Supporting Information

Precision Biotransformation of Emerging Pollutants by Human Cytochrome P450 Using Computational-Experimental Synergy: A Case Study of Tris(1,3-dichloro-2-propyl) Phosphate

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I. Detailed Experimental Data

1.1 Pre-experiments for determining the appropriate incubation time

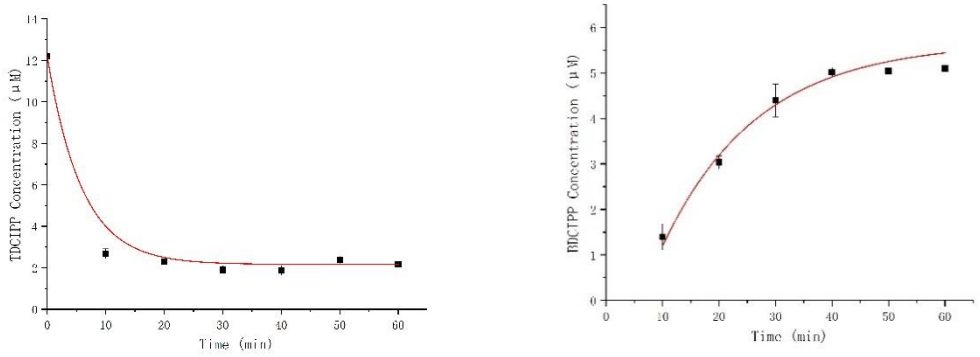
For kinetics studies, the concentration of TDCIPP and main metabolite BDCIPP was recorded every 10 minutes. The major metabolites of TDCIPP were identified by liquid chromatography-tandem mass spectrometry (Waters LC-MS/MS-0203). The LC-MS/MS analysis conditions: LC column: TSKgel ODS-100 V 3μm (2.0 x 150 mm), temperature: 40 °C, solvent: A: 10 mM ammonium acetate and 0.1% formic acid in water; B: acetonitrile, gradient: B: 15% (0 min)- 30% (0.5 min)-95% (10.0 min)-95%(12 min) -5% (12.5 min) -15% (15 min), flow rate: 0.3 mL/min, detection: MS/MS; ion source: ESI, polarity: positive ion mode, well Time: 0.330 sec, cone: 40.0 V, CE (Collision Energy): -22.0 V (428.99 > 98.83), -12.0 V (428.99 > 318.94) for TDCIPP and -16.0 V (319.2073 > 98.8985) for BDCIPP.

Table S1. The Kinetic Data for the Metabolism of TDCIPP in Human Liver Microsomes

Time(min)	0	10	20	30	40	50	60
Paralleled sample 1(μM)	11.71	2.69	2.30	1.76	2.10	2.56	2.10
Paralleled sample 2(μM)	12.68	2.22	2.30	2.10	1.64	2.20	2.22
Average(μM)	12.19	2.45	2.30	1.93	1.87	2.38	2.16
SD(μM)	0.48	0.23	0.00	0.17	0.23	0.18	0.06

Table S2. The Kinetic Data for the BDCIPP Production from TDCIPP in Human Liver Microsomes

Time(min)	0	10	20	30	40	50	60
Paralleled sample 1(μM)	0.0415	1.4386	2.9296	4.8007	5.0592	5.0882	4.655
Paralleled sample 2(μM)	0.0421	2.0166	3.2213	4.0792	5.2627	6.5727	5.1416
Average(μM)	0.0418	1.7276	3.07545	4.43995	5.16095	5.83045	4.8983
SD(μM)	0.0003	0.289	0.14585	0.36075	0.10175	0.74225	0.2433

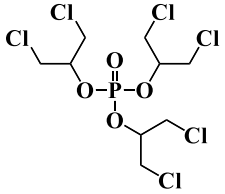
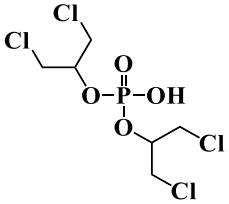
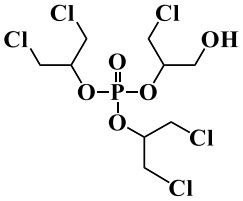
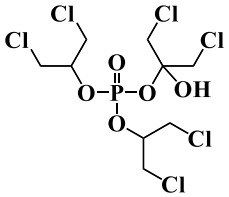


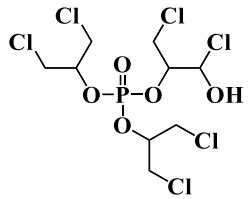
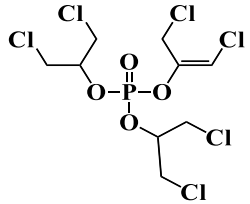
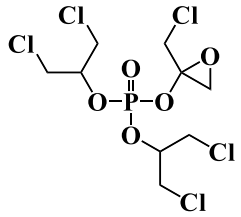
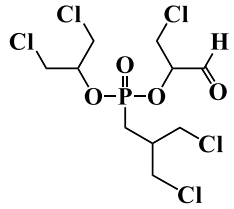
(a) **(b)**

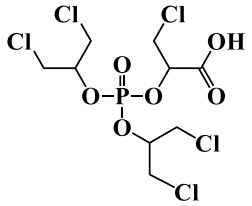
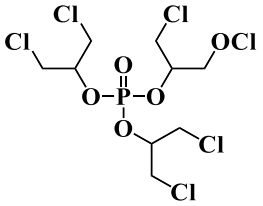
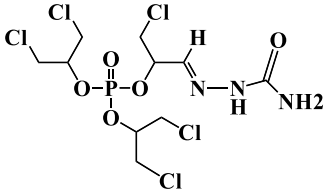
Figure S1. The curve of monitoring the metabolic process of TDCIPP (a) and the producing process of BDCIPP (b) in human liver microsomes

1.2 Detailed Experimental Information with LC-MS/MS

Table S3. Precursor and product ions in MS/MS, and retention time in LC of metabolites of tris(1,3-dichloro-2-propyl) phosphate (TDCIPP)

Compound	Structure	Formula	Reaction	Precursor ion $[M+H]^+$ (*m/z*)	Product ion (*m/z*)	Retention time (min)
TDCIPP		$C_9H_{15}Cl_6O_4P$	/	428.8917	99.0	10.8[a], 3.63[b]
M_{IV}		$C_6H_{11}O_4Cl_4P$	O-dealkylation	318.9227	99.0	6.8
M_{VIII}		$C_9H_{16}O_5Cl_5P$	Dehalogenation/Reduction	410.9256	99.0	9.3[a], 3.10[b]
M_I		$C_9H_{15}Cl_6O_5P$	α-Hydroxylation	444.8867	99.0	-

M_{II}		$C_9H_{15}Cl_6O_5P$	β-Hydroxylation	444.8867	99.0	-
M_{III}		$C_9H_{13}Cl_6O_4P$	Desaturation	426.8761	99.0	-
M_{V}		$C_9H_{14}O_5Cl_5P$	Epoxidation	408.9100	99.0	-
M_{VI}		$C_9H_{14}Cl_5O_5P$	Oxidative Dehalogenation	408.9100	99.0	-

M_{VII}		$C_9H_{14}O_6Cl_5P$	Oxidative Dehalogenation	424.9049	99.0	-
M_{IX}		$C_9H_{15}Cl_6O_5P$	Oxidative Halosylation	444.8867	99.0	-
Semicarbazide Adduct of M_{VI}		$C_{10}H_{17}N_3O_5Cl_5P$	Trapping Reactive Aldehyde	465.9427	99.0	4.10

[a] analyzed by Shimadzu LCMS-8030; [b] analyzed by Waters LC-MS/MS-0203

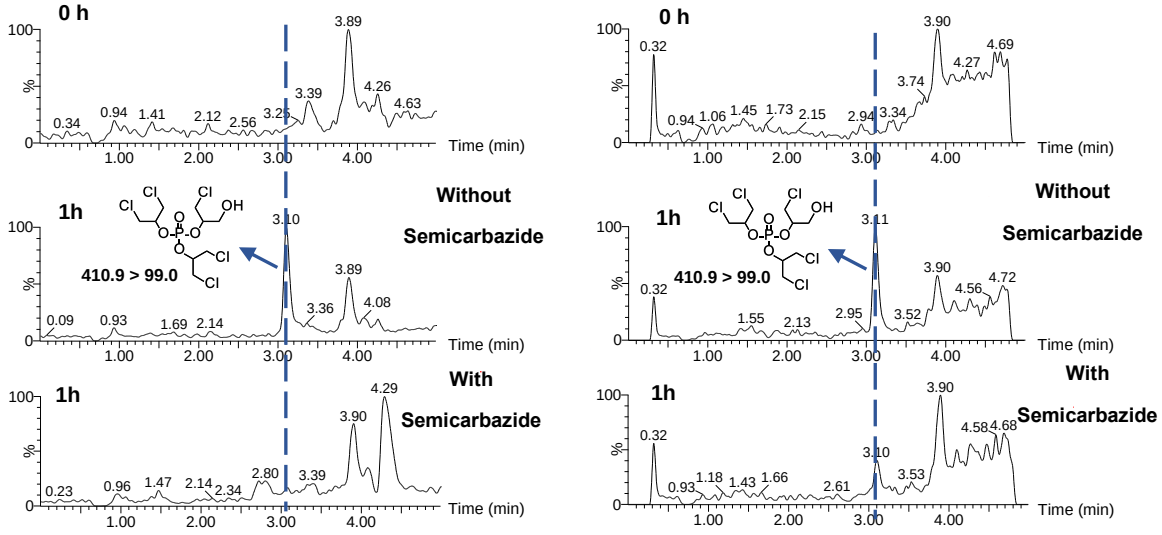


Figure S2. Ion chromatograms from LC-MS/MS analysis of the alcohol$_{\beta\text{-dehalogen}}$ with human liver microsomes **(a)** and recombinant human P450 enzymes CYP3A4 **(b)**. Incubation and LC-MS/MS conditions were as described under Materials and Methods.

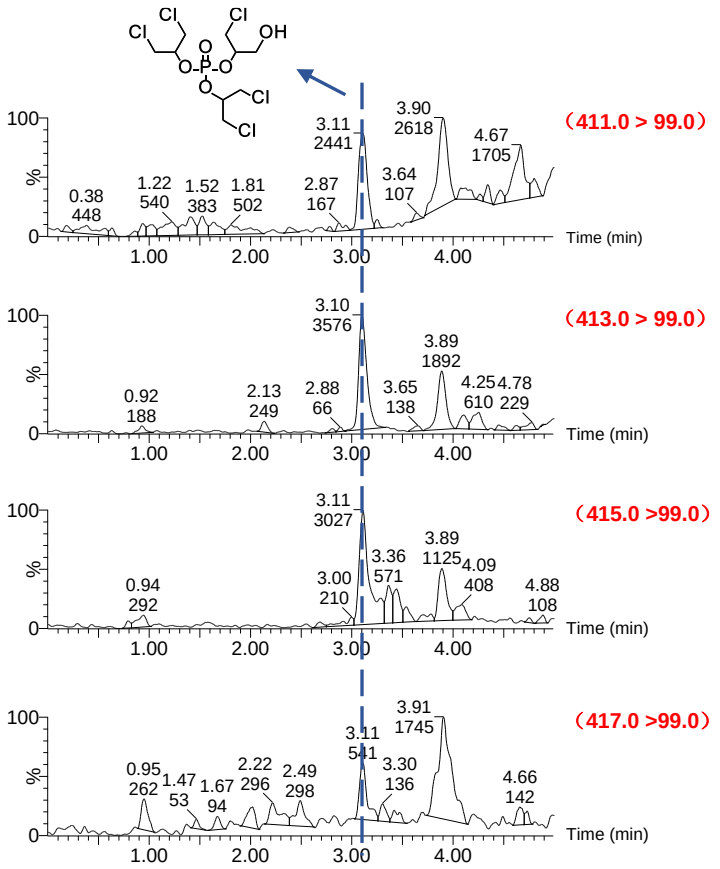
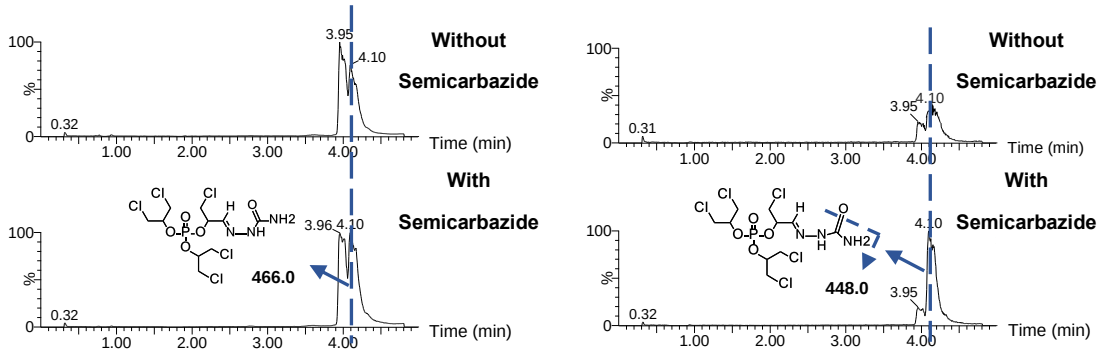


Figure S3. The chlorine isotope peaks of alcohol$_{\beta\text{-dehalogen}}$ with human liver microsomes

from LC-MS/MS analysis



（a） （b）

Figure S4. Ion chromatograms from LC-MS/MS analysis of the semicarbazide adducts of aldehyde$_{\beta\text{-dehalogen}}$ with recombinant human P450 enzymes CYP3A4 after 1 h incubation: **(a)** *m/z* 466.0 ($[M + H]^+$) and **(b)** *m/z* 448.0 ($[M + H - 18]^+$). Incubation and LC-MS/MS conditions were as described under Materials and Methods.

1.3 Detailed Experimental Information with LC/Q-TOF-MS Method

Metabolites of TDCIPP were identified by liquid chromatography-mass spectrometry (LC-MS) using an HPLC 1290 series coupled to a 6546 quadrupole-time-of-flight mass spectrometer (Q-TOF-MS) (Agilent Technologies). Chromatographic separation of the metabolites formed was achieved using an Eclipse Plus C18 column (50 mm × 2.1 mm × 1.8 μm, Agilent Technologies) and following mobile phase composition: 5 mM ammonium acetate in water (A) and methanol (B). Gradient elution was as follows: 10% B from 0 to 0.5 min, linear increase of B to 95%, from 0.5 to 10.5 min. The flow rate was 0.3 mL/min and the injection volume 10 μL. Total run time was 11 minutes. The Q-TOF-MS was run in ESI positive mode scanning *m*/*z* from 100 to 1000 amu at a scan rate of 1.00 spectra/s. The following MS parameters were used: gas temperature 320 ◦C, gas flow 8 L/min, nebulizer pressure 35 psi, sheath gas temperature 350 ◦C, sheath gas flow 11 L/min. Nozzle, capillary, fragmentor, and skimmer voltages were set to 1000 V, 3500 V, 125 V, and 65 V, respectively.

Table S4. LC/Q-TOF-MS Analysis of TDCIPP Metabolites in Human Liver Microsomes

Compound	**M + H^+ (*m/z*)**	**RT**	**Different (ppm)**	**Contribution (%)[a]**
BDCIPP	319.9222	6. 697	1.8	80.2
$Alcohol_{\beta\text{-dehalogen}}$	410.9251	8.235	1.5	16.8
$Carboxylic\text{-}acid_{\beta\text{-dehalogen}}$	424.9043	7.065	1.2	3.0

[a] Contributions were obtained by the peak area normalization method

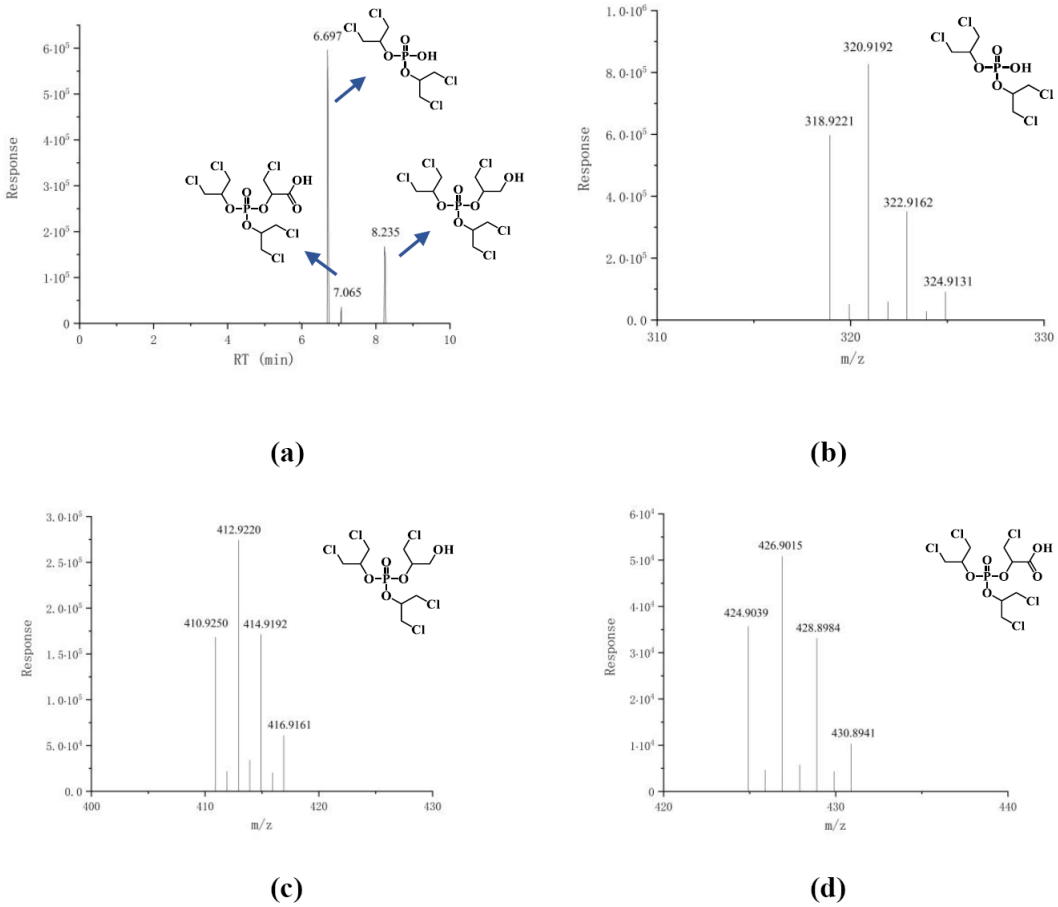


Figure S5. (a) Ion chromatograms from LC-Q-TOF analysis of the metabolites of TDCIPP in human liver microsomes; **(b)** The isotope peaks of BDCIPP; **(c)** The isotope peaks of Alcohol$_{\beta\text{-dehalogen}}$; **(d)** The isotope peaks of Carboxylic-acid$_{\beta\text{-dehalogen}}$

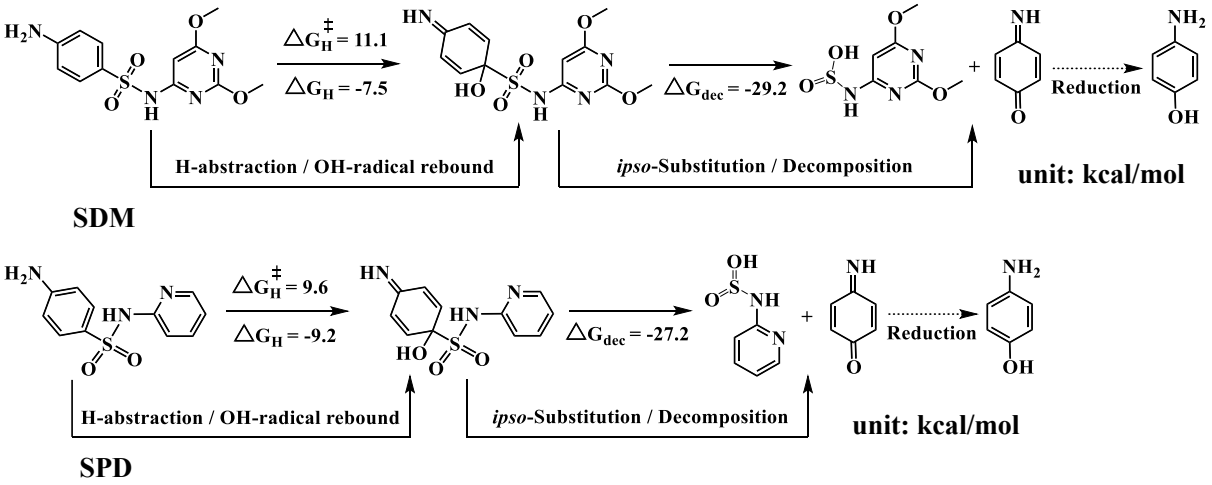
II. Investigation of the Emerging Pathways of Antibiotics, Antioxidants and Psychoactive Drugs by CYP450 with the Guidance of Experiments Using Computations

2.1 First-Step Computational Section

The computation methods (DFT functional and basis set) for optimization and enzymatic model for investigation of the emerging pathways of antibiotics, antioxidants and psychoactive drugs by CYP450 are as the same as for TDCIPP shown in the text. The relative free energies are reported below.

1) Antibiotics (Sulfadimethoxine, SDM; Sulfapyridine, SPD)-*ipso*-Substitution Mechanism

Scheme S1. *Ipso*-substitution Mechanism of SDM and SPD Catalyzed by CYP450

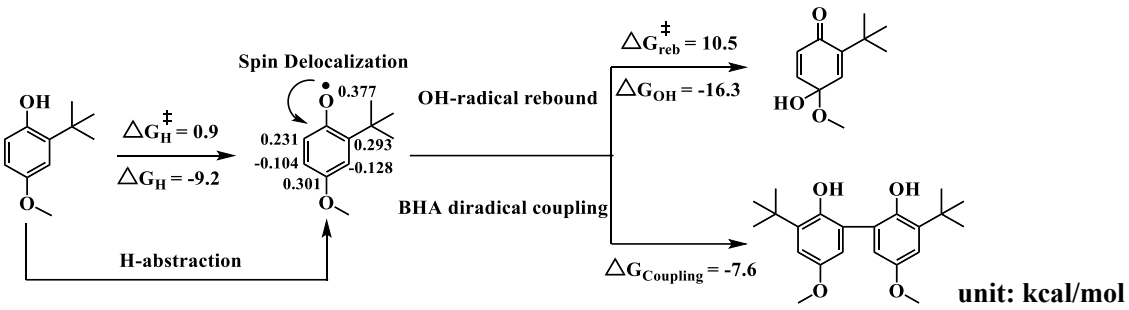


Important Enlightenments:

We find that the *ipso*-substitution proceeds via H-abstraction from SDM and SPD by Compound I of CYP450, followed by essentially barrierless radical rebound onto the *ipso*-position, resulting in fragmentation of SDM and SPD. And one fragment 4-iminocyclohexa-2,5-dienone may further evolve into the more stable 4-aminocyclohexa-2,5-dienol in the redox environment.

2) Antioxidants (butylated hydroxyanisole, BHA)−Coupling Mechanism

Scheme S2. Coupling Mechanism of BHA Catalyzed by CYP450

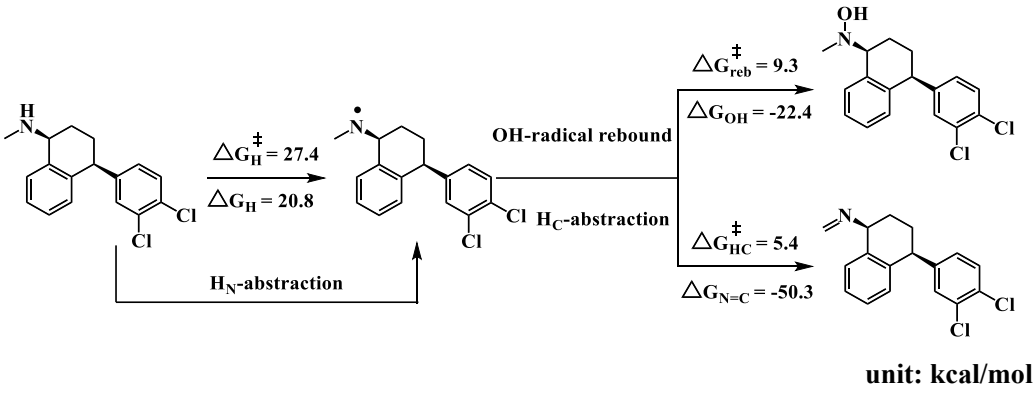


Important Enlightenments:

We find a diradical coupling pathway of BHA, which is characterized by significantly high rebound barrier of the phenoxy radical of BHA. A higher barrier for rebound than for H-abstraction in high-spin state can facilitate the phenoxy radical of BHA dissociation and thus enable phenol coupling. The high rebound barrier of phenoxy radicals, as a key for the mechanistic identification of phenol coupling, originates from the weak electron donor ability due to spin aromatic delocalization.

3) Psychoactive Drugs (Sertraline)-Desaturation Mechanism

Scheme S3. Desaturation Mechanism of Sertraline Catalyzed by CYP450



Important Enlightenments:

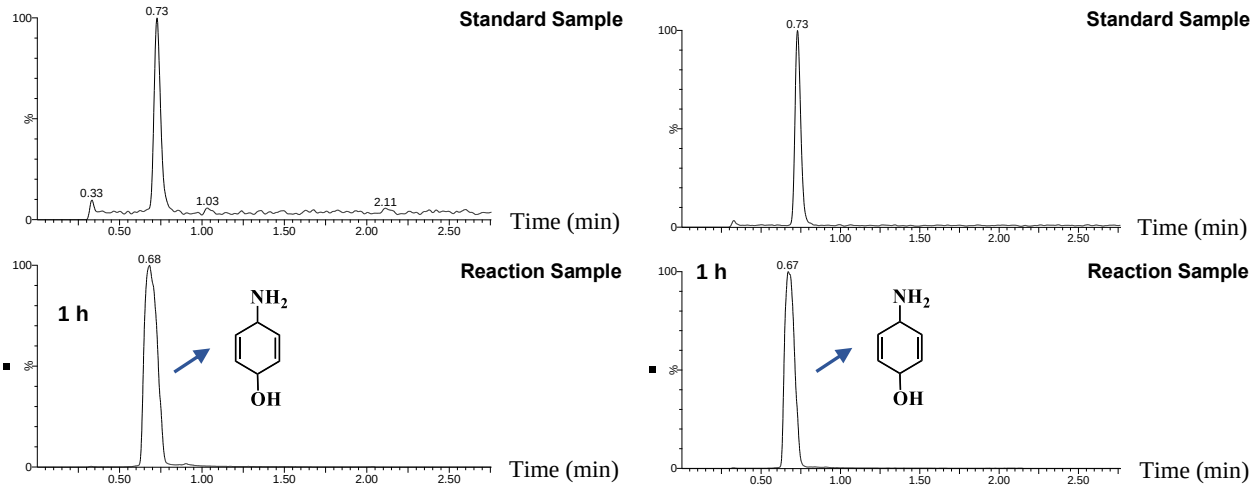
We find that the CYP450-catalyzed desaturation reaction can occur, which is competitive with hydroxylation reaction on the low-spin state thermodynamically.

2.2 Second-Step Experimental Section

1) Antibiotics (Sulfadimethoxine, SDM; Sulfapyridine, SPD)-*ipso*-Substitution Metabolites Detection

Analytical Methods. Sulfadimethoxine (SDM) and sulfapyridine (SPD) are purchased from Sigma-Aldrich (Shanghai, China). The *ipso*-substitution metabolites of SDM and SPD were identified by liquid chromatography-tandem mass spectrometry (Waters LC-MS/MS-0203), respectively. The LC-MS/MS analysis conditions: temperature: 40 °C, solvent: A: 0.1% formic acid in water; B: 0.1% formic acid in acetonitrile, gradient: B: 10% (0 min) - 90% (4.0 min) -10% (4.8 min) - 10% (5.5 min), flow rate: 0.3 mL/min, detection: MS/MS; ion source: ESI, polarity: positive ion mode, Dwell Time: 0.025 sec, SDM: cone: 8.0 V, CE (Collision Energy): -24.0 V (310.9618 > 108.1386), -18.0 V (310.9618 > 156.1440), -18.0 V (310.9618 > 245.0000); SPD: cone: 22.0 V, CE (Collision Energy): -22.0 V (249.9681 > 108.485), -14.0 V (249.9681 > 156.1651); PAP: cone: 40.0 V, CE (Collision Energy): -25.0 V (109.8404>39), -13.0 V (109.8404 > 92.9), cone: 15.0 V, CE (Collision Energy): -12.0 V (109.8404 > 64.9).

Detection Results:



(a) **(b)**

Figure S6. Ion chromatograms from LC-MS/MS analysis of the *ipso*-substitution metabolites of SDM **(a)** and SPD **(b)** in human liver microsomes after 1 h incubation

2) Antioxidants (butylated hydroxyanisole, BHA)-Coupling Metabolites Detection

Analytical Methods. Butylated hydroxyanisole (BHA) were purchased from Sigma-Aldrich (Shanghai, China). The metabolites of BHA are identified by liquid chromatography-mass spectrometry (LC-MS) using an HPLC 1290 series coupled to a 6546 quadrupole-time-of-flight mass spectrometer (Q-TOF-MS) (Agilent Technologies). Chromatographic separation of the metabolites formed was achieved using a EclipsePlus C18 column (50 mm × 2.1 mm × 1.8 μm, Agilent Technologies) and following mobile phase composition: 5 mM ammonium acetate in water (A) and acetonitrile (B). Gradient elution was as follows: B: 5% (5.0 min) - 30% (8.0 min) - 50% (12.0 min) - 90% (13.0 min) - 90% (2.0 min), flow rate: 0.25 mL/min, injection volume: 10 μL, the total run time:15 min. The Q-TOF-MS was run in ESI negative mode scanning *m/z* from 100 to 1000 amu at a scan rate of 1.00 spectra/s. The following MS parameters were used: gas temperature 320 ◦C, gas flow 8 L/min, nebulizer pressure 35 psi, sheath gas temperature 350 °C, sheath gas flow 11 L/min. Nozzle, capillary, fragmentor, and skimmer voltages were set to 1000 V, 3500 V, 125 V, and 65 V, respectively. For MS/MS analysis, the experimental conditions were the same as above except for the collision energy. The target *m/z* was 357.2072 $[M - H]^-$. Three levels of collision energy were applied: 10 V, 20 V, and 40 V, respectively.

Detection Results:

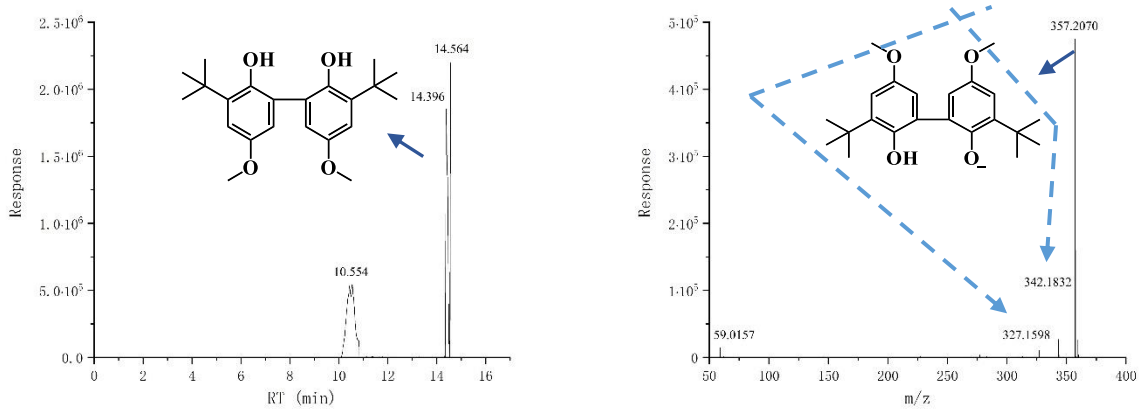


Figure S7. Ion chromatograms from LC-Q-TOF analysis of the coupling metabolites of BHA in human liver microsomes after 1 h incubation

3) Psychoactive Drugs (Sertraline)-Desaturation Metabolites Detection

Analytical Methods. The metabolites of sertraline is identified by the following mobile phase composition:0.1% formic acid in methanol (A) and 0.1% formic acid in ultrapure water (B). Gradient elution was as follows: B: 85% (1.0 min) - 55% (2 min) - 20% (4 min) - 0% (5.7-7.2 min) - 85 % (7.30-8.90 min). The flow rate was 0.2 mL/min and the injection volume 10 μL. Total run time was 9 min. The Q-TOF-MS was run in ESI positive mode scanning *m/z* from 100 to 400 amu at a scan rate of 1.00 spectra/s. The MS parameters were the same as for BPA shown above.

Detection Results:

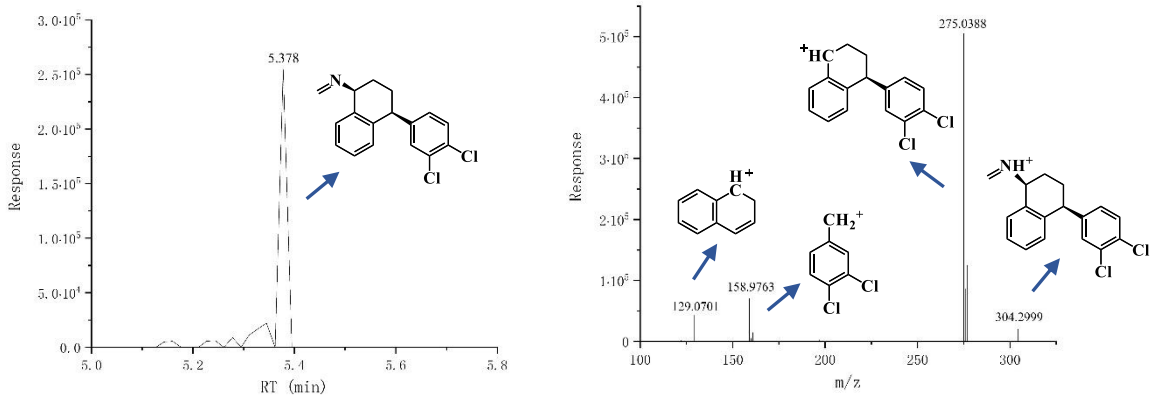


Figure S8. Ion chromatograms from LC-Q-TOF analysis of the desaturation metabolites of sertraline in human liver microsomes after 1 h incubation

III. Energies for Molecular Species Involved in Screening TDCIPP Metabolites by DFT Calculations

Table S5. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for molecular species involved in TDCIPP catalyzed by Cpd I of P450 at various levels of B3LYP-calculations

	BSI		BSI+G_{corr}		BSI+PCM		BSI+D_3		BSII/BSI		BSII/BSI+PCM + G_{corr}+D_3		BSII/BSI+PCM + G_{corr}		G_{corr}
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**
SUB+ ^{4}Cpd I	-5341.338321	**0.00**	-5340.909290	**0.00**	-5341.363524	**0.00**	-5341.451366	**0.00**	-5342.493376	**0.00**	-5342.202594	**0.00**	-5342.089548	**0.00**	0.429031
SUB+ ^{2}Cpd I	-5341.338352	**-0.02**	-5340.908831	**0.29**	-5341.363488	**0.02**	-5341.451264	**0.06**	-5342.493466	**-0.06**	-5342.201993	**0.38**	-5342.089081	**0.29**	0.429521
^{4}RC$_\alpha$	-5341.320666	**11.08**	-5340.872229	**23.26**	-5341.340327	**14.56**	-5341.453219	**-1.16**	-5342.511077	**-11.11**	-5342.214854	**-7.69**	-5342.082301	**4.55**	0.448437
^{2}RC$_\alpha$	-5341.320804	**10.99**	-5340.871890	**23.47**	-5341.340419	**14.50**	-5341.453404	**-1.28**	-5342.511718	**-11.51**	-5342.215018	**-7.80**	-5342.082419	**4.47**	0.448914
^{4}TS$_{\alpha H}$	-5341.277453	**38.20**	-5340.834489	**46.94**	-5341.297114	**41.67**	-5341.414374	**23.21**	-5342.470305	**14.48**	-5342.183924	**11.72**	-5342.047002	**26.70**	0.442964
^{2}TS$_{\alpha H}$	-5341.276420	**38.84**	-5340.832848	**47.97**	-5341.296281	**42.20**	-5341.412069	**24.66**	-5342.472161	**13.31**	-5342.184098	**11.61**	-5342.048449	**25.79**	0.443572
^{4}IM$_\alpha$	-5341.308203	**18.90**	-5340.862243	**29.52**	-5341.326882	**22.99**	-5341.442837	**5.35**	-5342.510010	**-10.44**	-5342.217363	**-9.27**	-5342.082728	**4.28**	0.445960
^{2}IM$_\alpha$	-5341.316526	**13.68**	-5340.871787	**23.53**	-5341.334568	**18.17**	-5341.448729	**1.65**	-5342.518643	**-15.86**	-5342.224150	**-13.53**	-5342.091947	**-1.50**	0.444739
^{4}TS$_{\alpha\text{-reb}}$	-5341.298810	**24.79**	-5340.852271	**35.78**	-5341.318471	**28.27**	-5341.438002	**8.39**	-5342.501060	**-4.82**	-5342.213374	**-6.76**	-5342.074182	**9.64**	0.446539
^{4}Pr$_\alpha$	-5341.398073	**-37.49**	-5340.951851	**-26.71**	-5341.420511	**-35.76**	-5341.531741	**-50.44**	-5342.595676	**-64.19**	-5342.305560	**-64.61**	-5342.171892	**-51.67**	0.446222
^{2}Pr$_\alpha$	-5341.398880	**-38.00**	-5340.950364	**-25.77**	-5341.420045	**-35.47**	-5341.530418	**-49.61**	-5342.594675	**-63.57**	-5342.298862	**-60.41**	-5342.167324	**-48.80**	0.448516
^{4}TS$_{2H}$	-5341.288656	**31.17**	-5340.848141	**38.37**	-5341.314668	**30.66**	-5341.424458	**16.89**	-5342.484411	**5.63**	-5342.205710	**-1.96**	-5342.069908	**12.32**	0.440515
^{2}TS$_{2H}$	-5341.301034	**23.40**	-5340.856161	**33.34**	-5341.321297	**26.50**	-5341.438177	**8.28**	-5342.496362	**-1.87**	-5342.208895	**-3.95**	-5342.071752	**11.17**	0.444873
^{4}P$_{2H}$	-5341.291069	**29.65**	-5340.849253	**37.67**	-5341.311344	**32.74**	-5341.416358	**21.97**	-5342.489230	**2.60**	-5342.192979	**6.03**	-5342.067690	**13.72**	0.441816
^{2}P$_{2H}$	-5341.291070	**29.65**	-5340.848603	**38.08**	-5341.311341	**32.75**	-5341.416373	**21.96**	-5342.488933	**2.79**	-5342.192040	**6.62**	-5342.066738	**14.31**	0.442467
^{4}RC$_\beta$	-5341.321820	**10.35**	-5340.875151	**21.42**	-5341.341351	**13.91**	-5341.449751	**1.01**	-5342.512319	**-11.89**	-5342.213111	**-6.60**	-5342.085180	**2.74**	0.446669

$^{2}RC_{\beta}$	-5341.321966	**10.26**	-5340.874653	**21.73**	-5341.341465	**13.84**	-5341.449958	**0.88**	-5342.512594	**-12.06**	-5342.212771	**-6.39**	-5342.084779	**2.99**	0.447313
$^{4}TS_{\beta H}$	-5341.276385	**38.87**	-5340.835364	**46.39**	-5341.296820	**41.86**	-5341.409978	**25.97**	-5342.467967	**15.94**	-5342.180974	**13.57**	-5342.047381	**26.46**	0.441021
$^{2}TS_{\beta H}$	-5341.275937	**39.15**	-5340.833951	**47.28**	-5341.296909	**41.80**	-5341.409234	**26.44**	-5342.466228	**17.04**	-5342.178511	**15.11**	-5342.045214	**27.82**	0.441986
$^{4}IM_{\beta}$	-5341.296270	**26.39**	-5340.849845	**37.30**	-5341.313377	**31.47**	-5341.429679	**13.61**	-5342.496015	**-1.66**	-5342.200105	**1.56**	-5342.066697	**14.34**	0.446425
$^{2}IM_{\beta}$	-5341.297838	**25.40**	-5340.852989	**35.33**	-5341.318440	**28.29**	-5341.424278	**17.00**	-5342.490915	**1.54**	-5342.193108	**5.95**	-5342.066667	**14.36**	0.444849
$^{4}TS_{\beta\text{-reb}}$	-5341.285702	**33.02**	-5340.838501	**44.42**	-5341.304186	**37.24**	-5341.417799	**21.06**	-5342.486670	**4.21**	-5342.190050	**7.87**	-5342.057953	**19.83**	0.447201
$^{4}Pr_{\beta}$	-5341.387286	**-30.73**	-5340.941181	**-20.01**	-5341.409860	**-29.08**	-5341.517997	**-41.81**	-5342.585836	**-58.02**	-5342.293015	**-56.74**	-5342.162305	**-45.66**	0.446105
$^{2}Pr_{\beta}$	-5341.395411	**-35.82**	-5340.943942	**-21.74**	-5341.414991	**-32.30**	-5341.528995	**-48.71**	-5342.590163	**-60.73**	-5342.291858	**-56.01**	-5342.158274	**-43.13**	0.451469
$^{4}TS_{cl}$	-5341.230307	**67.78**	-5340.784386	**78.38**	-5341.252700	**69.54**	-5341.359476	**57.66**	-5342.420741	**45.58**	-5342.126383	**47.82**	-5341.997213	**57.94**	0.445921
$^{2}TS_{cl}$	-5341.204661	**83.87**	-5340.753160	**97.97**	-5341.225984	**86.31**	-5341.343804	**67.50**	-5342.395430	**61.46**	-5342.104395	**61.62**	-5341.965252	**78.00**	0.451501
$^{4}P_{cl}$	-5341.234563	**65.11**	-5340.793660	**72.56**	-5341.255942	**67.51**	-5341.366185	**53.45**	-5342.425365	**42.68**	-5342.137464	**40.87**	-5342.005842	**52.53**	0.440903
$^{2}P_{cl}$	-5341.234985	**64.84**	-5340.793284	**72.79**	-5341.256323	**67.27**	-5341.366797	**53.07**	-5342.425812	**42.40**	-5342.137261	**41.00**	-5342.005450	**52.77**	0.441701

Table S6. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for molecular species involved in TDCIPP catalyzed by Cpd I of P450 using single-point calculations at the BSI level with different DFT functionals

	UB3LYP		UTPSSh		UB3PW91		UBLYP		MPW1PW91		M06L	
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**
SUB+^{4}Cpd I	-5341.338321	**0.00**	-5341.427932	**0.00**	-5340.302056	**0.00**	-5340.548619	**0.00**	-5340.992948	**0.00**	-5341.098148	**0.00**
SUB+^{2}Cpd I	-5341.338352	**-0.02**	-5341.428139	**-0.13**	-5340.302071	**-0.01**	-5340.550142	**-0.96**	-5340.992827	**0.08**	-5341.098886	**-0.46**
^{4}RC$_\alpha$	-5341.320666	**11.08**	-5341.422704	**3.28**	-5340.284317	**11.13**	-5340.521822	**16.82**	-5340.982585	**6.50**	-5341.100594	**-1.54**
^{2}RC$_\alpha$	-5341.320804	**10.99**	-5341.422999	**3.10**	-5340.284500	**11.02**	-5340.522986	**16.09**	-5340.982685	**6.44**	-5341.101364	**-2.02**
^{4}TS$_{\alpha H}$	-5341.277453	**38.20**	-5341.381792	**28.95**	-5340.243813	**36.55**	-5340.484573	**40.19**	-5340.942455	**31.69**	-5341.063102	**21.99**
^{2}TS$_{\alpha H}$	-5341.276420	**38.84**	-5341.383493	**27.89**	-5340.244783	**35.94**	-5340.489613	**37.03**	-5340.943237	**31.19**	-5341.064869	**20.88**
^{4}IM$_\alpha$	-5341.308203	**18.90**	-5341.411330	**10.42**	-5340.274734	**17.14**	-5340.510942	**23.64**	-5340.974242	**11.74**	-5341.091240	**4.33**
^{2}IM$_\alpha$	-5341.316526	**13.68**	-5341.405149	**14.30**	-5340.268277	**21.20**	-5340.507826	**25.60**	-5340.969388	**14.78**	-5341.085519	**7.92**
^{4}TS$_{\alpha\text{-reb}}$	-5341.298810	**24.79**	-5341.402709	**15.83**	-5340.266392	**22.38**	-5340.500041	**30.48**	-5340.967000	**16.28**	-5341.090249	**4.96**
^{4}Pr$_\alpha$	-5341.398073	**-37.49**	-5341.486517	**-36.76**	-5340.367334	**-40.96**	-5340.567838	**-12.06**	-5341.074036	**-50.88**	-5341.162634	**-40.47**
^{2}Pr$_\alpha$	-5341.398880	**-38.00**	-5341.491210	**-39.71**	-5340.368802	**-41.88**	-5340.577362	**-18.04**	-5341.072996	**-50.23**	-5341.160794	**-39.31**
^{4}TS$_{2H}$	-5341.288656	**31.17**	-5341.382172	**28.71**	-5340.249646	**32.89**	-5340.489558	**37.06**	-5340.949950	**26.98**	-5341.063894	**21.49**
^{2}TS$_{2H}$	-5341.301034	**23.40**	-5341.398542	**18.44**	-5340.265201	**23.13**	-5340.503125	**28.55**	-5340.965655	**17.13**	-5341.084317	**8.68**
^{4}P$_{2H}$	-5341.291069	**29.65**	-5341.384607	**27.19**	-5340.258840	**27.12**	-5340.476435	**45.30**	-5340.961482	**19.75**	-5341.052893	**28.40**
^{2}P$_{2H}$	-5341.291070	**29.65**	-5341.384607	**27.19**	-5340.258836	**27.12**	-5340.476436	**45.30**	-5340.961481	**19.75**	-5341.052901	**28.39**
^{4}RC$_\beta$	-5341.321820	**10.35**	-5341.423958	**2.49**	-5340.286498	**9.76**	-5340.523651	**15.67**	-5340.983811	**5.73**	-5341.097728	**0.26**
^{2}RC$_\beta$	-5341.321966	**10.26**	-5341.424234	**2.32**	-5340.286683	**9.65**	-5340.524718	**15.00**	-5340.983920	**5.66**	-5341.098507	**-0.23**
^{4}TS$_{\beta H}$	-5341.276385	**38.87**	-5341.380474	**29.78**	-5340.243693	**36.62**	-5340.483223	**41.04**	-5340.941844	**32.07**	-5341.060475	**23.64**
^{2}TS$_{\beta H}$	-5341.275937	**39.15**	-5341.377583	**31.59**	-5340.241885	**37.76**	-5340.484719	**40.10**	-5340.941128	**32.52**	-5341.058622	**24.80**

$^4IM_\beta$	-5341.296270	**26.39**	-5341.400442	**17.25**	-5340.265622	**22.86**	-5340.494579	**33.91**	-5340.966296	**16.72**	-5341.080470	**11.09**
$^2IM_\beta$	-5341.297838	**25.40**	-5341.394111	**21.22**	-5340.262911	**24.56**	-5340.493013	**34.89**	-5340.964482	**17.86**	-5341.070126	**17.58**
$^4TS_{\beta\text{-reb}}$	-5341.285702	**33.02**	-5341.390061	**23.76**	-5340.255203	**29.40**	-5340.485736	**39.46**	-5340.955105	**23.75**	-5341.070021	**17.65**
$^4Pr_\beta$	-5341.387286	**-30.73**	-5341.476215	**-30.30**	-5340.357084	**-34.53**	-5340.558443	**-6.16**	-5341.062944	**-43.92**	-5341.150999	**-33.16**
$^2Pr_\beta$	-5341.395411	**-35.82**	-5341.489053	**-38.35**	-5340.365525	**-39.83**	-5340.574044	**-15.95**	-5341.069523	**-48.05**	-5341.159049	**-38.22**
$^4TS_{cl}$	-5341.230307	**67.78**	-5341.334912	**58.37**	-5340.193206	**68.30**	-5340.438651	**69.01**	-5340.892225	**63.20**	-5341.009565	**55.59**
$^2TS_{cl}$	-5341.204661	**83.87**	-5341.310283	**73.83**	-5340.168085	**84.07**	-5340.408684	**87.81**	-5340.869323	**77.58**	-5340.990273	**67.69**
$^4P_{cl}$	-5341.234563	**65.11**	-5341.336090	**57.63**	-5340.196748	**66.08**	-5340.432532	**72.85**	-5340.898131	**59.50**	-5341.012725	**53.60**
$^2P_{cl}$	-5341.234985	**64.84**	-5341.336455	**57.40**	-5340.197204	**65.80**	-5340.431518	**73.48**	-5340.898760	**59.10**	-5341.009223	**55.80**

Table S7. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for molecular species involved in aldehyde$_{\beta\text{-dehalogen}}$ hydroxylation catalyzed by Cpd I of P450 at various levels of B3LYP-calculations

	BSI		**BSI+G_{corr}**		**BSI+PCM**		**BSI+D_3**		**BSII/BSI**		**BSII/BSI+PCM + G_{corr}+D_3**		**BSII/BSI+PCM + G_{corr}**		**G_{corr}**
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**
$^4RC_{c\alpha}$	-4955.715309	**0.00**	-4955.278492	**0.00**	-4955.735939	**0.00**	-4955.842904	**0.00**	-4956.899654	**0.00**	-4956.611061	**0.00**	-4956.483466	**0.00**	0.436817
$^2RC_{c\alpha}$	-4955.715460	**-0.09**	-4955.278072	**0.26**	-4955.736194	**-0.16**	-4955.843183	**-0.18**	-4956.899746	**-0.06**	-4956.610815	**0.15**	-4956.483092	**0.24**	0.437388
$^4TS_{c\alpha}$	-4955.694460	**13.08**	-4955.258706	**12.42**	-4955.714344	**13.55**	-4955.827491	**9.67**	-4956.880273	**12.16**	-4956.597433	**8.55**	-4956.464402	**11.96**	0.435754
$^2TS_{c\alpha}$	-4955.692908	**14.06**	-4955.256998	**13.49**	-4955.713417	**14.13**	-4955.825430	**10.97**	-4956.880432	**12.06**	-4956.597554	**8.48**	-4956.465031	**11.57**	0.435910
$^4IM_{c\alpha}$	-4955.711051	**2.67**	-4955.275751	**1.72**	-4955.729829	**3.83**	-4955.836738	**3.87**	-4956.905393	**-3.60**	-4956.614557	**-2.19**	-4956.488870	**-3.39**	0.435300
$^2IM_{c\alpha}$	-4955.711838	**2.18**	-4955.274510	**2.50**	-4955.732957	**1.87**	-4955.840006	**1.82**	-4956.899430	**0.14**	-4956.611389	**-0.21**	-4956.483220	**0.15**	0.437328
$^4Pr_{c\alpha}$	-4955.826520	**-69.79**	-4955.387304	**-68.28**	-4955.850222	**-71.71**	-4955.954268	**-69.88**	-4957.017350	**-73.86**	-4956.729584	**-74.37**	-4956.601836	**-74.28**	0.439216
$^2Pr_{c\alpha}$	-4955.835175	**-75.22**	-4955.392116	**-71.30**	-4955.855212	**-74.85**	-4955.957478	**-71.90**	-4957.021179	**-76.26**	-4956.720461	**-68.65**	-4956.598157	**-71.97**	0.443059

Table S8. Bond dissociation energies of TDCIPP and its metabolites at various reaction positions (kcal/mol)

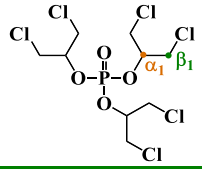
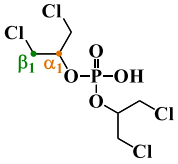
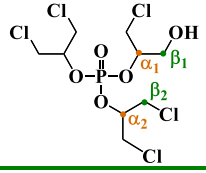
Compound	Structure	BDE			
		αC$_1$	**βC$_1$**	**αC$_2$**	**βC$_2$**
TDCIPP		78.4	85.7	/	/
BDCIPP (M_{IV})		75.2	82.6	/	/
Alcohol$_{β\text{-dehalogen}}$ (M_{VIII})		78.6	78.2	76.9	86.6

Table S9. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for calculations of bond dissociation energies of TDCIPP and its metabolites at various reaction positions. (kcal/mol)

	BSI	**BSI+G$_{corr}$**	**BSII/BSI**	**BSII/BSI+G$_{corr}$**	**G$_{corr}$**	**BDE**
	AE	**AE**	**AE**	**AE**	**AE**	**RE**
H·	-0.500273	-0.510927	-0.502257	-0.512911	-0.010654	
TDCIPP	-3755.524547	-3755.332737	-3755.894878	-3755.703068	0.191810	
αC$_1$-H·	-3754.868839	-3754.692883	-3755.241122	-3755.065166	0.175956	**78.43**

βC_1-H·	-3754.858855	-3754.682707	-3755.229743	-3755.053595	0.176148	**85.69**
BDCIPP	-2718.400653	-2718.266408	-2718.690236	-2718.555991	0.134245	
αC_1-H·	-2717.751846	-2717.632902	-2718.042230	-2717.923286	0.118944	**75.17**
βC_1-H·	-2717.737630	-2717.620523	-2718.028636	-2717.911529	0.117107	**82.55**
$Alcohol_{\beta\text{-dehalogen}}$	-3371.142194	-3370.935736	-3371.512481	-3371.306023	0.206458	
αC_1-H·	-3370.486810	-3370.298013	-3370.856614	-3370.667817	0.188797	**78.62**
βC_1-H·	-3370.484976	-3370.297273	-3370.856245	-3370.668542	0.187703	**78.17**
αC_2-H·	-3370.488619	-3370.298879	-3370.860285	-3370.670545	0.189740	**76.91**
βC_2-H·	-3370.472323	-3370.283548	-3370.843918	-3370.655143	0.188775	**86.58**

IV. Energies for Molecular Species Involved in Targeted High-Level Precision Computations

Table S10. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for molecular species involved in TDCIPP hydroxylation catalyzed by Cpd I of CYP3A4 cluster model at various levels of B3LYP-calculations

	BSI		**BSI+G_{corr}**		**BSI+PCM**		**BSI+D_3**		**BSII/BSI**		**BSII/BSI+PCM + G_{corr}+D_3**		**BSII/BSI+PCM + G_{corr}**		**G_{corr}**
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**
TDCIPP +^{2}Cpd I	-7683.424812	**0.00**	-7682.255269	**0.00**	-7683.481329	**0.00**	-7683.649682	**0.00**	-7685.295498	**0.00**	-7684.407344	**0.00**	-7684.182473	**0.00**	1.169543
TDCIPP +^{4}Cpd I	-7683.424745	**0.04**	-7682.255173	**0.06**	-7683.481322	**0.00**	-7683.649559	**0.08**	-7685.295270	**0.14**	-7684.407089	**0.16**	-7684.182275	**0.12**	1.169572
$^{2}TS_{\alpha H}$	-7683.366478	**36.61**	-7682.183139	**45.26**	-7683.417075	**40.32**	-7683.620572	**18.27**	-7685.271543	**15.03**	-7684.392896	**9.07**	-7684.138802	**27.40**	1.183339
$^{4}TS_{\alpha H}$	-7683.363075	**38.74**	-7682.178249	**48.33**	-7683.412777	**43.02**	-7683.617491	**20.20**	-7685.270174	**15.89**	-7684.389467	**11.22**	-7684.135051	**29.76**	1.184826
$^{2}IM_{\alpha}$	-7683.396865	**17.54**	-7682.202838	**32.90**	-7683.446043	**22.14**	-7683.645777	**2.45**	-7685.308937	**-8.43**	-7684.413000	**-3.55**	-7684.164088	**11.54**	1.194027
$^{4}IM_{\alpha}$	-7683.396737	**17.62**	-7682.200420	**34.42**	-7683.445929	**22.21**	-7683.645553	**2.59**	-7685.308931	**-8.43**	-7684.410622	**-2.06**	-7684.161807	**12.97**	1.196317
$^{4r}TS_{\alpha\text{-reb}}$	-7683.383796	**25.74**	-7682.189537	**41.25**	-7683.432767	**30.47**	-7683.639327	**6.50**	-7685.300089	**-2.88**	-7684.410331	**-1.87**	-7684.154801	**17.36**	1.194259
$^{2}P_{\alpha}$	-7683.491855	**-42.07**	-7682.287870	**-20.46**	-7683.540236	**-36.96**	-7683.747380	**-61.31**	-7685.397057	**-63.73**	-7684.496979	**-56.25**	-7684.241453	**-37.01**	1.203985
$^{4}P_{\alpha}$	-7683.491279	**-41.71**	-7682.290174	**-21.90**	-7683.542625	**-38.46**	-7683.744848	**-59.72**	-7685.401090	**-66.26**	-7684.504899	**-61.22**	-7684.251331	**-43.21**	1.201105
$^{2}TS_{\beta H}$	-7683.361868	**39.50**	-7682.170690	**53.07**	-7683.407691	**46.21**	-7683.626268	**14.69**	-7685.267391	**17.64**	-7684.386436	**13.12**	-7684.122036	**37.93**	1.191178
$^{4}TS_{\beta H}$	-7683.369256	**34.86**	-7682.176509	**49.42**	-7683.419832	**38.59**	-7683.625891	**14.93**	-7685.273596	**13.74**	-7684.388061	**12.10**	-7684.131426	**32.03**	1.192747
$^{2}IM_{\beta}$	-7683.395178	**18.60**	-7682.199380	**35.07**	-7683.441370	**25.07**	-7683.655606	**-3.72**	-7685.301304	**-3.64**	-7684.412127	**-3.00**	-7684.151698	**19.31**	1.195798
$^{4}IM_{\beta}$	-7683.395783	**18.22**	-7682.198035	**35.91**	-7683.441428	**25.04**	-7683.655755	**-3.81**	-7685.309220	**-8.61**	-7684.417088	**-6.12**	-7684.157116	**15.91**	1.197748
$^{4}TS_{\beta\text{-reb}}$	-7683.383282	**26.06**	-7682.189688	**41.15**	-7683.430723	**31.76**	-7683.644761	**3.09**	-7685.298069	**-1.61**	-7684.413395	**-3.80**	-7684.151916	**19.18**	1.193594
$^{2}P_{\beta}$	-7683.489279	**-40.45**	-7682.289857	**-21.70**	-7683.537300	**-35.12**	-7683.756296	**-66.90**	-7685.395873	**-62.99**	-7684.511490	**-65.35**	-7684.244472	**-38.91**	1.199422

$^4P_\beta$	-7683.485999	**-38.40**	-7682.288160	**-20.64**	-7683.537431	**-35.20**	-7683.747315	**-61.27**	-7685.398098	**-64.38**	-7684.513007	**-66.30**	-7684.251691	**-43.43**	1.197839

Table S11. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for dissociation of α-hydroxy-TDCIPP from resting state in the chlorobenzene environment

	BSI		**BSI+G_{corr}**		**BSII/BSI+PCM**		**BSI+D_3**		**BSII/BSI**		**BSII/BSI+PCM + G_{corr}+D_3**		**BSII/BSI+PCM + G_{corr}**		**G_{corr}**
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**
$^2Pr_\alpha$	-5341.398880	**0.00**	-5340.950364	**0.00**	-5341.420045	**0.00**	-5341.530418	**0.00**	-5342.594675	**0.00**	-5342.298862	**0.00**	-5341.167324	**0.00**	0.448516
α-hydroxy-TDCIPP	-3830.747777		-3830.554187		-3830.759703		-3830.808400		-3831.145475		-3831.024435		-3830.963812		0.193590
Resting State	-1510.678909	**-17.45**	-1510.441351	**-28.35**	-1510.689604	**-18.36**	-1510.732134	**-6.35**	-1511.442177	**4.41**	-1511.268538	**3.69**	-1511.215314	**-7.41**	0.237558
$^4Pr_\alpha$	-5341.398073	**0.00**	-5340.951851	**0.00**	-5341.420511	**0.00**	-5341.531741	**0.00**	-5342.595676	**0.00**	-5342.305560	**0.00**	-5342.171892	**0.00**	0.446222
α-hydroxy-TDCIPP	-3830.747777		-3830.554187		-3830.759703		-3830.808400		-3831.145475		-3831.024435		-3830.963812		0.193590
Resting State	-1510.662569	**-7.70**	-1510.430077	**-20.34**	-1510.673964	**-8.26**	-1510.714338	**5.65**	-1511.430375	**12.44**	-1511.261047	**12.60**	-1511.209278	**-0.75**	0.232492
Average		**-12.57**		**-24.34**		**-13.31**		**-0.35**		**8.42**		**8.15**		**-4.08**	

Table S12. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for dissociation of β-hydroxy-TDCIPP from resting state in the chlorobenzene environment

	BSI		**BSI+G_{corr}**		**BSII/BSI+PCM**		**BSI+D_3**		**BSII/BSI**		**BSII/BSI+PCM + G_{corr}+D_3**		**BSII/BSI+PCM + G_{corr}**		**G_{corr}**
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**
$^2Pr_\beta$	-5341.395411	**0.00**	-5340.943942	**0.00**	-5341.414991	**0.00**	-5341.528995	**0.00**	-5342.590163	**0.00**	-5342.291858	**0.00**	-5341.158274	**0.00**	0.451469
β-hydroxy-TDCIPP	-3830.743156		-3830.548943		-3830.755838		-3830.800814		-3831.141855		-3831.017983		-3830.960324		0.194213
Resting State	-1510.678909	**-16.73**	-1510.441351	**-29.09**	-1510.689604	**-19.11**	-1510.732134	**-2.48**	-1511.442177	**3.85**	-1511.268538	**3.35**	-1511.215314	**-10.09**	0.237558
$^4Pr_\beta$	-5341.387286	**0.00**	-5340.941181	**0.00**	-5341.409860	**0.00**	-5341.517997	**0.00**	-5342.585836	**0.00**	-5342.293015	**0.00**	-5342.162305	**0.00**	0.446105
β-hydroxy-TDCIPP	-3830.743156		-3830.548943		-3830.755838		-3830.800814		-3831.141855		-3831.017983		-3830.960324		0.194213
Resting State	-1510.662569	**-11.57**	-1510.430077	**-23.74**	-1510.673964	**-12.51**	-1510.714338	**1.79**	-1511.430375	**8.54**	-1511.261047	**8.78**	-1511.209278	**-4.58**	0.232492
Average		**-14.15**		**-26.42**		**-15.81**		**-0.35**		**6.19**		**6.06**		**-7.74**	

Table S13. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for the H-transfer reactions of α-hydroxy-TDCIPP in enzyme environment

	BSI		BSI+G_{corr}		BSI+PCM		BSI+D_3		BSII/BSI		BSII/BSI+PCM + G_{corr}+D_3		BSII/BSI+PCM + G_{corr}		G_{corr}
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**
^{2}RC	-5341.399705	**0.00**	-5340.947933	**0.00**	-5341.419530	**0.00**	-5341.537181	**0.00**	-5342.593577	**0.00**	-5342.299106	**0.00**	-5342.161630	**0.00**	0.451772
^{2}TS$_{H\text{-}transfer}$	-5341.379939	**12.40**	-5340.934231	**8.60**	-5341.399974	**12.27**	-5341.515419	**13.66**	-5342.573609	**12.53**	-5342.283418	**9.84**	-5342.147937	**8.59**	0.445708
^{2}Pr	-5341.412766	**-8.20**	-5340.969637	**-13.62**	-5341.431307	**-7.39**	-5341.548092	**-6.85**	-5342.610082	**-10.36**	-5342.320821	**-13.63**	-5342.185495	**-14.98**	0.443129
^{2}RC-H_2O	-5417.842009	**0.00**	-5417.368789	**0.00**	-5417.863569	**0.00**	-5417.984763	**0.00**	-5419.069148	**0.00**	-5418.760241	**0.00**	-5418.617488	**0.00**	0.473220
^{2}TS$_{H\text{-}transfer}$-H_2O	-5417.841969	**0.03**	-5417.369603	**-0.51**	-5417.860187	**2.12**	-5417.983318	**0.91**	-5419.067835	**0.82**	-5418.755036	**3.27**	-5418.613686	**2.39**	0.472366
^{2}Pr-H_2O	-5417.862511	**-12.87**	-5417.395732	**-16.91**	-5417.881288	**-11.12**	-5417.997345	**-7.90**	-5419.090683	**-13.51**	-5418.777515	**-10.84**	-5418.642681	**-15.81**	0.466779

Table S14. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for the H-transfer reactions of α-hydroxy-TDCIPP in water solution

	BSI+PCM		BSI+PCM+G_{corr}		BSI+PCM+D_3		BSII/BSI+PCM		BSII/BSI+PCM + G_{corr}+D_3		BSII/BSI+PCM + G_{corr}		G_{corr}
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**
RC	-3830.766581	**0.00**	-3830.573133	**0.00**	-3830.809331	**0.00**	-3831.164899	**0.00**	-3831.014201	**0.00**	-3830.971451	**0.00**	0.193448
TS$_{H\text{-}transfer}$	-3830.747571	**11.93**	-3830.559470	**8.57**	-3830.788441	**13.11**	-3831.145211	**12.35**	-3830.997980	**10.18**	-3830.957110	**9.00**	0.188101
Pr	-3830.770155	**-2.24**	-3830.583537	**-6.53**	-3830.802734	**4.14**	-3831.172559	**-4.81**	-3831.018520	**-2.71**	-3830.985941	**-9.09**	0.186618
RC-H_2O	-3907.216226	**0.00**	-3906.998533	**0.00**	-3907.263401	**0.00**	-3907.600000	**0.00**	-3907.475474	**0.00**	-3907.428300	**0.00**	0.217693
TS$_{H\text{-}transfer}$-H_2O	-3907.198382	**11.20**	-3906.987679	**6.81**	-3907.241555	**13.71**	-3907.627046	**11.89**	-3907.459516	**10.01**	-3907.416343	**7.50**	0.210703
Pr-H_2O	-3907.216321	**-0.06**	-3907.005524	**-4.39**	-3907.256672	**4.22**	-3907.647552	**-0.98**	-3907.477106	**-1.02**	-3907.436755	**-5.31**	0.210797

Table S15. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for the H-transfer reactions of β-hydroxy-TDCIPP in enzyme environment

	BSI		BSI+G_{corr}		BSI+PCM		BSI+D_3		BSII/BSI		BSII/BSI+PCM + G_{corr}+D_3		BSII/BSI+PCM + G_{corr}		G_{corr}
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE
^{2}RC	-5341.395411	0.00	-5340.943942	0.00	-5341.414991	0.00	-5341.528995	0.00	-5342.590163	0.00	-5342.291858	0.00	-5342.158274	0.00	0.451469
$^2TS_{H\text{-}transfer}$	-5341.339306	35.21	-5340.892763	32.12	-5341.364261	31.83	-5341.472923	35.19	-5342.533057	35.83	-5342.245086	29.35	-5342.111469	29.37	0.446543
^{2}Pr	-5341.386910	5.33	-5340.942880	0.67	-5341.407676	4.59	-5341.515875	8.23	-5342.583456	4.21	-5342.289155	1.70	-5342.160191	-1.20	0.444030
^{2}RC-H_2O	-5417.843435	0.00	-5417.366493	0.00	-5417.863136	0.00	-5417.985923	0.00	-5419.069312	0.00	-5418.754559	0.00	-5418.612072	0.00	0.476942
$^2TS_{H\text{-}transfer}$-H_2O	-5417.811160	20.25	-5417.338865	17.34	-5417.834634	17.89	-5417.955054	19.37	-5419.034255	22.00	-5418.729327	15.83	-5418.585433	16.72	0.472295
^{2}Pr-H_2O	-5417.833779	6.06	-5417.366966	-0.30	-5417.855694	4.67	-5417.975806	6.35	-5419.059541	6.13	-5418.756668	-1.32	-5418.614642	-1.61	0.466813

Table S16. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for the H-transfer reactions of β-hydroxy-TDCIPP in water solution

	BSI+PCM		BSI+PCM+G_{corr}		BSI+PCM+D_3		BSII/BSI+PCM		BSII/BSI+PCM + G_{corr}+D_3		BSII/BSI+PCM + G_{corr}		G_{corr}
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE
RC	-3830.755837	0.00	-3830.560949	0.00	-3830.796454	0.00	-3831.155164	0.00	-3831.000893	0.00	-3830.960276	0.00	0.194888
$TS_{H\text{-}transfer}$	-3830.719004	23.11	-3830.525677	22.13	-3830.744547	32.57	-3831.118664	22.90	-3830.950880	31.38	-3830.925337	21.92	0.193327
Pr	-3830.750767	3.18	-3830.565385	-2.78	-3830.788400	5.05	-3831.151307	2.42	-3831.003558	-1.67	-3830.965925	-3.55	0.185382
RC-H_2O	-3907.199706	0.00	-3830.984344	0.00	-3907.240697	0.00	-3907.630254	0.00	-3907.455883	0.00	-3907.414892	0.00	0.215362
$TS_{H\text{-}transfer}$-H_2O	-3907.193469	3.91	-3830.978810	3.47	-3907.230820	6.20	-3907.626186	2.55	-3907.448877	4.40	-3907.411527	2.11	0.214659
Pr-H_2O	-3907.196034	2.30	-3830.989071	-2.97	-3907.235027	3.56	-3907.626929	2.09	-3907.458959	-1.93	-3907.419966	-3.18	0.206963

Table S17. The standard reduction potentials referenced with respect to the standard hydrogen electrode (E_0 vs SHE, unit: V) of aldehydes at various levels of B3LYP-calculations

	BSI	BSII	BSII(+e)	ΔG	E_0 vs SHE
	(a.u.)	(a.u.)	(a.u.)	(kcal/mol)	(V)
Fe(II)	-1510.759930	-1511.537525	/	/	/
Fe(III)	-1510.676735	-1511.454300	/	-52.22	**-2.17**
4-Hydroxynonenal	-503.043305	-503.176429	-503.268134	-57.55	**-1.93**
4-Hydroxynonenal + H^+	-503.457360	-503.580514	-503.743949	-102.56	**0.02**
Aldehyde$_{\beta\text{-dehalogen}}$	-3369.938187	-3370.308920	-3370.378152	-43.44	**-2.55**
Aldehyde$_{\beta\text{-dehalogen}}$ + H^+	-3370.328758	-3370.691277	-3370.848530	-98.68	**-0.15**
Aldehyde$_{\beta\text{-dehalogen}}$ + H^+ + e^-	-3370.495085	-3370.867245	-3370.942282	-47.09	**-2.39**
Aldehyde$_{\beta\text{-dehalogen}}$ + H^+ + e^- + H^+	-3370.891050	-3371.253455	-3371.509712	-160.80	**2.54**

Table S18. Ionization potentials of phenols at various levels of B3LYP-calculations (AE: a.u., RE: eV)

	BSI	BSI(-e)	BSII/BSI + G_{corr}	BSII/BSI + G_{corr}(-e)	IP	G_{corr}	G_{corr}(-e)
	(a.u.)	(a.u.)	(a.u.)	(a.u.)	(eV)	(a.u.)	(a.u.)
Fe(II)	-1510.759930	-1510.678228	-1511.537525	-1511.453100	**2.37**	0.229322	0.234650

Table S19. Electron affinity of the aldehyde$_{\beta\text{-dehalogen}}$ at various levels of B3LYP-calculations (AE: a.u., RE: eV)

	BSI	**BSI(+e)**	**BSII/BSI**	**BSII/BSI(+e)**	**EA**
	(a.u.)	**(a.u.)**	**(a.u.)**	**(a.u.)**	**(eV)**
Aldehyde$_{\beta\text{-dehalogen}}$	-3369.921911	-3369.9058436	-3370.289893	-3370.297408	**0.20**
Aldehyde$_{\beta\text{-dehalogen}}$ + H^+	-3370.236499	-3370.456191	-3370.597173	-3370.827610	**6.07**
Aldehyde$_{\beta\text{-dehalogen}}$ + H^+ + e^-	-3370.481018	-3370.455751	-3370.850599	-3370.856203	**0.15**
Aldehyde$_{\beta\text{-dehalogen}}$ + H^+ + e^- + H^+	-3370.805571	-3371.122202	-3371.16587	-3371.492002	**8.60**

V. Mulliken Spin Densities and Charges

Table S20. Spin densities for TDCIPP hydroxylation catalyzed by CYP3A4 Cpd I cluster model

	Substrate					Cpd I			
	Sub	**αC**	**αH**	**βC**	**βH**	**O**	**Fe**	**Por**	**SH**
SUB+ ^{4}Cpd I	/	/	/	/	/	0.906933	1.110656	0.474841	0.505205
SUB+ ^{2}Cpd I	/	/	/	/	/	0.860838	1.229430	-0.537192	-0.553810
^{4}TS$_{\alpha H}$	0.436464	0.406226	-0.061699	-0.014935	0.000999	0.548514	1.123434	0.476779	0.414231
^{2}TS$_{\alpha H}$	0.436370	0.435217	-0.064392	-0.021103	0.000548	0.493249	1.130621	-0.660079	-0.400241
^{4}IM$_{\alpha}$	1.000054	0.790649	0.001952	-0.048840	0.003803	0.217360	1.803007	-0.103960	0.080928
^{2}IM$_{\alpha}$	-0.994791	-0.789600	0.002055	0.050447	-0.004475	0.217215	1.799754	-0.103664	0.083841
^{4}TS$_{\alpha\text{-reb}}$	0.769986	0.637083	0.003187	-0.026967	0.005156	0.006388	2.112234	-0.100876	0.212311
^{4}Pr$_{\alpha}$	-0.000206	0.000035	-0.000302	0.000000	0.000000	0.000009	2.466035	0.063358	0.470686
^{2}Pr$_{\alpha}$	0.000041	0.000009	-0.000045	0.000004	-0.000001	0.000055	1.201581	-0.129692	-0.071995
^{4}TS$_{\beta H}$	0.504728	-0.006396	0.002795	0.493503	-0.061256	0.559362	0.974792	0.565215	0.395053
^{2}TS$_{\beta H}$	-0.434584	0.006111	-0.000024	-0.430780	0.060718	-0.313436	1.212214	0.118951	0.416880
^{4}IM$_{\beta}$	1.004335	-0.025160	0.014613	0.898481	0.002177	0.175881	1.817822	-0.096598	0.098151
^{2}IM$_{\beta}$	-0.994353	0.021371	-0.012990	-0.888202	0.000612	0.109275	0.967728	0.461765	0.456617
^{4}TS$_{\beta\text{-reb}}$	0.798677	-0.016908	0.000745	0.735983	0.007917	0.023083	2.063139	-0.102511	0.216742
^{4}Pr$_{\beta}$	-0.000110	0.000074	-0.000013	-0.000407	-0.000608	0.001491	2.492491	0.033948	0.472035
^{2}Pr$_{\beta}$	0.000907	0.000031	-0.000023	0.000577	0.000229	-0.000900	1.136490	-0.100387	-0.036210

Table S21. Mulliken charges for TDCIPP hydroxylation catalyzed by CYP3A4 Cpd I cluster model

	Substrate					Cpd I			
	Sub	**αC**	**αH**	**βC**	**βH**	**O**	**Fe**	**Por**	**SH**
SUB+ ^{4}Cpd I	/	/	/	/	/	0.906933	1.110656	0.474841	0.505205
SUB+ ^{2}Cpd I	/	/	/	/	/	-0.419571	0.478284	-0.053011	-0.053297
^{4}TS$_{\alpha H}$	0.135616	0.157344	0.353997	-0.313067	0.172508	-0.572911	0.385154	0.012696	0.028485
^{2}TS$_{\alpha H}$	0.148122	0.159230	0.348626	-0.308332	0.191146	-0.572929	0.376177	0.032931	-0.005330
^{4}IM$_{\alpha}$	0.243670	0.365770	0.323744	-0.318065	0.229497	-0.588746	0.401622	-0.212759	0.061838
^{2}IM$_{\alpha}$	0.241065	0.366741	0.323700	-0.318747	0.229316	-0.588635	0.401165	-0.213032	0.062298
^{4}TS$_{\alpha\text{-reb}}$	0.361720	0.405449	0.333791	-0.286727	0.201085	-0.596788	0.428494	-0.240782	0.026888
^{4}Pr$_{\alpha}$	0.488531	0.513889	0.349242	-0.292537	0.183910	-0.488318	0.490802	-0.379788	-0.160833
^{2}Pr$_{\alpha}$	0.488804	0.514181	0.349410	-0.292427	0.184002	-0.485673	0.316341	-0.368009	-0.000032
^{4}TS$_{\beta H}$	0.157427	0.179539	0.166594	-0.365967	0.375180	-0.556992	0.381640	0.012941	-0.017632
^{2}TS$_{\beta H}$	0.199038	0.202829	0.161928	-0.363536	0.369398	-0.540305	0.377909	-0.142701	0.105141
^{4}IM$_{\beta}$	0.311633	0.184015	0.167905	-0.255308	0.317233	-0.617635	0.408959	-0.204899	0.095212
^{2}IM$_{\beta}$	0.307283	0.172749	0.166672	-0.257750	0.305114	-0.627080	0.364189	-0.071158	0.048542
^{4}TS$_{\beta\text{-reb}}$	0.365598	0.179816	0.175522	-0.142210	0.326169	-0.576980	0.403885	-0.234512	0.036076
^{4}Pr$_{\beta}$	0.492333	0.167443	0.181461	0.048499	0.351210	-0.442264	0.458362	-0.396683	-0.134290
^{2}Pr$_{\beta}$	0.543700	0.169729	0.184407	0.047980	0.360513	-0.444953	0.235563	-0.402394	0.060538

VI. Estimation of Activation Barriers for Electron Transfer Processes by Marcus Theory

The electron transfer treatment was based on the Marcus theory of electron-transfer reactions, which relies on the transition-state formalism defining the electron transfer (ET) free-energy activation barrier ($\Delta G^{\neq}_{ET}$) in terms of two thermodynamic parameters, the free energy of reaction (ΔG_{ET}) and the reorganization energy (λ):

$$\Delta G^{\neq}_{ET} = \frac{\lambda}{4}\left(1 + \frac{\Delta G_{ET}}{\lambda}\right)^2$$

The reorganization energy λ consists of two parts, the inner reorganization energy λ_i and the solvent reorganization energy λ_0, *i.e.* $\lambda = \lambda_i + \lambda_0$. The solvent reorganization energy λ_0 could be calculated by the following equation:

$$\lambda_0 = (332\ kcal/mol)\left(\frac{1}{2r_1} + \frac{1}{2r_2} - \frac{1}{R}\right)\left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon}\right)$$

Where ε_{op} is the optical dielectric constants (ε_{op} = 2.32), and ε is the static dielectric constant for the chlorobenzene solvent (ε = 5.70). ε_{op} is the vacuum permittivity, r_1 and r_2 are the hard sphere radii of the donor (Fe(II)) and acceptor (aldehyde$_{\beta\text{-dehalogen}}$) species, and $R = r_1 + r_2$.

For a self-exchange ET reaction $A^- + A \rightarrow A + A^-$, it is convenient to employ the four-point method developed by Nelsen for evaluating the inner reorganization energy λ_i by DFT calculations according to:

$$\lambda_i = \lambda_i\left(\frac{A}{A^-}\right) = E_0(A^-) - E_1(A^-) + E_1(A) - E_0(A)$$

Where the subscripts "0" and "1" refer to the equilibrium geometries of the neutral species and the ionic ones, respectively. For an electron

transfer from a donor *D* to an acceptor *A*, $D + A \rightarrow D^+ + A^-$, λ_i can be calculated by taking the average value of λ_i *(D /D*$^+$*)* and λ_i *(A /A*$^-$*)*:

$$\lambda_i = \lambda_i\left(\frac{D}{A}\right) = \frac{1}{2}\left[\lambda_i\left(\frac{D}{D^+}\right) + \lambda_i\left(\frac{A}{A^-}\right)\right]$$

For aldehyde$_{\beta\text{-dehalogen}}$:

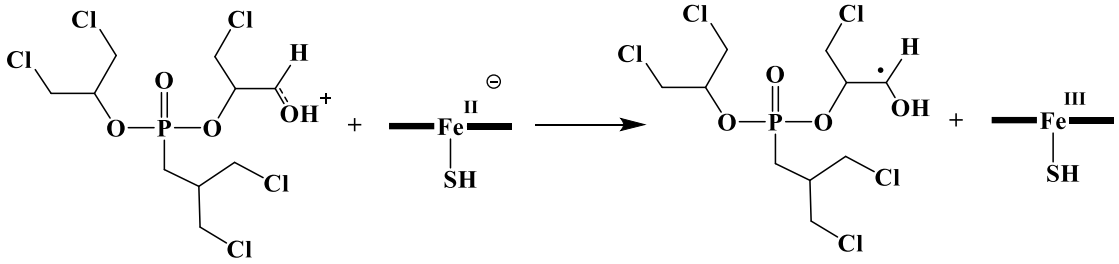


Table S22. Computed hard sphere radii (Units are presented in Å) of the donor and acceptor species

r_1 (Fe(II))	r_2 (aldehyde$_{\beta\text{-dehalogen}}$)
5.70	5.39

Table S23. Computed reorganization energies, free energies and activation barriers for the electron transfer from Fe(II) to aldehyde$_{\beta\text{-dehalogen}}$

λ_i	λ_0	$\Delta G^{\neq}_{ET}$	ΔG_{ET}
(kcal/mol)	(kcal/mol)	(kcal/mol)	(kcal/mol)
23.32	7.66	0.08	-27.79

Table S24. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for the aldehyde$_{\beta\text{-dehalogen}}$ in the outer-sphere electron transfer pathway

	BSI		BSI+G_{corr}		BSI+PCM		BSI+D_3		BSI+PCM + G_{corr}+D_3		BSI+PCM + G_{corr}		G_{corr}
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**
Fe(II)	-1510.759930		-1510.530608		-1510.827005		-1510.809370		-1510.647123		-1510.597683		0.229322
Aldehyde$_{\beta\text{-dehalogen}}$ + H^+	-3370.236499		-3370.042050		-3370.308462		-3370.291676		-3370.169189		-3370.114013		0.194449
Fe(III)	-1510.676735		-1510.444370		-1510.687781		-1510.727613		-1510.506295		-1510.455416		0.232365
Aldehyde$_{\beta\text{-dehalogen}}$ + H^+ + e^-	-3370.481018	**-101.23**	-3370.288994	**-100.84**	-3370.491151	**-27.27**	-3370.536196	**-102.14**	-3370.354305	**-27.79**	-3370.299127	**-26.89**	0.192024

Table S25. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for the aldehyde$_{\beta\text{-dehalogen}}$ in the hydrion transfer pathway

	BSI		BSI+G_{corr}		BSI+PCM		BSI+D_3		BSII/BSI		BSII/BSI+PCM + G_{corr}+D_3		BSII/BSI+PCM + G_{corr}		G_{corr}
	AE	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**	**RE**	**AE**
Aldehyde$_{\beta\text{-dehalogen}}$	-3369.921911		-3369.740914		-3369.933289		-3369.975928		-3370.289893		-3370.174291		-3370.120274		0.180997
H^+	0.000000		-0.010000		-0.137431		0.000000		0.000000		-0.147431		-0.147431		-0.010000
Aldehyde$_{\beta\text{-dehalogen}}$ + H^+	-3370.236499	**-197.41**	-3370.042050	**-182.69**	-3370.308462	**-149.19**	-3370.291676	**-198.13**	-3370.597173	**-192.82**	-3370.529863	**-130.61**	-3370.474687	**-129.88**	0.194449

VII. Description of Eyring Equation

The Eyring equation can be used to interpret the temperature dependence of rate constants. The most common form of the equation is:

$$k = \frac{k_B T}{h} exp\left(-\frac{\Delta G^{\ddagger}}{RT}\right)$$

where k is the rate constant, k_B is Boltzmann's constant, T is the absolute temperature, h is Planck's constant, R is the gas constant, $\Delta G^{\ddagger}$ is the free energy of activation. To explore the rates of different reactions, we can do the quotient of the equations to get a new form:

$$\frac{k_1}{k_2} = exp\left(-\frac{\Delta G_1^{\ddagger} - \Delta G_2^{\ddagger}}{RT}\right)$$

thus we estimate the ratio through this rate ratio, as shown in **Table S26.**

Table S26. Absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for computed the products ratio of different reaction paths of TDCIPP catalyzed by Cpd I of CYP3A4 cluster model through Eying equation

	BSII/BSI+PCM+G_{corr}+D_3		ΔG	Products ratio (C_β/C_α)
	AE	**RE**	**RE**	**/**
TDCIPP+^{2}Cpd I	-7684.407344	0.0		
$^2TS_{\alpha H}$	-7684.392896	9.1		
$^2TS_{\beta H}$	-7684.386436	13.1	4.0	**0.002**
TDCIPP+^{4}Cpd I	-7684.407089	0.0		
$^4TS_{\alpha H}$	-7684.389467	11.0		
$^4TS_{\beta H}$	-7684.388061	11.9	0.9	**0.23**

VIII. Cartesian Coordinates of All Structures

Optimization at the UB3LYP/BSI level of theory

For molecular structure of TDCIPP catalyzed by Cpd I of CYP450

^{4}Cpd I

1	26	0	0.220920	-0.344889	-0.185313
2	7	0	0.293749	-0.589383	1.817020
3	7	0	2.174531	0.163519	-0.179959
4	7	0	0.090610	0.193362	-2.123987
5	7	0	-1.782548	-0.580734	-0.121957
6	6	0	2.693422	-0.237358	2.180698
7	6	0	2.446828	0.706271	-2.554021
8	6	0	-2.311344	-0.134960	-2.472601
9	6	0	-2.046251	-1.190680	2.236359
10	6	0	1.415680	-0.547279	2.616247
11	6	0	3.043839	0.091718	0.874315
12	6	0	2.931134	0.521802	-1.266256
13	6	0	1.123333	0.551336	-2.948041
14	6	0	-1.027586	0.175801	-2.910054
15	6	0	-2.656468	-0.491094	-1.177916
16	6	0	-2.532855	-0.983055	0.951810
17	6	0	-0.736414	-0.987300	2.639205
18	6	0	-0.256374	-1.173965	3.986479
19	6	0	1.075106	-0.898143	3.973187
20	6	0	4.383018	0.420069	0.448385
21	6	0	4.312437	0.688238	-0.883882
22	6	0	0.644248	0.765813	-4.292642
23	6	0	-0.696191	0.533469	-4.268658
24	6	0	-3.992340	-0.835145	-0.753777
25	6	0	-3.914553	-1.146318	0.567754
26	1	0	3.488405	-0.253449	2.919531
27	1	0	5.249096	0.439582	1.096475
28	1	0	5.108532	0.974331	-1.558316
29	1	0	3.162052	0.995970	-3.317426
30	1	0	1.264530	1.059404	-5.129000
31	1	0	-1.407666	0.595471	-5.081316
32	1	0	-3.108059	-0.104497	-3.209118
33	1	0	-4.862078	-0.834189	-1.397199

34	1	0	-4.707310	-1.452261	1.237314
35	1	0	-2.754801	-1.516517	2.991089
36	1	0	-0.873643	-1.477490	4.821513
37	1	0	1.778587	-0.930110	4.794559
38	8	0	0.522943	-1.904461	-0.532417
39	16	0	-0.393823	2.020640	0.615831
40	1	0	0.765305	2.304482	1.246086

^{2}Cpd I

1	26	0	0.037823	-0.014556	-0.134641
2	7	0	0.370542	0.081953	1.846749
3	7	0	1.998819	0.303496	-0.478944
4	7	0	-0.328942	0.200892	-2.114700
5	7	0	-1.953935	-0.045885	0.206371
6	6	0	2.813079	0.268638	1.831369
7	6	0	1.974695	0.399868	-2.928599
8	6	0	-2.764285	-0.080960	-2.106918
9	6	0	-1.935600	-0.099010	2.654785
10	6	0	1.586224	0.151987	2.472955
11	6	0	2.999938	0.336552	0.457513
12	6	0	2.620179	0.393249	-1.695203
13	6	0	0.605662	0.313528	-3.120500
14	6	0	-1.546895	0.087986	-2.746091
15	6	0	-2.950501	-0.127089	-0.730830
16	6	0	-2.578679	-0.122074	1.426607
17	6	0	-0.560384	-0.008892	2.844452
18	6	0	0.081410	0.006273	4.137003
19	6	0	1.418653	0.104716	3.905510
20	6	0	4.285714	0.459262	-0.185348
21	6	0	4.049672	0.494307	-1.525111
22	6	0	-0.043739	0.304190	-4.408599
23	6	0	-1.376036	0.161310	-4.176632
24	6	0	-4.236789	-0.251174	-0.087476
25	6	0	-4.006378	-0.242576	1.252736
26	1	0	3.699169	0.312169	2.456780
27	1	0	5.232673	0.511896	0.335230
28	1	0	4.762284	0.581206	-2.334522
29	1	0	2.597417	0.476460	-3.814331
30	1	0	0.470283	0.390555	-5.356708
31	1	0	-2.183206	0.108022	-4.895029
32	1	0	-3.647639	-0.164344	-2.731843
33	1	0	-5.181205	-0.326387	-0.609833
34	1	0	-4.721717	-0.311344	2.061447
35	1	0	-2.556234	-0.164597	3.542843
36	1	0	-0.438340	-0.049980	5.084189
37	1	0	2.227327	0.147052	4.622934
38	8	0	0.169188	-1.631056	-0.221788
39	16	0	-0.403678	2.522090	-0.315099
40	1	0	0.644255	2.830430	-1.107653

TDCIPP

1	15	0	1.492306	-6.170516	-3.466904

2	8	0	1.290813	-7.052059	-2.289284
3	8	0	2.831807	-5.276938	-3.465103
4	8	0	0.344637	-5.068905	-3.702370
5	8	0	1.585235	-6.838388	-4.915685
6	6	0	2.040635	-8.153794	-5.305722
7	1	0	1.679024	-8.239322	-6.336028
8	6	0	1.356180	-9.237916	-4.471653
9	1	0	0.280323	-9.066425	-4.468418
10	1	0	1.733148	-9.273006	-3.452080
11	17	0	1.636223	-10.860129	-5.226338
12	6	0	-0.975674	-5.079756	-3.107094
13	1	0	-1.527524	-4.338244	-3.688770
14	6	0	-0.831965	-4.586034	-1.661143
15	1	0	-0.363111	-5.342081	-1.030171
16	1	0	-0.238236	-3.671831	-1.655620
17	17	0	-2.437521	-4.176461	-0.934299
18	6	0	3.233880	-4.563391	-2.272011
19	1	0	2.357718	-4.293265	-1.674381
20	6	0	3.954928	-3.303658	-2.722505
21	1	0	4.426120	-2.815220	-1.870443
22	17	0	2.824591	-2.105748	-3.466000
23	6	0	-1.694109	-6.421611	-3.183920
24	1	0	-1.114569	-7.206623	-2.699001
25	1	0	-2.667920	-6.331634	-2.703711
26	17	0	-1.999294	-6.941264	-4.891568
27	6	0	3.560202	-8.230732	-5.404260
28	1	0	3.838399	-9.112472	-5.980842
29	1	0	3.939189	-7.332484	-5.891319
30	17	0	4.419460	-8.374235	-3.815072
31	1	0	4.706803	-3.548533	-3.474457
32	6	0	4.130512	-5.506162	-1.462097
33	1	0	5.055625	-5.729078	-1.994532
34	1	0	3.589888	-6.429642	-1.260588
35	17	0	4.573199	-4.777116	0.135770

$^{4}RC_{\alpha}$

1	26	0	0.648025	-0.630358	-0.237139
2	7	0	0.667332	-1.277042	1.673485
3	7	0	2.637787	-0.312101	-0.133930
4	7	0	0.595595	0.299007	-2.026404
5	7	0	-1.369901	-0.670669	-0.210073
6	6	0	3.082803	-1.230886	2.093736
7	6	0	2.992651	0.684416	-2.345572
8	6	0	-1.820888	0.280353	-2.423101
9	6	0	-1.728483	-1.696295	1.986103
10	6	0	1.776333	-1.505620	2.459743
11	6	0	3.480841	-0.672064	0.882147
12	6	0	3.438570	0.197824	-1.124100
13	6	0	1.668256	0.726178	-2.761485
14	6	0	-0.506321	0.540316	-2.798205
15	6	0	-2.217759	-0.278161	-1.218281
16	6	0	-2.174022	-1.182613	0.775298

17	6	0	-0.408847	-1.723785	2.406870	43	8	0	2.816875	-5.271573	-3.461177
18	6	0	0.031440	-2.225661	3.685240	44	8	0	0.324315	-5.022722	-3.533614
19	6	0	1.383591	-2.087376	3.719561	45	8	0	1.475987	-6.791073	-4.857419
20	6	0	4.848411	-0.379302	0.531047	46	6	0	1.996540	-8.066322	-5.284883
21	6	0	4.822096	0.162671	-0.718205	47	1	0	1.642254	-8.138510	-6.319005
22	6	0	1.232670	1.247387	-4.034315	48	6	0	1.358182	-9.203913	-4.485216
23	6	0	-0.122762	1.131947	-4.057357	49	1	0	0.275587	-9.081008	-4.484708
24	6	0	-3.588287	-0.538389	-0.850735	50	1	0	1.730810	-9.247490	-3.464205
25	6	0	-3.560726	-1.104057	0.385262	51	17	0	1.710853	-10.793551	-5.278781
26	1	0	3.861477	-1.470249	2.810780	52	6	0	-1.005339	-5.131650	-2.962636
27	1	0	5.702352	-0.568353	1.167673	53	1	0	-1.549274	-4.300818	-3.417061
28	1	0	5.649702	0.515472	-1.319114	54	6	0	-0.896102	-4.897825	-1.449308
29	1	0	3.742400	1.055960	-3.036209	55	1	0	-0.407992	-5.736706	-0.953927
30	1	0	1.890564	1.645735	-4.794940	56	1	0	-0.355847	-3.968690	-1.255944
31	1	0	-0.812639	1.417333	-4.840240	57	17	0	-2.542928	-4.712785	-0.705338
32	1	0	-2.600423	0.537361	-3.133295	58	6	0	3.262744	-4.407986	-2.385862
33	1	0	-4.445026	-0.313568	-1.471826	59	1	0	2.422756	-3.824505	-1.993230
34	1	0	-4.389898	-1.441685	0.992231	60	6	0	4.311461	-3.481932	-2.985033
35	1	0	-2.477270	-2.087407	2.666988	61	1	0	4.704487	-2.820294	-2.214147
36	1	0	-0.624987	-2.626575	4.445914	62	17	0	3.647035	-2.434209	-4.298148
37	1	0	2.069025	-2.353326	4.513160	63	6	0	-1.709319	-6.442749	-3.293764
38	8	0	0.814852	-2.116269	-0.895234	64	1	0	-1.124171	-7.298404	-2.956228
39	16	0	0.252387	1.567652	0.991660	65	1	0	-2.683920	-6.456353	-2.808037
40	1	0	1.417722	1.607509	1.671028	66	17	0	-2.008931	-6.644919	-5.068198
41	15	0	1.469725	-6.139970	-3.391971	67	6	0	3.520258	-8.079383	-5.382793
42	8	0	1.306879	-7.065730	-2.240883	68	1	0	3.831286	-8.912730	-6.012248

69	1	0	3.863607	-7.138395	-5.812370
70	17	0	4.390531	-8.291950	-3.806932
71	1	0	5.122165	-4.065011	-3.426273
72	6	0	3.862173	-5.317093	-1.302412
73	1	0	4.710353	-5.875999	-1.700011
74	1	0	3.107625	-6.015698	-0.944440
75	17	0	4.450258	-4.376726	0.128584

$^{2}RC_{\alpha}$

1	26	0	0.621377	-1.507403	-0.416423
2	7	0	0.628841	-1.323920	1.598409
3	7	0	2.619562	-1.249500	-0.431135
4	7	0	0.593925	-1.381373	-2.424235
5	7	0	-1.398277	-1.438221	-0.390691
6	6	0	3.045500	-1.185658	1.982819
7	6	0	3.003871	-1.273897	-2.851216
8	6	0	-1.827854	-1.421711	-2.803177
9	6	0	-1.777451	-1.514386	2.030222
10	6	0	1.733083	-1.258934	2.419473
11	6	0	3.453510	-1.173138	0.652342
12	6	0	3.435027	-1.211136	-1.533973
13	6	0	1.678171	-1.356023	-3.260293
14	6	0	-0.506097	-1.409330	-3.237181
15	6	0	-2.238725	-1.435687	-1.478805
16	6	0	-2.212700	-1.498618	0.710860
17	6	0	-0.457849	-1.417879	2.438990
18	6	0	-0.027371	-1.391437	3.815340
19	6	0	1.328390	-1.288104	3.803570
20	6	0	4.827450	-1.067375	0.225381
21	6	0	4.815665	-1.091382	-1.134661
22	6	0	1.253239	-1.380613	-4.638629
23	6	0	-0.108650	-1.409629	-4.623952
24	6	0	-3.614965	-1.483816	-1.049243
25	6	0	-3.598007	-1.529458	0.310268
26	1	0	3.820640	-1.132486	2.740616
27	1	0	5.675496	-0.990181	0.892505
28	1	0	5.651708	-1.038393	-1.818939
29	1	0	3.763276	-1.247833	-3.625954
30	1	0	1.920095	-1.366139	-5.490250
31	1	0	-0.793831	-1.417659	-5.461190
32	1	0	-2.601554	-1.438271	-3.563475
33	1	0	-4.467099	-1.488332	-1.715402
34	1	0	-4.434523	-1.575342	0.994480
35	1	0	-2.535245	-1.584205	2.803573
36	1	0	-0.692251	-1.442989	4.667111
37	1	0	2.008403	-1.238810	4.643557
38	8	0	0.695323	-3.137054	-0.378032
39	16	0	0.320251	1.024415	-0.146080
40	1	0	1.505414	1.286635	0.443932
41	15	0	0.091241	-6.998127	-2.749662
42	8	0	-0.891222	-8.101227	-2.684783
43	8	0	1.381255	-7.257448	-1.835195

44	8	0	-0.485776	-5.544638	-2.335146	70	17	0	2.116159	-5.269851	-6.606839
45	8	0	0.760465	-6.654343	-4.168860	71	1	0	3.498456	-8.435743	-1.003568
46	6	0	-0.071329	-6.448981	-5.337179	72	6	0	2.903769	-5.662875	-0.925098
47	1	0	-1.109540	-6.266515	-5.035078	73	1	0	2.866473	-6.125519	0.062873
48	6	0	0.002455	-7.743689	-6.144061	74	1	0	2.148688	-4.877444	-0.989915
49	1	0	-0.340150	-8.573483	-5.526708	75	17	0	4.519822	-4.854737	-1.075344
50	1	0	1.016576	-7.927619	-6.497359						
51	17	0	-1.080503	-7.665415	-7.592998	**$^4TS_{\alpha H}$**					
52	6	0	-1.600658	-5.321947	-1.436659	1	26	0	-0.145857	0.950674	-1.356514
53	1	0	-1.641806	-4.236369	-1.344967	2	7	0	-1.561141	2.308778	-1.768964
54	6	0	-1.250810	-5.917507	-0.067041	3	7	0	-1.505585	-0.151461	-0.319078
55	1	0	-1.182755	-7.005614	-0.105900	4	7	0	1.307275	-0.299141	-0.711118
56	1	0	-0.314393	-5.477272	0.272494	5	7	0	1.225123	2.114354	-2.258728
57	17	0	-2.499698	-5.513720	1.183610	6	6	0	-3.511580	1.166994	-0.807616
58	6	0	2.707500	-6.708590	-2.027660	7	6	0	-0.021814	-1.838545	0.654872
59	1	0	2.782028	-6.242938	-3.012438	8	6	0	3.216174	0.753859	-1.834634
60	6	0	3.691140	-7.865189	-1.913899	9	6	0	-0.218750	3.928178	-3.030159
61	1	0	4.713707	-7.490309	-1.908261	10	6	0	-2.908504	2.206457	-1.496662
62	17	0	3.554541	-9.016751	-3.299009	11	6	0	-2.851239	0.085823	-0.229970
63	6	0	-2.912518	-5.854972	-2.001932	12	6	0	-1.267869	-1.260415	0.455996
64	1	0	-2.849421	-6.920591	-2.217197	13	6	0	1.174006	-1.394060	0.096525
65	1	0	-3.724055	-5.648934	-1.305872	14	6	0	2.630915	-0.233197	-1.043014
66	17	0	-3.351642	-5.031232	-3.562005	15	6	0	2.562210	1.841523	-2.393555
67	6	0	0.395530	-5.185723	-6.042156	16	6	0	1.012546	3.285446	-2.926778
68	1	0	-0.219430	-5.008745	-6.924522	17	6	0	-1.411957	3.472139	-2.490474
69	1	0	0.329761	-4.336091	-5.362502	18	6	0	-2.686486	4.129753	-2.646866

19	6	0	-3.613038	3.343194	-2.037148	45	8	0	0.188316	-5.323864	-1.727821
20	6	0	-3.486562	-0.910860	0.599837	46	6	0	1.349615	-5.573298	-2.567385
21	6	0	-2.498653	-1.741598	1.034373	47	1	0	1.337877	-4.898318	-3.431251
22	6	0	2.450740	-2.038310	0.288581	48	6	0	1.248893	-7.020390	-3.047860
23	6	0	3.358512	-1.317594	-0.429968	49	1	0	0.313520	-7.157087	-3.589632
24	6	0	3.208622	2.871222	-3.175967	50	1	0	1.313534	-7.716010	-2.211007
25	6	0	2.244901	3.771642	-3.505767	51	17	0	2.594136	-7.417109	-4.190422
26	1	0	-4.587062	1.221239	-0.672469	52	6	0	-1.318057	-2.182993	-3.348184
27	1	0	-4.543863	-0.941496	0.827130	53	1	0	-0.798521	-0.917959	-2.928601
28	1	0	-2.575701	-2.596448	1.692827	54	6	0	-2.830853	-2.115252	-3.236015
29	1	0	0.024003	-2.720270	1.286085	55	1	0	-3.290031	-3.043732	-3.591870
30	1	0	2.614742	-2.919837	0.894691	56	1	0	-3.121250	-1.950862	-2.198582
31	1	0	4.422709	-1.484051	-0.532431	57	17	0	-3.552809	-0.783133	-4.222523
32	1	0	4.283525	0.671786	-2.015182	58	6	0	-2.928737	-5.955352	-0.867899
33	1	0	4.261457	2.887806	-3.424456	59	1	0	-3.016894	-6.537463	-1.789977
34	1	0	2.339555	4.681567	-4.083256	60	6	0	-4.302698	-5.514640	-0.387488
35	1	0	-0.250489	4.857474	-3.590296	61	1	0	-4.865707	-6.372990	-0.022133
36	1	0	-2.835445	5.065205	-3.169568	62	17	0	-5.280967	-4.759134	-1.704036
37	1	0	-4.680158	3.500222	-1.953967	63	6	0	-0.773577	-2.356372	-4.746511
38	8	0	-0.354777	0.110364	-2.870251	64	1	0	-1.122717	-3.296976	-5.183773
39	16	0	-0.005821	2.224461	0.738344	65	1	0	-1.082087	-1.516093	-5.366074
40	1	0	0.134272	3.455820	0.204576	66	17	0	1.037924	-2.421400	-4.803589
41	15	0	-1.143178	-4.685685	-2.371889	67	6	0	2.588127	-5.217523	-1.763405
42	8	0	-1.614131	-5.298869	-3.635655	68	1	0	3.481785	-5.403040	-2.358809
43	8	0	-2.150844	-4.759640	-1.115737	69	1	0	2.547344	-4.170784	-1.462631
44	8	0	-0.792936	-3.115868	-2.409767	70	17	0	2.756530	-6.191805	-0.241188

71	1	0	-4.202064	-4.769107	0.403347
72	6	0	-2.173829	-6.756981	0.200165
73	1	0	-2.167727	-6.231796	1.156921
74	1	0	-1.146646	-6.925677	-0.120569
75	17	0	-2.931888	-8.376582	0.471103

$^{2}TS_{\alpha H}$

1	26	0	0.464084	-1.651131	-0.234799
2	7	0	0.262953	-1.545856	1.768721
3	7	0	2.429192	-1.999596	-0.015124
4	7	0	0.707589	-1.526036	-2.229384
5	7	0	-1.497260	-1.193591	-0.456139
6	6	0	2.560906	-2.069132	2.438950
7	6	0	3.123806	-1.928269	-2.371498
8	6	0	-1.628142	-1.151852	-2.901074
9	6	0	-2.140215	-1.050817	1.904537
10	6	0	1.230639	-1.785764	2.709629
11	6	0	3.115493	-2.133504	1.167977
12	6	0	3.372927	-2.050807	-1.013169
13	6	0	1.875881	-1.692750	-2.929953
14	6	0	-0.280889	-1.353737	-3.167488
15	6	0	-2.185127	-1.072139	-1.634817
16	6	0	-2.412535	-1.009455	0.546396
17	6	0	-0.896074	-1.306046	2.462326
18	6	0	-0.647507	-1.385571	3.881079
19	6	0	0.670030	-1.686786	4.034612
20	6	0	4.522455	-2.299543	0.906892
21	6	0	4.683356	-2.240004	-0.445903
22	6	0	1.622170	-1.605329	-4.346663
23	6	0	0.283347	-1.400521	-4.492679
24	6	0	-3.580182	-0.809669	-1.368484
25	6	0	-3.720109	-0.766781	-0.016875
26	1	0	3.225947	-2.212562	3.284032
27	1	0	5.280098	-2.414869	1.670911
28	1	0	5.599996	-2.300101	-1.018135
29	1	0	3.966332	-2.020740	-3.048436
30	1	0	2.380893	-1.700288	-5.111937
31	1	0	-0.285746	-1.286872	-5.405855
32	1	0	-2.292538	-1.032010	-3.750275
33	1	0	-4.335639	-0.673610	-2.130865
34	1	0	-4.615295	-0.589961	0.564313
35	1	0	-2.967183	-0.882117	2.586122
36	1	0	-1.398794	-1.233635	4.644514
37	1	0	1.227816	-1.831897	4.950096
38	8	0	-0.059764	-3.296839	-0.284333
39	16	0	0.845848	0.705684	-0.074770
40	1	0	0.641017	1.000027	-1.374947
41	15	0	2.768625	-6.962153	-1.875111
42	8	0	1.944954	-8.179140	-1.730715
43	8	0	4.175092	-7.029395	-1.104737
44	8	0	2.057623	-5.601729	-1.314065
45	8	0	3.213408	-6.507598	-3.345101

46	6	0	2.291244	-6.615629	-4.464062	72	6	0	5.987607	-5.625454	-0.539253
47	1	0	1.296033	-6.889610	-4.097778	73	1	0	6.184104	-6.123099	0.412149
48	6	0	2.834647	-7.738904	-5.343760	74	1	0	5.258014	-4.829770	-0.391488
49	1	0	2.901119	-8.656260	-4.760199	75	17	0	7.529633	-4.837416	-1.066578
50	1	0	3.811245	-7.482141	-5.752980						
51	17	0	1.722571	-8.061552	-6.733459	**$^4IM_\alpha$**					
52	6	0	0.974229	-5.565684	-0.403285	1	26	0	0.489676	-0.985670	-0.970737
53	1	0	0.580085	-4.274140	-0.368743	2	7	0	1.215722	-1.654214	0.779917
54	6	0	1.490109	-5.892993	0.990995	3	7	0	2.311403	-1.179877	-1.810021
55	1	0	1.861182	-6.923545	1.022464	4	7	0	-0.257944	-0.382780	-2.757850
56	1	0	2.299313	-5.208432	1.249237	5	7	0	-1.283493	-0.610642	-0.101575
57	17	0	0.239763	-5.758067	2.284344	6	6	0	3.533432	-2.108639	0.111263
58	6	0	5.473944	-6.615823	-1.588427	7	6	0	1.785899	-0.490324	-4.112771
59	1	0	5.375108	-6.125343	-2.558549	8	6	0	-2.554171	0.143792	-2.067290
60	6	0	6.368070	-7.843835	-1.693603	9	6	0	-0.775335	-1.356850	2.183576
61	1	0	7.396710	-7.540889	-1.888580	10	6	0	2.493300	-2.089428	1.027471
62	17	0	5.878289	-8.946367	-3.037459	11	6	0	3.437739	-1.680086	-1.205908
63	6	0	-0.273873	-6.301751	-0.841395	12	6	0	2.647405	-0.936717	-3.120005
64	1	0	-0.092294	-7.378114	-0.891892	13	6	0	0.435298	-0.233120	-3.934194
65	1	0	-1.086452	-6.076119	-0.153787	14	6	0	-1.537718	0.047554	-3.006056
66	17	0	-0.830347	-5.812411	-2.495173	15	6	0	-2.424120	-0.160140	-0.720202
67	6	0	2.159020	-5.249191	-5.113881	16	6	0	-1.615468	-0.834250	1.211184
68	1	0	1.474838	-5.306167	-5.960183	17	6	0	0.539973	-1.740371	1.970640
69	1	0	1.794387	-4.524005	-4.387208	18	6	0	1.408141	-2.273782	2.992334
70	17	0	3.733598	-4.607885	-5.750655	19	6	0	2.617422	-2.491725	2.408239
71	1	0	6.319463	-8.424831	-0.770992	20	6	0	4.524879	-1.719094	-2.150314

21	6	0	4.036547	-1.255317	-3.336062	47	1	0	3.616507	-4.046303	-4.060653
22	6	0	-0.443713	0.266142	-4.962480	48	6	0	2.721873	-5.713167	-5.072819
23	6	0	-1.665673	0.437907	-4.388221	49	1	0	1.691040	-5.380769	-4.957672
24	6	0	-3.498167	-0.073234	0.237398	50	1	0	2.763140	-6.799347	-5.110616
25	6	0	-2.997329	-0.488945	1.432991	51	17	0	3.309892	-5.084210	-6.670233
26	1	0	4.495015	-2.481655	0.446907	52	6	0	-0.172662	-5.771851	-1.251058
27	1	0	5.524793	-2.060375	-1.917415	53	1	0	-0.278422	-2.737772	-2.288301
28	1	0	4.553258	-1.134856	-4.279303	54	6	0	-0.860258	-5.184003	-0.097161
29	1	0	2.199752	-0.335660	-5.103389	55	1	0	-0.247584	-4.453102	0.422080
30	1	0	-0.144440	0.461001	-5.983703	56	1	0	-1.820145	-4.751776	-0.368557
31	1	0	-2.577734	0.804704	-4.839901	57	17	0	-1.254713	-6.506286	1.178725
32	1	0	-3.521031	0.496760	-2.409494	58	6	0	3.583321	-6.485239	0.392063
33	1	0	-4.501420	0.258067	0.004531	59	1	0	3.258905	-5.441711	0.376166
34	1	0	-3.504242	-0.571111	2.385219	60	6	0	5.077620	-6.582539	0.664115
35	1	0	-1.179569	-1.481046	3.182327	61	1	0	5.281290	-6.402542	1.718563
36	1	0	1.113094	-2.448773	4.018259	62	17	0	6.041421	-5.354997	-0.255817
37	1	0	3.521520	-2.882160	2.855609	63	6	0	-0.844580	-6.210044	-2.464397
38	8	0	0.041871	-2.673621	-1.373098	64	1	0	-0.362206	-7.048257	-2.960824
39	16	0	0.970953	1.208398	-0.432275	65	1	0	-1.902511	-6.390656	-2.289123
40	1	0	2.234802	1.248205	-0.901715	66	17	0	-0.863737	-4.860333	-3.832486
41	15	0	2.306923	-6.617436	-2.009444	67	6	0	5.042254	-5.587791	-3.928683
42	8	0	1.836400	-7.680857	-2.915850	68	1	0	5.538760	-5.242435	-4.835701
43	8	0	3.329984	-7.121889	-0.884043	69	1	0	5.538337	-5.180337	-3.048729
44	8	0	1.176507	-5.916180	-1.055619	70	17	0	5.260805	-7.382577	-3.862980
45	8	0	2.953618	-5.305276	-2.656071	71	1	0	5.450834	-7.564272	0.370022
46	6	0	3.587780	-5.135030	-3.951792	72	6	0	2.762956	-7.270817	1.424659

73	1	0	3.100108	-8.306750	1.486321
74	1	0	1.706420	-7.240053	1.162054
75	17	0	2.911419	-6.546988	3.077732

$^{2}IM_{\alpha}$

1	26	0	0.896214	-1.957240	-1.073579
2	7	0	1.822427	-2.257918	0.680632
3	7	0	2.639769	-1.406641	-1.910972
4	7	0	-0.030877	-1.724602	-2.864986
5	7	0	-0.884028	-2.326676	-0.208200
6	6	0	4.121090	-1.698437	0.028812
7	6	0	1.898280	-1.067666	-4.233084
8	6	0	-2.352998	-2.115259	-2.170592
9	6	0	-0.118184	-2.825192	2.073524
10	6	0	3.161190	-2.109210	0.940006
11	6	0	3.868950	-1.380718	-1.297755
12	6	0	2.860064	-1.101326	-3.233756
13	6	0	0.552562	-1.348200	-4.049767
14	6	0	-1.379058	-1.818261	-3.111215
15	6	0	-2.112105	-2.353936	-0.825116
16	6	0	-1.098635	-2.677542	1.102098
17	6	0	1.237717	-2.625658	1.866562
18	6	0	2.242414	-2.742546	2.895600
19	6	0	3.433164	-2.421309	2.322167
20	6	0	4.885669	-1.016620	-2.251326
21	6	0	4.261593	-0.844734	-3.449784
22	6	0	-0.450218	-1.242888	-5.080263
23	6	0	-1.646176	-1.532240	-4.498543
24	6	0	-3.129868	-2.712310	0.129688
25	6	0	-2.502189	-2.914509	1.322185
26	1	0	5.147373	-1.635000	0.372863
27	1	0	5.938527	-0.927716	-2.020039
28	1	0	4.696227	-0.580425	-4.404636
29	1	0	2.223018	-0.795029	-5.231456
30	1	0	-0.247500	-0.971687	-6.107757
31	1	0	-2.629249	-1.549320	-4.949746
32	1	0	-3.381510	-2.164181	-2.511543
33	1	0	-4.183324	-2.800117	-0.100869
34	1	0	-2.933208	-3.206062	2.270560
35	1	0	-0.437926	-3.114872	3.068506
36	1	0	2.040982	-3.028876	3.919171
37	1	0	4.414652	-2.389518	2.775895
38	8	0	1.175691	-3.699584	-1.463716
39	16	0	0.439798	0.244904	-0.552934
40	1	0	1.534917	0.799774	-1.111543
41	15	0	2.385414	-8.249003	-1.773617
42	8	0	1.775709	-9.000032	-2.885158
43	8	0	2.835477	-9.152407	-0.540033
44	8	0	1.415708	-7.104988	-1.092221
45	8	0	3.697846	-7.382288	-2.051089
46	6	0	3.756045	-6.406518	-3.129795
47	1	0	2.775855	-6.320346	-3.614167

48	6	0	4.762909	-6.975103	-4.127799	74	1	0	1.935699	-7.809082	1.491804
49	1	0	4.440540	-7.965616	-4.447475	75	17	0	3.612434	-7.801117	3.171079
50	1	0	5.759252	-7.026124	-3.689612						
51	17	0	4.863016	-5.937995	-5.606573	**$^4TS_{\alpha\text{-reb}}$**					
52	6	0	0.079423	-6.864563	-1.287199	1	26	0	1.277500	-0.301234	-0.969413
53	1	0	0.744695	-3.913069	-2.309629	2	7	0	2.554842	-0.776422	0.528189
54	6	0	-0.524153	-6.067293	-0.209146	3	7	0	2.768709	0.616206	-1.953770
55	1	0	0.160234	-5.309108	0.166908	4	7	0	0.018853	0.096776	-2.499476
56	1	0	-1.462567	-5.610600	-0.516417	5	7	0	-0.247333	-1.096402	0.086300
57	17	0	-0.951675	-7.134702	1.261530	6	6	0	4.606035	0.244240	-0.361178
58	6	0	3.671230	-8.715686	0.565255	7	6	0	1.568529	1.255686	-4.003543
59	1	0	4.177472	-7.783355	0.304535	8	6	0	-2.060505	-0.794405	-1.547646
60	6	0	4.685622	-9.819429	0.823904	9	6	0	0.970233	-1.812615	2.097021
61	1	0	5.244269	-9.604582	1.734439	10	6	0	3.883344	-0.432333	0.611575
62	17	0	5.885505	-9.978995	-0.514714	11	6	0	4.079729	0.719567	-1.554074
63	6	0	-0.583019	-7.161872	-2.547553	12	6	0	2.700240	1.180475	-3.204514
64	1	0	-0.212946	-8.052843	-3.046853	13	6	0	0.322885	0.749975	-3.664037
65	1	0	-1.665471	-7.155699	-2.445351	14	6	0	-1.323152	-0.179117	-2.548252
66	17	0	-0.252234	-5.788543	-3.855671	15	6	0	-1.550627	-1.218873	-0.327626
67	6	0	4.082359	-5.043865	-2.539781	16	6	0	-0.176286	-1.683563	1.325397
68	1	0	4.179004	-4.309454	-3.339485	17	6	0	2.231968	-1.371264	1.725779
69	1	0	3.297395	-4.726900	-1.851387	18	6	0	3.398517	-1.440699	2.568072
70	17	0	5.652155	-5.038809	-1.629016	19	6	0	4.421269	-0.857300	1.879831
71	1	0	4.178660	-10.781535	0.917246	20	6	0	4.851729	1.389013	-2.570394
72	6	0	2.730206	-8.505028	1.756188	21	6	0	3.997298	1.674964	-3.591357
73	1	0	2.287710	-9.448308	2.080677	22	6	0	-0.856809	0.864095	-4.488965

23	6	0	-1.877031	0.287572	-3.797838	49	1	0	5.230944	-2.934604	-2.041131
24	6	0	-2.326548	-1.886517	0.687320	50	1	0	5.996882	-4.548493	-1.975926
25	6	0	-1.475655	-2.173804	1.711215	51	17	0	7.255506	-2.892707	-0.812606
26	1	0	5.659661	0.419016	-0.172626	52	6	0	1.352766	-3.888296	-3.149324
27	1	0	5.911064	1.596678	-2.498459	53	1	0	2.175621	-2.444908	-1.159997
28	1	0	4.210739	2.165269	-4.531836	54	6	0	-0.079698	-3.626015	-3.289099
29	1	0	1.667845	1.743539	-4.967170	55	1	0	-0.572894	-3.556167	-2.323905
30	1	0	-0.881968	1.332588	-5.463807	56	1	0	-0.271931	-2.745910	-3.893712
31	1	0	-2.914831	0.185236	-4.085967	57	17	0	-0.939849	-5.046946	-4.176914
32	1	0	-3.118132	-0.953067	-1.729377	58	6	0	1.242545	-6.780930	-0.140772
33	1	0	-3.383162	-2.104845	0.607440	59	1	0	0.861173	-5.777578	0.063324
34	1	0	-1.689983	-2.675817	2.645349	60	6	0	1.479550	-7.537972	1.157191
35	1	0	0.869514	-2.282708	3.069344	61	1	0	0.529609	-7.859673	1.581552
36	1	0	3.412259	-1.865695	3.563064	62	17	0	2.282577	-6.519874	2.420568
37	1	0	5.446099	-0.706758	2.192512	63	6	0	2.337274	-3.777734	-4.275699
38	8	0	1.638590	-1.937170	-1.791955	64	1	0	3.354135	-3.652769	-3.907497
39	16	0	0.684272	1.711370	0.092177	65	1	0	2.315805	-4.682920	-4.893472
40	1	0	1.617534	2.496364	-0.483985	66	17	0	1.993344	-2.392070	-5.375199
41	15	0	3.037534	-5.474819	-1.712485	67	6	0	5.356742	-5.023389	0.781159
42	8	0	4.010804	-5.831599	-2.759860	68	1	0	6.223240	-4.598831	1.288106
43	8	0	2.510630	-6.709616	-0.841929	69	1	0	4.581932	-5.266364	1.507203
44	8	0	1.609901	-4.864750	-2.202901	70	17	0	5.899948	-6.586582	0.051919
45	8	0	3.476200	-4.315557	-0.677689	71	1	0	2.125064	-8.399324	0.980598
46	6	0	4.822411	-3.999741	-0.212138	72	6	0	0.277803	-7.525636	-1.073678
47	1	0	4.664488	-3.087217	0.369517	73	1	0	0.613547	-8.548992	-1.249028
48	6	0	5.725435	-3.665517	-1.401319	74	1	0	0.192194	-6.994483	-2.020679

75	17	0	-1.386283	-7.605517	-0.367371

$^{4}Pr_{\alpha}$

1	26	0	1.168006	-0.341782	-1.004511
2	7	0	1.901326	-1.074919	0.716792
3	7	0	3.043401	-0.270884	-1.740786
4	7	0	0.458869	-0.065896	-2.871620
5	7	0	-0.681023	-0.921163	-0.428015
6	6	0	4.308676	-0.825372	0.288712
7	6	0	2.560719	0.439225	-4.042626
8	6	0	-1.947856	-0.341664	-2.450750
9	6	0	-0.198774	-1.606429	1.879558
10	6	0	3.224763	-1.131354	1.097852
11	6	0	4.215414	-0.429116	-1.036476
12	6	0	3.422294	0.145941	-2.997747
13	6	0	1.178967	0.343590	-3.977118
14	6	0	-0.866425	-0.010693	-3.253351
15	6	0	-1.852823	-0.771851	-1.136489
16	6	0	-1.060131	-1.346267	0.825881
17	6	0	1.180729	-1.482371	1.819838
18	6	0	2.066279	-1.790139	2.910252
19	6	0	3.334495	-1.572238	2.462372
20	6	0	5.349268	-0.117152	-1.868943
21	6	0	4.856829	0.239380	-3.086105
22	6	0	0.292466	0.646665	-5.066640
23	6	0	-0.975926	0.427871	-4.617548
24	6	0	-2.984118	-1.125701	-0.317966
25	6	0	-2.492064	-1.482845	0.899493
26	1	0	5.299566	-0.905184	0.724475
27	1	0	6.381230	-0.177405	-1.551384
28	1	0	5.401038	0.533291	-3.973349
29	1	0	2.998407	0.766910	-4.979463
30	1	0	0.612574	0.980873	-6.044463
31	1	0	-1.909176	0.546406	-5.151742
32	1	0	-2.938988	-0.259522	-2.883821
33	1	0	-4.014001	-1.099165	-0.648103
34	1	0	-3.034024	-1.810342	1.776618
35	1	0	-0.634011	-1.937518	2.816411
36	1	0	1.745164	-2.134403	3.884333
37	1	0	4.268064	-1.700330	2.993981
38	8	0	1.599908	-3.370414	-2.790113
39	16	0	0.984059	1.986258	-0.374864
40	1	0	1.678292	1.857178	0.774803
41	15	0	2.898971	-6.088174	-2.620170
42	8	0	3.243066	-6.193376	-4.052307
43	8	0	2.885135	-7.501530	-1.857924
44	8	0	1.392696	-5.583785	-2.268878
45	8	0	3.791222	-5.113475	-1.712070
46	6	0	5.115619	-4.587528	-1.969795
47	1	0	5.159744	-3.704191	-1.323481
48	6	0	5.264350	-4.112251	-3.418676
49	1	0	4.441060	-3.446329	-3.672706

50	1	0	5.309505	-4.937727	-4.123853
51	17	0	6.800906	-3.161789	-3.592640
52	6	0	0.734409	-4.472511	-2.877182
53	1	0	1.260486	-2.654199	-3.351861
54	6	0	-0.495669	-4.184586	-2.005894
55	1	0	-0.159446	-3.985267	-0.989920
56	1	0	-1.031083	-3.320415	-2.395797
57	17	0	-1.672449	-5.556571	-1.936045
58	6	0	2.175151	-7.801512	-0.634282
59	1	0	1.884031	-6.883200	-0.119089
60	6	0	3.089612	-8.641909	0.245321
61	1	0	2.510595	-9.140979	1.021193
62	17	0	4.338011	-7.650044	1.102373
63	6	0	0.414066	-4.850677	-4.335051
64	1	0	1.332940	-5.120859	-4.852264
65	1	0	-0.301267	-5.670539	-4.366791
66	17	0	-0.324136	-3.450692	-5.219940
67	6	0	6.193364	-5.542225	-1.468957
68	1	0	7.156836	-5.032659	-1.464297
69	1	0	5.940888	-5.883876	-0.465937
70	17	0	6.390530	-7.025429	-2.486100
71	1	0	3.622735	-9.376267	-0.359855
72	6	0	0.919901	-8.571794	-1.064763
73	1	0	1.184457	-9.516241	-1.543049
74	1	0	0.335917	-7.957581	-1.747818
75	17	0	-0.150273	-8.950976	0.344913

$^{2}Pr_{\alpha}$

1	26	0	0.654156	-1.128870	-1.184387
2	7	0	1.590321	-1.855936	0.440649
3	7	0	2.427605	-0.673242	-2.002160
4	7	0	-0.209885	-0.775915	-2.954477
5	7	0	-1.054555	-1.926752	-0.498474
6	6	0	3.874482	-1.101522	-0.062833
7	6	0	1.718631	0.016563	-4.247061
8	6	0	-2.526658	-1.347024	-2.374858
9	6	0	-0.324255	-2.734288	1.699237
10	6	0	2.918392	-1.663917	0.767869
11	6	0	3.643315	-0.648902	-1.353495
12	6	0	2.675068	-0.165467	-3.260371
13	6	0	0.370056	-0.264284	-4.096042
14	6	0	-1.555472	-0.859689	-3.235446
15	6	0	-2.287503	-1.851311	-1.106535
16	6	0	-1.288701	-2.501809	0.731659
17	6	0	1.017514	-2.416656	1.565619
18	6	0	2.004723	-2.606676	2.594863
19	6	0	3.183283	-2.137829	2.101410
20	6	0	4.668222	-0.121382	-2.219004
21	6	0	4.067838	0.171941	-3.405829
22	6	0	-0.625543	-0.036398	-5.111772
23	6	0	-1.821576	-0.401135	-4.575789
24	6	0	-3.308711	-2.401218	-0.250043

25	6	0	-2.688012	-2.808267	0.889938	51	17	0	5.772680	-3.672947	-6.037061
26	1	0	4.885924	-1.019767	0.321669	52	6	0	1.740670	-6.125055	-1.070120
27	1	0	5.708000	-0.007455	-1.942215	53	1	0	1.732461	-4.236791	-0.599903
28	1	0	4.511883	0.581159	-4.303566	54	6	0	1.292483	-7.348522	-0.249899
29	1	0	2.046338	0.422366	-5.198524	55	1	0	1.982048	-7.467005	0.585256
30	1	0	-0.418317	0.351515	-6.100238	56	1	0	0.290583	-7.160695	0.134722
31	1	0	-2.801501	-0.376995	-5.033856	57	17	0	1.244143	-8.898498	-1.160803
32	1	0	-3.551767	-1.353921	-2.730919	58	6	0	5.763744	-8.267984	-1.114781
33	1	0	-4.358270	-2.462201	-0.505917	59	1	0	6.366921	-7.388565	-1.350369
34	1	0	-3.121349	-3.270832	1.766837	60	6	0	6.548683	-9.539717	-1.398409
35	1	0	-0.645622	-3.179101	2.635300	61	1	0	7.360556	-9.648366	-0.680061
36	1	0	1.805458	-3.042445	3.564826	62	17	0	7.292408	-9.521832	-3.043685
37	1	0	4.152083	-2.109206	2.582234	63	6	0	0.855807	-5.906106	-2.305431
38	8	0	1.657306	-5.097132	-0.152645	64	1	0	1.043228	-6.657869	-3.068787
39	16	0	0.275027	0.888397	-0.316885	65	1	0	-0.190231	-5.899654	-1.998904
40	1	0	0.686248	1.623156	-1.372783	66	17	0	1.180339	-4.291193	-3.059000
41	15	0	3.883408	-7.036534	-2.638264	67	6	0	5.336578	-3.676412	-2.792046
42	8	0	3.040705	-7.361496	-3.804667	68	1	0	5.222061	-2.748716	-3.351604
43	8	0	4.587916	-8.303476	-1.956817	69	1	0	4.671285	-3.668633	-1.929582
44	8	0	3.150506	-6.235294	-1.427947	70	17	0	7.029870	-3.698021	-2.141707
45	8	0	5.155618	-6.084956	-2.895982	71	1	0	5.889846	-10.408586	-1.352336
46	6	0	5.019169	-4.871815	-3.675172	72	6	0	5.267093	-8.195993	0.334310
47	1	0	3.981446	-4.755593	-4.008549	73	1	0	4.699840	-9.089934	0.599336
48	6	0	5.915271	-5.070089	-4.895452	74	1	0	4.643353	-7.311888	0.460697
49	1	0	5.602110	-5.963550	-5.434441	75	17	0	6.636192	-8.046957	1.508272
50	1	0	6.961983	-5.153227	-4.604168						

$^4TS_{2H}$

1	26	0	0.598764	-0.871784	-0.975881
2	7	0	1.082993	0.777408	0.080154
3	7	0	2.180270	-0.594495	-2.202413
4	7	0	0.104285	-2.517181	-2.039186
5	7	0	-0.985470	-1.146333	0.249880
6	6	0	3.049530	1.467229	-1.210379
7	6	0	1.926549	-2.532854	-3.670301
8	6	0	-1.916920	-3.150998	-0.805541
9	6	0	-0.671807	0.732761	1.783343
10	6	0	2.130425	1.621485	-0.176815
11	6	0	3.074001	0.438391	-2.150272
12	6	0	2.578410	-1.377260	-3.255274
13	6	0	0.765088	-3.059322	-3.105156
14	6	0	-0.978714	-3.325197	-1.819391
15	6	0	-1.916786	-2.144875	0.158209
16	6	0	-1.350861	-0.398491	1.338869
17	6	0	0.458413	1.286065	1.188371
18	6	0	1.124584	2.482656	1.641536
19	6	0	2.163915	2.693529	0.789059
20	6	0	4.063779	0.308074	-3.193735
21	6	0	3.756827	-0.825730	-3.880470
22	6	0	0.086846	-4.242458	-3.575814
23	6	0	-1.004019	-4.406398	-2.775849
24	6	0	-2.896134	-2.024324	1.211325
25	6	0	-2.541160	-0.937295	1.949478
26	1	0	3.831694	2.216324	-1.284623
27	1	0	4.881303	0.996490	-3.359685
28	1	0	4.268009	-1.260448	-4.728745
29	1	0	2.351914	-3.066276	-4.514713
30	1	0	0.411029	-4.851177	-4.409215
31	1	0	-1.761999	-5.177267	-2.816993
32	1	0	-2.718740	-3.880512	-0.750199
33	1	0	-3.730494	-2.696434	1.359000
34	1	0	-3.023356	-0.531535	2.828379
35	1	0	-1.060104	1.228964	2.667090
36	1	0	0.826438	3.067585	2.501052
37	1	0	2.897594	3.488173	0.803343
38	8	0	1.666260	-1.974187	0.172661
39	16	0	-0.656866	0.435777	-2.415285
40	1	0	-1.473505	1.005215	-1.504664
41	15	0	4.399065	-5.465002	0.301949
42	8	0	5.013293	-4.893131	-0.912419
43	8	0	3.172003	-6.450623	0.009166
44	8	0	3.694641	-4.451807	1.355854
45	8	0	5.390082	-6.234269	1.312941
46	6	0	6.630670	-6.916466	1.011548
47	1	0	7.066463	-7.078089	2.003619
48	6	0	7.578399	-6.011893	0.218572
49	1	0	7.621489	-5.025406	0.678699
50	1	0	7.284569	-5.918869	-0.823993
51	17	0	9.256599	-6.695467	0.266250

52	6	0	4.100656	-3.162631	1.687712
53	1	0	1.394476	-1.920595	1.113396
54	6	0	4.017805	-2.850170	3.029461
55	1	0	3.941953	-3.649781	3.752463
56	1	0	4.345131	-1.877103	3.363609
57	17	0	1.658799	-2.274064	3.376543
58	6	0	2.038146	-6.686691	0.880835
59	1	0	2.286757	-6.433366	1.913616
60	6	0	1.681181	-8.160467	0.762726
61	1	0	0.703625	-8.348416	1.203550
62	17	0	2.853424	-9.224673	1.641592
63	6	0	4.217010	-2.252799	0.573428
64	1	0	4.637987	-2.687164	-0.331666
65	1	0	2.930876	-2.023737	0.283615
66	17	0	5.025624	-0.696516	0.937281
67	6	0	6.399575	-8.310246	0.436840
68	1	0	7.332759	-8.872474	0.474644
69	1	0	5.628676	-8.819656	1.014330
70	17	0	5.852559	-8.327083	-1.287988
71	1	0	1.690448	-8.470470	-0.283109
72	6	0	0.922441	-5.763704	0.373341
73	1	0	0.674084	-5.986092	-0.665595
74	1	0	1.226073	-4.720430	0.464167
75	17	0	-0.593264	-5.958012	1.348813

$^{2}TS_{2H}$

1	26	0	0.667741	-1.029378	-0.917793
2	7	0	0.914579	0.740143	0.038062
3	7	0	2.437701	-0.810599	-1.853183
4	7	0	0.412538	-2.782209	-1.869267
5	7	0	-1.101850	-1.243016	0.034677
6	6	0	3.038456	1.406542	-0.992332
7	6	0	2.534490	-2.924414	-3.080720
8	6	0	-1.832211	-3.322627	-1.040660
9	6	0	-1.106597	0.777726	1.419697
10	6	0	1.951543	1.614250	-0.147790
11	6	0	3.265276	0.280820	-1.774100
12	6	0	3.056606	-1.694049	-2.696394
13	6	0	1.286586	-3.415754	-2.711275
14	6	0	-0.706923	-3.569192	-1.820935
15	6	0	-2.002613	-2.256801	-0.163142
16	6	0	-1.666515	-0.415550	0.972348
17	6	0	0.088353	1.324618	0.964404
18	6	0	0.620762	2.601539	1.377158
19	6	0	1.775779	2.784248	0.680713
20	6	0	4.439875	0.077019	-2.590861
21	6	0	4.314744	-1.153856	-3.156778
22	6	0	0.710075	-4.644878	-3.202727
23	6	0	-0.536030	-4.734170	-2.659949
24	6	0	-3.161100	-2.070628	0.678583
25	6	0	-2.948405	-0.930556	1.390987
26	1	0	3.789896	2.188947	-1.027263

27	1	0	5.247066	0.789398	-2.697870		53	1	0	1.139425	-1.656429	1.363582
28	1	0	4.994910	-1.661809	-3.827167		54	6	0	4.318691	-2.915390	3.511203
29	1	0	3.136291	-3.536440	-3.744104		55	1	0	4.791882	-3.734477	4.050004
30	1	0	1.201583	-5.328221	-3.882302		56	1	0	4.729868	-1.950911	3.794294
31	1	0	-1.280284	-5.506833	-2.802872		57	17	0	2.549152	-2.899303	4.141616
32	1	0	-2.642175	-4.042914	-1.101637		58	6	0	1.996832	-6.237594	1.159665
33	1	0	-4.012277	-2.737577	0.712638		59	1	0	2.409609	-6.040301	2.150705
34	1	0	-3.590604	-0.464909	2.126740		60	6	0	1.572391	-7.691715	1.030764
35	1	0	-1.663565	1.342564	2.160767		61	1	0	0.669564	-7.867844	1.613811
36	1	0	0.156936	3.259512	2.100035		62	17	0	2.823028	-8.841641	1.660411
37	1	0	2.458814	3.622563	0.716616		63	6	0	4.198149	-2.096797	1.047694
38	8	0	1.531572	-1.964608	0.531578		64	1	0	4.633992	-2.369633	0.085883
39	16	0	-0.317852	0.108774	-2.668745		65	1	0	3.032356	-1.966219	0.826019
40	1	0	-1.217763	0.819763	-1.957898		66	17	0	4.843388	-0.491139	1.550157
41	15	0	4.392704	-5.230747	0.306567		67	6	0	5.862567	-8.243912	-0.611432
42	8	0	4.819575	-4.427008	-0.854046		68	1	0	6.672399	-8.899332	-0.931880
43	8	0	2.997368	-5.978179	0.134582		69	1	0	5.173549	-8.783987	0.037068
44	8	0	4.165309	-4.436405	1.728444		70	17	0	4.935751	-7.795868	-2.100275
45	8	0	5.436927	-6.313669	0.866826		71	1	0	1.400456	-7.945899	-0.015897
46	6	0	6.449094	-7.054846	0.141115		72	6	0	0.843891	-5.272344	0.867690
47	1	0	7.055979	-7.485814	0.944553		73	1	0	0.371127	-5.505828	-0.086789
48	6	0	7.339657	-6.115200	-0.677209		74	1	0	1.185950	-4.234286	0.850983
49	1	0	7.656333	-5.273089	-0.062988		75	17	0	-0.430029	-5.396262	2.152154
50	1	0	6.842584	-5.749907	-1.572688							
51	17	0	8.839109	-6.992030	-1.190700	**$^4P_{2H}$**						
52	6	0	4.358862	-3.127913	2.061170	1	26	0	0.475713	-0.562218	-1.103584	

2	7	0	0.975170	-0.947213	0.802841	28	1	0	5.053482	0.303211	-3.507487
3	7	0	2.439439	-0.394018	-1.545084	29	1	0	2.806482	0.338824	-4.844378
4	7	0	0.001046	-0.385832	-3.066512	30	1	0	0.605136	0.377753	-6.264157
5	7	0	-1.464313	-0.916355	-0.712128	31	1	0	-2.012764	-0.045640	-5.713710
6	6	0	3.415320	-0.710873	0.682632	32	1	0	-3.358797	-0.630847	-3.518146
7	6	0	2.246904	0.082250	-3.950547	33	1	0	-4.740217	-1.138955	-1.337842
8	6	0	-2.435089	-0.644563	-2.948869	34	1	0	-4.094968	-1.468481	1.273377
9	6	0	-1.286161	-1.267030	1.711268	35	1	0	-1.851424	-1.454137	2.618486
10	6	0	2.227764	-0.936635	1.367859	36	1	0	0.346089	-1.502355	4.036263
11	6	0	3.506321	-0.447138	-0.677066	37	1	0	2.981033	-1.210944	3.463517
12	6	0	2.968644	-0.076195	-2.773701	38	8	0	0.668955	-2.714995	-1.563609
13	6	0	0.871363	-0.055380	-4.080542	39	16	0	0.219755	1.626758	-0.739411
14	6	0	-1.253519	-0.395877	-3.633771	40	1	0	1.350220	1.835144	-0.031647
15	6	0	-2.524438	-0.881937	-1.583046	41	15	0	3.290017	-8.109017	1.059690
16	6	0	-2.002068	-1.150363	0.528552	42	8	0	2.673911	-8.664251	-0.159431
17	6	0	0.094774	-1.172527	1.831866	43	8	0	3.235640	-9.086646	2.327605
18	6	0	0.811021	-1.319039	3.076404	44	8	0	2.570406	-6.779036	1.700472
19	6	0	2.136159	-1.175674	2.787971	45	8	0	4.791855	-7.563309	0.963814
20	6	0	4.735496	-0.171113	-1.378722	46	6	0	5.854171	-7.959844	0.053449
21	6	0	4.402090	0.061205	-2.677981	47	1	0	6.582175	-7.149859	0.166641
22	6	0	0.149317	0.121173	-5.316829	48	6	0	5.368639	-7.966389	-1.398113
23	6	0	-1.166958	-0.092039	-5.040387	49	1	0	4.836604	-7.041641	-1.616004
24	6	0	-3.762262	-1.112576	-0.875535	50	1	0	4.736694	-8.823812	-1.617761
25	6	0	-3.438306	-1.277175	0.434881	51	17	0	6.798732	-8.032915	-2.509705
26	1	0	4.337138	-0.725351	1.254992	52	6	0	1.776716	-5.832847	1.076266
27	1	0	5.716355	-0.158590	-0.921974	53	1	0	0.405634	-2.668665	-2.495768

54	6	0	1.193446	-4.869232	1.988068
55	1	0	1.648754	-3.937106	2.304965
56	1	0	1.624798	-2.896526	-1.570677
57	17	0	-0.317384	-5.239320	2.763685
58	6	0	3.231397	-8.684458	3.719371
59	1	0	3.591472	-7.658787	3.825452
60	6	0	4.125055	-9.647331	4.486695
61	1	0	3.931118	-9.566140	5.555518
62	17	0	5.884199	-9.293394	4.258567
63	6	0	1.695042	-5.727254	-0.371116
64	1	0	1.749709	-6.678135	-0.896174
65	1	0	0.856516	-5.108436	-0.681829
66	17	0	3.212122	-4.763345	-1.087211
67	6	0	6.559676	-9.224759	0.527173
68	1	0	7.479283	-9.355626	-0.043296
69	1	0	6.782908	-9.146223	1.590363
70	17	0	5.588768	-10.735856	0.310924
71	1	0	3.955146	-10.670831	4.149857
72	6	0	1.767938	-8.769875	4.172051
73	1	0	1.404794	-9.798262	4.137447
74	1	0	1.150330	-8.140167	3.533404
75	17	0	1.561622	-8.167882	5.864776

$^{2}P_{2H}$

1	26	0	0.474275	-0.563067	-1.101462
2	7	0	0.974096	-0.948072	0.804792
3	7	0	2.437912	-0.394319	-1.543229
4	7	0	-0.000689	-0.386885	-3.064359
5	7	0	-1.465583	-0.918019	-0.709861
6	6	0	3.414137	-0.710607	0.684403
7	6	0	2.244937	0.081754	-3.948701
8	6	0	-2.436715	-0.646518	-2.946480
9	6	0	-1.287007	-1.268904	1.713462
10	6	0	2.226753	-0.937057	1.369688
11	6	0	3.504898	-0.446771	-0.675290
12	6	0	2.966859	-0.076298	-2.771926
13	6	0	0.869424	-0.056349	-4.078532
14	6	0	-1.255299	-0.397436	-3.631507
15	6	0	-2.525832	-0.883979	-1.580663
16	6	0	-2.003114	-1.152362	0.530853
17	6	0	0.093903	-1.173935	1.833878
18	6	0	0.810357	-1.320414	3.078301
19	6	0	2.135394	-1.176379	2.789762
20	6	0	4.733865	-0.170174	-1.377067
21	6	0	4.400234	0.061862	-2.676322
22	6	0	0.147211	0.119786	-5.314778
23	6	0	-1.168974	-0.093778	-5.038173
24	6	0	-3.763473	-1.115209	-0.873036
25	6	0	-3.439309	-1.279725	0.437341
26	1	0	4.335998	-0.724608	1.256703
27	1	0	5.714755	-0.157105	-0.920403
28	1	0	5.051438	0.304116	-3.505904

29	1	0	2.804332	0.338423	-4.842620
30	1	0	0.602854	0.376370	-6.262189
31	1	0	-2.014859	-0.047732	-5.711419
32	1	0	-3.360482	-0.633151	-3.515671
33	1	0	-4.741465	-1.142001	-1.335240
34	1	0	-4.095803	-1.471352	1.275895
35	1	0	-1.852077	-1.456328	2.620735
36	1	0	0.345610	-1.504128	4.038173
37	1	0	2.980355	-1.211417	3.465210
38	8	0	0.668727	-2.716356	-1.561633
39	16	0	0.217616	1.625762	-0.737158
40	1	0	1.348568	1.834705	-0.030329
41	15	0	3.287654	-8.109797	1.058988
42	8	0	2.671327	-8.664249	-0.160367
43	8	0	3.231533	-9.087469	2.326836
44	8	0	2.569559	-6.778830	1.699444
45	8	0	4.790252	-7.566090	0.963863
46	6	0	5.852308	-7.963515	0.053587
47	1	0	6.581358	-7.154570	0.167491
48	6	0	5.367165	-7.968515	-1.398105
49	1	0	4.836430	-7.042912	-1.615549
50	1	0	4.734116	-8.824947	-1.618444
51	17	0	6.797434	-8.036258	-2.509389
52	6	0	1.775793	-5.832706	1.075185
53	1	0	0.404340	-2.670125	-2.493497
54	6	0	1.192001	-4.869376	1.986884
55	1	0	1.647660	-3.937973	2.305416
56	1	0	1.625007	-2.895577	-1.569997
57	17	0	-0.319026	-5.240022	2.761983
58	6	0	3.227973	-8.685261	3.718606
59	1	0	3.589637	-7.660146	3.824668
60	6	0	4.120134	-9.649508	4.485933
61	1	0	3.926235	-9.568094	5.554747
62	17	0	5.879839	-9.298229	4.257983
63	6	0	1.695000	-5.726560	-0.372247
64	1	0	1.749045	-6.677324	-0.897579
65	1	0	0.857501	-5.106483	-0.683206
66	17	0	3.213513	-4.763986	-1.087132
67	6	0	6.555942	-9.229652	0.526794
68	1	0	7.475541	-9.361449	-0.043480
69	1	0	6.778986	-9.152008	1.590089
70	17	0	5.583075	-10.739332	0.309462
71	1	0	3.948703	-10.672725	4.149010
72	6	0	1.764404	-8.768446	4.171334
73	1	0	1.399717	-9.796289	4.136808
74	1	0	1.147709	-8.137846	3.532691
75	17	0	1.559056	-8.166084	5.864058

$^{4}RC_{\beta}$

1	26	0	0.778537	-0.287494	-0.269846
2	7	0	0.816856	-1.184278	1.537114
3	7	0	2.709921	0.247593	-0.029084

4	7	0	0.668971	0.864811	-1.920871	30	1	0	1.871881	2.725877	-4.420256
5	7	0	-1.214163	-0.592094	-0.357096	31	1	0	-0.776178	2.175923	-4.630493
6	6	0	3.194771	-0.914290	2.072873	32	1	0	-2.486506	0.834639	-3.161072
7	6	0	3.009529	1.571812	-2.069590	33	1	0	-4.250530	-0.502976	-1.752367
8	6	0	-1.706922	0.588905	-2.447047	34	1	0	-4.134660	-1.943163	0.540908
9	6	0	-1.509896	-1.948543	1.661796	35	1	0	-2.222889	-2.522987	2.244259
10	6	0	1.920016	-1.384788	2.338855	36	1	0	-0.383824	-3.047337	4.040748
11	6	0	3.559659	-0.152555	0.966232	37	1	0	2.250373	-2.463893	4.274837
12	6	0	3.473741	0.977188	-0.904136	38	8	0	1.154609	-1.629532	-1.112436
13	6	0	1.703343	1.513826	-2.539674	39	16	0	0.063342	1.651232	1.240651
14	6	0	-0.428157	1.070768	-2.709378	40	1	0	1.209797	1.766776	1.943217
15	6	0	-2.066465	-0.185783	-1.355433	41	15	0	1.461795	-8.326526	-3.007244
16	6	0	-1.974026	-1.344368	0.500007	42	8	0	1.323713	-9.095818	-1.744537
17	6	0	-0.216948	-1.856754	2.149686	43	8	0	1.878055	-6.781451	-2.856561
18	6	0	0.240569	-2.469135	3.372858	44	8	0	0.134179	-8.255512	-3.914166
19	6	0	1.562852	-2.174987	3.491178	45	8	0	2.529652	-8.814686	-4.094169
20	6	0	4.892852	0.340976	0.720686	46	6	0	3.738530	-9.585060	-3.930601
21	6	0	4.838806	1.045360	-0.442761	47	1	0	3.956993	-9.917522	-4.951463
22	6	0	1.246434	2.148096	-3.752885	48	6	0	3.493955	-10.828702	-3.072798
23	6	0	-0.081903	1.872625	-3.858283	49	1	0	2.616074	-11.358431	-3.440831
24	6	0	-3.397171	-0.688566	-1.113922	50	1	0	3.372011	-10.587512	-2.019321
25	6	0	-3.338868	-1.412082	0.035953	51	17	0	4.901793	-11.959331	-3.224375
26	1	0	3.974074	-1.158025	2.787938	52	6	0	-1.078257	-9.014779	-3.715409
27	1	0	5.743955	0.165302	1.365070	53	1	0	-1.634841	-8.862507	-4.642963
28	1	0	5.636492	1.568527	-0.953161	54	6	0	-1.844581	-8.365842	-2.554372
29	1	0	3.728094	2.126032	-2.665158	55	1	0	-1.368814	-8.582517	-1.596715

56	1	0	-1.889527	-7.288811	-2.717408
57	17	0	-3.551435	-8.962729	-2.464500
58	6	0	1.266636	-5.955270	-1.829029
59	1	0	0.298191	-6.370266	-1.534519
60	6	0	1.083130	-4.565195	-2.410788
61	1	0	0.831169	-3.831792	-1.644844
62	17	0	-0.252143	-4.535283	-3.637113
63	6	0	-0.860446	-10.507757	-3.495282
64	1	0	-0.229782	-10.689939	-2.625956
65	1	0	-1.826570	-10.994619	-3.365794
66	17	0	-0.062977	-11.296285	-4.918247
67	6	0	4.922878	-8.711483	-3.529993
68	1	0	5.849610	-9.256287	-3.708729
69	1	0	4.911574	-7.792683	-4.116245
70	17	0	4.949798	-8.224374	-1.785295
71	1	0	1.991210	-4.247584	-2.925057
72	6	0	2.209860	-5.988389	-0.621983
73	1	0	3.145090	-5.468147	-0.832028
74	1	0	2.413107	-7.024974	-0.358389
75	17	0	1.456156	-5.205701	0.823682

$^{2}RC_{\beta}$

1	26	0	0.776734	-0.277536	-0.280945
2	7	0	0.811853	-1.180700	1.530408
3	7	0	2.708067	0.249424	-0.037449
4	7	0	0.669095	0.878604	-1.922724
5	7	0	-1.219490	-0.573164	-0.362722
6	6	0	3.190802	-0.921850	2.061675
7	6	0	3.012695	1.576026	-2.074745
8	6	0	-1.710277	0.617615	-2.446113
9	6	0	-1.515165	-1.943826	1.647789
10	6	0	1.915876	-1.392880	2.326818
11	6	0	3.555987	-0.156293	0.957850
12	6	0	3.475281	0.977019	-0.910870
13	6	0	1.704840	1.527176	-2.540794
14	6	0	-0.430090	1.096131	-2.706555
15	6	0	-2.071537	-0.161998	-1.358410
16	6	0	-1.978686	-1.330932	0.490326
17	6	0	-0.221541	-1.859559	2.135638
18	6	0	0.236554	-2.485644	3.351919
19	6	0	1.559433	-2.194518	3.471700
20	6	0	4.890867	0.333228	0.713656
21	6	0	4.840258	1.039343	-0.448919
22	6	0	1.246925	2.172582	-3.747309
23	6	0	-0.083290	1.904962	-3.850005
24	6	0	-3.402595	-0.665131	-1.119276
25	6	0	-3.343933	-1.395177	0.026432
26	1	0	3.971196	-1.171214	2.773612
27	1	0	5.740988	0.153447	1.358211
28	1	0	5.640162	1.560312	-0.958086
29	1	0	3.732667	2.128567	-2.670128
30	1	0	1.872909	2.752511	-4.412307

31	1	0	-0.778639	2.218068	-4.617321
32	1	0	-2.489311	0.870131	-3.158353
33	1	0	-4.256105	-0.475796	-1.756415
34	1	0	-4.139669	-1.928979	0.528617
35	1	0	-2.229001	-2.522005	2.225530
36	1	0	-0.387681	-3.070170	4.014449
37	1	0	2.247595	-2.492910	4.251234
38	8	0	1.134861	-1.639148	-1.096134
39	16	0	0.063867	1.651018	1.263291
40	1	0	1.215375	1.760584	1.958646
41	15	0	1.464480	-8.332725	-3.002244
42	8	0	1.329134	-9.103480	-1.740132
43	8	0	1.879109	-6.787351	-2.850383
44	8	0	0.135636	-8.262619	-3.907416
45	8	0	2.531419	-8.818415	-4.091238
46	6	0	3.740153	-9.589596	-3.930605
47	1	0	3.956432	-9.921583	-4.952092
48	6	0	3.497004	-10.833682	-3.073013
49	1	0	2.618175	-11.362955	-3.439422
50	1	0	3.377472	-10.593135	-2.019121
51	17	0	4.904190	-11.964655	-3.228394
52	6	0	-1.076587	-9.021541	-3.706457
53	1	0	-1.634740	-8.869277	-4.633070
54	6	0	-1.840865	-8.372378	-2.544199
55	1	0	-1.363640	-8.589255	-1.587307
56	1	0	-1.885690	-7.295320	-2.707115
57	17	0	-3.547722	-8.968854	-2.451625
58	6	0	1.270343	-5.963836	-1.819057
59	1	0	0.304296	-6.381568	-1.520551
60	6	0	1.080800	-4.573371	-2.397997
61	1	0	0.829905	-3.841516	-1.630143
62	17	0	-0.259633	-4.545515	-3.618851
63	6	0	-0.858624	-10.514527	-3.486535
64	1	0	-0.226605	-10.696685	-2.618196
65	1	0	-1.824584	-11.001316	-3.355573
66	17	0	-0.063332	-11.303231	-4.910662
67	6	0	4.925689	-8.716743	-3.531966
68	1	0	5.851828	-9.261954	-3.712523
69	1	0	4.913755	-7.797783	-4.117954
70	17	0	4.955989	-8.230028	-1.787214
71	1	0	1.985868	-4.252822	-2.915767
72	6	0	2.219224	-5.996594	-0.616498
73	1	0	3.152734	-5.474922	-0.830632
74	1	0	2.425176	-7.033115	-0.354762
75	17	0	1.471487	-5.216095	0.833371

$^{4}TS_{\beta H}$

1	26	0	1.183496	-0.660312	-0.743375
2	7	0	2.273784	-1.746872	0.605872
3	7	0	2.872959	0.021447	-1.562183
4	7	0	0.109675	0.477666	-1.988098
5	7	0	-0.496175	-1.199631	0.254510

6	6	0	4.511698	-1.273879	-0.265113	32	1	0	-3.197043	0.120541	-1.319844
7	6	0	1.922584	1.510063	-3.262003	33	1	0	-3.795143	-1.414261	0.720145
8	6	0	-2.136742	-0.051281	-1.163817	34	1	0	-2.338554	-2.848905	2.500637
9	6	0	0.466575	-2.632252	2.003563	35	1	0	0.231442	-3.266472	2.852356
10	6	0	3.636327	-1.892626	0.619407	36	1	0	2.797563	-3.764795	3.221168
11	6	0	4.155015	-0.373679	-1.258777	37	1	0	5.061529	-3.028542	1.927432
12	6	0	2.986362	0.908015	-2.604297	38	8	0	1.047799	-1.989274	-1.859924
13	6	0	0.579107	1.294860	-2.978082	39	16	0	1.554397	1.115420	0.845464
14	6	0	-1.258019	0.576657	-2.033318	40	1	0	0.781872	0.642056	1.844816
15	6	0	-1.778845	-0.874957	-0.098812	41	15	0	0.484069	-7.890460	-2.013084
16	6	0	-0.602075	-2.037227	1.337112	42	8	0	-0.417483	-8.970547	-1.551688
17	6	0	1.804250	-2.491686	1.663467	43	8	0	0.138805	-6.454613	-1.397083
18	6	0	2.902198	-3.124807	2.355262	44	8	0	0.508340	-7.604157	-3.600599
19	6	0	4.038578	-2.756780	1.703820	45	8	0	2.056997	-8.125367	-1.755757
20	6	0	5.096725	0.292038	-2.125272	46	6	0	2.725853	-8.858658	-0.712717
21	6	0	4.373401	1.092180	-2.954073	47	1	0	3.721667	-9.039618	-1.133159
22	6	0	-0.518857	1.917949	-3.682109	48	6	0	2.069986	-10.219607	-0.462281
23	6	0	-1.660426	1.468339	-3.097719	49	1	0	1.930073	-10.740698	-1.407903
24	6	0	-2.719903	-1.512440	0.787261	50	1	0	1.119328	-10.135670	0.058386
25	6	0	-1.987754	-2.233993	1.682521	51	17	0	3.169022	-11.250038	0.548927
26	1	0	5.569102	-1.488435	-0.148903	52	6	0	-0.061676	-8.480139	-4.601406
27	1	0	6.168984	0.153505	-2.088444	53	1	0	0.260189	-8.038487	-5.547195
28	1	0	4.728077	1.744362	-3.740919	54	6	0	-1.591602	-8.402093	-4.499362
29	1	0	2.159504	2.189941	-4.074007	55	1	0	-1.961743	-8.939714	-3.626557
30	1	0	-0.409169	2.606996	-4.508837	56	1	0	-1.896436	-7.358186	-4.442415
31	1	0	-2.685684	1.711985	-3.342356	57	17	0	-2.378731	-9.113108	-5.969009

58	6	0	0.334144	-5.140621	-1.992328
59	1	0	0.558198	-5.250209	-3.055326
60	6	0	1.461659	-4.424254	-1.276681
61	1	0	1.320564	-3.040725	-1.545580
62	17	0	3.086972	-4.847028	-1.835186
63	6	0	0.440876	-9.916809	-4.515462
64	1	0	0.227902	-10.344510	-3.536029
65	1	0	-0.043847	-10.511844	-5.289013
66	17	0	2.224207	-10.043504	-4.796340
67	6	0	2.963460	-7.997051	0.523712
68	1	0	3.675640	-8.495621	1.181009
69	1	0	3.350070	-7.025344	0.217602
70	17	0	1.478231	-7.684676	1.515252
71	1	0	1.410812	-4.487965	-0.191186
72	6	0	-0.966126	-4.362916	-1.804236
73	1	0	-0.835398	-3.340704	-2.155278
74	1	0	-1.268219	-4.362516	-0.756291
75	17	0	-2.342580	-5.080058	-2.739510

$^{2}TS_{\beta H}$

1	26	0	1.232851	-0.718795	-0.704511
2	7	0	2.380834	-1.691312	0.630384
3	7	0	2.886270	0.078732	-1.560377
4	7	0	0.089355	0.393068	-1.958475
5	7	0	-0.404663	-1.342403	0.274760
6	6	0	4.593031	-1.091530	-0.248906
7	6	0	1.839705	1.434351	-3.315381
8	6	0	-2.114214	-0.262834	-1.121265
9	6	0	0.640190	-2.647456	2.066271
10	6	0	3.750470	-1.753182	0.641461
11	6	0	4.191756	-0.233367	-1.261247
12	6	0	2.939932	0.922271	-2.647106
13	6	0	0.509451	1.186063	-2.989402
14	6	0	-1.280487	0.416954	-1.998435
15	6	0	-1.704358	-1.073121	-0.064172
16	6	0	-0.464523	-2.143407	1.385968
17	6	0	1.965624	-2.438822	1.707825
18	6	0	3.100662	-2.990177	2.406170
19	6	0	4.210158	-2.568348	1.739850
20	6	0	5.088333	0.454362	-2.160139
21	6	0	4.312936	1.170461	-3.017037
22	6	0	-0.623820	1.732517	-3.700608
23	6	0	-1.737525	1.254832	-3.083745
24	6	0	-2.607918	-1.732411	0.846248
25	6	0	-1.835811	-2.396557	1.751650
26	1	0	5.660301	-1.245731	-0.124873
27	1	0	6.167252	0.381356	-2.128204
28	1	0	4.623520	1.807410	-3.834466
29	1	0	2.031206	2.080941	-4.165815
30	1	0	-0.556207	2.393589	-4.554247
31	1	0	-2.775520	1.441032	-3.325110
32	1	0	-3.183977	-0.148333	-1.265929

33	1	0	-3.687048	-1.679989	0.791006
34	1	0	-2.150118	-3.001551	2.591589
35	1	0	0.450063	-3.264598	2.938706
36	1	0	3.038667	-3.615688	3.286611
37	1	0	5.248813	-2.773723	1.962136
38	8	0	1.208545	-1.996119	-1.899127
39	16	0	1.405003	1.373762	0.579157
40	1	0	2.457104	1.031628	1.352457
41	15	0	0.366606	-7.859544	-2.025384
42	8	0	-0.618256	-8.883950	-1.609773
43	8	0	0.063860	-6.400297	-1.442260
44	8	0	0.499778	-7.591373	-3.610410
45	8	0	1.905202	-8.178638	-1.669645
46	6	0	2.465518	-8.933261	-0.578113
47	1	0	3.470012	-9.184117	-0.937601
48	6	0	1.711891	-10.245515	-0.343183
49	1	0	1.593878	-10.777769	-1.285483
50	1	0	0.739999	-10.092021	0.118950
51	17	0	2.684276	-11.319340	0.749296
52	6	0	-0.043458	-8.454696	-4.637002
53	1	0	0.349573	-8.033726	-5.565161
54	6	0	-1.572788	-8.319212	-4.626142
55	1	0	-2.014123	-8.834503	-3.773258
56	1	0	-1.840657	-7.264248	-4.594241
57	17	0	-2.297399	-9.013937	-6.135278
58	6	0	0.353296	-5.103850	-2.035477
59	1	0	0.654925	-5.235238	-3.076648
60	6	0	1.448561	-4.421557	-1.240326
61	1	0	1.399320	-3.053199	-1.551549
62	17	0	3.093253	-4.937187	-1.637563
63	6	0	0.399232	-9.907977	-4.511825
64	1	0	0.110608	-10.320004	-3.544987
65	1	0	-0.059640	-10.491069	-5.309866
66	17	0	2.190046	-10.102878	-4.682702
67	6	0	2.687113	-8.064019	0.655809
68	1	0	3.329157	-8.592124	1.360500
69	1	0	3.149072	-7.123871	0.355869
70	17	0	1.171135	-7.641965	1.556203
71	1	0	1.297523	-4.445633	-0.162317
72	6	0	-0.923270	-4.270575	-1.953714
73	1	0	-0.719916	-3.257489	-2.296852
74	1	0	-1.305529	-4.251273	-0.932452
75	17	0	-2.252805	-4.934420	-2.990326

$^4IM_\beta$

1	26	0	0.478311	-1.334267	-0.161858
2	7	0	-0.164455	-1.957984	1.637460
3	7	0	2.261362	-0.813313	0.663562
4	7	0	1.059307	-0.518975	-1.906258
5	7	0	-1.249568	-1.916356	-0.990408
6	6	0	1.856831	-1.533288	2.975261
7	6	0	3.290156	0.298563	-1.268398

8	6	0	-0.881760	-1.123997	-3.284908	34	1	0	-4.308353	-3.244663	-1.053352
9	6	0	-2.385730	-2.792288	1.000566	35	1	0	-3.291493	-3.262223	1.367585
10	6	0	0.553048	-1.976018	2.810614	36	1	0	-2.295818	-3.355973	3.787948
11	6	0	2.640639	-0.981036	1.972803	37	1	0	0.086440	-2.671833	4.886388
12	6	0	3.286664	-0.136569	0.047900	38	8	0	1.173823	-2.956823	-0.576921
13	6	0	2.251037	0.112949	-2.168569	39	16	0	-0.344804	0.779250	0.278685
14	6	0	0.360529	-0.538501	-3.087329	40	1	0	-0.790464	0.546918	1.530274
15	6	0	-1.621379	-1.762142	-2.302602	41	15	0	1.542797	-7.105748	-2.927732
16	6	0	-2.309821	-2.510782	-0.354488	42	8	0	2.392385	-7.680271	-1.852384
17	6	0	-1.379133	-2.534085	1.918895	43	8	0	2.166417	-5.925014	-3.819489
18	6	0	-1.443924	-2.887200	3.313989	44	8	0	0.154234	-6.464483	-2.431649
19	6	0	-0.246907	-2.545554	3.864920	45	8	0	1.051650	-8.105855	-4.079872
20	6	0	3.960544	-0.438752	2.175417	46	6	0	1.768558	-9.194007	-4.700909
21	6	0	4.359100	0.086902	0.984294	47	1	0	1.010518	-9.640909	-5.353158
22	6	0	2.292022	0.523425	-3.548922	48	6	0	2.168024	-10.235635	-3.653652
23	6	0	1.122595	0.118243	-4.118132	49	1	0	1.299902	-10.490785	-3.046730
24	6	0	-2.937885	-2.314204	-2.508049	50	1	0	2.980583	-9.888436	-3.018675
25	6	0	-3.365599	-2.775343	-1.301400	51	17	0	2.708435	-11.759844	-4.469613
26	1	0	2.289184	-1.607432	3.967291	52	6	0	-0.511768	-6.805216	-1.187908
27	1	0	4.492059	-0.454445	3.117620	53	1	0	-1.483733	-6.314746	-1.274113
28	1	0	5.286435	0.590461	0.745671	54	6	0	0.274402	-6.173793	-0.030036
29	1	0	4.172522	0.820446	-1.622599	55	1	0	1.226735	-6.681408	0.120569
30	1	0	3.120699	1.045742	-4.008428	56	1	0	0.435167	-5.109732	-0.219251
31	1	0	0.794190	0.235337	-5.141998	57	17	0	-0.655637	-6.300570	1.524440
32	1	0	-1.308590	-1.070121	-4.280271	58	6	0	2.597338	-4.657988	-3.251084
33	1	0	-3.455807	-2.326544	-3.457778	59	1	0	1.864326	-4.334726	-2.496068

60	6	0	2.677821	-3.674034	-4.368220
61	1	0	2.125782	-2.935241	-0.381567
62	17	0	1.354815	-3.495303	-5.451595
63	6	0	-0.711224	-8.304863	-0.999880
64	1	0	0.241871	-8.833463	-1.032561
65	1	0	-1.191316	-8.484951	-0.039061
66	17	0	-1.786827	-9.027007	-2.264299
67	6	0	2.875627	-8.718277	-5.639432
68	1	0	3.129767	-9.524704	-6.326731
69	1	0	2.529963	-7.847392	-6.196189
70	17	0	4.425707	-8.247475	-4.827697
71	1	0	3.378818	-2.850348	-4.344861
72	6	0	3.966601	-4.888109	-2.592798
73	1	0	4.721756	-5.124663	-3.342307
74	1	0	3.898589	-5.699106	-1.869188
75	17	0	4.528438	-3.412258	-1.701184

$^{2}IM_{\beta}$

1	26	0	1.928283	-0.301128	0.257634
2	7	0	0.236882	-1.235538	0.786930
3	7	0	2.542164	-0.261712	2.189798
4	7	0	3.583931	0.760846	-0.236873
5	7	0	1.282366	-0.253088	-1.650444
6	6	0	0.703210	-1.546003	3.175734
7	6	0	4.630685	0.998887	1.964163
8	6	0	3.198052	0.898535	-2.655792
9	6	0	-0.884785	-1.348434	-1.386214
10	6	0	-0.081094	-1.698544	2.039455
11	6	0	1.908302	-0.855574	3.250691
12	6	0	3.677989	0.320695	2.710059
13	6	0	4.590560	1.193050	0.582731
14	6	0	3.946777	1.130702	-1.503998
15	6	0	1.961539	0.266053	-2.719201
16	6	0	0.108331	-0.734173	-2.148631
17	6	0	-0.817427	-1.587703	-0.021596
18	6	0	-1.828658	-2.278170	0.743292
19	6	0	-1.367968	-2.354819	2.020049
20	6	0	2.655102	-0.640846	4.468176
21	6	0	3.749299	0.094799	4.133784
22	6	0	5.614918	1.860561	-0.182179
23	6	0	5.215068	1.818287	-1.483961
24	6	0	1.193423	0.100121	-3.932379
25	6	0	0.034592	-0.519912	-3.575787
26	1	0	0.321375	-1.972141	4.098299
27	1	0	2.362253	-1.007120	5.443105
28	1	0	4.542071	0.453991	4.776350
29	1	0	5.488530	1.397526	2.496785
30	1	0	6.515524	2.292587	0.233261
31	1	0	5.719141	2.211068	-2.356885
32	1	0	3.614834	1.257171	-3.591908
33	1	0	1.508625	0.434294	-4.911844
34	1	0	-0.801934	-0.802458	-4.201183

35	1	0	-1.775937	-1.685009	-1.906745
36	1	0	-2.758026	-2.655368	0.338004
37	1	0	-1.842552	-2.804732	2.881843
38	8	0	2.793471	-1.865002	-0.071688
39	16	0	0.727467	1.709507	0.836560
40	1	0	1.771786	2.441272	1.277189
41	15	0	2.963224	-5.801021	-4.442005
42	8	0	4.356925	-6.063833	-4.883057
43	8	0	2.760190	-4.796668	-3.210647
44	8	0	2.147684	-7.110934	-3.967946
45	8	0	1.936483	-5.184976	-5.509575
46	6	0	2.190304	-4.318073	-6.632814
47	1	0	1.240752	-4.344226	-7.179013
48	6	0	3.273025	-4.904721	-7.541355
49	1	0	3.034782	-5.943820	-7.765736
50	1	0	4.263892	-4.832777	-7.098254
51	17	0	3.300805	-4.015109	-9.120100
52	6	0	2.533043	-8.477970	-4.231843
53	1	0	1.647659	-9.056157	-3.957284
54	6	0	3.683232	-8.831743	-3.277952
55	1	0	4.613375	-8.353086	-3.585887
56	1	0	3.416882	-8.519636	-2.268097
57	17	0	3.973351	-10.618508	-3.220681
58	6	0	3.612300	-4.925196	-2.001206
59	1	0	4.187870	-5.852865	-2.075395
60	6	0	2.749831	-4.919987	-0.799024
61	1	0	3.626311	-1.867653	0.424229
62	17	0	1.985785	-6.379922	-0.290342
63	6	0	2.893314	-8.765284	-5.685341
64	1	0	3.709644	-8.126226	-6.020818
65	1	0	3.179240	-9.812240	-5.781881
66	17	0	1.495396	-8.499863	-6.805900
67	6	0	2.373462	-2.859742	-6.220836
68	1	0	2.215521	-2.223337	-7.091475
69	1	0	1.661677	-2.603285	-5.436012
70	17	0	4.020343	-2.440921	-5.590231
71	1	0	2.435690	-3.999367	-0.315479
72	6	0	4.553004	-3.721774	-2.044603
73	1	0	4.000235	-2.796759	-1.878587
74	1	0	5.093132	-3.703932	-2.989169
75	17	0	5.787852	-3.842751	-0.718906

$^{4}TS_{\beta\text{-reb}}$

1	26	0	0.823664	-0.421283	0.511749
2	7	0	0.134419	-0.056611	2.373625
3	7	0	2.709356	-0.285828	1.184474
4	7	0	1.512257	-0.905132	-1.332232
5	7	0	-1.068656	-0.436671	-0.191590
6	6	0	2.270168	0.204876	3.554406
7	6	0	3.921895	-0.837107	-0.886282
8	6	0	-0.623941	-1.035225	-2.533990
9	6	0	-2.276420	0.017105	1.898018

10	6	0	0.884720	0.194644	3.497105	36	1	0	-2.182085	0.597551	4.683946
11	6	0	3.110243	-0.024097	2.473621	37	1	0	0.360780	0.705720	5.614101
12	6	0	3.858747	-0.497706	0.457624	38	8	0	0.727445	-2.263242	0.862999
13	6	0	2.822155	-1.022310	-1.712949	39	16	0	0.793956	1.866834	-0.044595
14	6	0	0.759143	-1.115707	-2.457758	40	1	0	2.077497	2.136664	0.270077
15	6	0	-1.463993	-0.717239	-1.475419	41	15	0	1.215836	-6.451418	-2.218424
16	6	0	-2.214629	-0.239519	0.534539	42	8	0	1.699818	-7.776500	-1.758863
17	6	0	-1.180527	0.106315	2.741958	43	8	0	1.600046	-5.175528	-1.320118
18	6	0	-1.259326	0.428048	4.145132	44	8	0	-0.388450	-6.318757	-2.333601
19	6	0	0.017974	0.482551	4.612531	45	8	0	1.669618	-5.941620	-3.666352
20	6	0	4.547852	-0.045369	2.554081	46	6	0	2.929289	-6.135511	-4.345887
21	6	0	5.010848	-0.338379	1.307040	47	1	0	2.728269	-5.733789	-5.344849
22	6	0	2.900782	-1.338682	-3.119519	48	6	0	3.235253	-7.627761	-4.486420
23	6	0	1.620540	-1.399701	-3.580448	49	1	0	2.361402	-8.139477	-4.888647
24	6	0	-2.902206	-0.669443	-1.566149	50	1	0	3.530510	-8.076406	-3.540079
25	6	0	-3.367268	-0.372443	-0.321051	51	17	0	4.585814	-7.872492	-5.667172
26	1	0	2.732376	0.408730	4.514211	52	6	0	-1.303778	-7.438565	-2.421147
27	1	0	5.114044	0.131583	3.458816	53	1	0	-2.256849	-6.974222	-2.684492
28	1	0	6.035385	-0.450750	0.978041	54	6	0	-1.416959	-8.069550	-1.025728
29	1	0	4.906767	-0.964399	-1.322962	55	1	0	-0.520578	-8.635498	-0.772022
30	1	0	3.824242	-1.467529	-3.669122	56	1	0	-1.582869	-7.285605	-0.286881
31	1	0	1.272577	-1.600200	-4.585116	57	17	0	-2.832221	-9.194528	-0.926831
32	1	0	-1.084868	-1.230699	-3.496352	58	6	0	1.389408	-5.196568	0.120265
33	1	0	-3.466594	-0.849967	-2.471427	59	1	0	1.327615	-6.233493	0.473274
34	1	0	-4.392047	-0.259184	0.006836	60	6	0	0.108657	-4.461311	0.396451
35	1	0	-3.258116	0.163074	2.335790	61	1	0	0.607193	-2.358724	1.822253

62	17	0	-0.930274	-5.035086	1.657612
63	6	0	-0.932451	-8.467241	-3.482940
64	1	0	0.063913	-8.871915	-3.305353
65	1	0	-1.663451	-9.275134	-3.467089
66	17	0	-0.955262	-7.772136	-5.153643
67	6	0	4.044953	-5.262906	-3.776687
68	1	0	4.839918	-5.174145	-4.516901
69	1	0	3.646260	-4.277446	-3.533172
70	17	0	4.830587	-5.907368	-2.276586
71	1	0	-0.399904	-3.960087	-0.412349
72	6	0	2.662819	-4.563114	0.696137
73	1	0	2.711401	-3.510390	0.429196
74	1	0	3.532328	-5.112180	0.337361
75	17	0	2.666793	-4.660149	2.501706

$^4Pr_\beta$

1	26	0	0.629715	-0.387325	0.154568
2	7	0	0.400916	-0.769095	2.124215
3	7	0	2.392027	-1.358968	0.196667
4	7	0	0.665609	-0.473645	-1.867051
5	7	0	-1.285535	0.211026	0.070198
6	6	0	2.589770	-1.764671	2.614699
7	6	0	2.938371	-1.340341	-2.201459
8	6	0	-1.532265	0.503066	-2.356892
9	6	0	-1.832762	0.189362	2.465554
10	6	0	1.343388	-1.284595	2.983668
11	6	0	3.070781	-1.798764	1.313646
12	6	0	3.232333	-1.599193	-0.870015
13	6	0	1.738326	-0.818941	-2.659209
14	6	0	-0.293374	0.006006	-2.729235
15	6	0	-1.987318	0.593513	-1.050234
16	6	0	-2.120005	0.460104	1.136383
17	6	0	-0.658425	-0.391855	2.916898
18	6	0	-0.381312	-0.688849	4.299487
19	6	0	0.860141	-1.244833	4.340733
20	6	0	4.357692	-2.321452	0.940397
21	6	0	4.458872	-2.196105	-0.414024
22	6	0	1.438207	-0.568365	-4.046047
23	6	0	0.177005	-0.058505	-4.089326
24	6	0	-3.283849	1.097586	-0.680067
25	6	0	-3.365409	1.016692	0.676920
26	1	0	3.235708	-2.144917	3.398913
27	1	0	5.079598	-2.731733	1.634125
28	1	0	5.277212	-2.489098	-1.057810
29	1	0	3.700968	-1.572223	-2.937467
30	1	0	2.116052	-0.761326	-4.866992
31	1	0	-0.395430	0.253023	-4.952888
32	1	0	-2.194218	0.846859	-3.144490
33	1	0	-4.025826	1.458125	-1.380068
34	1	0	-4.188343	1.296663	1.321084
35	1	0	-2.587244	0.439541	3.203843
36	1	0	-1.059806	-0.490994	5.118675

37	1	0	1.413229	-1.598280	5.200839	63	6	0	-0.273797	-9.887790	-3.633491
38	8	0	-0.473077	-3.188123	-0.147960	64	1	0	0.554971	-9.992738	-2.933932
39	16	0	1.490181	1.871573	0.379654	65	1	0	-0.948710	-10.737977	-3.539730
40	1	0	2.720423	1.497829	0.789084	66	17	0	0.415870	-9.947606	-5.306704
41	15	0	1.170110	-7.136303	-2.817452	67	6	0	4.333709	-6.000553	-3.887829
42	8	0	1.581046	-8.122465	-1.786841	68	1	0	5.331557	-6.092122	-4.316336
43	8	0	1.057834	-5.605326	-2.320152	69	1	0	3.860308	-5.082265	-4.235120
44	8	0	-0.268949	-7.391805	-3.484128	70	17	0	4.561929	-5.831150	-2.098814
45	8	0	2.079341	-6.955225	-4.118556	71	1	0	0.345270	-3.322183	-1.955721
46	6	0	3.490274	-7.197706	-4.312798	72	6	0	1.487412	-5.303121	0.034924
47	1	0	3.581777	-7.245352	-5.403399	73	1	0	2.094023	-4.398363	0.037847
48	6	0	3.905992	-8.556057	-3.743894	74	1	0	2.110807	-6.187074	-0.085330
49	1	0	3.226501	-9.326625	-4.106135	75	17	0	0.708510	-5.445691	1.672420
50	1	0	3.929386	-8.558986	-2.656511						
51	17	0	5.562069	-8.984453	-4.337710	**$^2Pr_\beta$**					
52	6	0	-1.054331	-8.603291	-3.378343	1	26	0	0.454184	-1.195545	-0.526043
53	1	0	-1.818633	-8.483133	-4.149253	2	7	0	0.312087	-2.126286	1.251762
54	6	0	-1.722337	-8.598116	-1.996604	3	7	0	2.448634	-1.144915	-0.296256
55	1	0	-0.997694	-8.803487	-1.207266	4	7	0	0.623887	-0.517380	-2.413699
56	1	0	-2.191772	-7.627696	-1.833810	5	7	0	-1.521425	-1.438845	-0.839625
57	17	0	-3.027903	-9.844974	-1.883141	6	6	0	2.667883	-2.123074	1.941851
58	6	0	0.417191	-5.298329	-1.063580	7	6	0	3.046165	-0.107834	-2.441078
59	1	0	-0.338123	-6.052214	-0.822897	8	6	0	-1.730870	-0.516239	-3.101414
60	6	0	-0.257060	-3.928541	-1.280996	9	6	0	-2.130378	-2.400273	1.337320
61	1	0	-0.851142	-3.728507	0.562374	10	6	0	1.321414	-2.386662	2.154155
62	17	0	-1.839683	-4.225693	-2.210346	11	6	0	3.186774	-1.537984	0.795295

12	6	0	3.350958	-0.614044	-1.185326	38	8	0	0.732797	-3.339729	-1.524373
13	6	0	1.779348	-0.063142	-3.005436	39	16	0	0.156004	0.846787	0.320183
14	6	0	-0.384352	-0.257102	-3.313934	40	1	0	1.024350	0.748542	1.349288
15	6	0	-2.255655	-1.061586	-1.938534	41	15	0	0.778642	-8.292266	-0.402026
16	6	0	-2.433871	-1.905534	0.075924	42	8	0	1.621565	-8.949125	0.619155
17	6	0	-0.855213	-2.498060	1.879610	43	8	0	0.709335	-6.696601	-0.252568
18	6	0	-0.571038	-3.022625	3.192162	44	8	0	-0.769859	-8.781459	-0.409079
19	6	0	0.778824	-2.955554	3.361539	45	8	0	1.185533	-8.448906	-1.944131
20	6	0	4.585056	-1.250628	0.587156	46	6	0	1.566705	-9.737387	-2.497514
21	6	0	4.686624	-0.675249	-0.641045	47	1	0	1.082544	-10.543260	-1.933406
22	6	0	1.494501	0.469659	-4.315471	48	6	0	3.083933	-9.847514	-2.355221
23	6	0	0.152536	0.347973	-4.507401	49	1	0	3.359508	-9.739452	-1.306679
24	6	0	-3.659802	-1.305023	-1.714077	50	1	0	3.587522	-9.094109	-2.960314
25	6	0	-3.771014	-1.828276	-0.463604	51	17	0	3.659676	-11.472649	-2.901483
26	1	0	3.362631	-2.381754	2.734212	52	6	0	-1.401946	-9.502509	0.679005
27	1	0	5.371381	-1.471473	1.296747	53	1	0	-2.449607	-9.560087	0.375074
28	1	0	5.574705	-0.325402	-1.150653	54	6	0	-1.298563	-8.682857	1.973458
29	1	0	3.868083	0.282072	-3.032871	55	1	0	-0.290768	-8.713138	2.388199
30	1	0	2.236818	0.881255	-4.986629	56	1	0	-1.583084	-7.649185	1.775642
31	1	0	-0.435240	0.639610	-5.367780	57	17	0	-2.433652	-9.312887	3.232630
32	1	0	-2.424649	-0.258706	-3.894990	58	6	0	0.379197	-5.761180	-1.305471
33	1	0	-4.442972	-1.097606	-2.431178	59	1	0	0.656674	-6.184849	-2.272733
34	1	0	-4.665329	-2.138451	0.060846	60	6	0	1.228595	-4.514207	-0.989818
35	1	0	-2.959403	-2.731812	1.954723	61	1	0	0.594251	-3.387204	-2.482730
36	1	0	-1.318846	-3.386337	3.884808	62	17	0	2.953593	-4.832109	-1.527145
37	1	0	1.366447	-3.254364	4.219589	63	6	0	-0.841153	-10.910524	0.842452

64	1	0	0.232132	-10.884098	1.027413
65	1	0	-1.352674	-11.416204	1.660923
66	17	0	-1.112329	-11.912562	-0.642912
67	6	0	1.017562	-9.812598	-3.913204
68	1	0	1.271668	-10.775872	-4.355088
69	1	0	-0.064817	-9.686108	-3.894631
70	17	0	1.679482	-8.531340	-5.006701
71	1	0	1.278712	-4.366079	0.087786
72	6	0	-1.130759	-5.489432	-1.265521
73	1	0	-1.403357	-4.750218	-0.511407
74	1	0	-1.659341	-6.425604	-1.091321
75	17	0	-1.705774	-4.866536	-2.867378

$^{4}TS_{Cl}$

1	26	0	-0.500750	-0.550801	-0.198162
2	7	0	-0.425540	-1.460615	1.598743
3	7	0	1.511307	-0.695287	-0.320969
4	7	0	-0.557290	0.483296	-1.935730
5	7	0	-2.483272	-0.264876	0.006736
6	6	0	1.986111	-1.842889	1.789356
7	6	0	1.821770	0.374293	-2.506008
8	6	0	-2.939340	1.019198	-2.026884
9	6	0	-2.824711	-1.481830	2.105682
10	6	0	0.685584	-1.936269	2.259634
11	6	0	2.368739	-1.267928	0.577180
12	6	0	2.288163	-0.280125	-1.368249
13	6	0	0.503543	0.730286	-2.764310
14	6	0	-1.644357	1.037757	-2.543166
15	6	0	-3.326839	0.408384	-0.843051
16	6	0	-3.275141	-0.745467	1.016690
17	6	0	-1.498777	-1.790291	2.387428
18	6	0	-1.056394	-2.489206	3.571062
19	6	0	0.299246	-2.573333	3.495127
20	6	0	3.725390	-1.209966	0.091276
21	6	0	3.674396	-0.596719	-1.124366
22	6	0	0.069007	1.454690	-3.936745
23	6	0	-1.270162	1.650173	-3.796937
24	6	0	-4.683035	0.357993	-0.349066
25	6	0	-4.652382	-0.366105	0.801039
26	1	0	2.770729	-2.263367	2.410915
27	1	0	4.589031	-1.591153	0.619881
28	1	0	4.488294	-0.371068	-1.800481
29	1	0	2.560641	0.644270	-3.254363
30	1	0	0.716308	1.767793	-4.745094
31	1	0	-1.952936	2.155818	-4.466607
32	1	0	-3.713321	1.509286	-2.609471
33	1	0	-5.533708	0.816357	-0.835499
34	1	0	-5.472106	-0.625156	1.457515
35	1	0	-3.571798	-1.820927	2.815235
36	1	0	-1.712001	-2.854774	4.350105
37	1	0	0.987028	-3.029510	4.194574
38	8	0	-0.813645	-2.042109	-1.129273

39	16	0	-0.334569	1.480902	1.083770
40	1	0	0.863895	1.245080	1.656790
41	15	0	-0.955323	-7.927933	-0.390424
42	8	0	-1.075335	-8.615120	0.921742
43	8	0	0.451758	-7.214692	-0.690380
44	8	0	-2.016053	-6.746974	-0.646462
45	8	0	-1.132152	-8.793164	-1.725195
46	6	0	-0.958013	-10.207955	-1.948199
47	1	0	-1.522987	-10.384373	-2.870183
48	6	0	-1.600825	-11.038118	-0.835297
49	1	0	-2.619525	-10.692940	-0.664093
50	1	0	-1.029608	-10.998537	0.088992
51	17	0	-1.708211	-12.771174	-1.353115
52	6	0	-3.213511	-6.495052	0.123634
53	1	0	-3.777666	-5.791987	-0.492912
54	6	0	-2.774558	-5.796534	1.417489
55	1	0	-2.239842	-6.486184	2.071961
56	1	0	-2.146233	-4.943346	1.160770
57	17	0	-4.194156	-5.158289	2.349023
58	6	0	1.097089	-6.411625	0.329245
59	1	0	0.353406	-5.972702	1.006979
60	6	0	1.862398	-5.335004	-0.357886
61	1	0	2.426665	-4.649563	0.260966
62	17	0	0.170998	-3.563327	-0.854262
63	6	0	-4.060067	-7.733958	0.393274
64	1	0	-3.484918	-8.496533	0.917468
65	1	0	-4.929701	-7.452339	0.985515
66	17	0	-4.689079	-8.480350	-1.133519
67	6	0	0.488195	-10.549423	-2.288977
68	1	0	0.533097	-11.550906	-2.716400
69	1	0	0.875275	-9.820665	-3.001041
70	17	0	1.615131	-10.548212	-0.870370
71	1	0	2.178829	-5.497031	-1.381716
72	6	0	1.972159	-7.372640	1.163837
73	1	0	2.782190	-7.790751	0.567276
74	1	0	1.346360	-8.167349	1.569033
75	17	0	2.712965	-6.506036	2.573178

$^{2}TS_{Cl}$

1	26	0	-0.494179	-0.848154	-0.119520
2	7	0	-0.227911	-1.931837	1.566479
3	7	0	1.500183	-0.734873	-0.336185
4	7	0	-0.764053	0.361177	-1.706203
5	7	0	-2.496646	-0.829510	0.201637
6	6	0	2.216836	-2.011234	1.630491
7	6	0	1.575642	0.599264	-2.390579
8	6	0	-3.198503	0.617770	-1.638849
9	6	0	-2.581182	-2.300503	2.158543
10	6	0	0.961598	-2.328737	2.130308
11	6	0	2.464589	-1.268428	0.477366
12	6	0	2.172374	-0.109971	-1.352307
13	6	0	0.212783	0.822992	-2.547368

14	6	0	-1.942122	0.847326	-2.197767	40	1	0	0.606245	0.770587	2.117281
15	6	0	-3.454538	-0.166973	-0.523053	41	15	0	-0.849550	-7.523120	-0.428418
16	6	0	-3.171609	-1.505858	1.183480	42	8	0	-1.225987	-7.641722	1.003290
17	6	0	-1.215329	-2.478804	2.348411	43	8	0	0.696372	-7.229920	-0.744238
18	6	0	-0.633215	-3.242145	3.426976	44	8	0	-1.584750	-6.353034	-1.250195
19	6	0	0.717760	-3.141850	3.297012	45	8	0	-1.098658	-8.788955	-1.379333
20	6	0	3.779668	-0.977147	-0.039055	46	6	0	-1.295457	-10.186218	-1.092052
21	6	0	3.597179	-0.260081	-1.182481	47	1	0	-1.903552	-10.533018	-1.935241
22	6	0	-0.366718	1.615378	-3.605874	48	6	0	-2.103335	-10.415496	0.187845
23	6	0	-1.709683	1.634936	-3.384847	49	1	0	-3.020669	-9.831211	0.154361
24	6	0	-4.767326	-0.423989	0.022241	50	1	0	-1.542237	-10.178296	1.088206
25	6	0	-4.592398	-1.263305	1.076975	51	17	0	-2.600486	-12.156106	0.287092
26	1	0	3.077437	-2.389381	2.173771	52	6	0	-2.907626	-5.824044	-0.992953
27	1	0	4.707696	-1.286484	0.423174	53	1	0	-3.178069	-5.324346	-1.925747
28	1	0	4.344847	0.141345	-1.853541	54	6	0	-2.770408	-4.777118	0.119963
29	1	0	2.236771	1.037643	-3.131788	55	1	0	-2.541782	-5.246722	1.077291
30	1	0	0.193763	2.090140	-4.400146	56	1	0	-1.991939	-4.063891	-0.145321
31	1	0	-2.481760	2.127717	-3.960509	57	17	0	-4.307443	-3.831616	0.324421
32	1	0	-4.050248	1.080724	-2.127405	58	6	0	1.484262	-6.360381	0.111239
33	1	0	-5.689137	-0.015154	-0.369410	59	1	0	0.839853	-5.818056	0.814808
34	1	0	-5.339706	-1.689163	1.732642	60	6	0	2.243957	-5.410832	-0.741021
35	1	0	-3.245210	-2.793481	2.861718	61	1	0	2.862376	-4.691499	-0.221571
36	1	0	-1.198442	-3.773701	4.180905	62	17	0	0.508890	-3.618886	-1.189417
37	1	0	1.488239	-3.579115	3.917355	63	6	0	-3.958764	-6.875688	-0.658429
38	8	0	-0.721356	-2.294310	-1.135165	64	1	0	-3.645794	-7.488623	0.187478
39	16	0	-0.535325	1.040332	1.450744	65	1	0	-4.894712	-6.376056	-0.412886

66	17	0	-4.315754	-7.983441	-2.046983
67	6	0	0.019886	-10.952079	-1.192680
68	1	0	-0.181054	-12.021563	-1.247042
69	1	0	0.561182	-10.626327	-2.080652
70	17	0	1.133472	-10.712169	0.216878
71	1	0	2.477866	-5.700365	-1.758714
72	6	0	2.371415	-7.311616	0.941028
73	1	0	3.071724	-7.857480	0.309146
74	1	0	1.735849	-8.009600	1.485061
75	17	0	3.339769	-6.398631	2.173584

$^{4}P_{Cl}$

1	26	0	-0.209775	-0.070300	-0.267856
2	7	0	-0.183375	-1.172125	1.418337
3	7	0	1.772113	-0.376630	-0.469483
4	7	0	-0.222977	1.124282	-1.902229
5	7	0	-2.166939	0.339464	0.008136
6	6	0	2.191561	-1.767170	1.501429
7	6	0	2.128579	0.889992	-2.540355
8	6	0	-2.559189	1.840623	-1.883750
9	6	0	-2.565887	-1.053217	1.983675
10	6	0	0.896497	-1.800789	1.997105
11	6	0	2.596777	-1.103796	0.342267
12	6	0	2.560981	0.085072	-1.488321
13	6	0	0.838580	1.372258	-2.729075
14	6	0	-1.274613	1.814114	-2.427377
15	6	0	-2.972057	1.150155	-0.752998
16	6	0	-2.977570	-0.182265	0.982866
17	6	0	-1.263225	-1.492151	2.199633
18	6	0	-0.858322	-2.339013	3.297205
19	6	0	0.484594	-2.525981	3.174816
20	6	0	3.944285	-1.102696	-0.170219
21	6	0	3.920854	-0.362988	-1.314904
22	6	0	0.441350	2.238528	-3.815123
23	6	0	-0.876920	2.517154	-3.625035
24	6	0	-4.320733	1.150288	-0.235818
25	6	0	-4.326186	0.315892	0.837207
26	1	0	2.947299	-2.322185	2.047769
27	1	0	4.781652	-1.606037	0.293832
28	1	0	4.738004	-0.132075	-1.985291
29	1	0	2.874269	1.178281	-3.275079
30	1	0	1.096893	2.581123	-4.604588
31	1	0	-1.530533	3.134882	-4.226261
32	1	0	-3.303831	2.439084	-2.399499
33	1	0	-5.142514	1.714290	-0.656395
34	1	0	-5.152804	0.053548	1.483819
35	1	0	-3.322875	-1.399783	2.679721
36	1	0	-1.527545	-2.727591	4.052819
37	1	0	1.148845	-3.100840	3.806210
38	8	0	-0.678733	-1.432133	-1.387848
39	16	0	0.146908	1.811487	1.163314
40	1	0	1.210581	1.336908	1.843891

41	15	0	0.650401	-7.520749	-0.127314	67	6	0	2.525579	-10.165773	-1.393702
42	8	0	0.416426	-7.999728	1.260380	68	1	0	2.750902	-11.184449	-1.708066
43	8	0	2.046392	-6.794055	-0.433356	69	1	0	2.922789	-9.454904	-2.118119
44	8	0	-0.418160	-6.437487	-0.659034	70	17	0	3.431863	-9.906656	0.154252
45	8	0	0.612006	-8.609321	-1.303264	71	1	0	2.906072	-4.088328	-1.070026
46	6	0	1.012288	-9.994883	-1.290616	72	6	0	3.285592	-6.369269	1.581823
47	1	0	0.614225	-10.371457	-2.239242	73	1	0	4.151757	-6.919190	1.213494
48	6	0	0.321456	-10.750900	-0.153950	74	1	0	2.623572	-7.039264	2.128002
49	1	0	-0.749034	-10.551436	-0.184813	75	17	0	3.896511	-5.132173	2.763840
50	1	0	0.724189	-10.484738	0.820820						
51	17	0	0.533594	-12.535250	-0.380325	**$^{2}P_{Cl}$**					
52	6	0	-1.768598	-6.280446	-0.153546	1	26	0	-0.181747	-0.063986	-0.291869
53	1	0	-2.249919	-5.639544	-0.895031	2	7	0	-0.124836	-1.174128	1.392458
54	6	0	-1.671958	-5.527635	1.180959	3	7	0	1.789155	-0.362405	-0.527995
55	1	0	-1.217706	-6.148925	1.952668	4	7	0	-0.228317	1.143737	-1.910079
56	1	0	-1.095726	-4.615027	1.033011	5	7	0	-2.147673	0.334934	0.018649
57	17	0	-3.307052	-5.017698	1.778856	6	6	0	2.246121	-1.781702	1.416265
58	6	0	2.541488	-5.695808	0.429255	7	6	0	2.118528	0.947994	-2.575595
59	1	0	1.677378	-5.140662	0.810230	8	6	0	-2.579062	1.822684	-1.871307
60	6	0	3.378548	-4.817101	-0.422863	9	6	0	-2.499671	-1.061161	2.000364
61	1	0	4.442717	-5.002589	-0.521586	10	6	0	0.960089	-1.818667	1.938345
62	17	0	-0.011634	-3.012062	-1.221515	11	6	0	2.629292	-1.099499	0.261678
63	6	0	-2.541745	-7.587176	-0.021562	12	6	0	2.566638	0.127327	-1.544955
64	1	0	-2.015405	-8.291583	0.622830	13	6	0	0.820405	1.419534	-2.742605
65	1	0	-3.524807	-7.377326	0.397819	14	6	0	-1.298822	1.820140	-2.421565
66	17	0	-2.819432	-8.396876	-1.616145	15	6	0	-2.973337	1.125457	-0.736303

16	6	0	-2.936342	-0.194695	1.005942	42	8	0	0.346731	-8.035373	1.257046
17	6	0	-1.192512	-1.498239	2.190053	43	8	0	2.032478	-6.797585	-0.355881
18	6	0	-0.770033	-2.360500	3.268606	44	8	0	-0.424514	-6.449681	-0.670037
19	6	0	0.568816	-2.556293	3.115319	45	8	0	0.641799	-8.604874	-1.307371
20	6	0	3.971074	-1.077563	-0.265750	46	6	0	1.041488	-9.990838	-1.297801
21	6	0	3.931345	-0.314239	-1.393272	47	1	0	0.679659	-10.354948	-2.265627
22	6	0	0.400610	2.291084	-3.815173	48	6	0	0.309109	-10.762206	-0.198045
23	6	0	-0.921548	2.542258	-3.613861	49	1	0	-0.759359	-10.560810	-0.264892
24	6	0	-4.316282	1.107997	-0.203820	50	1	0	0.676592	-10.511254	0.794561
25	6	0	-4.294643	0.281785	0.875615	51	17	0	0.528515	-12.543323	-0.443184
26	1	0	3.012404	-2.341802	1.942240	52	6	0	-1.782640	-6.279790	-0.190185
27	1	0	4.817296	-1.582656	0.180054	53	1	0	-2.246163	-5.641436	-0.945085
28	1	0	4.740143	-0.062382	-2.066233	54	6	0	-1.702652	-5.516980	1.139561
29	1	0	2.853557	1.255938	-3.312974	55	1	0	-1.265719	-6.136155	1.923022
30	1	0	1.044391	2.654043	-4.605198	56	1	0	-1.116701	-4.610177	0.993694
31	1	0	-1.590531	3.154123	-4.204086	57	17	0	-3.342390	-4.990020	1.708131
32	1	0	-3.336132	2.410671	-2.380993	58	6	0	2.487185	-5.711786	0.541103
33	1	0	-5.152047	1.656041	-0.617880	59	1	0	1.605244	-5.171962	0.903863
34	1	0	-5.108667	0.010663	1.534480	60	6	0	3.341304	-4.809108	-0.268174
35	1	0	-3.242408	-1.415163	2.707969	61	1	0	4.417320	-4.943552	-0.290276
36	1	0	-1.425800	-2.753870	4.033588	62	17	0	-0.001391	-2.999113	-1.269207
37	1	0	1.242143	-3.144593	3.724192	63	6	0	-2.567358	-7.579879	-0.061086
38	8	0	-0.725160	-1.439136	-1.364028	64	1	0	-2.061343	-8.279946	0.603843
39	16	0	0.160471	1.801601	1.173215	65	1	0	-3.559410	-7.358602	0.330376
40	1	0	1.240449	1.331283	1.830969	66	17	0	-2.808868	-8.407245	-1.652871
41	15	0	0.628668	-7.535193	-0.114092	67	6	0	2.557672	-10.159920	-1.346156

68	1	0	2.795528	-11.175643	-1.660891	72	6	0	3.200157	-6.397219	1.706049
69	1	0	2.980914	-9.442339	-2.048886	73	1	0	4.079330	-6.938336	1.355979
70	17	0	3.404919	-9.913595	0.236870	74	1	0	2.525227	-7.077786	2.222526
71	1	0	2.880155	-4.118442	-0.963484	75	17	0	3.769745	-5.174307	2.922860

For hydroxylation of tris(1, 3-dichloro-2-propyl) phosphate catalyzed by Cpd I of CYP450 using the cluster models

^{2}Cpd I						19	6	0	-0.774070	6.672338	-0.675539
1	7	0	-10.881403	-3.526250	3.052921	20	8	0	-0.473379	6.346132	0.459220
2	6	0	-11.213848	-3.282438	1.654946	21	6	0	-2.896785	8.020006	-1.339323
3	6	0	-12.477209	-4.023397	1.211175	22	6	0	-3.760836	7.662812	-0.105016
4	8	0	-12.991960	-4.938791	1.816237	23	6	0	-3.296591	7.225196	-2.591927
5	6	0	-10.034174	-3.686299	0.733346	24	6	0	-3.889785	6.180005	0.273498
6	6	0	-8.763800	-2.869973	1.001104	25	1	0	-0.626124	8.010327	-2.974364
7	6	0	-7.562205	-3.346513	0.176329	26	7	0	2.416249	5.462801	1.153395
8	7	0	-6.389670	-2.534391	0.474415	27	6	0	2.664769	4.020861	1.015614
9	6	0	-5.177711	-2.724928	-0.186911	28	6	0	4.114236	3.756552	0.627121
10	7	0	-4.155610	-1.961642	0.376994	29	8	0	4.640916	2.645441	0.751343
11	7	0	-4.931407	-3.490075	-1.192825	30	6	0	1.737440	3.424897	-0.055148
12	1	0	-10.970677	-4.525310	3.233450	31	7	0	4.737598	4.829445	0.104522
13	1	0	-6.272344	-2.323921	1.458214	32	6	0	6.069899	4.752714	-0.430352
14	1	0	-3.301788	-2.011566	-0.164667	33	6	0	7.035040	3.935977	0.445407
15	1	0	-4.414767	-1.007767	0.596372	34	8	0	7.797468	3.113231	-0.027191
16	1	0	-5.724294	-4.092912	-1.406188	35	1	0	1.424118	5.670181	1.053573
17	7	0	-0.658223	8.653763	-2.187886	36	1	0	4.182148	5.680186	0.094187
18	6	0	-1.363675	8.029553	-1.062700	37	7	0	8.266043	2.109332	2.899260

38	6	0	7.753216	1.199247	3.931559
39	6	0	8.499094	-0.131883	4.051090
40	8	0	8.172464	-1.027758	4.798408
41	6	0	6.237022	0.924721	3.675039
42	8	0	6.060428	0.585099	2.306956
43	6	0	5.353839	2.092367	4.111118
44	1	0	8.138160	1.658375	1.991766
45	1	0	5.570805	1.289002	1.844306
46	7	0	1.273116	-5.896432	4.002640
47	6	0	1.321637	-5.468050	5.396436
48	6	0	1.211581	-6.634745	6.381849
49	8	0	0.873003	-7.762428	6.093244
50	6	0	0.211528	-4.441432	5.677737
51	1	0	0.439917	-6.468986	3.873618
52	16	0	1.757419	-1.839158	-4.705649
53	26	0	0.969251	-0.386352	-2.732882
54	6	0	-1.837162	-2.365368	-2.722730
55	6	0	2.363266	-2.346528	-0.316331
56	6	0	3.880704	1.387997	-2.974279
57	6	0	-0.354652	1.444940	-5.309412
58	7	0	0.405355	-2.056848	-1.762899
59	6	0	-0.792576	-2.714718	-1.870812
60	6	0	-0.840649	-3.827218	-0.953124
61	6	0	0.335180	-3.817570	-0.265730
62	6	0	1.101980	-2.706822	-0.776828
63	7	0	2.763678	-0.466547	-1.830759
64	6	0	3.130356	-1.296056	-0.803463
65	6	0	4.445728	-0.948048	-0.316437
66	6	0	4.877415	0.094423	-1.074238
67	6	0	3.820769	0.383547	-2.015611
68	7	0	1.646623	1.090355	-3.937151
69	6	0	2.867404	1.713733	-3.866773
70	6	0	2.940530	2.780542	-4.834610
71	6	0	1.742639	2.805147	-5.481157
72	6	0	0.942516	1.747768	-4.913656
73	7	0	-0.727090	-0.482142	-3.839217
74	6	0	-1.125212	0.405046	-4.814096
75	6	0	-2.467476	0.101911	-5.246050
76	6	0	-2.885467	-0.967386	-4.515790
77	6	0	-1.799086	-1.322367	-3.636709
78	1	0	-3.835300	-1.483950	-4.550286
79	1	0	-3.003920	0.647300	-6.011309
80	1	0	1.418216	3.463330	-6.276355
81	1	0	3.803611	3.414915	-4.987716
82	1	0	5.798271	0.654722	-0.988805
83	1	0	4.949530	-1.417932	0.516992
84	1	0	-1.688087	-4.492004	-0.850177
85	1	0	0.664328	-4.479738	0.524934
86	1	0	2.784889	-2.938437	0.489851
87	1	0	-0.794630	2.063591	-6.085279
88	1	0	4.793995	1.972808	-3.020277
89	1	0	-2.756835	-2.941015	-2.643818

90	8	0	0.322846	0.633932	-1.641440	116	1	0	0.308581	8.839522	-1.932072
91	1	0	-7.379990	-4.417430	0.370989	117	8	0	-0.575029	5.861302	-1.737001
92	1	0	-7.781731	-3.251289	-0.894447	118	1	0	-0.189310	5.030721	-1.407057
93	1	0	-8.948079	-1.811218	0.778750	119	1	0	-1.203199	8.656752	-0.180354
94	1	0	-8.530970	-2.934303	2.070398	120	1	0	-3.050670	6.163221	-2.511412
95	1	0	-9.829613	-4.754963	0.888347	121	1	0	-4.376061	7.309698	-2.757666
96	1	0	-10.346719	-3.572325	-0.310686	122	1	0	-2.802050	7.619133	-3.484973
97	1	0	-11.399072	-2.209977	1.517980	123	1	0	-3.094204	9.077249	-1.558136
98	1	0	-11.575014	-3.084607	3.651663	124	1	0	-4.579567	6.070894	1.117012
99	1	0	0.313704	-3.603798	4.984276	125	1	0	-4.290548	5.583218	-0.551959
100	1	0	-0.775797	-4.891879	5.525268	126	1	0	-2.935937	5.744242	0.579297
101	1	0	0.266355	-4.071861	6.704430	127	1	0	-3.386358	8.223977	0.761210
102	1	0	2.051102	-6.526566	3.818329	128	1	0	-4.767839	8.053667	-0.300885
103	1	0	2.289577	-4.985385	5.578722	129	1	0	0.693477	3.531839	0.257976
104	1	0	7.849874	1.674439	4.915490	130	1	0	1.884062	3.943768	-1.010460
105	1	0	5.609100	3.008681	3.572514	131	1	0	1.931817	2.363288	-0.213133
106	1	0	4.306029	1.854459	3.904032	132	1	0	2.501286	3.461182	1.949027
107	1	0	5.455775	2.276941	5.185599	133	1	0	2.701580	5.787322	2.073697
108	1	0	5.980626	0.042564	4.273588	134	1	0	6.090491	4.285976	-1.421022
109	1	0	9.268734	2.238584	3.009804	135	1	0	6.468464	5.768452	-0.522799
110	8	0	9.591248	-0.206243	3.254453	136	8	0	6.982392	4.268986	1.735849
111	1	0	9.980876	-1.082527	3.414273	137	1	0	7.511497	3.588597	2.260890
112	8	0	1.525154	-6.267143	7.647382	138	1	0	0.933697	-2.886183	-4.490815
113	1	0	1.408616	-7.059092	8.199300						
114	8	0	-12.959783	-3.557031	0.035722	**^{4}Cpd I**					
115	1	0	-13.736237	-4.101330	-0.180109	1	7	0	-10.883332	-3.525779	3.053462

2	6	0	-11.213848	-3.282438	1.654946	28	6	0	4.114190	3.756465	0.626924
3	6	0	-12.477221	-4.022657	1.209986	29	8	0	4.640778	2.645289	0.750760
4	8	0	-12.993310	-4.937461	1.814799	30	6	0	1.737389	3.427150	-0.056350
5	6	0	-10.033357	-3.687807	0.734982	31	7	0	4.737525	4.829411	0.104368
6	6	0	-8.762369	-2.872911	1.004246	32	6	0	6.069898	4.752714	-0.430352
7	6	0	-7.560205	-3.350915	0.181079	33	6	0	7.035065	3.936184	0.445556
8	7	0	-6.386995	-2.540468	0.481091	34	8	0	7.797703	3.113581	-0.026951
9	6	0	-5.174520	-2.731617	-0.179067	35	1	0	1.425109	5.670988	1.056540
10	7	0	-4.152315	-1.969693	0.386647	36	1	0	4.182558	5.680478	0.095330
11	7	0	-4.927651	-3.496104	-1.185319	37	7	0	8.265890	2.109446	2.899295
12	1	0	-10.973819	-4.524643	3.234471	38	6	0	7.753216	1.199247	3.931559
13	1	0	-6.270572	-2.330746	1.465151	39	6	0	8.498965	-0.132002	4.050682
14	1	0	-3.297931	-2.020253	-0.154079	40	8	0	8.172488	-1.027885	4.798054
15	1	0	-4.410829	-1.015651	0.606097	41	6	0	6.236960	0.924907	3.675371
16	1	0	-5.720737	-4.098168	-1.400132	42	8	0	6.060143	0.585233	2.307336
17	7	0	-0.658127	8.655262	-2.186971	43	6	0	5.353974	2.092678	4.111508
18	6	0	-1.363675	8.029553	-1.062700	44	1	0	8.137772	1.658636	1.991759
19	6	0	-0.770510	6.674454	-0.673735	45	1	0	5.570011	1.288843	1.844812
20	8	0	-0.470675	6.349842	0.461717	46	7	0	1.273362	-5.896967	4.002825
21	6	0	-2.896228	8.015105	-1.342149	47	6	0	1.321637	-5.468050	5.396436
22	6	0	-3.761508	7.656450	-0.109142	48	6	0	1.211548	-6.634337	6.382322
23	6	0	-3.291326	7.217995	-2.594795	49	8	0	0.872616	-7.762046	6.094238
24	6	0	-3.886275	6.173661	0.270809	50	6	0	0.211274	-4.441532	5.677191
25	1	0	-0.622882	8.011598	-2.973118	51	1	0	0.440437	-6.469964	3.873939
26	7	0	2.417155	5.462763	1.155548	52	16	0	1.779630	-1.851670	-4.690270
27	6	0	2.664770	4.020862	1.015614	53	26	0	0.973277	-0.393199	-2.746897

54	6	0	-1.834427	-2.367874	-2.727582	80	1	0	1.436468	3.441504	-6.301575
55	6	0	2.369274	-2.354541	-0.327783	81	1	0	3.815481	3.400268	-5.000883
56	6	0	3.885059	1.384362	-2.978210	82	1	0	5.797738	0.658701	-0.982489
57	6	0	-0.340778	1.427496	-5.331501	83	1	0	4.950833	-1.420092	0.516046
58	7	0	0.408209	-2.062503	-1.770897	84	1	0	-1.689944	-4.488981	-0.846056
59	6	0	-0.791458	-2.717077	-1.873637	85	1	0	0.667416	-4.481792	0.520738
60	6	0	-0.840649	-3.827219	-0.953124	86	1	0	2.790917	-2.947813	0.477423
61	6	0	0.337817	-3.820265	-0.270271	87	1	0	-0.777436	2.039941	-6.114121
62	6	0	1.106455	-2.712729	-0.786004	88	1	0	4.797266	1.970953	-3.023419
63	7	0	2.770724	-0.472094	-1.838210	89	1	0	-2.755336	-2.941480	-2.648613
64	6	0	3.135899	-1.301997	-0.811330	90	8	0	0.353907	0.617827	-1.628605
65	6	0	4.448682	-0.950495	-0.318548	91	1	0	-7.379734	-4.422122	0.375746
66	6	0	4.879409	0.094996	-1.072511	92	1	0	-7.778015	-3.255119	-0.889990
67	6	0	3.825022	0.381346	-2.017855	93	1	0	-8.945123	-1.813962	0.781565
68	7	0	1.652646	1.082453	-3.946984	94	1	0	-8.531004	-2.937402	2.073847
69	6	0	2.874110	1.705531	-3.874990	95	1	0	-9.830216	-4.756670	0.890481
70	6	0	2.951520	2.766983	-4.848241	96	1	0	-10.344423	-3.573709	-0.309479
71	6	0	1.756884	2.787987	-5.500942	97	1	0	-11.398019	-2.209905	1.517169
72	6	0	0.954179	1.733990	-4.931314	98	1	0	-11.577211	-3.083080	3.651113
73	7	0	-0.719369	-0.488128	-3.847484	99	1	0	0.313396	-3.604168	4.983397
74	6	0	-1.111846	0.389172	-4.833894	100	1	0	-0.775936	-4.892242	5.524762
75	6	0	-2.449941	0.079555	-5.273331	101	1	0	0.265887	-4.071537	6.703744
76	6	0	-2.871239	-0.984329	-4.537182	102	1	0	2.051685	-6.526730	3.818693
77	6	0	-1.790924	-1.330391	-3.647425	103	1	0	2.289444	-4.985118	5.578669
78	1	0	-3.819580	-1.503387	-4.574884	104	1	0	7.850179	1.674262	4.915544
79	1	0	-2.981513	0.617288	-6.047333	105	1	0	5.609165	3.008897	3.572706

106	1	0	4.306091	1.854793	3.904745
107	1	0	5.456192	2.277416	5.185934
108	1	0	5.980569	0.042830	4.274047
109	1	0	9.268625	2.238560	3.009614
110	8	0	9.590810	-0.206409	3.253647
111	1	0	9.980364	-1.082781	3.413168
112	8	0	1.525457	-6.266315	7.647655
113	1	0	1.408790	-7.058011	8.199906
114	8	0	-12.958065	-3.556438	0.033766
115	1	0	-13.734627	-4.100301	-0.182780
116	1	0	0.307686	8.844035	-1.929651
117	8	0	-0.567105	5.863429	-1.734394
118	1	0	-0.178772	5.034559	-1.403250
119	1	0	-1.206741	8.657754	-0.180430
120	1	0	-3.042628	6.156777	-2.512815
121	1	0	-4.370697	7.299353	-2.762742
122	1	0	-2.796112	7.612436	-3.487249
123	1	0	-3.096435	9.071556	-1.562259
124	1	0	-4.577164	6.063225	1.113240
125	1	0	-4.283643	5.574651	-0.554674
126	1	0	-2.931513	5.741404	0.578735
127	1	0	-3.390532	8.219821	0.757156
128	1	0	-4.769402	8.043786	-0.307409
129	1	0	0.693397	3.535172	0.256459
130	1	0	1.885386	3.947018	-1.010959
131	1	0	1.930167	2.365387	-0.215482
132	1	0	2.500766	3.459797	1.948081
133	1	0	2.703231	5.785807	2.076139
134	1	0	6.090574	4.285804	-1.420932
135	1	0	6.468336	5.768479	-0.523000
136	8	0	6.982125	4.269100	1.736000
137	1	0	7.511305	3.588790	2.261054
138	1	0	0.965857	-2.905060	-4.469240

Tris(1, 3-dichloro-2-propyl) phosphate

1	15	0	-1.222145	1.483582	-6.874175
2	8	0	-1.776382	2.859973	-6.932266
3	8	0	0.385555	1.393831	-6.847603
4	8	0	-1.589216	0.499580	-8.077938
5	8	0	-1.611253	0.623500	-5.574794
6	6	0	-1.492518	1.188671	-4.245693
7	1	0	-0.606254	1.833997	-4.199158
8	6	0	-1.269675	-0.021263	-3.341650
9	1	0	-0.429057	-0.606197	-3.712234
10	1	0	-2.162432	-0.643828	-3.292247
11	17	0	-0.868795	0.504995	-1.658742
12	6	0	-2.905695	0.310459	-8.662936
13	1	0	-2.713809	-0.367507	-9.496804
14	6	0	-3.425107	1.644983	-9.217144
15	1	0	-3.756833	2.323412	-8.432793
16	1	0	-2.640438	2.128703	-9.797855
17	17	0	-4.819165	1.365470	-10.338416

18	6	0	1.179717	2.181667	-7.772202
19	1	0	0.628076	2.339240	-8.703747
20	6	0	2.452375	1.398293	-8.049243
21	1	0	3.154437	2.013619	-8.610841
22	17	0	2.137356	-0.085141	-9.026794
23	6	0	-3.878370	-0.346943	-7.692002
24	1	0	-3.965055	0.209190	-6.757593
25	1	0	-4.858266	-0.421248	-8.163197
26	17	0	-3.370405	-2.026872	-7.263670
27	6	0	-2.694422	2.062345	-3.905602
28	1	0	-2.584431	2.464923	-2.898629
29	1	0	-2.777707	2.871144	-4.630442
30	17	0	-4.262997	1.155336	-3.945074
31	1	0	2.909114	1.077796	-7.111165
32	6	0	1.446617	3.530678	-7.095144
33	1	0	2.058539	3.406295	-6.199899
34	1	0	0.495963	3.996420	-6.838020
35	17	0	2.319046	4.666785	-8.200362

$^{2}TS_{\alpha H}$

1	7	0	-11.055185	-2.804008	3.022553
2	6	0	-11.213837	-3.282436	1.654941
3	6	0	-12.394552	-4.243681	1.500475
4	8	0	-12.957696	-4.802205	2.417105
5	6	0	-9.919011	-3.980659	1.165229
6	6	0	-8.711453	-3.036189	1.127375
7	6	0	-7.405289	-3.749764	0.758374
8	7	0	-6.300819	-2.800332	0.729257
9	6	0	-5.013958	-3.185545	0.352512
10	7	0	-4.086284	-2.163586	0.564595
11	7	0	-4.628581	-4.312487	-0.133347
12	1	0	-11.146500	-3.600242	3.652083
13	1	0	-6.303680	-2.139954	1.497322
14	1	0	-3.181971	-2.397561	0.172940
15	1	0	-4.395852	-1.250487	0.253593
16	1	0	-5.373146	-5.007148	-0.100604
17	7	0	-1.425689	8.823656	-2.294183
18	6	0	-1.363646	8.029516	-1.062673
19	6	0	-1.204965	6.529641	-1.322275
20	8	0	-0.397643	5.801491	-0.769469
21	6	0	-2.559148	8.400171	-0.133976
22	6	0	-2.450277	7.825350	1.300353
23	6	0	-3.935777	8.153468	-0.770251
24	6	0	-2.866731	6.363391	1.518381
25	1	0	-2.147217	8.451525	-2.906263
26	7	0	2.302711	5.438225	0.855127
27	6	0	2.664746	4.020917	1.015585
28	6	0	4.136639	3.782578	0.695645
29	8	0	4.683162	2.693170	0.908446
30	6	0	1.819908	3.129868	0.090291
31	7	0	4.747320	4.835913	0.129577
32	6	0	6.069879	4.752687	-0.430329

33	6	0	7.036321	3.903118	0.410125	59	6	0	-0.341610	-3.373994	-2.227066
34	8	0	7.726583	3.028942	-0.081761	60	6	0	-0.840571	-3.827313	-0.952855
35	1	0	1.386967	5.548776	0.424281	61	6	0	0.047593	-3.399950	-0.009776
36	1	0	4.142693	5.646388	0.009842	62	6	0	1.081072	-2.676302	-0.708208
37	7	0	8.243044	2.024099	2.819719	63	7	0	3.203237	-1.097722	-2.088378
38	6	0	7.753227	1.199245	3.931559	64	6	0	3.114829	-1.278113	-0.729908
39	6	0	8.361531	-0.202904	4.016194	65	6	0	4.199446	-0.593579	-0.060659
40	8	0	8.037809	-1.033006	4.837012	66	6	0	4.947907	-0.005875	-1.030462
41	6	0	6.199642	1.079906	3.857420	67	6	0	4.330740	-0.341576	-2.294122
42	8	0	5.830105	0.681078	2.545535	68	7	0	3.125125	-1.064740	-4.926012
43	6	0	5.492912	2.359457	4.301359	69	6	0	4.281991	-0.348966	-4.758859
44	1	0	7.998105	1.558167	1.944924	70	6	0	4.827719	0.015062	-6.040484
45	1	0	5.459822	1.437975	2.052860	71	6	0	3.979034	-0.482173	-6.986692
46	7	0	0.404310	-4.876009	4.427203	72	6	0	2.909216	-1.142438	-6.282958
47	6	0	1.321551	-5.467947	5.396152	73	7	0	0.628493	-2.476650	-4.895171
48	6	0	0.613582	-5.959833	6.661079	74	6	0	0.762826	-2.361825	-6.253979
49	8	0	-0.514974	-5.662833	6.989507	75	6	0	-0.331187	-3.027034	-6.920180
50	6	0	2.419521	-4.460249	5.776681	76	6	0	-1.121350	-3.555126	-5.946571
51	1	0	-0.152213	-4.168736	4.905505	77	6	0	-0.506273	-3.214685	-4.685185
52	16	0	3.099547	-3.785450	-3.830662	78	1	0	-2.032259	-4.128569	-6.053732
53	26	0	1.939370	-1.773076	-3.470052	79	1	0	-0.458465	-3.076012	-7.992971
54	6	0	-0.975476	-3.617160	-3.438683	80	1	0	4.055802	-0.420348	-8.064307
55	6	0	2.143741	-2.028053	-0.085077	81	1	0	5.745474	0.570704	-6.182355
56	6	0	4.842228	0.003781	-3.534324	82	1	0	5.827804	0.612634	-0.912655
57	6	0	1.816037	-1.732066	-6.903731	83	1	0	4.360693	-0.562276	1.008957
58	7	0	0.839111	-2.687581	-2.056640	84	1	0	-1.766354	-4.374308	-0.811434

85	1	0	0.022467	-3.552548	1.062003	111	1	0	9.633041	-1.334944	3.237664
86	1	0	2.207162	-2.104077	0.995471	112	8	0	1.403211	-6.768524	7.407763
87	1	0	1.786324	-1.698456	-7.987408	113	1	0	0.884493	-7.007066	8.194824
88	1	0	5.757794	0.586067	-3.552092	114	8	0	-12.740173	-4.429498	0.204995
89	1	0	-1.896543	-4.190507	-3.407383	115	1	0	-13.470455	-5.071642	0.203302
90	8	0	1.081569	-0.249101	-3.303375	116	1	0	-0.550416	8.739413	-2.805514
91	1	0	-7.220474	-4.575477	1.467028	117	8	0	-2.045356	6.079489	-2.270749
92	1	0	-7.494474	-4.200962	-0.237778	118	1	0	-1.876386	5.127280	-2.412815
93	1	0	-8.890801	-2.231649	0.402857	119	1	0	-0.450481	8.314854	-0.530208
94	1	0	-8.612376	-2.562051	2.110773	120	1	0	-4.108452	7.099961	-1.005633
95	1	0	-9.711360	-4.824830	1.837759	121	1	0	-4.726989	8.480357	-0.086836
96	1	0	-10.100994	-4.405182	0.171557	122	1	0	-4.049602	8.728447	-1.693929
97	1	0	-11.403960	-2.423326	0.999995	123	1	0	-2.445575	9.487661	-0.039516
98	1	0	-11.827546	-2.186425	3.260680	124	1	0	-2.802804	6.112860	2.582607
99	1	0	2.935616	-4.132052	4.871802	125	1	0	-3.900504	6.186392	1.206039
100	1	0	1.981546	-3.579061	6.258922	126	1	0	-2.223509	5.662420	0.981811
101	1	0	3.143044	-4.904412	6.464452	127	1	0	-1.421602	7.965214	1.658542
102	1	0	-0.269693	-5.578261	4.129406	128	1	0	-3.077493	8.456705	1.942920
103	1	0	1.800404	-6.340008	4.934880	129	1	0	0.764156	3.185398	0.369753
104	1	0	8.011184	1.684705	4.880929	130	1	0	1.914427	3.469476	-0.946870
105	1	0	5.771077	3.207882	3.670692	131	1	0	2.157201	2.093325	0.148549
106	1	0	4.409754	2.220449	4.230942	132	1	0	2.521340	3.669385	2.047502
107	1	0	5.738436	2.601256	5.340724	133	1	0	2.288244	5.916570	1.749947
108	1	0	5.924283	0.264957	4.536381	134	1	0	6.064300	4.307485	-1.431243
109	1	0	9.259259	2.064973	2.833438	135	1	0	6.482628	5.764508	-0.505538
110	8	0	9.326894	-0.423466	3.093640	136	8	0	7.077347	4.269717	1.691859

137	1	0	7.584036	3.563570	2.202952
138	1	0	2.366228	-4.587464	-3.031064
139	15	0	-1.301597	1.232897	-6.836521
140	8	0	-2.205021	2.399827	-6.975094
141	8	0	0.271244	1.604855	-6.882873
142	8	0	-1.476402	0.098216	-7.958556
143	8	0	-1.390352	0.320126	-5.523594
144	6	0	-1.130580	0.551332	-4.147251
145	1	0	-0.021299	-0.040708	-3.833202
146	6	0	-2.276460	-0.126591	-3.410506
147	1	0	-2.322358	-1.178869	-3.687287
148	1	0	-3.220328	0.363425	-3.660815
149	17	0	-2.093096	-0.039738	-1.617383
150	6	0	-2.576881	0.029365	-8.899827
151	1	0	-2.437210	-0.940036	-9.382953
152	6	0	-2.391109	1.142046	-9.941291
153	1	0	-2.653036	2.117912	-9.531916
154	1	0	-1.355820	1.144189	-10.283006
155	17	0	-3.430607	0.857737	-11.395545
156	6	0	0.717420	2.726530	-7.686451
157	1	0	-0.034388	2.981345	-8.437945
158	6	0	2.024384	2.332918	-8.353425
159	1	0	2.504779	3.208302	-8.788776
160	17	0	1.763565	1.158619	-9.708583
161	6	0	-3.954319	0.077441	-8.247839
162	1	0	-4.071670	0.976174	-7.642672
163	1	0	-4.716145	0.054610	-9.026976
164	17	0	-4.257157	-1.347938	-7.176198
165	6	0	-0.754915	1.943617	-3.720771
166	1	0	-0.389159	1.909376	-2.697101
167	1	0	0.011681	2.360274	-4.369167
168	17	0	-2.162206	3.132309	-3.724663
169	1	0	2.691596	1.847399	-7.639073
170	6	0	0.871694	3.910962	-6.725453
171	1	0	1.647534	3.718269	-5.981987
172	1	0	-0.084950	4.096730	-6.237604
173	17	0	1.319364	5.430307	-7.599513

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1	7	0	-11.056528	-2.838844	3.034481
2	6	0	-11.213838	-3.282436	1.654944
3	6	0	-12.400436	-4.231640	1.473489
4	8	0	-12.969819	-4.808951	2.374514
5	6	0	-9.922140	-3.977228	1.152249
6	6	0	-8.708408	-3.040055	1.142291
7	6	0	-7.405314	-3.751357	0.758125
8	7	0	-6.294889	-2.808588	0.764253
9	6	0	-5.009439	-3.185855	0.375721
10	7	0	-4.077541	-2.176828	0.626902
11	7	0	-4.628119	-4.295805	-0.151064
12	1	0	-11.157607	-3.649461	3.643860
13	1	0	-6.296302	-2.174045	1.553768

14	1	0	-3.174970	-2.397373	0.223977	40	8	0	8.017688	-1.034439	4.840109
15	1	0	-4.383422	-1.250540	0.353596	41	6	0	6.197715	1.101256	3.883053
16	1	0	-5.375747	-4.987911	-0.145088	42	8	0	5.801956	0.693659	2.581252
17	7	0	-1.431120	8.830646	-2.289761	43	6	0	5.514946	2.394728	4.323764
18	6	0	-1.363647	8.029509	-1.062677	44	1	0	7.976342	1.546340	1.939768
19	6	0	-1.224768	6.529097	-1.333066	45	1	0	5.434751	1.450451	2.085657
20	8	0	-0.412863	5.791059	-0.799364	46	7	0	0.493126	-5.157230	4.235548
21	6	0	-2.543738	8.409367	-0.118445	47	6	0	1.321627	-5.468033	5.396404
22	6	0	-2.424298	7.826570	1.311707	48	6	0	0.694595	-6.526202	6.307865
23	6	0	-3.930787	8.181256	-0.738900	49	8	0	-0.463227	-6.883055	6.269035
24	6	0	-2.846879	6.365845	1.526044	50	6	0	1.607842	-4.192024	6.206083
25	1	0	-2.162942	8.467709	-2.895235	51	1	0	-0.445064	-4.931977	4.563989
26	7	0	2.296175	5.434261	0.834918	52	16	0	3.016370	-3.916749	-3.561477
27	6	0	2.664743	4.020922	1.015579	53	26	0	1.964739	-1.726437	-3.423145
28	6	0	4.137872	3.784898	0.701020	54	6	0	-0.911297	-3.619138	-3.444501
29	8	0	4.687286	2.698422	0.923013	55	6	0	2.114249	-2.010652	-0.029278
30	6	0	1.824487	3.112992	0.102545	56	6	0	4.893816	0.021592	-3.417471
31	7	0	4.747231	4.835871	0.129830	57	6	0	1.962056	-1.733123	-6.845043
32	6	0	6.069883	4.752693	-0.430334	58	7	0	0.848385	-2.660194	-2.025332
33	6	0	7.033150	3.894869	0.405245	59	6	0	-0.318644	-3.369109	-2.217360
34	8	0	7.709440	3.010440	-0.088284	60	6	0	-0.840649	-3.827231	-0.953099
35	1	0	1.384672	5.535427	0.392316	61	6	0	0.020532	-3.390257	0.007332
36	1	0	4.138615	5.642133	0.000026	62	6	0	1.061792	-2.652438	-0.667576
37	7	0	8.238285	2.012571	2.809328	63	7	0	3.242745	-1.116699	-2.011620
38	6	0	7.753230	1.199245	3.931563	64	6	0	3.124031	-1.288424	-0.657096
39	6	0	8.342983	-0.211093	4.013219	65	6	0	4.203185	-0.622209	0.037065

66	6	0	4.978466	-0.040852	-0.916333	92	1	0	-7.492061	-4.170678	-0.252036
67	6	0	4.379522	-0.362038	-2.190634	93	1	0	-8.880693	-2.215393	0.439051
68	7	0	3.194347	-1.008696	-4.850301	94	1	0	-8.609152	-2.592763	2.138191
69	6	0	4.341938	-0.292129	-4.658562	95	1	0	-9.722394	-4.839285	1.804134
70	6	0	4.913533	0.088962	-5.925392	96	1	0	-10.103570	-4.375509	0.147671
71	6	0	4.092850	-0.416808	-6.890927	97	1	0	-11.396167	-2.406287	1.020682
72	6	0	3.019320	-1.093596	-6.205454	98	1	0	-11.824453	-2.220442	3.284542
73	7	0	0.744801	-2.496502	-4.859463	99	1	0	2.077635	-3.451356	5.555122
74	6	0	0.908334	-2.384204	-6.217368	100	1	0	0.675440	-3.765398	6.592794
75	6	0	-0.163444	-3.056918	-6.908542	101	1	0	2.267697	-4.400603	7.051614
76	6	0	-0.978862	-3.579647	-5.952524	102	1	0	0.375158	-5.997322	3.672878
77	6	0	-0.397195	-3.231841	-4.679830	103	1	0	2.277984	-5.872504	5.043771
78	1	0	-1.887837	-4.151697	-6.079207	104	1	0	8.032725	1.685010	4.874697
79	1	0	-0.262797	-3.110617	-7.984055	105	1	0	5.791945	3.231852	3.677767
80	1	0	4.192910	-0.355470	-7.966604	106	1	0	4.429024	2.268413	4.274912
81	1	0	5.829381	0.652815	-6.044315	107	1	0	5.782081	2.646224	5.355445
82	1	0	5.859524	0.571927	-0.780027	108	1	0	5.922145	0.297184	4.574746
83	1	0	4.341887	-0.591043	1.109755	109	1	0	9.255026	2.040890	2.809334
84	1	0	-1.762177	-4.385623	-0.831112	110	8	0	9.294574	-0.447343	3.080182
85	1	0	-0.023829	-3.545988	1.078019	111	1	0	9.591240	-1.361896	3.224628
86	1	0	2.153435	-2.079550	1.053184	112	8	0	1.584103	-7.025027	7.199440
87	1	0	1.957171	-1.712412	-7.929625	113	1	0	1.095742	-7.664799	7.745000
88	1	0	5.808091	0.606728	-3.410802	114	8	0	-12.743470	-4.383062	0.172905
89	1	0	-1.831611	-4.194706	-3.441693	115	1	0	-13.477842	-5.020225	0.153192
90	8	0	1.128757	-0.214988	-3.319384	116	1	0	-0.562608	8.738408	-2.811251
91	1	0	-7.229546	-4.599800	1.441718	117	8	0	-2.087907	6.095140	-2.266590

118	1	0	-1.938302	5.140613	-2.422185	144	6	0	-1.194835	0.555042	-4.010319
119	1	0	-0.441062	8.302227	-0.539807	145	1	0	0.070961	-0.050509	-3.689123
120	1	0	-4.118445	7.130938	-0.976625	146	6	0	-2.287690	-0.145747	-3.228334
121	1	0	-4.709789	8.514722	-0.044653	147	1	0	-2.321187	-1.202518	-3.492422
122	1	0	-4.048851	8.761258	-1.658903	148	1	0	-3.259448	0.313524	-3.431608
123	1	0	-2.416983	9.495091	-0.019992	149	17	0	-2.026783	-0.040975	-1.442489
124	1	0	-2.775205	6.109457	2.588432	150	6	0	-2.677743	-0.147927	-8.725720
125	1	0	-3.884194	6.195980	1.221621	151	1	0	-2.524377	-1.126435	-9.185991
126	1	0	-2.212172	5.664372	0.980094	152	6	0	-2.533093	0.940905	-9.798777
127	1	0	-1.391253	7.958578	1.660401	153	1	0	-2.810511	1.921056	-9.410733
128	1	0	-3.041342	8.458255	1.963802	154	1	0	-1.503384	0.957054	-10.156649
129	1	0	0.768268	3.169073	0.380044	155	17	0	-3.586906	0.594600	-11.229649
130	1	0	1.918967	3.436778	-0.939615	156	6	0	0.588487	2.638860	-7.622119
131	1	0	2.164934	2.078538	0.176520	157	1	0	-0.166207	2.855407	-8.382683
132	1	0	2.521747	3.684122	2.052456	158	6	0	1.905686	2.256197	-8.275414
133	1	0	2.268522	5.922815	1.723829	159	1	0	2.370314	3.130545	-8.729468
134	1	0	6.062743	4.314090	-1.434195	160	17	0	1.673984	1.046630	-9.605666
135	1	0	6.485689	5.763748	-0.498776	161	6	0	-4.046321	-0.112890	-8.054511
136	8	0	7.089313	4.267054	1.684577	162	1	0	-4.171230	0.794360	-7.463675
137	1	0	7.592252	3.557577	2.194716	163	1	0	-4.819665	-0.163845	-8.820809
138	1	0	3.420225	-3.998877	-2.276536	164	17	0	-4.307691	-1.524203	-6.953056
139	15	0	-1.404343	1.143962	-6.717265	165	6	0	-0.832965	1.945427	-3.628954
140	8	0	-2.318881	2.296556	-6.899381	166	1	0	-0.470140	1.959299	-2.604222
141	8	0	0.165729	1.530988	-6.788951	167	1	0	-0.085894	2.368662	-4.294710
142	8	0	-1.567179	-0.030188	-7.803175	168	17	0	-2.269686	3.146920	-3.648399
143	8	0	-1.477221	0.276626	-5.377035	169	1	0	2.580485	1.800819	-7.548470

170	6	0	0.714768	3.854086	-6.695894
171	1	0	1.493774	3.700940	-5.946526
172	1	0	-0.246424	4.032657	-6.214346
173	17	0	1.130502	5.357192	-7.613783

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1	7	0	9.980175	6.761197	2.879376
2	6	0	9.060732	6.027884	3.741221
3	6	0	9.612807	5.830570	5.155209
4	8	0	10.775173	5.968787	5.469666
5	6	0	8.719522	4.649217	3.129334
6	6	0	8.015275	4.772203	1.775217
7	6	0	7.761679	3.412861	1.120287
8	7	0	7.080443	3.582070	-0.153054
9	6	0	6.540536	2.517682	-0.850739
10	7	0	5.988773	2.902600	-2.068120
11	7	0	6.510812	1.277893	-0.485294
12	1	0	10.917868	6.388611	3.023325
13	1	0	7.419775	4.338095	-0.733303
14	1	0	5.499983	2.140566	-2.523807
15	1	0	5.422307	3.740180	-2.014760
16	1	0	7.086593	1.113496	0.337611
17	7	0	0.319010	-7.095527	3.538532
18	6	0	-0.181886	-6.073090	4.457368
19	6	0	-0.317496	-4.675787	3.838942
20	8	0	-1.184696	-3.870546	4.119998
21	6	0	0.670564	-6.099303	5.767726
22	6	0	-0.077791	-5.632146	7.039965
23	6	0	2.050313	-5.437577	5.620409
24	6	0	-0.277048	-4.124956	7.247756
25	1	0	1.271485	-6.883710	3.253186
26	7	0	-4.193745	-3.214966	3.675027
27	6	0	-4.377879	-2.029921	2.825409
28	6	0	-5.655728	-2.147885	2.004028
29	8	0	-6.161180	-1.174899	1.431618
30	6	0	-3.193366	-1.877457	1.858804
31	7	0	-6.132162	-3.402161	1.916693
32	6	0	-7.199027	-3.762603	1.019844
33	6	0	-8.326234	-2.720182	0.962264
34	8	0	-8.776966	-2.312471	-0.092447
35	1	0	-3.209704	-3.367160	3.883668
36	1	0	-5.600009	-4.088497	2.446109
37	7	0	-10.101780	-0.013365	1.558985
38	6	0	-9.920899	1.314883	2.158929
39	6	0	-10.462350	2.481072	1.328715
40	8	0	-10.349155	3.645842	1.642510
41	6	0	-8.408065	1.556288	2.459949
42	8	0	-7.648653	1.240387	1.302936
43	6	0	-7.931334	0.799283	3.698678
44	1	0	-9.585267	-0.038107	0.678515
45	1	0	-7.209850	0.376304	1.415762
46	7	0	-3.146541	7.669304	0.790707

47	6	0	-3.837555	8.445053	1.816292	73	7	0	0.132388	0.618311	-4.566574
48	6	0	-4.200770	9.856207	1.347088	74	6	0	0.485181	-0.183921	-5.624774
49	8	0	-3.727120	10.411203	0.378881	75	6	0	1.721509	0.279648	-6.200328
50	6	0	-2.977307	8.533034	3.088634	76	6	0	2.100254	1.379874	-5.490965
51	1	0	-2.384410	8.237919	0.423656	77	6	0	1.095318	1.591882	-4.480029
52	16	0	-2.675969	1.699252	-5.104659	78	1	0	2.969887	2.007237	-5.634731
53	26	0	-1.578119	0.495823	-3.456835	79	1	0	2.219693	-0.183923	-7.041315
54	6	0	1.090307	2.650768	-3.583271	80	1	0	-1.841670	-3.498250	-6.839262
55	6	0	-3.005200	2.396323	-0.999689	81	1	0	-4.063171	-3.722529	-5.299425
56	6	0	-4.227960	-1.648697	-3.354547	82	1	0	-6.161467	-0.929777	-1.378834
57	6	0	-0.242084	-1.270240	-6.088924	83	1	0	-5.503569	1.341197	-0.098206
58	7	0	-1.084693	2.203022	-2.518094	84	1	0	0.893301	4.755014	-1.686283
59	6	0	0.077448	2.922628	-2.676250	85	1	0	-1.420728	4.649851	-0.273136
60	6	0	0.090756	4.033302	-1.759955	86	1	0	-3.463078	2.999856	-0.223508
61	6	0	-1.069112	3.979323	-1.047238	87	1	0	0.168871	-1.829877	-6.922286
62	6	0	-1.789990	2.823261	-1.516091	88	1	0	-5.070471	-2.330859	-3.316392
63	7	0	-3.234497	0.360303	-2.351227	89	1	0	1.934513	3.331433	-3.606633
64	6	0	-3.670784	1.249304	-1.398298	90	8	0	-0.668634	-0.516614	-2.266821
65	6	0	-4.944170	0.825791	-0.867839	91	1	0	8.714750	2.868483	1.007761
66	6	0	-5.279239	-0.320069	-1.519620	92	1	0	7.119805	2.802445	1.767082
67	6	0	-4.217117	-0.595535	-2.456317	93	1	0	7.055038	5.288227	1.900417
68	7	0	-2.143124	-1.108434	-4.533461	94	1	0	8.631099	5.398058	1.119151
69	6	0	-3.258431	-1.877126	-4.321457	95	1	0	9.653652	4.081528	3.015608
70	6	0	-3.285042	-2.972030	-5.256907	96	1	0	8.093489	4.092681	3.835874
71	6	0	-2.170221	-2.858386	-6.030985	97	1	0	8.128758	6.599275	3.831101
72	6	0	-1.455384	-1.696084	-5.569035	98	1	0	10.030316	7.731677	3.179710

99	1	0	-2.738521	7.523396	3.430261	125	1	0	0.677906	-3.590201	7.277845
100	1	0	-2.036511	9.054597	2.879772	126	1	0	-0.888618	-3.681121	6.460135
101	1	0	-3.500433	9.070809	3.883217	127	1	0	-1.054016	-6.133695	7.070102
102	1	0	-3.770366	7.529141	-0.001438	128	1	0	0.485067	-6.027451	7.895967
103	1	0	-4.774615	7.934993	2.068375	129	1	0	-2.267341	-1.712464	2.415790
104	1	0	-10.466938	1.357988	3.109338	130	1	0	-3.076226	-2.785754	1.258088
105	1	0	-8.061844	-0.279894	3.581914	131	1	0	-3.359642	-1.035454	1.184008
106	1	0	-6.867920	0.999709	3.860642	132	1	0	-4.471855	-1.096036	3.399711
107	1	0	-8.479573	1.123171	4.589535	133	1	0	-4.680046	-3.101614	4.560065
108	1	0	-8.300726	2.632549	2.635743	134	1	0	-6.845674	-3.888624	-0.009204
109	1	0	-11.077417	-0.156698	1.309737	135	1	0	-7.629418	-4.712831	1.353799
110	8	0	-11.112489	2.084974	0.209769	136	8	0	-8.781700	-2.372066	2.166773
111	1	0	-11.404678	2.899262	-0.233794	137	1	0	-9.376101	-1.565170	2.055683
112	8	0	-5.110801	10.447189	2.157082	138	1	0	-2.342161	2.934467	-4.677918
113	1	0	-5.258651	11.339218	1.799367	139	15	0	3.904227	-2.284397	-0.480654
114	8	0	8.654318	5.453533	6.032897	140	8	0	4.994298	-1.977066	0.474280
115	1	0	9.097859	5.322796	6.888437	141	8	0	2.867357	-3.434444	-0.044358
116	1	0	-0.240164	-7.119976	2.689670	142	8	0	4.338990	-2.763037	-1.942661
117	8	0	0.623834	-4.404147	2.906125	143	8	0	2.853733	-1.085925	-0.795590
118	1	0	0.477381	-3.490888	2.581925	144	6	0	2.441516	-0.153072	0.136385
119	1	0	-1.205747	-6.348967	4.732358	145	1	0	0.176772	-0.756492	-2.679807
120	1	0	1.979499	-4.362940	5.425600	146	6	0	3.433637	0.790202	0.696857
121	1	0	2.626149	-5.566943	6.542826	147	1	0	4.436731	0.649150	0.291816
122	1	0	2.636865	-5.886133	4.812169	148	1	0	3.449232	0.759774	1.788476
123	1	0	0.839290	-7.175272	5.899641	149	17	0	2.974842	2.543464	0.302045
124	1	0	-0.776823	-3.944810	8.205464	150	6	0	5.622176	-2.523741	-2.583612

151	1	0	5.492917	-2.982700	-3.566197
152	6	0	6.710531	-3.285413	-1.812918
153	1	0	6.961767	-2.791391	-0.875253
154	1	0	6.371940	-4.303201	-1.616605
155	17	0	8.224127	-3.422860	-2.795375
156	6	0	3.327411	-4.774234	0.254426
157	1	0	4.158681	-5.038762	-0.407254
158	6	0	2.157675	-5.713280	0.003381
159	1	0	2.415698	-6.719787	0.331551
160	17	0	1.735513	-5.817744	-1.747977
161	6	0	5.957298	-1.049931	-2.743273
162	1	0	6.019749	-0.503290	-1.796382
163	1	0	6.912898	-0.963080	-3.260960
164	17	0	4.730525	-0.197948	-3.772073
165	6	0	1.039877	-0.185832	0.521809
166	1	0	0.658296	0.797077	0.787718
167	1	0	0.387370	-0.684823	-0.193367
168	17	0	0.819701	-1.147824	2.179565
169	1	0	1.274178	-5.362870	0.538168
170	6	0	3.789469	-4.778728	1.717150
171	1	0	2.954823	-4.575360	2.387003
172	1	0	4.574486	-4.036501	1.856759
173	17	0	4.481381	-6.389357	2.185730

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1	7	0	-10.087427	-3.679041	2.491035
2	6	0	-11.213843	-3.282438	1.654945
3	6	0	-12.565021	-3.640846	2.278238
4	8	0	-12.722865	-4.426500	3.187673
5	6	0	-11.108212	-3.928163	0.254322
6	6	0	-9.851601	-3.489341	-0.503358
7	6	0	-9.707024	-4.200944	-1.849669
8	7	0	-8.514253	-3.744624	-2.547692
9	6	0	-8.227987	-4.212100	-3.831819
10	7	0	-6.954851	-3.820689	-4.257288
11	7	0	-8.970265	-4.918187	-4.605329
12	1	0	-10.245666	-4.635099	2.806628
13	1	0	-7.690784	-3.680797	-1.960426
14	1	0	-6.826670	-4.047167	-5.235337
15	1	0	-6.725655	-2.853250	-4.058675
16	1	0	-9.806271	-5.246405	-4.125149
17	7	0	-1.224152	8.537347	-2.428262
18	6	0	-1.363652	8.029509	-1.062666
19	6	0	-1.166984	6.514334	-0.939827
20	8	0	-0.524822	5.960761	-0.067568
21	6	0	-2.695708	8.556623	-0.444566
22	6	0	-2.751609	8.509116	1.101953
23	6	0	-3.956820	7.967546	-1.097010
24	6	0	-3.063200	7.162085	1.769455
25	1	0	-1.928247	8.136098	-3.041351
26	7	0	2.354515	5.458207	1.012214
27	6	0	2.664874	4.020978	1.015484

28	6	0	4.135856	3.783280	0.699783	54	6	0	-0.852847	-3.879129	-3.451116
29	8	0	4.679857	2.690385	0.897845	55	6	0	2.056115	-1.886008	-0.121771
30	6	0	1.819650	3.289098	-0.038472	56	6	0	4.725084	0.074080	-3.647698
31	7	0	4.749478	4.838521	0.137091	57	6	0	2.135583	-2.362859	-6.944252
32	6	0	6.069766	4.752631	-0.430228	58	7	0	0.857238	-2.753305	-2.081066
33	6	0	7.037679	3.903044	0.409394	59	6	0	-0.296800	-3.486086	-2.242761
34	8	0	7.730556	3.031640	-0.083192	60	6	0	-0.840666	-3.827233	-0.953138
35	1	0	1.379969	5.622487	0.770847	61	6	0	-0.004493	-3.300775	-0.014328
36	1	0	4.158050	5.660439	0.039397	62	6	0	1.042506	-2.615251	-0.728006
37	7	0	8.254340	2.033404	2.830434	63	7	0	3.107535	-1.032387	-2.168514
38	6	0	7.753228	1.199263	3.931539	64	6	0	3.005845	-1.142965	-0.802059
39	6	0	8.360948	-0.203320	4.009935	65	6	0	4.034197	-0.358919	-0.162142
40	8	0	8.033413	-1.038133	4.824377	66	6	0	4.761456	0.221148	-1.154732
41	6	0	6.200349	1.078563	3.841354	67	6	0	4.193328	-0.222337	-2.404502
42	8	0	5.844342	0.687029	2.524074	68	7	0	3.215577	-1.316963	-4.994194
43	6	0	5.486489	2.354433	4.286179	69	6	0	4.272057	-0.454985	-4.848737
44	1	0	8.025696	1.570246	1.949215	70	6	0	4.864488	-0.184881	-6.133142
45	1	0	5.501167	1.453156	2.026914	71	6	0	4.152512	-0.891833	-7.054695
46	7	0	0.892688	-5.342975	4.006670	72	6	0	3.113516	-1.587077	-6.339441
47	6	0	1.321641	-5.468040	5.396443	73	7	0	0.825505	-2.879141	-4.934780
48	6	0	1.623132	-6.915018	5.795932	74	6	0	1.071682	-2.959860	-6.283376
49	8	0	1.294506	-7.895253	5.163015	75	6	0	0.051460	-3.754073	-6.920240
50	6	0	0.256704	-4.882000	6.338748	76	6	0	-0.806621	-4.156042	-5.940456
51	1	0	0.141103	-6.012652	3.845939	77	6	0	-0.304722	-3.620689	-4.699998
52	16	0	3.348629	-3.830764	-3.520309	78	1	0	-1.693613	-4.768793	-6.030426
53	26	0	1.990009	-1.956002	-3.533359	79	1	0	0.010354	-3.966149	-7.980190

80	1	0	4.296342	-0.940169	-8.125977	106	1	0	4.404465	2.214466	4.200160
81	1	0	5.716512	0.462970	-6.290739	107	1	0	5.718632	2.589098	5.330252
82	1	0	5.606824	0.888887	-1.055634	108	1	0	5.919375	0.258760	4.512021
83	1	0	4.180075	-0.269776	0.906081	109	1	0	9.270333	2.076233	2.859832
84	1	0	-1.742243	-4.407020	-0.804655	110	8	0	9.330011	-0.417867	3.089701
85	1	0	-0.068350	-3.364639	1.064519	111	1	0	9.633844	-1.331185	3.226861
86	1	0	2.091132	-1.876359	0.962237	112	8	0	2.295500	-6.992971	6.968918
87	1	0	2.196554	-2.495985	-8.019078	113	1	0	2.421722	-7.939855	7.150354
88	1	0	5.586394	0.732516	-3.680379	114	8	0	-13.593899	-2.994289	1.681312
89	1	0	-1.761407	-4.470560	-3.414584	115	1	0	-14.405469	-3.305346	2.117420
90	8	0	0.919890	-0.504946	-3.696454	116	1	0	-0.316628	8.288160	-2.812215
91	1	0	-9.701747	-5.293910	-1.694851	117	8	0	-1.759928	5.807493	-1.931447
92	1	0	-10.575844	-3.976100	-2.480505	118	1	0	-1.580313	4.860219	-1.770574
93	1	0	-9.878698	-2.405808	-0.675095	119	1	0	-0.546855	8.453538	-0.469192
94	1	0	-8.976137	-3.688869	0.125092	120	1	0	-4.037266	6.886750	-0.950079
95	1	0	-11.107380	-5.020118	0.378398	121	1	0	-4.850156	8.429638	-0.663673
96	1	0	-12.006257	-3.676004	-0.320743	122	1	0	-3.986419	8.161331	-2.173605
97	1	0	-11.191755	-2.193040	1.528330	123	1	0	-2.659434	9.619237	-0.715458
98	1	0	-10.077815	-3.118172	3.339664	124	1	0	-3.132161	7.292705	2.854443
99	1	0	0.066113	-3.842617	6.062175	125	1	0	-4.022174	6.754944	1.432735
100	1	0	-0.683690	-5.437258	6.247962	126	1	0	-2.289330	6.416219	1.577223
101	1	0	0.583403	-4.926248	7.380505	127	1	0	-1.805110	8.899261	1.498868
102	1	0	1.646599	-5.651376	3.395765	128	1	0	-3.521272	9.229251	1.408778
103	1	0	2.248772	-4.897469	5.528025	129	1	0	0.756493	3.383384	0.197100
104	1	0	8.001869	1.677467	4.887163	130	1	0	1.989462	3.724979	-1.028784
105	1	0	5.771778	3.207808	3.665196	131	1	0	2.088053	2.231510	-0.075060

132	1	0	2.482842	3.543540	1.989950
133	1	0	2.517187	5.863019	1.929823
134	1	0	6.058608	4.306965	-1.430762
135	1	0	6.482973	5.764045	-0.507660
136	8	0	7.074607	4.266243	1.692344
137	1	0	7.586173	3.563537	2.204408
138	1	0	2.539565	-4.632865	-2.797965
139	15	0	-2.620135	2.343833	-6.009184
140	8	0	-4.081933	2.520479	-6.192541
141	8	0	-1.826263	3.634059	-5.474167
142	8	0	-1.786161	1.889677	-7.290482
143	8	0	-2.133148	1.249395	-4.915284
144	6	0	-2.729577	0.988991	-3.699651
145	1	0	0.454692	-0.591456	-4.544431
146	6	0	-4.171022	0.723930	-3.618827
147	1	0	-4.752231	1.285429	-4.346809
148	1	0	-4.540895	0.883379	-2.607255
149	17	0	-4.548175	-1.074516	-3.992887
150	6	0	-2.348191	1.357864	-8.523077
151	1	0	-1.465489	1.053434	-9.088722
152	6	0	-3.047788	2.509450	-9.257336
153	1	0	-3.989607	2.775488	-8.776925
154	1	0	-2.382180	3.373051	-9.282343
155	17	0	-3.406061	2.067661	-10.973030
156	6	0	-2.167642	4.959679	-5.959780
157	1	0	-2.634921	4.898811	-6.947108
158	6	0	-0.872351	5.751116	-6.042682
159	1	0	-1.085426	6.802453	-6.232236
160	17	0	0.184713	5.172116	-7.387141
161	6	0	-3.255044	0.153903	-8.306410
162	1	0	-4.072011	0.388600	-7.622832
163	1	0	-3.666635	-0.155904	-9.267151
164	17	0	-2.351109	-1.253474	-7.631440
165	6	0	-1.812106	0.828185	-2.571583
166	1	0	-2.130770	0.044660	-1.885559
167	1	0	-0.770531	0.686284	-2.864648
168	17	0	-1.841844	2.370647	-1.463180
169	1	0	-0.308102	5.644286	-5.114709
170	6	0	-3.163133	5.534891	-4.948715
171	1	0	-2.705267	5.623841	-3.964180
172	1	0	-4.043476	4.894367	-4.908146
173	17	0	-3.727827	7.187912	-5.433890

$^{4}TS_{\alpha\text{-reb}}$

1	7	0	9.046929	7.282203	2.998278
2	6	0	9.060716	6.027869	3.741200
3	6	0	10.339491	5.844739	4.562219
4	8	0	11.360937	6.477530	4.403194
5	6	0	8.890152	4.824239	2.783944
6	6	0	7.548095	4.851360	2.045874
7	6	0	7.417088	3.725734	1.017314
8	7	0	6.121902	3.792118	0.355569

9	6	0	5.721380	2.819264	-0.553741	35	1	0	-3.231320	-3.432660	3.824327
10	7	0	4.513025	3.145947	-1.170463	36	1	0	-5.633364	-4.068334	2.494087
11	7	0	6.327431	1.722970	-0.851911	37	7	0	-10.163978	-0.046407	1.662599
12	1	0	9.959175	7.403352	2.560258	38	6	0	-9.920886	1.314875	2.158926
13	1	0	5.829808	4.726837	0.097685	39	6	0	-10.537772	2.433556	1.317022
14	1	0	4.171806	2.388993	-1.751704	40	8	0	-10.388939	3.614059	1.545758
15	1	0	3.804315	3.490969	-0.534423	41	6	0	-8.380898	1.552365	2.290703
16	1	0	7.258751	1.685886	-0.442585	42	8	0	-7.742190	1.133505	1.094370
17	7	0	-0.104401	-7.372130	3.782449	43	6	0	-7.795119	0.884880	3.533990
18	6	0	-0.181885	-6.073095	4.457371	44	1	0	-9.748140	-0.122566	0.733007
19	6	0	-0.449892	-4.908219	3.505217	45	1	0	-7.283444	0.284907	1.235858
20	8	0	-1.250896	-4.014100	3.711376	46	7	0	-3.265123	7.543656	0.821339
21	6	0	1.069115	-5.882979	5.369643	47	6	0	-3.837416	8.444858	1.816142
22	6	0	0.923300	-4.766764	6.432848	48	6	0	-4.337232	9.758664	1.209578
23	6	0	2.391529	-5.790060	4.592108	49	8	0	-4.037612	10.176746	0.111904
24	6	0	1.127416	-3.312840	5.982883	50	6	0	-2.806611	8.749232	2.916854
25	1	0	0.609279	-7.349909	3.058136	51	1	0	-2.596251	8.071894	0.262208
26	7	0	-4.214421	-3.214531	3.680737	52	16	0	-2.788937	2.159112	-5.375567
27	6	0	-4.377897	-2.029910	2.825418	53	26	0	-1.468890	0.773925	-4.006984
28	6	0	-5.615869	-2.158985	1.939973	54	6	0	1.113076	3.009241	-3.797896
29	8	0	-6.070119	-1.203128	1.295801	55	6	0	-2.920407	2.166843	-1.237271
30	6	0	-3.155239	-1.829122	1.923195	56	6	0	-3.921914	-1.608386	-4.087523
31	7	0	-6.118966	-3.403114	1.896255	57	6	0	-0.180227	-0.438294	-6.944751
32	6	0	-7.199031	-3.762604	1.019846	58	7	0	-1.026445	2.310930	-2.799401
33	6	0	-8.358347	-2.752876	1.020742	59	6	0	0.106643	3.087616	-2.844752
34	8	0	-8.921695	-2.417029	-0.003654	60	6	0	0.090641	4.033515	-1.759793

61	6	0	-1.064043	3.829709	-1.065891	87	1	0	0.211911	-0.809209	-7.885709
62	6	0	-1.744631	2.734899	-1.707288	88	1	0	-4.697976	-2.365843	-4.115385
63	7	0	-3.049710	0.317170	-2.841439	89	1	0	1.938168	3.708878	-3.714485
64	6	0	-3.513609	1.031025	-1.764123	90	8	0	-0.389211	-0.405513	-2.986816
65	6	0	-4.716382	0.425517	-1.243233	91	1	0	8.250272	3.781240	0.295854
66	6	0	-4.978367	-0.656406	-2.025458	92	1	0	7.494211	2.752415	1.517535
67	6	0	-3.949576	-0.702075	-3.038323	93	1	0	6.725011	4.769546	2.767129
68	7	0	-1.974776	-0.696842	-5.283626	94	1	0	7.444040	5.824842	1.552968
69	6	0	-3.009460	-1.587401	-5.135127	95	1	0	9.716302	4.841758	2.059454
70	6	0	-3.022167	-2.509787	-6.241644	96	1	0	8.991157	3.896517	3.358265
71	6	0	-1.986251	-2.165710	-7.057514	97	1	0	8.218364	6.024122	4.443723
72	6	0	-1.327663	-1.040108	-6.446290	98	1	0	8.956534	8.062047	3.645024
73	7	0	0.180324	1.160396	-5.115842	99	1	0	-2.469230	7.810438	3.361860
74	6	0	0.518147	0.582660	-6.317189	100	1	0	-1.934245	9.260307	2.494216
75	6	0	1.720204	1.188899	-6.829502	101	1	0	-3.235197	9.386099	3.694667
76	6	0	2.099673	2.140825	-5.931697	102	1	0	-3.990637	7.266138	0.163346
77	6	0	1.122166	2.131095	-4.872660	103	1	0	-4.700268	7.951846	2.279095
78	1	0	2.952521	2.805124	-5.973536	104	1	0	-10.367937	1.421644	3.154874
79	1	0	2.200161	0.909647	-7.758050	105	1	0	-7.956924	-0.196326	3.519748
80	1	0	-1.675738	-2.629048	-7.984630	106	1	0	-6.717051	1.068208	3.571132
81	1	0	-3.739836	-3.310073	-6.365052	107	1	0	-8.243767	1.293562	4.445483
82	1	0	-5.802004	-1.352238	-1.938678	108	1	0	-8.244934	2.636937	2.370624
83	1	0	-5.280146	0.784846	-0.393085	109	1	0	-11.160884	-0.201979	1.534501
84	1	0	0.863277	4.769585	-1.578544	110	8	0	-11.298487	1.976863	0.294933
85	1	0	-1.431949	4.357966	-0.195695	111	1	0	-11.629846	2.765789	-0.166600
86	1	0	-3.390420	2.624937	-0.373693	112	8	0	-5.149642	10.436841	2.054637

113	1	0	-5.393634	11.260417	1.598852	139	15	0	2.637515	-3.386391	-1.769379
114	8	0	10.218893	4.865757	5.488886	140	8	0	3.016862	-3.255170	-0.340573
115	1	0	11.079871	4.800408	5.936310	141	8	0	2.155659	-4.845390	-2.236732
116	1	0	-0.981988	-7.571915	3.308684	142	8	0	3.761675	-3.020331	-2.845821
117	8	0	0.273724	-4.972723	2.369780	143	8	0	1.385192	-2.485716	-2.278464
118	1	0	-0.023497	-4.253045	1.779685	144	6	0	0.386898	-1.925818	-1.493505
119	1	0	-1.055272	-6.093492	5.117269	145	1	0	0.437143	-0.469734	-3.494352
120	1	0	2.431418	-4.917155	3.934931	146	6	0	0.901509	-1.029367	-0.410004
121	1	0	3.231432	-5.721758	5.292008	147	1	0	1.591456	-0.308455	-0.852792
122	1	0	2.557514	-6.678522	3.975387	148	1	0	1.436014	-1.608128	0.349473
123	1	0	1.089081	-6.830719	5.922406	149	17	0	-0.375946	-0.097615	0.443990
124	1	0	1.054823	-2.643144	6.846478	150	6	0	4.937755	-2.193619	-2.593000
125	1	0	2.116540	-3.160808	5.539167	151	1	0	5.342628	-2.022208	-3.592159
126	1	0	0.375237	-2.994011	5.258325	152	6	0	5.924494	-3.041653	-1.780178
127	1	0	-0.062096	-4.861954	6.907927	153	1	0	5.600007	-3.143088	-0.744237
128	1	0	1.655535	-4.985661	7.221167	154	1	0	6.009263	-4.025806	-2.241859
129	1	0	-2.265663	-1.624097	2.522676	155	17	0	7.576997	-2.311462	-1.778733
130	1	0	-2.963633	-2.732505	1.335890	156	6	0	2.757961	-6.031316	-1.655316
131	1	0	-3.326751	-0.995894	1.239442	157	1	0	3.748529	-5.800762	-1.252814
132	1	0	-4.525743	-1.108043	3.407669	158	6	0	2.871498	-7.068071	-2.760588
133	1	0	-4.639405	-3.066094	4.590747	159	1	0	3.142749	-8.036597	-2.342064
134	1	0	-6.874058	-3.848636	-0.022417	160	17	0	4.147850	-6.631457	-3.962922
135	1	0	-7.594237	-4.734617	1.333450	161	6	0	4.618851	-0.865042	-1.928030
136	8	0	-8.701850	-2.341914	2.243774	162	1	0	4.096227	-1.016029	-0.983055
137	1	0	-9.337991	-1.566823	2.149400	163	1	0	5.512804	-0.261665	-1.743044
138	1	0	-2.542961	3.319670	-4.733963	164	17	0	3.546104	0.158349	-2.980669

165	6	0	-0.915885	-2.565399	-1.555115
166	1	0	-1.709053	-1.930028	-1.176999
167	1	0	-1.135250	-2.953737	-2.544067
168	17	0	-1.007308	-4.136404	-0.447175
169	1	0	1.928760	-7.146749	-3.304417
170	6	0	1.835561	-6.466503	-0.511678
171	1	0	0.846641	-6.737796	-0.881895
172	1	0	1.746777	-5.660459	0.213807
173	17	0	2.505570	-7.897675	0.376198

$^{2}P_{\alpha}$

1	7	0	9.275240	7.010307	2.685725
2	6	0	9.060715	6.027868	3.741199
3	6	0	10.337014	5.722637	4.529292
4	8	0	11.459366	5.994703	4.161549
5	6	0	8.495036	4.712696	3.156519
6	6	0	7.130108	4.900693	2.484949
7	6	0	6.642332	3.614899	1.815027
8	7	0	5.336146	3.803697	1.197028
9	6	0	4.690624	2.736612	0.582725
10	7	0	3.533115	3.124422	-0.092787
11	7	0	5.054436	1.502181	0.586613
12	1	0	10.134847	6.768496	2.194390
13	1	0	5.225629	4.681265	0.703570
14	1	0	3.024026	2.324405	-0.449583
15	1	0	2.936507	3.756395	0.427235
16	1	0	5.981785	1.376399	0.984851
17	7	0	0.159840	-7.478582	4.211306
18	6	0	-0.181896	-6.073090	4.457367
19	6	0	0.168434	-5.149645	3.285012
20	8	0	-0.575792	-4.294723	2.829644
21	6	0	0.409876	-5.625060	5.828371
22	6	0	-0.156409	-4.285626	6.360702
23	6	0	1.943888	-5.683329	5.888551
24	6	0	0.423692	-2.983859	5.788136
25	1	0	1.134137	-7.555872	3.929875
26	7	0	-3.593724	-3.263085	2.648534
27	6	0	-4.377854	-2.029888	2.825448
28	6	0	-5.663217	-2.128937	2.009980
29	8	0	-6.255197	-1.143096	1.558800
30	6	0	-3.634476	-0.719900	2.534863
31	7	0	-6.097854	-3.396141	1.871625
32	6	0	-7.199070	-3.762611	1.019826
33	6	0	-8.301461	-2.697160	0.943903
34	8	0	-8.687091	-2.238900	-0.116934
35	1	0	-3.119087	-3.241245	1.746814
36	1	0	-5.429720	-4.095076	2.187874
37	7	0	-10.022276	0.008623	1.498282
38	6	0	-9.920866	1.314859	2.158916
39	6	0	-10.359620	2.508414	1.306254
40	8	0	-10.307500	3.661018	1.675857
41	6	0	-8.464548	1.556938	2.657381

42	8	0	-7.562747	1.367777	1.577146	68	7	0	-2.792208	-0.846785	-4.393024
43	6	0	-8.111085	0.702288	3.873634	69	6	0	-3.982840	-1.493752	-4.152994
44	1	0	-9.409099	0.010573	0.682362	70	6	0	-4.158966	-2.589217	-5.072979
45	1	0	-7.121934	0.500642	1.651470	71	6	0	-3.068863	-2.594805	-5.887530
46	7	0	-3.241911	7.699073	0.710792	72	6	0	-2.219253	-1.514502	-5.452466
47	6	0	-3.837413	8.444857	1.816142	73	7	0	-0.344846	0.574627	-4.455774
48	6	0	-4.450209	9.775150	1.370770	74	6	0	-0.089450	-0.287130	-5.504284
49	8	0	-4.231474	10.322232	0.311465	75	6	0	1.242522	-0.083854	-6.009530
50	6	0	-2.789369	8.702860	2.912102	76	6	0	1.799556	0.914182	-5.267903
51	1	0	-2.626078	8.329688	0.198819	77	6	0	0.801673	1.334027	-4.320256
52	16	0	-2.995200	2.182434	-5.104840	78	1	0	2.789597	1.342947	-5.348714
53	26	0	-2.117125	0.842760	-3.552971	79	1	0	1.683859	-0.646128	-6.821912
54	6	0	0.953722	2.398247	-3.443526	80	1	0	-2.838656	-3.267782	-6.703092
55	6	0	-3.234639	2.884471	-1.074506	81	1	0	-5.014438	-3.251748	-5.083436
56	6	0	-4.899411	-1.136751	-3.175555	82	1	0	-6.660565	-0.192200	-1.147465
57	6	0	-0.970526	-1.243462	-5.986982	83	1	0	-5.784097	2.093947	-0.028089
58	7	0	-1.296755	2.318259	-2.469824	84	1	0	0.984242	4.640291	-1.689051
59	6	0	-0.040412	2.871537	-2.601309	85	1	0	-1.398478	4.956232	-0.411299
60	6	0	0.090625	4.033513	-1.759788	86	1	0	-3.623520	3.581440	-0.339066
61	6	0	-1.101872	4.191152	-1.118524	87	1	0	-0.636293	-1.855993	-6.818112
62	6	0	-1.954417	3.114675	-1.559155	88	1	0	-5.798988	-1.735862	-3.078536
63	7	0	-3.703020	0.835929	-2.341766	89	1	0	1.905804	2.919173	-3.443364
64	6	0	-4.031875	1.803720	-1.415557	90	8	0	-0.078193	-2.869028	-3.079895
65	6	0	-5.308666	1.513539	-0.807787	91	1	0	7.392780	3.273933	1.081398
66	6	0	-5.758027	0.360460	-1.371606	92	1	0	6.549081	2.820179	2.565469
67	6	0	-4.767264	-0.041650	-2.337994	93	1	0	6.389123	5.221575	3.228142

94	1	0	7.212666	5.706145	1.746187	120	1	0	2.416651	-5.003899	5.174632
95	1	0	9.217965	4.323272	2.426025	121	1	0	2.289735	-5.413622	6.892550
96	1	0	8.424451	3.969633	3.958791	122	1	0	2.309361	-6.693616	5.681790
97	1	0	8.326373	6.427499	4.451325	123	1	0	0.036123	-6.405707	6.503130
98	1	0	9.452331	7.922933	3.098468	124	1	0	-0.027738	-2.121825	6.291088
99	1	0	-2.373491	7.748489	3.242930	125	1	0	1.505030	-2.919195	5.945790
100	1	0	-1.969517	9.316109	2.521392	126	1	0	0.228588	-2.877730	4.718729
101	1	0	-3.230714	9.221891	3.766441	127	1	0	-1.246141	-4.286300	6.224095
102	1	0	-3.969557	7.451660	0.043105	128	1	0	0.006354	-4.281658	7.446500
103	1	0	-4.646319	7.843471	2.247349	129	1	0	-2.764271	-0.631753	3.192601
104	1	0	-10.581989	1.325458	3.034438	130	1	0	-3.287466	-0.688273	1.498016
105	1	0	-8.171398	-0.364771	3.644625	131	1	0	-4.286710	0.142080	2.694029
106	1	0	-7.088722	0.927309	4.192417	132	1	0	-4.701172	-2.014812	3.877067
107	1	0	-8.783166	0.917540	4.710949	133	1	0	-2.846730	-3.335142	3.334356
108	1	0	-8.414790	2.615346	2.937173	134	1	0	-6.874849	-3.941728	-0.011577
109	1	0	-10.960298	-0.125987	1.128446	135	1	0	-7.646622	-4.685886	1.404851
110	8	0	-10.842177	2.149789	0.093915	136	8	0	-8.823788	-2.397723	2.133200
111	1	0	-11.080429	2.977618	-0.356814	137	1	0	-9.388313	-1.569738	2.019827
112	8	0	-5.264815	10.304203	2.314178	138	1	0	-1.959237	3.042580	-5.210050
113	1	0	-5.585562	11.150018	1.957441	139	15	0	2.605797	-4.270700	-0.765975
114	8	0	10.080506	5.082331	5.693661	140	8	0	2.257102	-4.011802	0.663427
115	1	0	10.942315	4.902921	6.107017	141	8	0	2.908971	-5.809255	-1.124294
116	1	0	-0.389468	-7.838048	3.434449	142	8	0	3.918937	-3.515035	-1.268800
117	8	0	1.389230	-5.394696	2.784972	143	8	0	1.550058	-3.900308	-1.885287
118	1	0	1.588963	-4.778820	2.034580	144	6	0	0.105559	-3.618108	-1.943359
119	1	0	-1.271312	-6.008745	4.546988	145	1	0	0.277955	-1.973892	-2.964547

146	6	0	-0.306846	-2.893118	-0.652797		172	1	0	1.803166	-6.973489	0.918084
147	1	0	0.284026	-1.982045	-0.549979		173	17	0	3.264574	-8.664839	1.688638
148	1	0	-0.186596	-3.511624	0.234431							
149	17	0	-2.041054	-2.395819	-0.736828	$^4\mathbf{P}_\alpha$						
150	6	0	4.578948	-2.378581	-0.640276		1	7	0	9.268629	7.015021	2.688842
151	1	0	5.253293	-2.018855	-1.419881		2	6	0	9.060710	6.027861	3.741198
152	6	0	5.401781	-2.936824	0.529792		3	6	0	10.341727	5.719639	4.520450
153	1	0	4.770464	-3.153550	1.392508		4	8	0	11.461794	5.993418	4.147112
154	1	0	5.909185	-3.843586	0.200909		5	6	0	8.492358	4.714935	3.153963
155	17	0	6.686147	-1.784732	1.069918		6	6	0	7.123934	4.905241	2.490181
156	6	0	3.617831	-6.677675	-0.208403		7	6	0	6.632167	3.621528	1.819098
157	1	0	4.105312	-6.095498	0.579026		8	7	0	5.322489	3.812465	1.209067
158	6	0	4.649401	-7.460529	-1.006464		9	6	0	4.671248	2.747002	0.598337
159	1	0	5.054203	-8.271884	-0.402717		10	7	0	3.508596	3.137074	-0.067602
160	17	0	6.047204	-6.436231	-1.518501		11	7	0	5.033186	1.512086	0.597755
161	6	0	3.645942	-1.260022	-0.208889		12	1	0	10.125525	6.775921	2.191481
162	1	0	2.912613	-1.611988	0.516463		13	1	0	5.209496	4.690993	0.717899
163	1	0	4.216684	-0.411240	0.190157		14	1	0	2.996234	2.337495	-0.420805
164	17	0	2.714655	-0.567692	-1.612199		15	1	0	2.916904	3.767797	0.459562
165	6	0	-0.644221	-4.920532	-2.247121		16	1	0	5.963604	1.384452	0.988180
166	1	0	-1.686899	-4.686601	-2.452560		17	7	0	0.162848	-7.479744	4.220888
167	1	0	-0.182455	-5.388132	-3.115158		18	6	0	-0.181892	-6.073082	4.457366
168	17	0	-0.617551	-6.112815	-0.894966		19	6	0	0.176562	-5.157389	3.281934
169	1	0	4.195984	-7.861350	-1.914449		20	8	0	-0.569130	-4.313225	2.809045
170	6	0	2.553613	-7.584491	0.420991		21	6	0	0.398445	-5.617893	5.830615
171	1	0	2.081231	-8.218708	-0.330248		22	6	0	-0.170642	-4.274418	6.349475

23	6	0	1.931772	-5.677833	5.905616	49	8	0	-4.203125	10.326164	0.309594
24	6	0	0.413381	-2.977372	5.770157	50	6	0	-2.794881	8.697168	2.918718
25	1	0	1.139619	-7.557374	3.948198	51	1	0	-2.619279	8.321978	0.204934
26	7	0	-3.606526	-3.276759	2.694319	52	16	0	-3.029301	2.292377	-5.349895
27	6	0	-4.377856	-2.029889	2.825459	53	26	0	-2.100881	0.876644	-3.615812
28	6	0	-5.653653	-2.133890	1.995944	54	6	0	0.973330	2.417147	-3.444981
29	8	0	-6.232740	-1.151022	1.521476	55	6	0	-3.216027	2.848589	-1.051017
30	6	0	-3.613778	-0.737577	2.509678	56	6	0	-4.876314	-1.114391	-3.265212
31	7	0	-6.097536	-3.399028	1.872057	57	6	0	-0.861915	-1.285309	-5.964752
32	6	0	-7.199065	-3.762608	1.019817	58	7	0	-1.289247	2.326171	-2.484993
33	6	0	-8.305077	-2.700027	0.954260	59	6	0	-0.034612	2.884375	-2.615039
34	8	0	-8.710572	-2.252207	-0.103476	60	6	0	0.090618	4.033508	-1.759786
35	1	0	-3.115320	-3.285312	1.801283	61	6	0	-1.098404	4.172724	-1.103962
36	1	0	-5.445333	-4.100689	2.213588	62	6	0	-1.945128	3.098446	-1.549461
37	7	0	-10.038402	0.000740	1.516490	63	7	0	-3.678063	0.830027	-2.367420
38	6	0	-9.920859	1.314860	2.158914	64	6	0	-4.004749	1.768672	-1.411852
39	6	0	-10.374777	2.499233	1.301407	65	6	0	-5.283272	1.463840	-0.818245
40	8	0	-10.311209	3.655877	1.656271	66	6	0	-5.735006	0.331706	-1.422117
41	6	0	-8.453179	1.558508	2.622862	67	6	0	-4.742299	-0.043878	-2.397192
42	8	0	-7.575175	1.344397	1.527340	68	7	0	-2.737504	-0.837904	-4.441188
43	6	0	-8.077755	0.723911	3.846347	69	6	0	-3.943919	-1.467014	-4.229660
44	1	0	-9.447889	-0.006450	0.683991	70	6	0	-4.104585	-2.562360	-5.147962
45	1	0	-7.135637	0.477327	1.609519	71	6	0	-2.984865	-2.594257	-5.924008
46	7	0	-3.239361	7.694135	0.715283	72	6	0	-2.133387	-1.527921	-5.470542
47	6	0	-3.837414	8.444859	1.816143	73	7	0	-0.282951	0.560307	-4.450278
48	6	0	-4.437483	9.779155	1.365549	74	6	0	0.006008	-0.325557	-5.468254

75	6	0	1.348221	-0.121666	-5.943571	101	1	0	-3.238218	9.220703	3.769293
76	6	0	1.874095	0.902838	-5.215366	102	1	0	-3.964939	7.448439	0.044645
77	6	0	0.848379	1.335290	-4.303466	103	1	0	-4.653199	7.849400	2.242475
78	1	0	2.860146	1.342682	-5.283918	104	1	0	-10.563084	1.337296	3.048089
79	1	0	1.815050	-0.698107	-6.731230	105	1	0	-8.147670	-0.346755	3.637508
80	1	0	-2.738137	-3.278797	-6.724806	106	1	0	-7.047819	0.949482	4.139387
81	1	0	-4.969346	-3.211759	-5.183424	107	1	0	-8.730811	0.956933	4.693869
82	1	0	-6.642221	-0.221922	-1.219967	108	1	0	-8.391939	2.621458	2.882201
83	1	0	-5.761241	2.023220	-0.024875	109	1	0	-10.986257	-0.139855	1.175056
84	1	0	0.980141	4.645877	-1.686113	110	8	0	-10.883806	2.127518	0.104130
85	1	0	-1.393676	4.925529	-0.383301	111	1	0	-11.128763	2.950435	-0.352024
86	1	0	-3.603759	3.527849	-0.299239	112	8	0	-5.259298	10.311953	2.300485
87	1	0	-0.507229	-1.914234	-6.774256	113	1	0	-5.570672	11.160335	1.941512
88	1	0	-5.780926	-1.708775	-3.192893	114	8	0	10.092244	5.074469	5.683662
89	1	0	1.920154	2.946736	-3.434563	115	1	0	10.956521	4.893561	6.091179
90	8	0	-0.105781	-2.950450	-3.062843	116	1	0	-0.379825	-7.843205	3.441224
91	1	0	7.378327	3.282496	1.080249	117	8	0	1.405432	-5.397587	2.799917
92	1	0	6.542830	2.824631	2.567688	118	1	0	1.609543	-4.787157	2.046146
93	1	0	6.386975	5.224069	3.238250	119	1	0	-1.272035	-6.009418	4.537872
94	1	0	7.202737	5.712909	1.753441	120	1	0	2.412523	-5.003055	5.192675
95	1	0	9.211612	4.328726	2.418158	121	1	0	2.268228	-5.403328	6.911495
96	1	0	8.426120	3.968568	3.953542	122	1	0	2.297604	-6.689778	5.707957
97	1	0	8.330306	6.423969	4.457322	123	1	0	0.017499	-6.393742	6.506903
98	1	0	9.447498	7.925971	3.104506	124	1	0	-0.039589	-2.111149	6.264461
99	1	0	-2.387908	7.740473	3.253930	125	1	0	1.494002	-2.912643	5.932514
100	1	0	-1.968215	9.304009	2.532423	126	1	0	0.223722	-2.878853	4.698984

127	1	0	-1.259643	-4.275874	6.206709
128	1	0	-0.014250	-4.262110	7.436137
129	1	0	-2.749751	-0.643850	3.174764
130	1	0	-3.255191	-0.737473	1.476237
131	1	0	-4.256354	0.136474	2.639340
132	1	0	-4.715660	-1.981476	3.871515
133	1	0	-2.872517	-3.336047	3.394967
134	1	0	-6.877541	-3.933312	-0.013824
135	1	0	-7.642578	-4.689972	1.399319
136	8	0	-8.806320	-2.389991	2.150046
137	1	0	-9.379848	-1.567937	2.038590
138	1	0	-2.220410	3.340060	-5.087359
139	15	0	2.622734	-4.279230	-0.753520
140	8	0	2.275868	-4.023742	0.676878
141	8	0	2.946457	-5.814006	-1.110241
142	8	0	3.920690	-3.503096	-1.263181
143	8	0	1.557604	-3.923402	-1.869343
144	6	0	0.104590	-3.693000	-1.925930
145	1	0	0.236576	-2.049420	-2.952277
146	6	0	-0.330455	-2.980545	-0.636041
147	1	0	0.223263	-2.045464	-0.539790
148	1	0	-0.182180	-3.589177	0.253825
149	17	0	-2.084536	-2.555993	-0.713809
150	6	0	4.571630	-2.362095	-0.632590
151	1	0	5.234258	-1.988740	-1.415800
152	6	0	5.411690	-2.918289	0.526145
153	1	0	4.790555	-3.148730	1.392735
154	1	0	5.927131	-3.816457	0.186357
155	17	0	6.686863	-1.755036	1.063773
156	6	0	3.674354	-6.668901	-0.196192
157	1	0	4.163101	-6.076137	0.582508
158	6	0	4.707246	-7.443604	-1.000374
159	1	0	5.129996	-8.244716	-0.395242
160	17	0	6.084478	-6.403736	-1.535954
161	6	0	3.628380	-1.258207	-0.185493
162	1	0	2.907256	-1.623180	0.545482
163	1	0	4.193468	-0.404536	0.211068
164	17	0	2.672892	-0.571529	-1.574919
165	6	0	-0.601620	-5.019657	-2.229667
166	1	0	-1.648654	-4.818606	-2.446887
167	1	0	-0.116891	-5.477640	-3.090297
168	17	0	-0.554660	-6.203857	-0.871250
169	1	0	4.249100	-7.857579	-1.900052
170	6	0	2.628055	-7.584794	0.449818
171	1	0	2.156199	-8.229722	-0.292568
172	1	0	1.874575	-6.980341	0.950379
173	17	0	3.365547	-8.647399	1.717094

$^{2}TS_{\beta H}$

1	7	0	-11.013352	-2.928054	3.054389
2	6	0	-11.213849	-3.282436	1.654939
3	6	0	-12.403936	-4.222340	1.449887

4	8	0	-12.941824	-4.860687	2.328777	30	6	0	1.739530	2.869168	0.598393
5	6	0	-9.937406	-3.940697	1.068990	31	7	0	4.731206	4.830342	0.083774
6	6	0	-8.722422	-3.004122	1.079762	32	6	0	6.069862	4.752681	-0.430288
7	6	0	-7.430369	-3.696949	0.629112	33	6	0	7.032166	3.958222	0.466339
8	7	0	-6.313845	-2.760374	0.658911	34	8	0	7.831563	3.160805	0.011596
9	6	0	-5.028408	-3.144631	0.280803	35	1	0	1.655530	5.327888	-0.243831
10	7	0	-4.085293	-2.154428	0.570882	36	1	0	4.165202	5.673559	0.047102
11	7	0	-4.652337	-4.247325	-0.264956	37	7	0	8.279754	2.145725	2.940260
12	1	0	-11.096478	-3.776034	3.613525	38	6	0	7.753196	1.199245	3.931518
13	1	0	-6.318172	-2.137958	1.457995	39	6	0	8.502511	-0.132069	4.023486
14	1	0	-3.174927	-2.400546	0.201828	40	8	0	8.163832	-1.052955	4.734242
15	1	0	-4.364358	-1.219403	0.296710	41	6	0	6.241330	0.926720	3.639149
16	1	0	-5.409417	-4.928776	-0.288652	42	8	0	6.079083	0.635194	2.256950
17	7	0	-1.604802	9.075731	-2.063121	43	6	0	5.342827	2.071582	4.103491
18	6	0	-1.363654	8.029542	-1.062677	44	1	0	8.203486	1.716766	2.016596
19	6	0	-1.257150	6.625478	-1.675549	45	1	0	5.651299	1.383129	1.799834
20	8	0	-0.381713	5.818380	-1.398677	46	7	0	0.469198	-5.045690	4.288598
21	6	0	-2.407329	8.154961	0.087193	47	6	0	1.321512	-5.467914	5.396034
22	6	0	-2.070480	7.321683	1.348196	48	6	0	0.523651	-5.976462	6.599635
23	6	0	-3.860884	7.969048	-0.374823	49	8	0	-0.665651	-5.813022	6.767976
24	6	0	-2.405363	5.822844	1.328590	50	6	0	2.240753	-4.314766	5.832369
25	1	0	-2.403585	8.818681	-2.637416	51	1	0	-0.213266	-4.378963	4.647100
26	7	0	2.213000	5.362634	0.608320	52	16	0	2.450714	-3.320474	-4.411482
27	6	0	2.664795	4.020919	1.015575	53	26	0	1.489224	-1.348859	-3.558665
28	6	0	4.099625	3.749726	0.569072	54	6	0	-1.422937	-3.201999	-3.300462
29	8	0	4.629486	2.636924	0.689503	55	6	0	2.208431	-2.032107	-0.306542

56	6	0	4.468086	0.257491	-3.904438	82	1	0	5.867742	0.536579	-1.412334
57	6	0	0.697287	-0.648985	-6.815525	83	1	0	4.601556	-0.714675	0.597858
58	7	0	0.605590	-2.452111	-2.118357	84	1	0	-1.721022	-4.428796	-0.757558
59	6	0	-0.572933	-3.160296	-2.201982	85	1	0	0.314841	-3.779818	0.930587
60	6	0	-0.840511	-3.827368	-0.952721	86	1	0	2.428967	-2.229565	0.737363
61	6	0	0.171780	-3.485226	-0.101877	87	1	0	0.453201	-0.396609	-7.842197
62	6	0	1.062281	-2.622346	-0.838258	88	1	0	5.413440	0.778812	-4.013405
63	7	0	3.004872	-0.922492	-2.340793	89	1	0	-2.334709	-3.781369	-3.195526
64	6	0	3.096753	-1.230484	-1.004401	90	8	0	0.735107	0.159496	-3.064610
65	6	0	4.300595	-0.656248	-0.440306	91	1	0	-7.241472	-4.578004	1.266298
66	6	0	4.944500	-0.025537	-1.455699	92	1	0	-7.542083	-4.066306	-0.398150
67	6	0	4.135216	-0.207364	-2.640779	93	1	0	-8.909923	-2.143441	0.425254
68	7	0	2.429725	-0.453597	-5.073420	94	1	0	-8.598652	-2.611202	2.095645
69	6	0	3.667673	0.135663	-5.036195	95	1	0	-9.717775	-4.841463	1.659282
70	6	0	3.988143	0.691711	-6.326501	96	1	0	-10.150201	-4.275944	0.047706
71	6	0	2.915550	0.456295	-7.135749	97	1	0	-11.417059	-2.367999	1.084218
72	6	0	1.940889	-0.252956	-6.345569	98	1	0	-11.771581	-2.326677	3.367507
73	7	0	-0.097161	-1.786377	-4.798276	99	1	0	2.821817	-3.973228	4.972899
74	6	0	-0.245577	-1.373574	-6.094317	100	1	0	1.648219	-3.470263	6.202056
75	6	0	-1.492090	-1.863123	-6.633117	101	1	0	2.921789	-4.630697	6.626121
76	6	0	-2.081516	-2.601340	-5.650711	102	1	0	-0.086107	-5.837868	3.971797
77	6	0	-1.197467	-2.553374	-4.509562	103	1	0	1.950912	-6.298335	5.053885
78	1	0	-3.017391	-3.143558	-5.682524	104	1	0	7.828012	1.643758	4.931480
79	1	0	-1.846290	-1.672515	-7.637461	105	1	0	5.600126	3.009188	3.603578
80	1	0	2.781056	0.732825	-8.173145	106	1	0	4.300692	1.834590	3.868898
81	1	0	4.913251	1.200036	-6.564592	107	1	0	5.424886	2.218100	5.185460

108	1	0	5.981337	0.020099	4.197155	134	1	0	6.104247	4.271647	-1.413302
109	1	0	9.272518	2.302910	3.095033	135	1	0	6.463571	5.769269	-0.533802
110	8	0	9.610831	-0.176103	3.247732	136	8	0	6.937371	4.279270	1.758939
111	1	0	10.000149	-1.056317	3.385398	137	1	0	7.484033	3.620558	2.288219
112	8	0	1.305140	-6.631978	7.490875	138	1	0	1.957818	-4.199807	-3.514904
113	1	0	0.723615	-6.894137	8.224720	139	15	0	-1.720624	3.080131	-4.932301
114	8	0	-12.789521	-4.288486	0.154103	140	8	0	-2.269147	4.039455	-3.929132
115	1	0	-13.523133	-4.925722	0.116263	141	8	0	-0.132350	2.914216	-4.966835
116	1	0	-0.810683	9.136415	-2.695961	142	8	0	-2.097110	3.449409	-6.448951
117	8	0	-2.217235	6.378874	-2.577170	143	8	0	-2.175355	1.562175	-4.856171
118	1	0	-2.126094	5.463064	-2.941018	144	6	0	-2.663630	0.732753	-3.768740
119	1	0	-0.379699	8.214903	-0.619870	145	1	0	-2.792147	-0.238209	-4.253578
120	1	0	-4.046741	6.971746	-0.781960	146	6	0	-4.041398	1.271025	-3.357884
121	1	0	-4.544048	8.123627	0.467500	147	1	0	-4.648568	1.428822	-4.249046
122	1	0	-4.125194	8.701093	-1.143796	148	1	0	-3.951995	2.194882	-2.788341
123	1	0	-2.300233	9.207760	0.378224	149	17	0	-4.920522	0.071901	-2.325810
124	1	0	-2.174539	5.376421	2.301884	150	6	0	-3.036379	4.459081	-6.883724
125	1	0	-3.469100	5.648680	1.138747	151	1	0	-3.094690	4.304818	-7.963361
126	1	0	-1.831486	5.278991	0.575018	152	6	0	-2.427604	5.843300	-6.612833
127	1	0	-1.004121	7.450902	1.578625	153	1	0	-2.453678	6.098633	-5.553133
128	1	0	-2.612023	7.780508	2.185713	154	1	0	-1.400675	5.855462	-6.978179
129	1	0	0.751196	2.993122	1.050519	155	17	0	-3.324571	7.138192	-7.505097
130	1	0	1.613365	2.841088	-0.488430	156	6	0	0.798526	4.014154	-4.833107
131	1	0	2.157361	1.908770	0.907134	157	1	0	0.275643	4.974117	-4.890589
132	1	0	2.725870	4.021571	2.113252	158	6	0	1.822451	3.901638	-5.951441
133	1	0	1.605014	5.756566	1.319045	159	1	0	2.649226	4.586999	-5.773941

160	17	0	1.127587	4.338444	-7.567729
161	6	0	-4.426756	4.311189	-6.277639
162	1	0	-4.388031	4.333733	-5.188902
163	1	0	-5.063551	5.117765	-6.639752
164	17	0	-5.220921	2.759165	-6.766175
165	6	0	-1.687688	0.504893	-2.632663
166	1	0	-1.926339	-0.405331	-2.085578
167	1	0	-0.453686	0.289186	-3.037844
168	17	0	-1.491008	1.841005	-1.479548
169	1	0	2.192351	2.879214	-6.032939
170	6	0	1.408611	3.849480	-3.437069
171	1	0	1.861308	2.863775	-3.324608
172	1	0	0.635003	4.004740	-2.685492
173	17	0	2.684233	5.101112	-3.123219

$^{4}TS_{\beta H}$

1	7	0	-10.989657	-2.856767	3.030686
2	6	0	-11.213862	-3.282432	1.654931
3	6	0	-12.359825	-4.288686	1.528355
4	8	0	-12.840635	-4.910538	2.451006
5	6	0	-9.923442	-3.900796	1.056058
6	6	0	-8.757542	-2.905912	0.989572
7	6	0	-7.447070	-3.552021	0.522969
8	7	0	-6.380733	-2.559585	0.468015
9	6	0	-5.090752	-2.898528	0.059569
10	7	0	-4.190467	-1.850121	0.264002
11	7	0	-4.679074	-4.008570	-0.443596
12	1	0	-11.005600	-3.682670	3.627553
13	1	0	-6.386169	-1.905750	1.241701
14	1	0	-3.280064	-2.066227	-0.122847
15	1	0	-4.525087	-0.943170	-0.039296
16	1	0	-5.400064	-4.727194	-0.402783
17	7	0	-1.770791	9.271189	-1.734711
18	6	0	-1.363584	8.029460	-1.062637
19	6	0	-1.143182	6.880618	-2.050103
20	8	0	-0.116320	6.217764	-2.104345
21	6	0	-2.342494	7.721296	0.108475
22	6	0	-1.858791	6.597788	1.056453
23	6	0	-3.803395	7.534720	-0.330084
24	6	0	-2.032922	5.145988	0.588085
25	1	0	-2.567892	9.081907	-2.337307
26	7	0	2.180019	5.286159	0.433814
27	6	0	2.664663	4.020986	1.015525
28	6	0	4.111782	3.754836	0.613319
29	8	0	4.664538	2.663388	0.798596
30	6	0	1.787043	2.793427	0.732158
31	7	0	4.729838	4.823247	0.082269
32	6	0	6.069899	4.752679	-0.430304
33	6	0	7.021230	3.914265	0.437397
34	8	0	7.747797	3.059588	-0.036689
35	1	0	1.719590	5.132119	-0.462100
36	1	0	4.141829	5.645983	-0.021630

37	7	0	8.251377	2.071066	2.860839	63	7	0	3.274317	-1.120992	-1.743159
38	6	0	7.753199	1.199235	3.931526	64	6	0	3.293425	-1.623168	-0.474567
39	6	0	8.399639	-0.187310	3.994154	65	6	0	4.430781	-1.114604	0.261066
40	8	0	8.072265	-1.053256	4.775607	66	6	0	5.098601	-0.287539	-0.584643
41	6	0	6.208395	1.038508	3.807069	67	6	0	4.374633	-0.304755	-1.836107
42	8	0	5.898364	0.644661	2.477548	68	7	0	2.953715	-0.301612	-4.475624
43	6	0	5.447983	2.290036	4.241267	69	6	0	4.113816	0.367193	-4.206602
44	1	0	8.058489	1.622087	1.964606	70	6	0	4.600048	1.029721	-5.390788
45	1	0	5.452859	1.367436	1.997480	71	6	0	3.718414	0.738375	-6.390074
46	7	0	0.513106	-5.247185	4.199580	72	6	0	2.693838	-0.088130	-5.803515
47	6	0	1.321370	-5.467812	5.395570	73	7	0	0.485955	-1.695604	-4.600814
48	6	0	0.533206	-6.127034	6.530577	74	6	0	0.541300	-1.300940	-5.918725
49	8	0	-0.673862	-6.229062	6.574340	75	6	0	-0.648798	-1.721418	-6.616405
50	6	0	1.926956	-4.141758	5.884939	76	6	0	-1.428288	-2.368588	-5.704398
51	1	0	-0.327199	-4.738601	4.471708	77	6	0	-0.703048	-2.359880	-4.457547
52	16	0	2.829977	-3.442565	-3.956407	78	1	0	-2.395501	-2.830414	-5.851458
53	26	0	1.849332	-1.356118	-3.139339	79	1	0	-0.848414	-1.537371	-7.663731
54	6	0	-1.131235	-2.987897	-3.289591	80	1	0	3.746721	1.045748	-7.427185
55	6	0	2.331430	-2.486229	0.048117	81	1	0	5.503929	1.622391	-5.439717
56	6	0	4.764840	0.386425	-2.971117	82	1	0	5.978275	0.308876	-0.387164
57	6	0	1.576851	-0.568953	-6.484799	83	1	0	4.662574	-1.324120	1.295693
58	7	0	0.852892	-2.567263	-1.904861	84	1	0	-1.805229	-4.314138	-0.863981
59	6	0	-0.394665	-3.108522	-2.122348	85	1	0	0.182409	-4.113618	0.984514
60	6	0	-0.840336	-3.827445	-0.952231	86	1	0	2.463632	-2.821292	1.072164
61	6	0	0.148042	-3.716903	-0.022639	87	1	0	1.494433	-0.325478	-7.539631
62	6	0	1.190889	-2.913764	-0.616077	88	1	0	5.671315	0.979445	-2.896971

89	1	0	-2.108871	-3.459555	-3.303376	115	1	0	-13.477874	-5.108481	0.262026
90	8	0	1.039318	0.055220	-2.512733	116	1	0	-1.023117	9.588797	-2.347510
91	1	0	-7.190296	-4.391835	1.191502	117	8	0	-2.175753	6.713874	-2.883244
92	1	0	-7.575136	-3.974583	-0.481640	118	1	0	-2.007369	5.980574	-3.524727
93	1	0	-9.009042	-2.083261	0.308018	119	1	0	-0.379167	8.204882	-0.617224
94	1	0	-8.622040	-2.465430	1.984199	120	1	0	-3.936124	6.679971	-0.997765
95	1	0	-9.640919	-4.764222	1.674770	121	1	0	-4.439954	7.382403	0.548541
96	1	0	-10.149465	-4.288847	0.056579	122	1	0	-4.172870	8.425746	-0.846409
97	1	0	-11.480834	-2.405155	1.052942	123	1	0	-2.305748	8.651142	0.690775
98	1	0	-11.771224	-2.286284	3.344267	124	1	0	-1.710631	4.455573	1.375055
99	1	0	2.508339	-3.691628	5.077224	125	1	0	-3.080041	4.915981	0.368311
100	1	0	1.135343	-3.439175	6.168878	126	1	0	-1.441768	4.920462	-0.302444
101	1	0	2.573795	-4.299755	6.751042	127	1	0	-0.801737	6.776865	1.299376
102	1	0	0.172061	-6.142865	3.856417	128	1	0	-2.403001	6.720373	2.001968
103	1	0	2.143583	-6.146964	5.139420	129	1	0	0.784063	2.943605	1.142932
104	1	0	7.967772	1.662962	4.902383	130	1	0	1.691492	2.615044	-0.343740
105	1	0	5.710994	3.153076	3.624427	131	1	0	2.223737	1.897377	1.177996
106	1	0	4.372155	2.114280	4.143796	132	1	0	2.705786	4.170238	2.104041
107	1	0	5.658883	2.531268	5.288279	133	1	0	1.481239	5.707273	1.037566
108	1	0	5.935421	0.208598	4.469503	134	1	0	6.103647	4.309117	-1.431543
109	1	0	9.263576	2.153650	2.915759	135	1	0	6.473727	5.768842	-0.492301
110	8	0	9.403440	-0.349249	3.100930	136	8	0	7.011375	4.271261	1.722641
111	1	0	9.733893	-1.254586	3.229244	137	1	0	7.534043	3.583675	2.242218
112	8	0	1.342402	-6.583622	7.516054	138	1	0	3.122773	-3.997899	-2.762366
113	1	0	0.759749	-6.961055	8.196861	139	15	0	-1.577375	4.029689	-5.956521
114	8	0	-12.776848	-4.434641	0.248888	140	8	0	-2.145239	4.887923	-4.873818

141	8	0	-0.035294	4.312675	-6.313418
142	8	0	-2.318266	4.205215	-7.368878
143	8	0	-1.608858	2.457084	-5.778805
144	6	0	-1.344962	1.629281	-4.569000
145	1	0	-1.405636	0.620772	-4.983746
146	6	0	-2.516848	1.862958	-3.615867
147	1	0	-3.449379	1.779565	-4.173517
148	1	0	-2.453822	2.837513	-3.135298
149	17	0	-2.558389	0.613884	-2.312821
150	6	0	-3.618868	4.800756	-7.590259
151	1	0	-3.851766	4.533055	-8.623169
152	6	0	-3.458176	6.324153	-7.489593
153	1	0	-3.323391	6.642286	-6.455385
154	1	0	-2.602653	6.630254	-8.092007
155	17	0	-4.905922	7.187909	-8.146130
156	6	0	0.473980	5.663732	-6.443227
157	1	0	-0.350821	6.376818	-6.532229
158	6	0	1.344112	5.709202	-7.690513
159	1	0	1.907472	6.640928	-7.721656
160	17	0	0.375309	5.627421	-9.214405
161	6	0	-4.715337	4.273544	-6.671791
162	1	0	-4.457891	4.421727	-5.623274
163	1	0	-5.646770	4.792179	-6.897483
164	17	0	-5.024145	2.508085	-6.915667
165	6	0	0.046579	1.819119	-4.041738
166	1	0	0.492190	0.720720	-3.198849
167	1	0	0.806885	1.776797	-4.818002
168	17	0	0.300830	3.235951	-3.014178
169	1	0	2.028132	4.859030	-7.698818
170	6	0	1.270150	5.970414	-5.169695
171	1	0	2.162134	5.346203	-5.099459
172	1	0	0.657775	5.829487	-4.279727
173	17	0	1.812787	7.701750	-5.158628

$^{2}IM_{\beta}$

1	7	0	-10.966960	-3.437750	3.082881
2	6	0	-11.213818	-3.282431	1.654932
3	6	0	-12.511893	-3.955588	1.204454
4	8	0	-13.120283	-4.785564	1.844999
5	6	0	-10.030871	-3.854422	0.829314
6	6	0	-8.707303	-3.128896	1.102354
7	6	0	-7.510417	-3.763052	0.381191
8	7	0	-6.291940	-3.029044	0.691973
9	6	0	-5.066106	-3.331744	0.105928
10	7	0	-4.024026	-2.605383	0.685438
11	7	0	-4.818280	-4.160416	-0.848358
12	1	0	-11.150453	-4.407737	3.336098
13	1	0	-6.213292	-2.739759	1.658779
14	1	0	-3.150266	-2.747530	0.194502
15	1	0	-4.226991	-1.623783	0.834884
16	1	0	-5.637994	-4.722096	-1.074074
17	7	0	-1.414990	8.886786	-2.253375

18	6	0	-1.363666	8.029587	-1.062665	44	1	0	8.114509	1.654320	1.981530
19	6	0	-1.590827	6.549096	-1.378057	45	1	0	5.587774	1.395696	1.909896
20	8	0	-0.903367	5.639676	-0.936202	46	7	0	0.604347	-4.624022	4.444524
21	6	0	-2.303467	8.606260	0.038861	47	6	0	1.321447	-5.467867	5.395821
22	6	0	-2.104444	7.973335	1.438454	48	6	0	0.803863	-5.319466	6.828906
23	6	0	-3.781240	8.665553	-0.377942	49	8	0	0.069966	-4.436537	7.218030
24	6	0	-2.781256	6.622862	1.714783	50	6	0	2.827883	-5.160978	5.351648
25	1	0	-2.275954	8.705746	-2.763259	51	1	0	0.619359	-3.666872	4.794460
26	7	0	2.131863	5.139713	0.222108	52	16	0	2.782249	-3.232521	-3.950492
27	6	0	2.664847	4.020892	1.015563	53	26	0	1.342703	-1.298145	-3.606255
28	6	0	4.119236	3.763339	0.636894	54	6	0	-1.414896	-3.271301	-3.320475
29	8	0	4.682459	2.680609	0.834877	55	6	0	2.160928	-1.962221	-0.327809
30	6	0	1.849950	2.722373	0.958223	56	6	0	4.094168	0.697378	-3.859045
31	7	0	4.733112	4.830855	0.094272	57	6	0	0.723077	-0.906749	-6.953722
32	6	0	6.069838	4.752602	-0.430255	58	7	0	0.574868	-2.442142	-2.139506
33	6	0	7.029343	3.934557	0.447078	59	6	0	-0.584185	-3.172571	-2.211068
34	8	0	7.770946	3.090657	-0.022391	60	6	0	-0.840389	-3.827386	-0.952470
35	1	0	1.938590	4.827485	-0.728723	61	6	0	0.166862	-3.466838	-0.107962
36	1	0	4.134556	5.636033	-0.063648	62	6	0	1.038238	-2.591999	-0.855842
37	7	0	8.256081	2.102264	2.888292	63	7	0	2.843355	-0.754833	-2.340836
38	6	0	7.753091	1.199275	3.931455	64	6	0	3.001360	-1.103286	-1.021679
39	6	0	8.462751	-0.154437	4.014855	65	6	0	4.154928	-0.438119	-0.456015
40	8	0	8.140414	-1.042952	4.772732	66	6	0	4.691132	0.321298	-1.446948
41	6	0	6.221091	0.969050	3.735637	67	6	0	3.869266	0.116277	-2.620389
42	8	0	5.969334	0.630822	2.378721	68	7	0	2.233900	-0.317196	-5.113067
43	6	0	5.389503	2.161906	4.204799	69	6	0	3.347578	0.477218	-5.018403

70	6	0	3.672385	1.034925	-6.306894	96	1	0	-10.284266	-3.797307	-0.235288
71	6	0	2.745902	0.559402	-7.188227	97	1	0	-11.301501	-2.213462	1.425644
72	6	0	1.848676	-0.276117	-6.432360	98	1	0	-11.644564	-2.891521	3.609234
73	7	0	-0.092563	-1.913219	-4.876165	99	1	0	3.191159	-5.291893	4.329967
74	6	0	-0.192268	-1.653387	-6.220111	100	1	0	3.018505	-4.124393	5.651375
75	6	0	-1.379481	-2.264876	-6.765125	101	1	0	3.385056	-5.820074	6.021508
76	6	0	-1.996163	-2.904835	-5.733408	102	1	0	-0.380311	-4.882471	4.442853
77	6	0	-1.175101	-2.694001	-4.565443	103	1	0	1.175848	-6.516498	5.109174
78	1	0	-2.910083	-3.483544	-5.747227	104	1	0	7.901925	1.664764	4.913510
79	1	0	-1.685336	-2.204298	-7.801071	105	1	0	5.642306	3.068224	3.647865
80	1	0	2.661913	0.754367	-8.249099	106	1	0	4.327269	1.950621	4.049751
81	1	0	4.508063	1.694627	-6.499743	107	1	0	5.547198	2.352382	5.271448
82	1	0	5.549175	0.977532	-1.388351	108	1	0	5.964261	0.093215	4.341910
83	1	0	4.493440	-0.525581	0.568520	109	1	0	9.261663	2.221930	2.983188
84	1	0	-1.694351	-4.466737	-0.764046	110	8	0	9.516154	-0.258771	3.171298
85	1	0	0.321994	-3.757539	0.923703	111	1	0	9.883425	-1.148392	3.309031
86	1	0	2.397002	-2.158540	0.713132	112	8	0	1.273551	-6.292611	7.645762
87	1	0	0.530038	-0.782955	-8.014631	113	1	0	0.916244	-6.103687	8.530078
88	1	0	4.948542	1.361567	-3.944944	114	8	0	-12.908726	-3.539024	-0.020764
89	1	0	-2.319013	-3.861189	-3.201878	115	1	0	-13.715190	-4.038553	-0.234743
90	8	0	0.364095	0.144877	-3.075224	116	1	0	-0.657286	8.639326	-2.885625
91	1	0	-7.430932	-4.828533	0.658018	117	8	0	-2.615621	6.352830	-2.218118
92	1	0	-7.665744	-3.728438	-0.704532	118	1	0	-2.754894	5.386887	-2.380468
93	1	0	-8.787442	-2.078716	0.794471	119	1	0	-0.344820	8.077615	-0.664802
94	1	0	-8.531286	-3.129470	2.184333	120	1	0	-4.199559	7.675235	-0.576223
95	1	0	-9.928441	-4.921010	1.074254	121	1	0	-4.375656	9.130777	0.416077

122	1	0	-3.912436	9.273556	-1.278042	148	1	0	-4.531626	2.634817	-1.015298
123	1	0	-1.954385	9.643760	0.117264	149	17	0	-5.068001	0.878146	0.484478
124	1	0	-2.596010	6.318124	2.750355	150	6	0	-4.908610	3.721069	-5.643994
125	1	0	-3.866633	6.679264	1.584554	151	1	0	-5.272841	3.338734	-6.599837
126	1	0	-2.401334	5.828514	1.068592	152	6	0	-4.242109	5.086005	-5.870669
127	1	0	-1.027405	7.883467	1.633064	153	1	0	-3.962783	5.560920	-4.929576
128	1	0	-2.479706	8.698451	2.172403	154	1	0	-3.360658	4.951443	-6.497718
129	1	0	0.835311	2.897385	1.326147	155	17	0	-5.351530	6.217393	-6.744379
130	1	0	1.781118	2.348582	-0.068636	156	6	0	-0.622663	3.377306	-4.509128
131	1	0	2.318010	1.942981	1.563612	157	1	0	-1.110913	4.347894	-4.638432
132	1	0	2.693289	4.362960	2.060859	158	6	0	0.121589	2.982389	-5.773556
133	1	0	1.229439	5.440214	0.582055	159	1	0	0.994895	3.616689	-5.912057
134	1	0	6.096821	4.290974	-1.423401	160	17	0	-0.902670	3.172548	-7.255897
135	1	0	6.470144	5.768602	-0.514991	161	6	0	-6.065714	3.799358	-4.655232
136	8	0	7.003313	4.291570	1.731883	162	1	0	-5.715953	4.067018	-3.658448
137	1	0	7.522916	3.607087	2.258301	163	1	0	-6.780906	4.543947	-5.003808
138	1	0	3.854605	-2.575044	-4.438546	164	17	0	-6.959644	2.232878	-4.520255
139	15	0	-3.134928	2.686910	-3.856514	165	6	0	-2.231479	1.015422	-1.271711
140	8	0	-3.316474	3.888764	-2.988803	166	1	0	-1.378300	0.466867	-1.666066
141	8	0	-1.616297	2.347689	-4.243487	167	1	0	-0.294460	0.304481	-3.768560
142	8	0	-3.877829	2.773067	-5.271876	168	17	0	-1.831924	2.323561	-0.229418
143	8	0	-3.662119	1.299301	-3.288867	169	1	0	0.428238	1.937956	-5.725994
144	6	0	-3.587454	0.867851	-1.856624	170	6	0	0.276545	3.408692	-3.267945
145	1	0	-3.803423	-0.200132	-1.950467	171	1	0	0.724757	2.428039	-3.091289
146	6	0	-4.744926	1.576206	-1.153680	172	1	0	-0.298533	3.735533	-2.401676
147	1	0	-5.653202	1.447440	-1.740764	173	17	0	1.611185	4.628578	-3.465796

$^4IM_\beta$

1	7	0	-11.078907	-3.270642	3.106143
2	6	0	-11.213836	-3.282434	1.654934
3	6	0	-12.438135	-4.069886	1.183232
4	8	0	-13.058807	-4.858216	1.863416
5	6	0	-9.941764	-3.873643	0.991957
6	6	0	-8.678890	-3.047364	1.269884
7	6	0	-7.405856	-3.708448	0.726509
8	7	0	-6.238077	-2.880618	1.003802
9	6	0	-4.961032	-3.264838	0.592675
10	7	0	-3.971834	-2.431406	1.122682
11	7	0	-4.630893	-4.246077	-0.170395
12	1	0	-11.239124	-4.216762	3.449390
13	1	0	-6.243025	-2.454561	1.922853
14	1	0	-3.068985	-2.638770	0.712874
15	1	0	-4.189869	-1.443657	1.056676
16	1	0	-5.427737	-4.848264	-0.371034
17	7	0	-1.625847	9.010237	-2.122971
18	6	0	-1.363662	8.029535	-1.062695
19	6	0	-1.352334	6.583642	-1.573331
20	8	0	-0.477976	5.769616	-1.317134
21	6	0	-2.325854	8.282712	0.136413
22	6	0	-1.964259	7.492974	1.418355
23	6	0	-3.814025	8.168915	-0.228903
24	6	0	-2.394088	6.020251	1.496708
25	1	0	-2.467425	8.746858	-2.629260
26	7	0	2.188743	5.319130	0.508965
27	6	0	2.664869	4.020885	1.015614
28	6	0	4.106770	3.754591	0.594803
29	8	0	4.650152	2.653830	0.755520
30	6	0	1.769607	2.822187	0.672865
31	7	0	4.729701	4.827586	0.082148
32	6	0	6.069850	4.752643	-0.430258
33	6	0	7.024744	3.935050	0.452841
34	8	0	7.784558	3.104540	-0.011458
35	1	0	1.683812	5.209799	-0.369202
36	1	0	4.149036	5.658195	0.003134
37	7	0	8.264186	2.109219	2.898885
38	6	0	7.753086	1.199269	3.931444
39	6	0	8.457693	-0.157356	4.009660
40	8	0	8.128440	-1.049219	4.760603
41	6	0	6.221623	0.975520	3.722176
42	8	0	5.981692	0.645099	2.360742
43	6	0	5.387324	2.167476	4.188413
44	1	0	8.134298	1.666524	1.987872
45	1	0	5.577709	1.400626	1.894405
46	7	0	0.586128	-4.602989	4.477800
47	6	0	1.321469	-5.467877	5.395850
48	6	0	0.827849	-5.355743	6.840588
49	8	0	0.108485	-4.477619	7.266159
50	6	0	2.825967	-5.154093	5.335471

51	1	0	0.597153	-3.656407	4.855515	77	6	0	-0.853648	-2.844185	-4.610833
52	16	0	2.799452	-3.594860	-3.857958	78	1	0	-2.523128	-3.598916	-5.898632
53	26	0	1.713269	-1.586840	-3.515667	79	1	0	-1.057481	-2.505411	-7.900606
54	6	0	-1.227330	-3.341539	-3.369038	80	1	0	3.488317	0.113774	-8.153199
55	6	0	2.221956	-2.122328	-0.186708	81	1	0	5.263311	1.043733	-6.325455
56	6	0	4.562123	0.283072	-3.668640	82	1	0	5.748257	0.695017	-1.103504
57	6	0	1.352917	-1.323159	-6.932724	83	1	0	4.497029	-0.693105	0.824846
58	7	0	0.732421	-2.577538	-2.085625	84	1	0	-1.758241	-4.380165	-0.785421
59	6	0	-0.468050	-3.238517	-2.213683	85	1	0	0.219190	-3.775873	0.985947
60	6	0	-0.840425	-3.827350	-0.952508	86	1	0	2.392614	-2.306137	0.868382
61	6	0	0.142472	-3.510204	-0.061347	87	1	0	1.248556	-1.241511	-8.009206
62	6	0	1.112191	-2.714931	-0.771912	88	1	0	5.455853	0.896320	-3.707701
63	7	0	3.063886	-0.976152	-2.184902	89	1	0	-2.160265	-3.890964	-3.301416
64	6	0	3.111688	-1.291137	-0.848427	90	8	0	0.786570	-0.036339	-3.263267
65	6	0	4.238419	-0.638907	-0.224688	91	1	0	-7.301616	-4.718880	1.158155
66	6	0	4.877019	0.061292	-1.199829	92	1	0	-7.485536	-3.834312	-0.360529
67	6	0	4.155846	-0.175246	-2.427288	93	1	0	-8.779522	-2.050685	0.821798
68	7	0	2.788465	-0.761775	-5.011797	94	1	0	-8.591084	-2.903232	2.353069
69	6	0	3.931669	-0.013609	-4.871223	95	1	0	-9.806759	-4.897205	1.368912
70	6	0	4.380541	0.440055	-6.161105	96	1	0	-10.112136	-3.954370	-0.087534
71	6	0	3.490108	-0.031130	-7.081057	97	1	0	-11.331990	-2.250625	1.302187
72	6	0	2.486500	-0.765650	-6.355750	98	1	0	-11.822231	-2.709251	3.514722
73	7	0	0.292114	-2.135561	-4.872530	99	1	0	3.173436	-5.258705	4.305300
74	6	0	0.332081	-1.951283	-6.234216	100	1	0	3.017411	-4.124370	5.657491
75	6	0	-0.843354	-2.523676	-6.840240	101	1	0	3.396026	-5.827204	5.980166
76	6	0	-1.581303	-3.070340	-5.834136	102	1	0	-0.396193	-4.870125	4.478859

103	1	0	1.174684	-6.509472	5.085633	129	1	0	0.770176	2.961297	1.094809
104	1	0	7.895328	1.656849	4.918149	130	1	0	1.669527	2.714969	-0.411597
105	1	0	5.646202	3.076127	3.638187	131	1	0	2.198532	1.895502	1.059439
106	1	0	4.326599	1.957126	4.021032	132	1	0	2.715389	4.103903	2.110833
107	1	0	5.533619	2.352959	5.257539	133	1	0	1.518090	5.721635	1.155863
108	1	0	5.956964	0.097728	4.322398	134	1	0	6.103939	4.291194	-1.422926
109	1	0	9.267755	2.234983	3.005690	135	1	0	6.469362	5.769106	-0.511505
110	8	0	9.514060	-0.260068	3.169925	136	8	0	6.974682	4.277341	1.741672
111	1	0	9.877173	-1.152165	3.302687	137	1	0	7.507497	3.602234	2.266412
112	8	0	1.302518	-6.354826	7.622472	138	1	0	3.674761	-3.176792	-4.795113
113	1	0	0.961791	-6.187306	8.517586	139	15	0	-2.398074	2.749897	-4.388986
114	8	0	-12.751440	-3.809022	-0.107459	140	8	0	-2.625931	3.837438	-3.393562
115	1	0	-13.513882	-4.371755	-0.325888	141	8	0	-0.870014	2.302822	-4.580804
116	1	0	-0.869580	8.992483	-2.803094	142	8	0	-2.891554	3.091602	-5.874327
117	8	0	-2.401553	6.303218	-2.360156	143	8	0	-3.108665	1.354422	-4.126445
118	1	0	-2.372231	5.354322	-2.639663	144	6	0	-3.327222	0.713934	-2.795636
119	1	0	-0.347048	8.202681	-0.695147	145	1	0	-3.454483	-0.333042	-3.085569
120	1	0	-4.085098	7.168040	-0.574421	146	6	0	-4.652369	1.271648	-2.280718
121	1	0	-4.432959	8.405999	0.643391	147	1	0	-5.364138	1.312828	-3.103838
122	1	0	-4.079101	8.880817	-1.016170	148	1	0	-4.527110	2.262868	-1.846440
123	1	0	-2.136907	9.339822	0.363262	149	17	0	-5.365625	0.193865	-1.017301
124	1	0	-2.133318	5.607447	2.477226	150	6	0	-3.684033	4.229859	-6.288353
125	1	0	-3.476248	5.908615	1.377061	151	1	0	-3.938827	3.998555	-7.324784
126	1	0	-1.902796	5.402969	0.740960	152	6	0	-2.781224	5.471367	-6.258713
127	1	0	-0.879713	7.562951	1.579367	153	1	0	-2.591101	5.806515	-5.238269
128	1	0	-2.423508	8.026196	2.260891	154	1	0	-1.841852	5.236912	-6.760290

155	17	0	-3.531958	6.853587	-7.152073
156	6	0	0.225692	3.255096	-4.662994
157	1	0	-0.155036	4.252115	-4.905246
158	6	0	1.160150	2.770088	-5.758478
159	1	0	2.083655	3.345924	-5.751210
160	17	0	0.426937	2.972139	-7.402890
161	6	0	-4.964743	4.423474	-5.484652
162	1	0	-4.753016	4.553564	-4.423886
163	1	0	-5.494321	5.297016	-5.864280
164	17	0	-6.088000	3.014633	-5.647731
165	6	0	-2.148878	0.795203	-1.894684
166	1	0	-1.212024	0.300528	-2.134414
167	1	0	0.152783	0.052786	-3.993137
168	17	0	-2.076946	1.875297	-0.557882
169	1	0	1.382317	1.711258	-5.628223
170	6	0	0.875288	3.272007	-3.275794
171	1	0	1.227988	2.273705	-3.008577
172	1	0	0.163869	3.651766	-2.542044
173	17	0	2.288081	4.412506	-3.236682

$^{4r}TS_{\beta\text{-reb}}$

1	7	0	-11.065610	-2.824338	3.030710
2	6	0	-11.213841	-3.282434	1.654934
3	6	0	-12.392924	-4.241669	1.477609
4	8	0	-12.961229	-4.815277	2.381680
5	6	0	-9.915222	-3.973562	1.164974
6	6	0	-8.705355	-3.030806	1.150220
7	6	0	-7.399441	-3.745859	0.783285
8	7	0	-6.286335	-2.805613	0.778064
9	6	0	-4.999168	-3.205158	0.419347
10	7	0	-4.057535	-2.199868	0.657796
11	7	0	-4.621089	-4.332465	-0.070250
12	1	0	-11.165028	-3.629393	3.647679
13	1	0	-6.294759	-2.150178	1.550306
14	1	0	-3.151313	-2.456345	0.284846
15	1	0	-4.344334	-1.277735	0.350460
16	1	0	-5.375870	-5.016584	-0.059339
17	7	0	-1.339567	9.099576	-2.067152
18	6	0	-1.363655	8.029524	-1.062690
19	6	0	-1.232142	6.633410	-1.687514
20	8	0	-0.414108	5.794817	-1.331531
21	6	0	-2.591096	8.212721	-0.122516
22	6	0	-2.573833	7.293837	1.123158
23	6	0	-3.942688	8.196663	-0.853399
24	6	0	-3.024525	5.836785	0.942270
25	1	0	-2.031908	8.907272	-2.786619
26	7	0	2.215041	5.369097	0.623080
27	6	0	2.664862	4.020916	1.015597
28	6	0	4.108580	3.759754	0.596976
29	8	0	4.650017	2.658166	0.762271
30	6	0	1.758381	2.884396	0.530228
31	7	0	4.726762	4.827830	0.072913

32	6	0	6.069834	4.752632	-0.430246	58	7	0	0.629798	-2.477723	-2.112878
33	6	0	7.021687	3.938492	0.459357	59	6	0	-0.501379	-3.245522	-2.230476
34	8	0	7.786331	3.110815	-0.001804	60	6	0	-0.840392	-3.827343	-0.952488
35	1	0	1.527678	5.339226	-0.127966	61	6	0	0.113791	-3.417507	-0.069694
36	1	0	4.141973	5.656219	-0.009002	62	6	0	1.031830	-2.580858	-0.806957
37	7	0	8.264999	2.123273	2.911480	63	7	0	2.987617	-0.898032	-2.312190
38	6	0	7.753081	1.199251	3.931431	64	6	0	3.053745	-1.189142	-0.967385
39	6	0	8.478007	-0.146364	4.012264	65	6	0	4.182963	-0.519703	-0.371207
40	8	0	8.149510	-1.049355	4.750070	66	6	0	4.786652	0.194307	-1.360627
41	6	0	6.227836	0.953697	3.697593	67	6	0	4.035978	-0.043139	-2.567608
42	8	0	6.010198	0.640668	2.328480	68	7	0	2.473408	-0.442142	-5.077451
43	6	0	5.369121	2.125264	4.171253	69	6	0	3.622521	0.303554	-4.968379
44	1	0	8.154501	1.683738	1.996271	70	6	0	4.005389	0.805038	-6.263833
45	1	0	5.611004	1.402013	1.868000	71	6	0	3.088690	0.335113	-7.158548
46	7	0	0.591795	-4.583201	4.492760	72	6	0	2.143454	-0.455616	-6.414675
47	6	0	1.321461	-5.467876	5.395842	73	7	0	0.243483	-2.219365	-4.939049
48	6	0	0.818973	-5.388443	6.839708	74	6	0	0.194091	-1.952319	-6.284057
49	8	0	0.098750	-4.518921	7.281279	75	6	0	-0.947651	-2.604844	-6.871973
50	6	0	2.826191	-5.152118	5.352245	76	6	0	-1.597005	-3.250417	-5.862591
51	1	0	0.596820	-3.645829	4.892824	77	6	0	-0.849160	-3.001013	-4.656245
52	16	0	2.818929	-3.427499	-4.125194	78	1	0	-2.500230	-3.844057	-5.912223
53	26	0	1.584614	-1.502053	-3.605951	79	1	0	-1.210713	-2.555879	-7.920305
54	6	0	-1.207416	-3.477369	-3.400973	80	1	0	3.051061	0.490887	-8.228421
55	6	0	2.159643	-1.981376	-0.263498	81	1	0	4.880159	1.413627	-6.453028
56	6	0	4.339656	0.518583	-3.798647	82	1	0	5.643291	0.849563	-1.277230
57	6	0	1.081938	-1.143894	-6.981465	83	1	0	4.462280	-0.565308	0.673615

84	1	0	-1.711668	-4.446589	-0.771922	110	8	0	9.551531	-0.225029	3.191868
85	1	0	0.211803	-3.659118	0.981535	111	1	0	9.927154	-1.111906	3.324830
86	1	0	2.354293	-2.138770	0.791903	112	8	0	1.286803	-6.406418	7.601156
87	1	0	0.932163	-1.040557	-8.050772	113	1	0	0.940753	-6.259047	8.497774
88	1	0	5.221338	1.148104	-3.856620	114	8	0	-12.730335	-4.406978	0.177234
89	1	0	-2.096485	-4.095014	-3.331068	115	1	0	-13.460001	-5.049618	0.160703
90	8	0	0.462465	-0.040081	-3.248489	116	1	0	-0.436984	9.111789	-2.536279
91	1	0	-7.226696	-4.582745	1.481820	117	8	0	-2.085345	6.434781	-2.698359
92	1	0	-7.482302	-4.182434	-0.219900	118	1	0	-1.975677	5.528807	-3.079359
93	1	0	-8.876077	-2.216478	0.434711	119	1	0	-0.468623	8.139891	-0.442203
94	1	0	-8.613325	-2.570258	2.140737	120	1	0	-4.140338	7.243190	-1.349487
95	1	0	-9.713538	-4.827794	1.826541	121	1	0	-4.754206	8.384148	-0.141765
96	1	0	-10.089698	-4.383327	0.163774	122	1	0	-3.987471	8.986240	-1.609365
97	1	0	-11.399163	-2.413807	1.011293	123	1	0	-2.446244	9.235834	0.247821
98	1	0	-11.837947	-2.207604	3.271081	124	1	0	-3.027654	5.324504	1.910196
99	1	0	3.180062	-5.233148	4.322146	125	1	0	-4.040238	5.774710	0.539625
100	1	0	3.014897	-4.129770	5.698519	126	1	0	-2.361591	5.273721	0.281080
101	1	0	3.392642	-5.839329	5.985180	127	1	0	-1.564804	7.308012	1.557029
102	1	0	-0.389589	-4.853154	4.477662	128	1	0	-3.225683	7.761137	1.872615
103	1	0	1.177424	-6.502360	5.061539	129	1	0	0.758482	2.982449	0.960987
104	1	0	7.873633	1.653228	4.922663	130	1	0	1.659616	2.904635	-0.559524
105	1	0	5.624785	3.047199	3.641897	131	1	0	2.176627	1.914725	0.806831
106	1	0	4.314546	1.903598	3.981424	132	1	0	2.695218	3.979091	2.113477
107	1	0	5.494960	2.293070	5.245888	133	1	0	1.760199	5.832844	1.401911
108	1	0	5.969209	0.062585	4.280398	134	1	0	6.112119	4.290418	-1.422231
109	1	0	9.264997	2.262984	3.033627	135	1	0	6.468932	5.769266	-0.512268

136	8	0	6.963868	4.281065	1.747600
137	1	0	7.496624	3.608075	2.275738
138	1	0	3.844754	-3.210538	-3.276738
139	15	0	-1.423136	3.057561	-4.956079
140	8	0	-2.059509	4.118293	-4.120531
141	8	0	0.182095	2.979888	-4.883311
142	8	0	-1.712578	3.217764	-6.525579
143	8	0	-1.804734	1.543092	-4.701366
144	6	0	-2.337207	0.835446	-3.526513
145	1	0	-2.395031	-0.195720	-3.879201
146	6	0	-3.753612	1.377782	-3.285991
147	1	0	-4.309634	1.388250	-4.223306
148	1	0	-3.728992	2.374006	-2.846035
149	17	0	-4.660534	0.298532	-2.149676
150	6	0	-2.685185	4.093795	-7.143362
151	1	0	-2.655694	3.803301	-8.195682
152	6	0	-2.190250	5.541713	-7.011600
153	1	0	-2.302344	5.913377	-5.992905
154	1	0	-1.145163	5.587933	-7.317612
155	17	0	-3.112401	6.651467	-8.103558
156	6	0	1.014708	4.168075	-4.919684
157	1	0	0.409170	5.051269	-5.143702
158	6	0	2.086434	3.973367	-5.981010
159	1	0	2.859274	4.732857	-5.871457
160	17	0	1.441762	4.132863	-7.664903
161	6	0	-4.101660	3.917427	-6.610352
162	1	0	-4.143959	4.085586	-5.534226
163	1	0	-4.763838	4.619597	-7.116092
164	17	0	-4.750107	2.259695	-6.934930
165	6	0	-1.432752	0.825440	-2.342982
166	1	0	-1.377165	-0.065984	-1.738155
167	1	0	0.641164	0.629886	-3.929902
168	17	0	-1.170158	2.293884	-1.459566
169	1	0	2.524699	2.977132	-5.906113
170	6	0	1.599291	4.305106	-3.509459
171	1	0	2.234037	3.452275	-3.263094
172	1	0	0.793683	4.407763	-2.782307
173	17	0	2.610638	5.803720	-3.367272

$^2P_\beta$

1	7	0	-11.051332	-2.856927	3.039627
2	6	0	-11.213810	-3.282436	1.654938
3	6	0	-12.400883	-4.229586	1.465765
4	8	0	-12.966117	-4.819193	2.361388
5	6	0	-9.924253	-3.970122	1.138361
6	6	0	-8.709695	-3.033872	1.136332
7	6	0	-7.410684	-3.744985	0.739603
8	7	0	-6.294590	-2.808789	0.750379
9	6	0	-5.014309	-3.199396	0.357079
10	7	0	-4.068523	-2.202046	0.608772
11	7	0	-4.646557	-4.311618	-0.172506
12	1	0	-11.149908	-3.675610	3.638561

13	1	0	-6.287957	-2.183095	1.546975	39	6	0	8.500247	-0.134020	4.011566
14	1	0	-3.164916	-2.443205	0.219984	40	8	0	8.172412	-1.051986	4.731056
15	1	0	-4.360490	-1.267772	0.348063	41	6	0	6.237656	0.930171	3.658475
16	1	0	-5.401088	-4.996027	-0.166219	42	8	0	6.057668	0.636611	2.279737
17	7	0	-1.621476	9.113714	-2.016575	43	6	0	5.347531	2.077912	4.132180
18	6	0	-1.363667	8.029504	-1.062716	44	1	0	8.187116	1.715911	2.012330
19	6	0	-1.177476	6.664923	-1.741107	45	1	0	5.646789	1.393824	1.823080
20	8	0	-0.280145	5.878260	-1.472105	46	7	0	1.161646	-5.432692	3.946586
21	6	0	-2.445778	8.049236	0.058563	47	6	0	1.321653	-5.468048	5.396404
22	6	0	-2.102367	7.179373	1.292741	48	6	0	1.600969	-6.875272	5.931346
23	6	0	-3.873162	7.808935	-0.456980	49	8	0	1.450535	-7.902515	5.305918
24	6	0	-2.356467	5.667539	1.199697	50	6	0	0.073412	-4.890304	6.084603
25	1	0	-2.394047	8.855969	-2.625210	51	1	0	0.459099	-6.123003	3.684820
26	7	0	2.217725	5.370632	0.626267	52	16	0	2.748973	-3.379769	-4.198322
27	6	0	2.664835	4.020906	1.015601	53	26	0	1.555905	-1.573365	-3.668568
28	6	0	4.103970	3.754715	0.581731	54	6	0	-1.287109	-3.435229	-3.379321
29	8	0	4.639897	2.648158	0.726221	55	6	0	2.124986	-1.916841	-0.297386
30	6	0	1.748165	2.883836	0.550440	56	6	0	4.329024	0.383611	-3.935142
31	7	0	4.726119	4.827692	0.069940	57	6	0	0.799658	-0.949566	-6.974177
32	6	0	6.069848	4.752677	-0.430289	58	7	0	0.596490	-2.450945	-2.141024
33	6	0	7.028143	3.958940	0.471252	59	6	0	-0.529706	-3.239843	-2.234125
34	8	0	7.824496	3.158003	0.017647	60	6	0	-0.840715	-3.827204	-0.953101
35	1	0	1.584727	5.347208	-0.171332	61	6	0	0.111396	-3.391752	-0.079957
36	1	0	4.153806	5.666313	0.017449	62	6	0	1.005198	-2.542513	-0.828732
37	7	0	8.270001	2.145972	2.934965	63	7	0	2.916217	-0.877519	-2.371719
38	6	0	7.753205	1.199271	3.931543	64	6	0	3.014231	-1.138516	-1.023573

65	6	0	4.188224	-0.507589	-0.466828	91	1	0	-7.235907	-4.601498	1.413376
66	6	0	4.809657	0.130123	-1.493610	92	1	0	-7.503365	-4.153379	-0.274464
67	6	0	4.017195	-0.110602	-2.677506	93	1	0	-8.882614	-2.200806	0.443250
68	7	0	2.365588	-0.464641	-5.146606	94	1	0	-8.606648	-2.598746	2.137206
69	6	0	3.563947	0.207300	-5.082336	95	1	0	-9.722304	-4.840970	1.777786
70	6	0	3.906673	0.740209	-6.377678	96	1	0	-10.109347	-4.354976	0.129231
71	6	0	2.902801	0.384105	-7.230596	97	1	0	-11.399037	-2.398026	1.033055
72	6	0	1.953239	-0.375185	-6.459174	98	1	0	-11.818653	-2.242345	3.300755
73	7	0	0.045375	-2.056753	-4.916972	99	1	0	-0.105437	-3.878982	5.712655
74	6	0	-0.084147	-1.738218	-6.250269	100	1	0	-0.808074	-5.499179	5.854151
75	6	0	-1.263954	-2.356290	-6.800885	101	1	0	0.198046	-4.861722	7.169746
76	6	0	-1.842392	-3.066585	-5.792297	102	1	0	2.020048	-5.756368	3.505481
77	6	0	-1.017273	-2.879745	-4.624093	103	1	0	2.183036	-4.845463	5.667103
78	1	0	-2.741740	-3.667692	-5.819721	104	1	0	7.842446	1.642229	4.931006
79	1	0	-1.590138	-2.254974	-7.827650	105	1	0	5.600911	3.014047	3.627325
80	1	0	2.807122	0.600961	-8.286264	106	1	0	4.302155	1.842628	3.910671
81	1	0	4.808050	1.298808	-6.595425	107	1	0	5.443219	2.226462	5.212767
82	1	0	5.707192	0.732963	-1.455186	108	1	0	5.982091	0.024843	4.220459
83	1	0	4.485654	-0.533946	0.573580	109	1	0	9.264277	2.302718	3.080691
84	1	0	-1.701155	-4.457781	-0.761026	110	8	0	9.592243	-0.183416	3.213568
85	1	0	0.218725	-3.622059	0.972938	111	1	0	9.980019	-1.065576	3.342890
86	1	0	2.329068	-2.061684	0.758433	112	8	0	2.029719	-6.857724	7.216519
87	1	0	0.584701	-0.789209	-8.025636	113	1	0	2.160031	-7.786238	7.473996
88	1	0	5.247278	0.954556	-4.030482	114	8	0	-12.749451	-4.363604	0.164733
89	1	0	-2.166625	-4.064229	-3.288239	115	1	0	-13.483440	-5.001032	0.139552
90	8	0	0.299439	0.490744	-3.301627	116	1	0	-0.814010	9.240312	-2.622109

117	8	0	-2.089564	6.427779	-2.692480	143	8	0	-1.615136	1.641509	-5.013580
118	1	0	-1.941223	5.540295	-3.098570	144	6	0	-2.034232	0.781840	-3.925635
119	1	0	-0.402349	8.233999	-0.580628	145	1	0	-2.057897	-0.205634	-4.394471
120	1	0	-3.992848	6.823109	-0.913870	146	6	0	-3.444382	1.172354	-3.492788
121	1	0	-4.587972	7.888005	0.369283	147	1	0	-4.085787	1.225033	-4.372384
122	1	0	-4.154827	8.560505	-1.200599	148	1	0	-3.454966	2.120182	-2.957063
123	1	0	-2.402387	9.092169	0.397302	149	17	0	-4.136559	-0.091944	-2.400798
124	1	0	-2.131502	5.192004	2.160425	150	6	0	-2.534841	4.365540	-7.240590
125	1	0	-3.403325	5.446538	0.969128	151	1	0	-2.500949	4.133477	-8.307023
126	1	0	-1.732503	5.186370	0.443250	152	6	0	-2.051921	5.806366	-7.023268
127	1	0	-1.051808	7.353551	1.562680	153	1	0	-2.159997	6.112029	-5.981926
128	1	0	-2.692076	7.572451	2.131087	154	1	0	-1.009021	5.880681	-7.332088
129	1	0	0.751677	2.991715	0.987736	155	17	0	-2.991773	6.972788	-8.035846
130	1	0	1.639462	2.892997	-0.538191	156	6	0	1.179037	4.291521	-4.994155
131	1	0	2.162861	1.914453	0.833726	157	1	0	0.589492	5.189178	-5.201041
132	1	0	2.709371	3.990628	2.113333	158	6	0	2.257091	4.106003	-6.050963
133	1	0	1.698551	5.803246	1.382753	159	1	0	3.053663	4.832953	-5.899237
134	1	0	6.116483	4.274222	-1.414167	160	17	0	1.635039	4.362893	-7.731035
135	1	0	6.462338	5.770277	-0.529339	161	6	0	-3.948139	4.140526	-6.716980
136	8	0	6.935871	4.285852	1.762149	162	1	0	-3.998281	4.274886	-5.636655
137	1	0	7.478284	3.623612	2.292885	163	1	0	-4.623236	4.842768	-7.205344
138	1	0	3.132432	-3.720586	-2.949417	164	17	0	-4.555499	2.478290	-7.090669
139	15	0	-1.283559	3.194289	-5.120686	165	6	0	-0.974609	0.675947	-2.815382
140	8	0	-1.965803	4.153623	-4.208364	166	1	0	-1.209267	-0.170350	-2.172661
141	8	0	0.320372	3.115635	-5.010177	167	1	0	0.488036	1.082847	-4.049982
142	8	0	-1.546297	3.468643	-6.672796	168	17	0	-1.032470	2.142595	-1.686577

169	1	0	2.659414	3.091872	-6.015655
170	6	0	1.743491	4.375987	-3.572252
171	1	0	2.359751	3.505589	-3.340412
172	1	0	0.928737	4.475688	-2.854718
173	17	0	2.778468	5.850343	-3.379431

$^4P_\beta$

1	7	0	-10.970083	-2.921880	3.046097
2	6	0	-11.213821	-3.282436	1.654939
3	6	0	-12.386456	-4.252645	1.494951
4	8	0	-12.874695	-4.902862	2.393853
5	6	0	-9.944130	-3.907653	1.021345
6	6	0	-8.757171	-2.937196	0.985457
7	6	0	-7.465934	-3.589665	0.477564
8	7	0	-6.382905	-2.615002	0.448441
9	6	0	-5.110406	-2.952672	-0.010586
10	7	0	-4.190871	-1.923474	0.208429
11	7	0	-4.726217	-4.044488	-0.570980
12	1	0	-11.010622	-3.771643	3.607285
13	1	0	-6.360649	-1.997756	1.251282
14	1	0	-3.298895	-2.130733	-0.223304
15	1	0	-4.527928	-0.998621	-0.030621
16	1	0	-5.453156	-4.757409	-0.538543
17	7	0	-1.342940	9.199883	-1.951645
18	6	0	-1.363666	8.029504	-1.062717
19	6	0	-1.099381	6.727250	-1.827544
20	8	0	-0.217942	5.929414	-1.536970
21	6	0	-2.656046	8.052837	-0.196470
22	6	0	-2.624889	7.089633	1.013901
23	6	0	-3.957863	7.941404	-1.005365
24	6	0	-2.831321	5.592892	0.741099
25	1	0	-1.984915	9.050479	-2.726023
26	7	0	2.210478	5.361194	0.604692
27	6	0	2.664833	4.020904	1.015609
28	6	0	4.103760	3.752826	0.583453
29	8	0	4.642698	2.648750	0.737250
30	6	0	1.753536	2.868533	0.573749
31	7	0	4.723258	4.823307	0.063384
32	6	0	6.069847	4.752682	-0.430301
33	6	0	7.019543	3.940721	0.463735
34	8	0	7.794008	3.120701	0.005417
35	1	0	1.563650	5.322344	-0.180966
36	1	0	4.145622	5.657626	-0.003779
37	7	0	8.260073	2.124356	2.910412
38	6	0	7.753175	1.199250	3.931525
39	6	0	8.477474	-0.147162	4.006858
40	8	0	8.154624	-1.048864	4.748772
41	6	0	6.227413	0.953575	3.704745
42	8	0	6.007280	0.629462	2.338459
43	6	0	5.369804	2.128798	4.171013
44	1	0	8.145261	1.686022	1.995192
45	1	0	5.584243	1.376200	1.875447

46	7	0	1.201000	-5.494654	3.941808	72	6	0	2.281859	-0.363627	-6.243587
47	6	0	1.321638	-5.468047	5.396375	73	7	0	0.206648	-1.933358	-4.794475
48	6	0	1.592247	-6.850843	5.995135	74	6	0	0.133339	-1.553375	-6.115566
49	8	0	1.453008	-7.903290	5.410287	75	6	0	-1.104682	-2.004477	-6.697485
50	6	0	0.051389	-4.871546	6.025953	76	6	0	-1.779750	-2.672297	-5.719518
51	1	0	0.522599	-6.212906	3.691448	77	6	0	-0.950730	-2.633541	-4.541687
52	16	0	3.037015	-3.661927	-4.261163	78	1	0	-2.744212	-3.159479	-5.776097
53	26	0	1.796020	-1.705652	-3.550072	79	1	0	-1.402500	-1.828360	-7.722699
54	6	0	-1.278501	-3.233313	-3.333390	80	1	0	3.209553	0.650891	-8.008724
55	6	0	2.263483	-2.201110	-0.191038	81	1	0	5.165744	1.265783	-6.234600
56	6	0	4.578814	0.298242	-3.618448	82	1	0	5.840720	0.558858	-1.071998
57	6	0	1.104307	-0.839340	-6.802217	83	1	0	4.577413	-0.847792	0.834387
58	7	0	0.730705	-2.555141	-2.080845	84	1	0	-1.764592	-4.368876	-0.786986
59	6	0	-0.482366	-3.202928	-2.198872	85	1	0	0.248187	-3.838651	0.970057
60	6	0	-0.840657	-3.827187	-0.953050	86	1	0	2.442965	-2.417481	0.856705
61	6	0	0.161431	-3.547360	-0.069605	87	1	0	0.924987	-0.626492	-7.850750
62	6	0	1.128268	-2.747359	-0.774495	88	1	0	5.500252	0.869892	-3.657310
63	7	0	3.104609	-1.028288	-2.173191	89	1	0	-2.225449	-3.758475	-3.262642
64	6	0	3.166305	-1.376511	-0.843048	90	8	0	0.370342	0.851521	-3.141278
65	6	0	4.313390	-0.767682	-0.212033	91	1	0	-7.217290	-4.460659	1.108172
66	6	0	4.957363	-0.056962	-1.175349	92	1	0	-7.613407	-3.968082	-0.541758
67	6	0	4.209285	-0.236772	-2.396025	93	1	0	-8.996823	-2.080805	0.342240
68	7	0	2.658248	-0.510888	-4.923844	94	1	0	-8.602686	-2.542656	1.996488
69	6	0	3.860046	0.150483	-4.798381	95	1	0	-9.677868	-4.801422	1.602953
70	6	0	4.250916	0.713230	-6.062949	96	1	0	-10.186436	-4.249623	0.008917
71	6	0	3.269889	0.395899	-6.959102	97	1	0	-11.461671	-2.373996	1.092357

98	1	0	-11.731885	-2.340717	3.387536	124	1	0	-2.862468	5.040740	1.686340
99	1	0	-0.122163	-3.876725	5.609629	125	1	0	-3.776259	5.400401	0.223276
100	1	0	-0.820002	-5.494631	5.795208	126	1	0	-2.023423	5.165039	0.142643
101	1	0	0.145337	-4.799524	7.112221	127	1	0	-1.675773	7.230431	1.548863
102	1	0	2.078491	-5.815938	3.537926	128	1	0	-3.407995	7.424848	1.706408
103	1	0	2.171530	-4.828929	5.664138	129	1	0	0.756134	2.980709	1.007713
104	1	0	7.878198	1.651729	4.922877	130	1	0	1.643387	2.850308	-0.514964
105	1	0	5.619918	3.045489	3.630208	131	1	0	2.175446	1.909679	0.881494
106	1	0	4.314323	1.902825	3.991041	132	1	0	2.712312	4.008639	2.113649
107	1	0	5.502247	2.308307	5.242965	133	1	0	1.705303	5.810944	1.360495
108	1	0	5.970230	0.067685	4.296374	134	1	0	6.121263	4.290802	-1.421956
109	1	0	9.260648	2.264283	3.027410	135	1	0	6.465840	5.770664	-0.509447
110	8	0	9.542337	-0.227967	3.175850	136	8	0	6.949257	4.277010	1.753095
111	1	0	9.917317	-1.115835	3.304005	137	1	0	7.485498	3.606343	2.281065
112	8	0	1.995728	-6.778880	7.286242	138	1	0	2.578726	-4.463479	-3.277394
113	1	0	2.120457	-7.695504	7.585762	139	15	0	-0.833606	3.439911	-5.390459
114	8	0	-12.818024	-4.330683	0.214498	140	8	0	-1.588775	4.512058	-4.683150
115	1	0	-13.535675	-4.986863	0.204091	141	8	0	0.735840	3.325944	-5.047999
116	1	0	-0.418654	9.303584	-2.363990	142	8	0	-0.865616	3.567253	-6.983631
117	8	0	-1.897627	6.577348	-2.890159	143	8	0	-1.250602	1.917031	-5.192944
118	1	0	-1.685701	5.746235	-3.377574	144	6	0	-1.840674	1.168540	-4.101994
119	1	0	-0.516431	8.124569	-0.376232	145	1	0	-1.844349	0.144945	-4.487118
120	1	0	-4.046300	6.987315	-1.530283	146	6	0	-3.278364	1.636784	-3.898206
121	1	0	-4.819821	8.042739	-0.336865	147	1	0	-3.796362	1.627088	-4.857181
122	1	0	-4.031348	8.740752	-1.748960	148	1	0	-3.320769	2.628441	-3.450726
123	1	0	-2.630663	9.067716	0.220964	149	17	0	-4.160165	0.496851	-2.804197

150	6	0	-1.756633	4.402847	-7.765589	162	1	0	-3.428579	4.424406	-6.380609
151	1	0	-1.570397	4.078897	-8.791606	163	1	0	-3.826432	4.876880	-8.056823
152	6	0	-1.306798	5.861962	-7.607645	164	17	0	-3.796007	2.526865	-7.766046
153	1	0	-1.569055	6.255503	-6.625226	165	6	0	-0.938154	1.134015	-2.857185
154	1	0	-0.229162	5.920032	-7.761233	166	1	0	-1.307876	0.376297	-2.168662
155	17	0	-2.081136	6.923469	-8.850012	167	1	0	0.677567	1.368787	-3.904033
156	6	0	1.619298	4.481647	-4.991933	168	17	0	-1.079119	2.719758	-1.893157
157	1	0	1.083837	5.378605	-5.315888	169	1	0	3.181286	3.195688	-5.747484
158	6	0	2.814249	4.213260	-5.893994	170	6	0	2.015067	4.637092	-3.520423
159	1	0	3.604360	4.933609	-5.686156	171	1	0	2.609150	3.788100	-3.177368
160	17	0	2.414380	4.374827	-7.651137	172	1	0	1.125438	4.756841	-2.901270
161	6	0	-3.231118	4.212337	-7.431260	173	17	0	3.011031	6.133366	-3.286506

For molecular structure of aldehyde$_{\beta\text{-dehalogen}}$ hydroxylation catalyzed by Cpd I of CYP450

$^4RC_{c\alpha}$						11	6	0	3.566656	-0.161569	0.993383
1	26	0	0.926528	-0.285654	-0.521496	12	6	0	3.600583	1.149785	-0.758199
2	7	0	0.839376	-1.358581	1.184840	13	6	0	1.966906	1.778707	-2.498923
3	7	0	2.793725	0.307101	-0.035659	14	6	0	-0.114278	1.265831	-2.924097
4	7	0	0.912835	1.025957	-2.053692	15	6	0	-1.805169	-0.192656	-1.871127
5	7	0	-1.029662	-0.666180	-0.839563	16	6	0	-1.824483	-1.538871	-0.143902
6	6	0	3.138421	-1.045612	1.980650	17	6	0	-0.209862	-2.140297	1.617738
7	6	0	3.218592	1.842118	-1.898913	18	6	0	0.162636	-2.857592	2.812125
8	6	0	-1.385971	0.706333	-2.838797	19	6	0	1.448699	-2.518803	3.092987
9	6	0	-1.440988	-2.240993	0.992381	20	6	0	4.895032	0.396860	0.921484
10	6	0	1.869703	-1.592347	2.071580	21	6	0	4.914705	1.214817	-0.167235

22	6	0	1.596926	2.510463	-3.685668	48	1	0	1.510487	-2.850571	-5.772986
23	6	0	0.299595	2.191993	-3.950029	49	6	0	3.379799	-2.731212	-6.819701
24	6	0	-3.123196	-0.776970	-1.815459	50	1	0	3.239719	-3.674750	-7.346811
25	6	0	-3.133494	-1.617140	-0.746143	51	1	0	4.438173	-2.557460	-6.630817
26	1	0	3.861831	-1.339970	2.733420	52	17	0	2.788901	-1.414293	-7.912459
27	1	0	5.693336	0.179802	1.618216	53	6	0	4.538486	-7.108310	-4.444530
28	1	0	5.732548	1.812315	-0.547200	54	1	0	3.935308	-7.983227	-4.191510
29	1	0	3.962670	2.477514	-2.367900	55	6	0	5.923683	-7.243909	-3.795822
30	1	0	2.253574	3.176540	-4.229050	56	1	0	6.588363	-6.437846	-4.106325
31	1	0	-0.331841	2.544669	-4.754595	57	1	0	5.813572	-7.238503	-2.711087
32	1	0	-2.107274	0.993433	-3.597309	58	17	0	6.708501	-8.815260	-4.232906
33	1	0	-3.922150	-0.560700	-2.512096	59	6	0	4.731460	-3.950590	-1.473601
34	1	0	-3.943155	-2.233955	-0.379787	60	1	0	5.175998	-4.950077	-1.434702
35	1	0	-2.173301	-2.906291	1.438105	61	6	0	3.820812	-3.751146	-0.259167
36	1	0	-0.488370	-3.534710	3.348690	62	6	0	4.629082	-6.979605	-5.961166
37	1	0	2.076414	-2.864051	3.903103	63	1	0	5.125790	-6.052909	-6.248316
38	8	0	1.454700	-1.520829	-1.448275	64	1	0	5.183227	-7.830026	-6.357610
39	16	0	-0.037705	1.442309	1.090167	65	17	0	3.001502	-7.000840	-6.750868
40	1	0	1.023024	1.524635	1.920216	66	6	0	2.665429	-1.516887	-4.631889
41	8	0	4.051975	-4.238046	0.822958	67	1	0	2.112369	-0.703676	-5.101426
42	15	0	4.160282	-4.452137	-4.047883	68	1	0	2.257758	-1.715435	-3.638496
43	8	0	5.489250	-4.179372	-4.650249	69	17	0	4.353013	-0.885512	-4.393662
44	8	0	3.853459	-3.810122	-2.608209	70	1	0	2.942548	-3.107207	-0.467916
45	8	0	3.846923	-6.014413	-3.795209	71	6	0	5.824627	-2.876048	-1.573031
46	8	0	2.849987	-4.000634	-4.839358	72	1	0	5.400408	-1.876409	-1.472958
47	6	0	2.571757	-2.753676	-5.521450	73	1	0	6.330252	-2.963791	-2.534421

74	17	0	7.065006	-3.082872	-0.276373

$^{2}RC_{c\alpha}$

1	26	0	0.735668	-0.229998	-0.402724
2	7	0	0.262443	-1.476932	1.120138
3	7	0	2.658411	-0.243915	0.203272
4	7	0	1.162929	1.237631	-1.709310
5	7	0	-1.232179	-0.009782	-0.800965
6	6	0	2.510044	-1.905861	2.000105
7	6	0	3.592639	1.353071	-1.404245
8	6	0	-1.089904	1.682364	-2.567329
9	6	0	-2.153241	-1.673590	0.747240
10	6	0	1.139491	-2.105229	1.976847
11	6	0	3.214340	-1.039121	1.169930
12	6	0	3.704387	0.437194	-0.367651
13	6	0	2.405297	1.721715	-2.025817
14	6	0	0.287846	1.873397	-2.547682
15	6	0	-1.791450	0.801795	-1.758179
16	6	0	-2.269058	-0.732179	-0.268653
17	6	0	-0.978757	-2.003915	1.402369
18	6	0	-0.881384	-2.960993	2.476837
19	6	0	0.429072	-3.021271	2.834928
20	6	0	4.644047	-0.850429	1.217507
21	6	0	4.948809	0.065766	0.259124
22	6	0	2.313293	2.682677	-3.097866
23	6	0	0.993841	2.779433	-3.420510
24	6	0	-3.216617	0.590317	-1.823871
25	6	0	-3.512703	-0.366638	-0.902556
26	1	0	3.083689	-2.475914	2.723917
27	1	0	5.310584	-1.363312	1.897957
28	1	0	5.917326	0.459893	-0.016793
29	1	0	4.508036	1.807626	-1.767379
30	1	0	3.155456	3.204687	-3.531575
31	1	0	0.526754	3.400798	-4.172841
32	1	0	-1.660993	2.257765	-3.288515
33	1	0	-3.885982	1.111826	-2.494746
34	1	0	-4.477371	-0.789484	-0.655469
35	1	0	-3.061149	-2.173986	1.068318
36	1	0	-1.718894	-3.506515	2.890794
37	1	0	0.891121	-3.628345	3.602005
38	8	0	0.941229	-1.435523	-1.481439
39	16	0	0.162405	1.428311	1.467790
40	1	0	1.172629	1.103474	2.301524
41	8	0	4.852324	-1.086855	-3.448616
42	15	0	1.400533	-3.842734	-5.545120
43	8	0	1.047415	-3.434034	-6.928169
44	8	0	2.005529	-2.718976	-4.571005
45	8	0	2.518211	-5.002507	-5.453843
46	8	0	0.255353	-4.443111	-4.608787
47	6	0	-1.099755	-3.976154	-4.401035
48	1	0	-1.451206	-4.618296	-3.586742
49	6	0	-1.913164	-4.293827	-5.656255

50	1	0	-1.745288	-5.332326	-5.940563
51	1	0	-1.655653	-3.630020	-6.480139
52	17	0	-3.683974	-4.109397	-5.327681
53	6	0	2.846814	-5.910742	-6.532727
54	1	0	3.481593	-6.661317	-6.056405
55	6	0	3.672194	-5.136707	-7.571397
56	1	0	3.049038	-4.451214	-8.145499
57	1	0	4.461309	-4.583205	-7.061736
58	17	0	4.487817	-6.258608	-8.734406
59	6	0	3.117863	-1.874447	-4.928454
60	1	0	3.877288	-2.432650	-5.485319
61	6	0	3.698049	-1.419102	-3.586913
62	6	0	1.638552	-6.596230	-7.161120
63	1	0	0.922056	-5.863977	-7.533323
64	1	0	1.975030	-7.228419	-7.982470
65	17	0	0.772891	-7.672032	-5.992720
66	6	0	-1.195898	-2.551298	-3.862281
67	1	0	-2.177596	-2.412327	-3.410028
68	1	0	-0.416878	-2.358328	-3.121637
69	17	0	-1.055008	-1.254757	-5.128625
70	1	0	2.953312	-1.407005	-2.765360
71	6	0	2.587265	-0.700237	-5.765391
72	1	0	1.950494	-0.048326	-5.166195
73	1	0	2.019906	-1.088822	-6.610781
74	17	0	3.940834	0.299976	-6.420103

$^4TS_{c\alpha}$

1	26	0	1.397613	-0.172530	-0.502613
2	7	0	1.336267	-0.514852	1.490461
3	7	0	2.663436	1.346108	-0.228202
4	7	0	1.256033	0.287373	-2.445168
5	7	0	0.017008	-1.664701	-0.755105
6	6	0	3.018232	1.127239	2.187405
7	6	0	2.747418	2.233303	-2.507300
8	6	0	-0.245869	-1.516727	-3.184989
9	6	0	-0.274986	-2.367177	1.570917
10	6	0	2.116819	0.097005	2.434222
11	6	0	3.259702	1.709875	0.952040
12	6	0	3.122794	2.227659	-1.170737
13	6	0	1.882495	1.320193	-3.098567
14	6	0	0.552509	-0.402156	-3.405804
15	6	0	-0.515182	-2.085156	-1.947027
16	6	0	-0.555445	-2.449465	0.214359
17	6	0	0.616520	-1.474250	2.156311
18	6	0	0.935436	-1.449855	3.562767
19	6	0	1.871277	-0.476188	3.735056
20	6	0	4.140220	2.836229	0.741080
21	6	0	4.049653	3.162423	-0.575276
22	6	0	1.556733	1.290833	-4.502678
23	6	0	0.740465	0.215894	-4.694341
24	6	0	-1.438534	-3.173478	-1.725349
25	6	0	-1.468899	-3.394451	-0.383265

26	1	0	3.565173	1.521344	3.038003	52	17	0	6.052621	-0.398145	-6.520819
27	1	0	4.730490	3.309053	1.514676	53	6	0	2.014901	-6.016572	-5.327596
28	1	0	4.552017	3.957202	-1.110459	54	1	0	0.936771	-6.167956	-5.417444
29	1	0	3.176307	2.999870	-3.144856	55	6	0	2.643539	-7.259694	-4.680739
30	1	0	1.914310	2.004461	-5.233274	56	1	0	3.731403	-7.200149	-4.671695
31	1	0	0.290654	-0.133406	-5.614170	57	1	0	2.269634	-7.362196	-3.661573
32	1	0	-0.729161	-1.956855	-4.051082	58	17	0	2.170602	-8.766639	-5.564885
33	1	0	-1.991243	-3.680000	-2.505343	59	6	0	3.324717	-4.542071	-1.422146
34	1	0	-2.045830	-4.125239	0.167616	60	1	0	2.801583	-5.483280	-1.626499
35	1	0	-0.776913	-3.069723	2.227819	61	6	0	2.568813	-3.784870	-0.310091
36	1	0	0.500605	-2.107029	4.303894	62	6	0	2.598618	-5.730001	-6.706503
37	1	0	2.360910	-0.164897	4.648183	63	1	0	3.649018	-5.445445	-6.639714
38	8	0	2.707262	-1.269504	-0.712943	64	1	0	2.502439	-6.620354	-7.327289
39	16	0	-0.568645	1.208824	-0.300141	65	17	0	1.718247	-4.399546	-7.559133
40	1	0	-0.931823	0.847001	0.947361	66	6	0	4.707611	-1.092790	-3.602159
41	8	0	2.092438	-4.324445	0.644602	67	1	0	5.020946	-0.057792	-3.733176
42	15	0	3.509035	-4.137025	-4.073911	68	1	0	3.953094	-1.153840	-2.815466
43	8	0	4.737592	-4.914417	-4.369941	69	17	0	6.175447	-1.974353	-2.993385
44	8	0	3.272339	-3.668973	-2.555039	70	1	0	2.555022	-2.465026	-0.515913
45	8	0	2.130504	-4.909388	-4.401388	71	6	0	4.789601	-4.800020	-1.040072
46	8	0	3.276871	-2.752367	-4.827958	72	1	0	5.260886	-3.890746	-0.666319
47	6	0	4.160054	-1.602971	-4.933925	73	1	0	5.328782	-5.151564	-1.919896
48	1	0	3.483399	-0.818846	-5.286940	74	17	0	4.917418	-6.069850	0.233520
49	6	0	5.185555	-1.907760	-6.025044						
50	1	0	4.672239	-2.288133	-6.907682	**$^{2}TS_{c\alpha}$**					
51	1	0	5.932817	-2.623630	-5.684764	1	26	0	1.317911	-0.251122	-0.482465

2	7	0	1.309399	-0.562243	1.502440	28	1	0	4.520220	3.852765	-1.182733
3	7	0	2.602458	1.292599	-0.229691	29	1	0	3.116719	2.886836	-3.181618
4	7	0	1.163631	0.205628	-2.444989	30	1	0	1.844162	1.889212	-5.245143
5	7	0	-0.036998	-1.713801	-0.720232	31	1	0	0.185808	-0.227779	-5.605163
6	6	0	3.020553	1.068209	2.172698	32	1	0	-0.875528	-2.017538	-4.000152
7	6	0	2.681342	2.135800	-2.530388	33	1	0	-2.121142	-3.694959	-2.418159
8	6	0	-0.363611	-1.577504	-3.150992	34	1	0	-2.142545	-4.110515	0.261330
9	6	0	-0.335394	-2.377036	1.621585	35	1	0	-0.853051	-3.057975	2.288423
10	6	0	2.111460	0.052682	2.432886	36	1	0	0.455965	-2.086623	4.345122
11	6	0	3.236226	1.648989	0.930923	37	1	0	2.363413	-0.183644	4.646774
12	6	0	3.060278	2.150337	-1.196825	38	8	0	2.673996	-1.250911	-0.744065
13	6	0	1.804935	1.224284	-3.104328	39	16	0	-0.442959	1.356748	-0.205976
14	6	0	0.451001	-0.478685	-3.394276	40	1	0	-0.181508	1.672565	1.078729
15	6	0	-0.604544	-2.129121	-1.902353	41	8	0	2.076773	-4.309317	0.601873
16	6	0	-0.618260	-2.469345	0.266657	42	15	0	3.555438	-4.106188	-4.095454
17	6	0	0.572030	-1.492483	2.188120	43	8	0	4.783796	-4.887600	-4.380699
18	6	0	0.902031	-1.452194	3.591027	44	8	0	3.306207	-3.648694	-2.573507
19	6	0	1.861101	-0.498517	3.741789	45	8	0	2.177193	-4.870420	-4.439712
20	6	0	4.128576	2.758419	0.689366	46	8	0	3.335547	-2.715699	-4.839934
21	6	0	4.014033	3.073641	-0.628470	47	6	0	4.217420	-1.563715	-4.929447
22	6	0	1.477194	1.186281	-4.508776	48	1	0	3.542724	-0.779557	-5.286243
23	6	0	0.643167	0.123686	-4.689981	49	6	0	5.256856	-1.860083	-6.009627
24	6	0	-1.543788	-3.194159	-1.652439	50	1	0	4.755510	-2.237602	-6.900325
25	6	0	-1.557394	-3.400205	-0.307267	51	1	0	6.002205	-2.575361	-5.663873
26	1	0	3.588365	1.456037	3.012014	52	17	0	6.125267	-0.345521	-6.486507
27	1	0	4.745996	3.226319	1.444541	53	6	0	2.064157	-5.970348	-5.375665

54	1	0	0.986024	-6.112203	-5.479478
55	6	0	2.675391	-7.222099	-4.729003
56	1	0	3.763444	-7.169676	-4.704904
57	1	0	2.287006	-7.328852	-3.715691
58	17	0	2.204660	-8.719806	-5.629282
59	6	0	3.342112	-4.529872	-1.449209
60	1	0	2.812994	-5.465761	-1.662382
61	6	0	2.579562	-3.773880	-0.340978
62	6	0	2.667061	-5.679288	-6.745392
63	1	0	3.718861	-5.403690	-6.664039
64	1	0	2.571681	-6.565148	-7.372722
65	17	0	1.807962	-4.336962	-7.600483
66	6	0	4.747641	-1.060085	-3.588610
67	1	0	5.066586	-0.025808	-3.711287
68	1	0	3.981793	-1.120824	-2.813139
69	17	0	6.203697	-1.949598	-2.962731
70	1	0	2.567866	-2.500686	-0.530768
71	6	0	4.800199	-4.801185	-1.050674
72	1	0	5.275774	-3.896586	-0.670957
73	1	0	5.344826	-5.155368	-1.926238
74	17	0	4.900903	-6.073803	0.221646

$^{4}IM_{c\alpha}$

1	26	0	0.792275	0.011814	-0.497378
2	7	0	0.974436	-1.317342	1.021770
3	7	0	2.516179	0.887233	0.075930
4	7	0	0.655173	1.282707	-2.048600
5	7	0	-1.014431	-0.744181	-0.945834
6	6	0	3.084306	-0.533477	2.001742
7	6	0	2.738618	2.540988	-1.728602
8	6	0	-1.537083	0.613363	-2.925544
9	6	0	-1.153921	-2.512181	0.757429
10	6	0	1.984735	-1.376574	1.950186
11	6	0	3.325854	0.511194	1.120826
12	6	0	3.171076	1.903859	-0.574639
13	6	0	1.566937	2.243226	-2.407023
14	6	0	-0.376365	1.371465	-2.948233
15	6	0	-1.823453	-0.368776	-1.988922
16	6	0	-1.646125	-1.791335	-0.320696
17	6	0	0.062823	-2.279640	1.380479
18	6	0	0.533848	-2.993642	2.541293
19	6	0	1.723292	-2.434475	2.894205
20	6	0	4.504514	1.340010	1.150474
21	6	0	4.409096	2.201315	0.100021
22	6	0	1.111750	2.936975	-3.587344
23	6	0	-0.092926	2.397787	-3.921781
24	6	0	-3.012555	-1.182977	-2.004165
25	6	0	-2.902138	-2.064311	-0.972434
26	1	0	3.813739	-0.707888	2.785229
27	1	0	5.298350	1.250929	1.880161
28	1	0	5.108420	2.965894	-0.211216
29	1	0	3.365432	3.329439	-2.130875

30	1	0	1.652002	3.737332	-4.075364
31	1	0	-0.747431	2.664006	-4.741226
32	1	0	-2.274588	0.799481	-3.698953
33	1	0	-3.812760	-1.086201	-2.725822
34	1	0	-3.593082	-2.840383	-0.671191
35	1	0	-1.772947	-3.312139	1.149122
36	1	0	0.003858	-3.808303	3.016622
37	1	0	2.375966	-2.696884	3.715914
38	8	0	1.651473	-1.129222	-1.583219
39	16	0	-0.389543	1.433075	0.885464
40	1	0	0.653692	2.147904	1.353916
41	8	0	4.272897	-3.948852	0.621282
42	15	0	3.429243	-4.100545	-4.249446
43	8	0	4.704671	-4.151099	-5.007073
44	8	0	3.489236	-3.481229	-2.759554
45	8	0	2.760711	-5.541529	-3.967054
46	8	0	2.201310	-3.290488	-4.851439
47	6	0	2.176586	-1.999911	-5.520447
48	1	0	1.106247	-1.844845	-5.688958
49	6	0	2.869124	-2.145029	-6.876013
50	1	0	2.479573	-3.023968	-7.389296
51	1	0	3.950633	-2.216010	-6.770927
52	17	0	2.509033	-0.713148	-7.922664
53	6	0	3.020927	-6.735813	-4.744749
54	1	0	2.250766	-7.435138	-4.411639
55	6	0	4.401868	-7.272974	-4.340471
56	1	0	5.203563	-6.657901	-4.749153
57	1	0	4.471725	-7.299407	-3.252626
58	17	0	4.645739	-8.969252	-4.920261
59	6	0	4.475581	-3.894582	-1.810178
60	1	0	4.645172	-4.977482	-1.860391
61	6	0	3.880248	-3.572495	-0.429726
62	6	0	2.906800	-6.539777	-6.252371
63	1	0	3.580879	-5.756409	-6.599394
64	1	0	3.151951	-7.477149	-6.751263
65	17	0	1.230875	-6.095447	-6.765058
66	6	0	2.619554	-0.842086	-4.635366
67	1	0	2.256262	0.089855	-5.068178
68	1	0	2.231920	-0.959525	-3.619886
69	17	0	4.422988	-0.650065	-4.493106
70	1	0	1.972272	-1.909040	-1.098851
71	6	0	5.781642	-3.125866	-2.058333
72	1	0	5.653877	-2.063608	-1.850019
73	1	0	6.068997	-3.262677	-3.100752
74	17	0	7.118517	-3.754888	-1.026161

$^{2}IM_{c\alpha}$

1	26	0	0.588971	-0.287623	-0.291199
2	7	0	0.087157	-1.589624	1.173584
3	7	0	2.553359	-0.513203	0.154531
4	7	0	1.101189	1.090927	-1.668181
5	7	0	-1.367403	0.015971	-0.652649

6	6	0	2.341143	-2.253926	1.870500	32	1	0	-1.706403	2.246780	-3.181944
7	6	0	3.541128	1.067251	-1.430797	33	1	0	-3.985865	1.326367	-2.263548
8	6	0	-1.151355	1.648005	-2.466653	34	1	0	-4.661134	-0.417858	-0.300693
9	6	0	-2.349215	-1.486357	1.010983	35	1	0	-3.281810	-1.869680	1.413546
10	6	0	0.954816	-2.327636	1.934216	36	1	0	-1.951865	-3.418415	3.091704
11	6	0	3.080192	-1.397173	1.062817	37	1	0	0.680369	-3.872286	3.541543
12	6	0	3.630947	0.123657	-0.417770	38	8	0	0.644268	-1.652842	-1.488739
13	6	0	2.356618	1.510244	-2.020434	39	16	0	0.630778	1.312040	1.521879
14	6	0	0.235917	1.762874	-2.491797	40	1	0	1.653561	2.076565	1.085454
15	6	0	-1.892580	0.841716	-1.609713	41	8	0	4.937084	-0.326228	-4.373778
16	6	0	-2.435959	-0.567397	-0.033570	42	15	0	1.396499	-3.550913	-5.391867
17	6	0	-1.170932	-1.968633	1.564214	43	8	0	0.960584	-3.367896	-6.799196
18	6	0	-1.096659	-2.963229	2.610177	44	8	0	2.012590	-2.249550	-4.653444
19	6	0	0.224395	-3.191621	2.834930	45	8	0	2.597268	-4.612415	-5.197256
20	6	0	4.521762	-1.306713	1.071597	46	8	0	0.345352	-4.043947	-4.309029
21	6	0	4.863345	-0.359502	0.156927	47	6	0	-1.080254	-3.780293	-4.195677
22	6	0	2.286758	2.468167	-3.096617	48	1	0	-1.366091	-4.401984	-3.341430
23	6	0	0.964296	2.624485	-3.390863	49	6	0	-1.787508	-4.309792	-5.444515
24	6	0	-3.335598	0.771081	-1.600875	50	1	0	-1.465230	-5.332253	-5.640155
25	6	0	-3.674532	-0.105053	-0.615766	51	1	0	-1.600601	-3.680736	-6.313036
26	1	0	2.899575	-2.906290	2.534794	52	17	0	-3.576833	-4.363351	-5.174301
27	1	0	5.171632	-1.897144	1.703727	53	6	0	2.912623	-5.677051	-6.127770
28	1	0	5.850132	-0.014159	-0.121012	54	1	0	3.602863	-6.313948	-5.569982
29	1	0	4.469933	1.475482	-1.815653	55	6	0	3.650477	-5.053778	-7.321896
30	1	0	3.141434	2.949231	-3.553244	56	1	0	2.969402	-4.489404	-7.959048
31	1	0	0.511463	3.265149	-4.135975	57	1	0	4.441141	-4.400365	-6.952097

58	17	0	4.451573	-6.317356	-8.339311
59	6	0	2.994843	-1.448936	-5.326116
60	1	0	3.632929	-2.062204	-5.974098
61	6	0	3.880928	-0.844005	-4.228903
62	6	0	1.711072	-6.504064	-6.571478
63	1	0	0.947581	-5.875323	-7.030196
64	1	0	2.042941	-7.253557	-7.289440
65	17	0	0.943563	-7.397166	-5.199319
66	6	0	-1.391110	-2.351458	-3.778063
67	1	0	-2.425347	-2.300642	-3.438094
68	1	0	-0.712858	-2.032503	-2.978013
69	17	0	-1.256269	-1.137209	-5.128607
70	1	0	1.443736	-1.565098	-2.030320
71	6	0	2.276877	-0.367345	-6.144931
72	1	0	1.766534	0.341770	-5.492809
73	1	0	1.557868	-0.857927	-6.800597
74	17	0	3.434182	0.551223	-7.178709

$^{4}Pr_{c\alpha}$

1	26	0	0.808962	-0.275721	0.204852
2	7	0	0.835418	-1.281856	1.950443
3	7	0	2.518676	0.636779	0.735963
4	7	0	1.145737	0.301731	-1.721311
5	7	0	-0.637749	-1.498716	-0.458225
6	6	0	2.720182	-0.163712	3.051810
7	6	0	3.031885	1.833991	-1.352444
8	6	0	-0.772014	-0.784345	-2.807642
9	6	0	-1.121840	-2.722732	1.616712
10	6	0	1.657879	-1.052275	3.028105
11	6	0	3.117608	0.618070	1.977793
12	6	0	3.256036	1.527245	-0.017850
13	6	0	2.040788	1.266039	-2.138993
14	6	0	0.317237	0.072561	-2.801986
15	6	0	-1.205044	-1.518038	-1.713747
16	6	0	-1.367248	-2.393047	0.292480
17	6	0	-0.086508	-2.207997	2.378710
18	6	0	0.169934	-2.576864	3.748566
19	6	0	1.253500	-1.860715	4.151284
20	6	0	4.238464	1.518058	2.006049
21	6	0	4.323733	2.083401	0.769294
22	6	0	1.789248	1.621999	-3.509548
23	6	0	0.721526	0.879109	-3.921371
24	6	0	-2.315622	-2.432223	-1.746706
25	6	0	-2.416566	-2.974691	-0.501563
26	1	0	3.287253	-0.078642	3.972539
27	1	0	4.875841	1.678618	2.865254
28	1	0	5.045081	2.803226	0.405949
29	1	0	3.678019	2.574041	-1.812854
30	1	0	2.349552	2.363810	-4.063791
31	1	0	0.227543	0.883036	-4.884088
32	1	0	-1.328766	-0.885914	-3.732964
33	1	0	-2.924319	-2.628045	-2.619378

34	1	0	-3.125235	-3.708247	-0.140983	60	1	0	5.289289	-3.382598	-2.737646
35	1	0	-1.779347	-3.447800	2.084163	61	6	0	3.679591	-3.189107	-1.331980
36	1	0	-0.412659	-3.294220	4.310942	62	6	0	2.254970	-6.008766	-5.764310
37	1	0	1.747349	-1.866235	5.113774	63	1	0	3.180014	-5.695459	-6.248213
38	8	0	2.524911	-2.532388	-1.125341	64	1	0	2.151808	-7.091028	-5.835225
39	16	0	-0.730796	1.475027	0.830719	65	17	0	0.880009	-5.286280	-6.694336
40	1	0	0.202931	2.258595	1.409011	66	6	0	3.741357	-0.240697	-6.448745
41	8	0	3.984070	-4.166115	-0.693677	67	1	0	3.752279	0.443779	-7.296805
42	15	0	3.486660	-3.225861	-4.746406	68	1	0	3.213451	0.210674	-5.608266
43	8	0	4.667392	-3.926902	-5.302536	69	17	0	5.470210	-0.445331	-5.946221
44	8	0	3.768718	-2.175534	-3.542625	70	1	0	2.381151	-1.830883	-1.786061
45	8	0	2.367567	-4.170053	-4.083982	71	6	0	5.349955	-1.349721	-1.994173
46	8	0	2.607468	-2.313158	-5.719017	72	1	0	4.666638	-0.577913	-1.636796
47	6	0	3.034431	-1.529075	-6.858847	73	1	0	5.913895	-0.971594	-2.846736
48	1	0	2.084048	-1.211855	-7.301018	74	17	0	6.513344	-1.709390	-0.668273
49	6	0	3.761691	-2.410173	-7.876398						
50	1	0	3.168174	-3.302021	-8.075213	**$^{2}Pr_{c\alpha}$**					
51	1	0	4.758114	-2.689156	-7.539793	1	26	0	0.997036	0.485752	0.294743
52	17	0	3.929962	-1.522127	-9.444737	2	7	0	1.336994	-1.503717	0.298096
53	6	0	2.239611	-5.602112	-4.295890	3	7	0	2.978591	0.774532	0.321298
54	1	0	1.266762	-5.837298	-3.859488	4	7	0	0.713525	2.412237	-0.153634
55	6	0	3.342146	-6.307086	-3.492223	5	7	0	-0.935171	0.141858	-0.122311
56	1	0	4.317502	-6.183255	-3.963909	6	6	0	3.778632	-1.534817	0.562940
57	1	0	3.369759	-5.914987	-2.475512	7	6	0	3.006220	3.224302	0.176590
58	17	0	3.012299	-8.082860	-3.368439	8	6	0	-1.702955	2.425723	-0.572909
59	6	0	4.587920	-2.605320	-2.426964	9	6	0	-0.994208	-2.285801	0.250246

10	6	0	2.541746	-2.156529	0.516327	36	1	0	0.434343	-4.695620	0.762582
11	6	0	3.976670	-0.165739	0.473054	37	1	0	3.107973	-4.286730	0.881479
12	6	0	3.621343	1.992503	0.333973	38	8	0	1.307882	-1.233320	-2.704359
13	6	0	1.654832	3.414019	-0.064202	39	16	0	0.689664	0.695602	2.487015
14	6	0	-0.474830	3.052034	-0.434016	40	1	0	1.792208	0.031180	2.896038
15	6	0	-1.913909	1.065089	-0.418442	41	8	0	2.686152	-3.017150	-2.864942
16	6	0	-1.592334	-1.064386	-0.018678	42	15	0	0.046861	-3.890917	-5.571080
17	6	0	0.367357	-2.490614	0.403138	43	8	0	0.924853	-4.603243	-6.530055
18	6	0	0.977367	-3.766078	0.654055	44	8	0	0.439186	-2.369461	-5.204985
19	6	0	2.323531	-3.560508	0.716544	45	8	0	-0.072900	-4.565471	-4.115849
20	6	0	5.264348	0.473448	0.568732	46	8	0	-1.496461	-3.701388	-5.952960
21	6	0	5.043062	1.813163	0.489799	47	6	0	-2.094279	-3.504124	-7.252918
22	6	0	1.049168	4.699481	-0.303729	48	1	0	-3.166442	-3.570269	-7.038472
23	6	0	-0.271600	4.473984	-0.540130	49	6	0	-1.725475	-4.654950	-8.191341
24	6	0	-3.201548	0.426013	-0.517378	50	1	0	-1.915389	-5.604237	-7.691205
25	6	0	-3.003108	-0.895126	-0.262199	51	1	0	-0.688618	-4.602828	-8.517053
26	1	0	4.651671	-2.162505	0.706735	52	17	0	-2.777510	-4.611803	-9.664497
27	1	0	6.203961	-0.050959	0.680525	53	6	0	0.282102	-5.936567	-3.805818
28	1	0	5.764308	2.619046	0.520400	54	1	0	-0.066533	-6.063255	-2.778723
29	1	0	3.637188	4.106509	0.210443	55	6	0	1.811409	-6.073427	-3.838865
30	1	0	1.582374	5.640911	-0.296879	56	1	0	2.187801	-6.117027	-4.860719
31	1	0	-1.049622	5.191529	-0.764509	57	1	0	2.265871	-5.234948	-3.311925
32	1	0	-2.563620	3.047652	-0.796358	58	17	0	2.332940	-7.592926	-2.996658
33	1	0	-4.126135	0.937708	-0.749434	59	6	0	1.809467	-2.023157	-4.891918
34	1	0	-3.729886	-1.696392	-0.245414	60	1	0	2.497983	-2.715260	-5.382263
35	1	0	-1.641141	-3.153740	0.324860	61	6	0	2.004903	-2.152319	-3.374585

62	6	0	-0.397542	-6.962237	-4.704499
63	1	0	-0.147500	-6.790574	-5.751568
64	1	0	-0.075566	-7.961475	-4.412433
65	17	0	-2.201480	-6.927021	-4.557848
66	6	0	-1.879041	-2.093389	-7.794597
67	1	0	-2.600154	-1.902631	-8.589095
68	1	0	-2.012176	-1.370550	-6.989691
69	17	0	-0.244619	-1.791895	-8.516173
70	1	0	1.409401	-1.384902	-1.736831
71	6	0	1.994996	-0.606061	-5.422554
72	1	0	1.335734	0.086607	-4.900913
73	1	0	1.798700	-0.585566	-6.493957
74	17	0	3.694259	-0.056400	-5.154353