000
6	2.382462000	1.463805000	1.842765000
6	3.362985000	2.317770000	2.332727000
1	4.293783000	1.919315000	2.715666000
6	3.113382000	3.697936000	2.312624000
1	3.859470000	4.388531000	2.686131000
6	1.899071000	4.174028000	1.808086000
1	1.679487000	5.233354000	1.785530000
6	0.954458000	3.265023000	1.326660000
1	-0.002650000	3.572788000	0.930021000
6	0.189354000	-2.200137000	-0.202799000
6	-0.060486000	-3.432477000	-0.844615000
1	0.754132000	-4.132549000	-0.979407000
6	-1.330767000	-3.715033000	-1.291502000
1	-1.545010000	-4.648077000	-1.800815000
6	-2.375993000	-2.782801000	-1.076305000
6	-2.076598000	-1.542973000	-0.410873000
6	2.424718000	-0.052998000	1.828822000
1	3.431545000	-0.451796000	1.963777000
6	2.513134000	0.107316000	-0.701212000
1	3.186028000	0.906647000	-0.374901000
1	3.139393000	-0.657714000	-1.166486000
6	1.559946000	-1.933260000	0.359856000
1	1.631248000	-2.400759000	1.347010000
1	2.334707000	-2.390987000	-0.259952000
7	1.805843000	-0.458737000	0.495508000
8	-1.368789000	1.337386000	1.090441000
6	-4.427814000	-0.942691000	-0.554929000
6	-4.720392000	-2.148483000	-1.238515000
6	-3.139084000	-0.642124000	-0.151319000
1	-5.736500000	-2.359243000	-1.551707000
1	-2.934341000	0.272923000	0.383686000
6	-3.709826000	-3.052996000	-1.489511000
1	-3.913313000	-3.989753000	-1.997387000
1	-5.225740000	-0.239921000	-0.340810000
6	-2.318124000	2.987886000	-3.928060000
6	-2.660539000	2.839933000	-2.561445000
6	-1.103847000	2.517362000	-4.382169000
1	-3.608253000	3.225262000	-2.201196000
1	-0.814759000	2.632039000	-5.421505000
6	-1.805230000	2.213589000	-1.672144000

6	-0.195815000	1.878449000	-3.493327000
1	-2.071004000	2.122711000	-0.629963000
6	-0.557978000	1.705550000	-2.111757000
1	-3.006516000	3.476976000	-4.607689000
1	-5.498430000	5.221904000	-1.113841000
6	-3.567575000	5.400474000	0.819275000
1	-2.702732000	5.106474000	0.208747000
1	-3.220478000	5.497728000	1.852950000
1	-3.885711000	6.389319000	0.471596000
6	-4.685482000	4.386624000	0.704616000
6	-4.838109000	3.365409000	1.659941000
6	-5.858747000	2.412607000	1.539774000
6	-6.748652000	2.465818000	0.458717000
6	-6.610446000	3.480291000	-0.498418000
6	-5.590380000	4.431547000	-0.373577000
1	-4.158302000	3.321713000	2.506534000
1	-5.964069000	1.637972000	2.293292000
1	-7.544986000	1.733738000	0.368784000
1	-7.299661000	3.535608000	-1.335478000

³ TS _{HA,Tot} :			
26	-0.178703000	0.392955000	0.322052000
7	-0.363692000	-0.329474000	2.166159000
7	0.509835000	0.921558000	-1.565798000
7	0.721677000	1.976494000	1.125530000
7	-0.621182000	-1.475306000	-0.467848000
6	0.833496000	-0.422440000	2.807965000
6	0.933595000	-0.941393000	4.093832000
1	1.896499000	-1.008670000	4.583875000
6	-0.238051000	-1.380833000	4.726905000
1	-0.191793000	-1.791412000	5.728143000
6	-1.460866000	-1.295504000	4.053143000
1	-2.378847000	-1.634371000	4.515243000
6	-1.494172000	-0.764850000	2.762000000
1	-2.406998000	-0.679301000	2.190162000
6	1.811629000	0.615993000	-1.720926000
6	2.484625000	0.718539000	-2.958950000
1	3.529477000	0.440899000	-3.017649000
6	1.798320000	1.161974000	-4.065734000
1	2.288651000	1.237568000	-5.030166000
6	1.796006000	1.628787000	1.886594000
6	2.590329000	2.585500000	2.508117000
1	3.441981000	2.286255000	3.105603000
6	2.265031000	3.937988000	2.329723000
1	2.866412000	4.706570000	2.799628000
6	1.169110000	4.285597000	1.533213000
1	0.900977000	5.321600000	1.372299000
6	0.411212000	3.276541000	0.935322000
1	-0.442011000	3.483884000	0.305406000
6	0.433989000	-2.306979000	-0.391392000
6	0.452063000	-3.585189000	-0.993689000
1	1.340874000	-4.197445000	-0.907903000
6	-0.656474000	-4.024282000	-1.679773000
1	-0.663309000	-4.996705000	-2.159955000
6	-1.807868000	-3.200960000	-1.752746000
6	-1.777659000	-1.908868000	-1.121734000
6	1.967410000	0.123414000	1.961478000
1	2.952497000	-0.173705000	2.326992000
6	2.593516000	0.211190000	-0.499007000
1	3.082923000	1.097936000	-0.084589000
1	3.389195000	-0.492102000	-0.757316000
6	1.619603000	-1.878182000	0.433248000
1	1.523427000	-2.306520000	1.435873000

1	2.548855000	-2.271712000	0.013603000
7	1.693402000	-0.383376000	0.543709000
8	-1.789576000	1.141492000	0.288334000
6	-4.081629000	-1.558219000	-1.806480000
6	-4.108061000	-2.820044000	-2.451038000
6	-2.945782000	-1.107278000	-1.157837000
1	-5.008426000	-3.149555000	-2.957173000
1	-2.928695000	-0.150759000	-0.653533000
6	-2.989175000	-3.626497000	-2.420982000
1	-2.991819000	-4.601291000	-2.897325000
1	-4.969385000	-0.934986000	-1.818719000
6	-1.621777000	2.409048000	-4.903992000
6	-2.239759000	2.316014000	-3.631926000
6	-0.305176000	2.025679000	-5.053678000
1	-3.270090000	2.634869000	-3.515780000
1	0.191377000	2.100238000	-6.015428000
6	-1.552721000	1.829833000	-2.533803000
6	0.435842000	1.532541000	-3.944322000
1	-2.018398000	1.772963000	-1.559408000
6	-0.203556000	1.414977000	-2.661212000
1	-2.182578000	2.788241000	-5.750805000
1	-5.012427000	0.999399000	2.710348000
6	-2.797616000	2.499983000	2.227552000
1	-2.698541000	1.845652000	3.095110000
1	-2.143399000	3.371575000	2.283144000
1	-2.233307000	1.793973000	1.271155000
6	-4.166828000	2.764735000	1.782944000
6	-4.464545000	3.898655000	0.985906000
6	-5.764165000	4.136465000	0.537983000
6	-6.798264000	3.246371000	0.868697000
6	-6.521233000	2.114991000	1.652307000
6	-5.222460000	1.873765000	2.101348000
1	-3.667010000	4.590580000	0.731508000
1	-5.975956000	5.013322000	-0.065152000
1	-7.808682000	3.432621000	0.520118000
1	-7.319233000	1.427123000	1.912212000

⁵Re_{Tol}:

26	-0.084150000	0.590429000	0.724273000
7	0.191889000	-0.270095000	2.643063000
7	0.273172000	1.193886000	-1.311296000
7	1.263354000	2.078589000	1.425719000
7	-0.843742000	-1.280348000	-0.034340000
6	1.508666000	-0.488963000	2.906367000
6	1.925887000	-1.049645000	4.108529000
1	2.977718000	-1.219913000	4.300794000
6	0.949758000	-1.388322000	5.057882000
1	1.244639000	-1.828893000	6.002514000
6	-0.401013000	-1.155795000	4.778385000
1	-1.171898000	-1.406252000	5.495373000
6	-0.754049000	-0.590930000	3.550692000
1	-1.780728000	-0.388102000	3.277201000
6	1.473321000	0.767521000	-1.743851000
6	1.884701000	0.890904000	-3.089435000
1	2.857290000	0.518642000	-3.385513000
6	1.037094000	1.481596000	-4.001047000
1	1.327399000	1.580264000	-5.041289000
6	2.429300000	1.527719000	1.859123000
6	3.463078000	2.311962000	2.358778000
1	4.385512000	1.855946000	2.695515000
6	3.277027000	3.701716000	2.411635000
1	4.065553000	4.338427000	2.793945000
6	2.072324000	4.257666000	1.968468000

1	1.903846000	5.326111000	2.001536000
6	1.074184000	3.413957000	1.475111000
1	0.123133000	3.785607000	1.118156000
6	0.153200000	-2.157046000	-0.252475000
6	-0.043796000	-3.378002000	-0.934070000
1	0.797569000	-4.039637000	-1.096181000
6	-1.305945000	-3.701720000	-1.383271000
1	-1.480639000	-4.628905000	-1.918005000
6	-2.391748000	-2.822372000	-1.142528000
6	-2.137851000	-1.591457000	-0.445722000
6	2.415397000	0.009930000	1.793985000
1	3.418724000	-0.417308000	1.852692000
6	2.436211000	0.212945000	-0.727660000
1	3.094304000	1.021978000	-0.396040000
1	3.077549000	-0.550583000	-1.174433000
6	1.504202000	-1.844888000	0.335282000
1	1.563650000	-2.303383000	1.327116000
1	2.305132000	-2.284487000	-0.263988000
7	1.728564000	-0.358901000	0.477056000
8	-1.466612000	1.414073000	1.103536000
6	-4.499980000	-1.052109000	-0.589422000
6	-4.752841000	-2.256323000	-1.293765000
6	-3.222611000	-0.721325000	-0.173816000
1	-5.761812000	-2.491294000	-1.612956000
1	-3.040702000	0.193709000	0.372132000
6	-3.716088000	-3.126314000	-1.562728000
1	-3.892133000	-4.056755000	-2.092168000
1	-5.319997000	-0.376627000	-0.371280000
6	-2.342741000	3.080042000	-4.035917000
6	-2.698736000	2.940826000	-2.670740000
6	-1.126729000	2.603839000	-4.481576000
1	-3.651555000	3.325279000	-2.323306000
1	-0.834596000	2.708076000	-5.521204000
6	-1.849477000	2.322643000	-1.770187000
6	-0.226407000	1.969589000	-3.581675000
1	-2.123152000	2.227912000	-0.729044000
6	-0.598563000	1.817589000	-2.202023000
1	-3.026272000	3.564780000	-4.723598000
1	-5.285597000	5.301556000	-0.873229000
6	-3.534417000	4.994137000	1.206524000
1	-2.734485000	4.897687000	0.460533000
1	-3.117135000	4.717490000	2.179639000
1	-3.809284000	6.054890000	1.245099000
6	-4.723433000	4.127296000	0.851287000
6	-5.059046000	3.001698000	1.623869000
6	-6.157369000	2.197178000	1.287801000
6	-6.939663000	2.506213000	0.168099000
6	-6.616986000	3.626783000	-0.610601000
6	-5.521547000	4.428771000	-0.270010000
1	-4.460872000	2.758371000	2.497619000
1	-6.404155000	1.337922000	1.904074000
1	-7.793233000	1.887938000	-0.091066000
1	-7.220982000	3.878419000	-1.477011000

⁵TS_{HA,Tol}:

26	-0.376492000	0.229114000	0.535758000
7	0.042909000	-0.577922000	2.508792000
7	0.108833000	0.897413000	-1.496754000
7	0.630548000	1.981679000	1.329856000
7	-0.522501000	-1.802573000	-0.264467000
6	1.353792000	-0.480824000	2.851506000
6	1.820022000	-0.933927000	4.082533000
1	2.869607000	-0.851478000	4.335933000

6	0.900257000	-1.499300000	4.977565000	6	-5.401906000	5.243450000	-0.407477000
1	1.235571000	-1.862744000	5.941555000	6	-5.905771000	3.980489000	-0.760338000
6	-0.448439000	-1.591649000	4.617228000	6	-5.527883000	2.849584000	-0.036425000
1	-1.179257000	-2.021653000	5.289920000	1	-3.465952000	4.335538000	2.249166000
6	-0.849563000	-1.118352000	3.365844000	1	-4.134259000	6.343202000	0.954311000
1	-1.877498000	-1.159610000	3.031482000	1	-5.695078000	6.122070000	-0.972243000
6	1.403428000	0.727854000	-1.811867000	1	-6.592821000	3.884982000	-1.594506000
6	1.895055000	0.917528000	-3.124969000				
1	2.945936000	0.751452000	-3.326682000				
6	1.029504000	1.308125000	-4.122505000				
1	1.383435000	1.452035000	-5.137604000				
6	1.858339000	1.699281000	1.838355000				
6	2.664918000	2.692534000	2.387011000				
1	3.642885000	2.448185000	2.782850000				
6	2.180973000	4.008583000	2.410090000				
1	2.788557000	4.801977000	2.828481000				
6	0.912790000	4.288302000	1.890028000				
1	0.513858000	5.294401000	1.898273000				
6	0.155208000	3.245092000	1.352440000				
1	-0.833419000	3.399018000	0.940516000				
6	0.665573000	-2.422833000	-0.351147000				
6	0.820510000	-3.677748000	-0.986278000				
1	1.803974000	-4.128193000	-1.037834000				
6	-0.279248000	-4.301559000	-1.531869000				
1	-0.181317000	-5.259535000	-2.031019000				
6	-1.556275000	-3.690344000	-1.441556000				
6	-1.659522000	-2.417252000	-0.785651000				
6	2.200779000	0.216730000	1.797029000				
1	3.268168000	0.050670000	1.968184000				
6	2.383814000	0.408310000	-0.708148000				
1	2.806422000	1.352510000	-0.349810000				
1	3.220737000	-0.176219000	-1.102122000				
6	1.867087000	-1.795268000	0.315794000				
1	1.969024000	-2.232578000	1.314160000				
1	2.778831000	-2.056233000	-0.230545000				
7	1.753286000	-0.307422000	0.446247000				
8	-1.987360000	0.751429000	0.868979000				
6	-4.052542000	-2.429201000	-1.190472000				
6	-3.953813000	-3.678951000	-1.852849000				
6	-2.933197000	-1.806703000	-0.667530000				
1	-4.844820000	-4.145445000	-2.257539000				
1	-3.010594000	-0.857321000	-0.154875000				
6	-2.726400000	-4.298392000	-1.973850000				
1	-2.633381000	-5.258267000	-2.471013000				
1	-5.022571000	-1.954364000	-1.090720000				
6	-2.589587000	2.187367000	-4.473297000				
6	-3.023263000	1.990209000	-3.137756000				
6	-1.269915000	1.961697000	-4.808917000				
1	-4.057830000	2.185328000	-2.877668000				
1	-0.918769000	2.114889000	-5.824065000				
6	-2.146423000	1.561194000	-2.157638000				
6	-0.339149000	1.531058000	-3.823783000				
1	-2.475511000	1.418326000	-1.137403000				
6	-0.787456000	1.317863000	-2.476588000				
1	-3.296255000	2.520614000	-5.224896000				
1	-5.920118000	1.873988000	-0.307114000				
6	-4.228467000	1.761345000	1.819700000				
1	-4.926193000	0.922188000	1.753215000				
1	-3.941169000	1.960632000	2.856149000				
1	-3.216593000	1.322037000	1.347633000				
6	-4.643519000	2.956681000	1.065982000				
6	-4.142899000	4.238602000	1.405632000				
6	-4.519851000	5.367507000	0.678224000				